The Art of BART:
On Flexibility of Bayesian Forests

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Abstract

Considerable effort has been directed to developing asymptotically minimax procedures in problems of recovering functions and densities. These methods often rely on somewhat arbitrary and restrictive assumptions such as isotropy or spatial homogeneity. This work enhances theoretical understanding of Bayesian forests (including BART) under substantially relaxed smoothness assumptions. In particular, we provide a comprehensive study of asymptotic optimality and posterior contraction of Bayesian forests when the regression function has anisotropic smoothness that possibly varies over the function domain. The regression function can also be possibly discontinuous. We introduce a new class of sparse piecewise heterogeneous anisotropic Hölder functions and derive their minimax rate of estimation in high-dimensional scenarios under the $L_2$-loss. Next, we find that the default Bayesian tree priors, coupled with a subset selection prior for sparse estimation in high-dimensional scenarios, adapt to unknown heterogeneous smoothness, discontinuity, and sparsity. These results show that Bayesian forests are uniquely suited for more general estimation problems which would render other default machine learning tools, such as Gaussian processes, suboptimal. Beyond nonparametric regression, we also show that Bayesian forests can be successfully applied to many other problems including density estimation and binary classification.

Keywords: Adaptive Bayesian procedure; BART; Bayesian CART; High-dimensional inference; Posterior contraction; Sparsity priors

1 Introduction

Many of the existing asymptotic minimaxity results for estimating regression functions are predicated on the assumption that certain smoothness conditions hold, which can be rarely satisfied/verified when confronted with real data. This creates a disconnect between theory

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and practice, limiting the scope of many of the theoretical results. For example, in nonparametric regression involving multiple predictors, the assumption of isotropic smoothness can be unnecessarily restrictive. A more realistic scenario is when the function exerts different degrees of smoothness in different directions and areas, while discontinuities are allowed for further flexibility. This work evaluates theoretical performance of Bayesian forests, one of the workhorses of Bayesian machine learning, in such broad scenarios.

Bayesian trees and their ensembles have achieved a notable empirical success in statistics and machine learning (Chipman et al., 1998; Denison et al., 1998; Chipman et al., 2010). Relative to other Bayesian machine learning alternatives, tree-based methods require comparatively less tuning and can be scaled to higher dimensions (Lakshminarayanan et al., 2013; Bleich et al., 2014; He et al., 2019). The popularity of Bayesian forests such as Bayesian Additive Regression Trees (BART) (Chipman et al., 2010) is growing rapidly in many areas including causal inference (Hill, 2011; Hahn et al., 2020), mean-variance function estimation (Pratola et al., 2019), smooth function estimation (Linero and Yang, 2018), variable selection (Bleich et al., 2014; Linero, 2018), interaction detection (Du and Linero, 2019), survival analysis (Sparapani et al., 2016) and time series (Taddy et al., 2011), to list a few. Despite the remarkable success in empirical studies, theoretical properties of Bayesian forests were unavailable for a long time with first studies emerging only very recently (Roˇckov´a and van der Pas, 2017; Linero and Yang, 2018; Roˇckov´a and Saha, 2019; Castillo and Roˇckov´a, 2019). Although these pioneering findings divulge why tree-based methods perform very well, they are limited to isotropic regression function surfaces, which exhibit the same level of smoothness in every direction. Isotropy is one of the archetypal assumptions in theoretical studies, but can be restrictive in real-world applications. This assumption is particularly unattractive in higher dimensions where the function can behave very poorly in certain directions.

From the plentiful empirical evidence, however, Bayesian forests are expected to adapt to more intricate smoothness situations. This is for at least three reasons: (i) tree methods are based on top-down recursive partitioning, where splits occur more often in areas where the function is locally uneven or bumpy, making the procedure spatially adaptive; (ii) the choice of coordinates for split is data-driven, making the domain divided more often in directions in which the function is less smooth; and (iii) tree-based learners are piecewise constant and, as such, are expected to adapt to discontinuous functions by detecting smoothness boundaries and jumps. These considerations naturally create an expectation that Bayesian forests achieve optimal estimation in more complex function classes without any prior modification.

The main goal of this paper is to study optimality and posterior contraction of Bayesian forests under relaxed smoothness assumptions. More specifically, we introduce a class of functions whose domain has been cleaved into hyper-rectangles where each rectangular piece has its own anisotropic smoothness (with the same harmonic mean). We allow for possible discontinuities at the boundaries of the pieces. We call this new class piecewise heterogeneous anisotropic functions (see Definition 2 in Section 2.1). We establish approximation theory for this general class which blends anisotropy with spatial inhomogeneity and which, to the best of our knowledge, has not yet been pursued in the literature. Our results complement the body of existing work on piecewise isotropic smoothness classes (e.g., Cand`es and Donoho, 2000, 2004; Le Pennec and Mallat, 2005; Petersen and Voigtlaender, 2018; Imaizumi and Fukumizu, 2019). Our function class subsumes the usual (homogeneous) anisotropic space for which adaptive procedures exist with optimal convergence rate guarantees, including the Dyadic CART of Donoho (1997). We refer to Barron et al. (1999), Neumann and von Sachs
There are also adaptive Bayesian procedures for anisotropic function estimation with desired asymptotic properties (e.g., Bhattacharya et al., 2014; Shen and Ghosal, 2015). There appear to be no theoretical properties for adaptation in the more general case of piecewise heterogeneous anisotropic smoothness. Indeed, existing theoretical studies for discontinuous piecewise smooth classes impose the isotropy assumption (e.g., Candès and Donoho, 2000, 2004; Le Pennec and Mallat, 2005; Petersen and Voigtlaender, 2018; Imaizumi and Fukumizu, 2019) and the convergence rates in spatially adaptive estimation depend on global smoothness parameters (e.g., Pintore et al., 2006; Liu and Guo, 2010; Wang et al., 2013; Tibshirani, 2014). In this respect, our study appears to be the first theoretical investigation of piecewise anisotropic function classes.

The majority of frequentist/Bayesian methods for anisotropic function estimation rely on multiple scaling (bandwidth) parameters, one for each direction. As noted by Bhattacharya et al. (2014), selecting optimal scaling parameters in a frequentist way can be computationally difficult as adaptation in anisotropic spaces presents several challenges (Lepski and Levit, 1999). The Bayesian paradigm provides an effective remedy by assigning priors over these unknown parameters. One such example is the generalized Gaussian process priors or spline basis representations (Bhattacharya et al., 2014; Shen and Ghosal, 2015). Although these priors enjoy elegant theoretical guarantees in typical anisotropic spaces, it is unclear whether they can adapt to piecewise heterogeneous anisotropic spaces without substantial modification. Bayesian forests, on the other hand, are expected to work in these more complex scenarios without any additional scaling parameters. The approximability is controlled merely by the depth of a tree and the orientation of its branches, where no prior modifications should be required to achieve optimal performance. Moreover, computation with Gaussian processes can be quite costly (Banerjee et al., 2013; Liu et al., 2020), while Bayesian forests are more scalable and faster than their (Bayesian) competitors.

In the context of regression or classification, Bayesian forests often rely on observed covariate values for splits in recursive partitioning (Chipman et al., 1998; Denison et al., 1998; Chipman et al., 2010). This facilitates theoretical investigation under the fixed regression design. In the context of nonparametric Gaussian regression, Ročková and van der Pas (2017) and Ročková and Saha (2019) investigated posterior contraction for BART based on this conventional manner of partitioning. Dyadic CART (Donoho, 1997), on the other hand, splits at dyadic midpoints of the domain and can achieve optimal performance as well (Castillo and Ročková, 2019). We generalize Dyadic CART by introducing the notion of split-nets which form a collection of candidate split-points that are not necessarily observed covariate values and/or dyadic midpoints. Our findings show that optimality can be achieved with split-nets which are sufficiently evenly distributed. By allowing the split-points occur beyond observed values, we show that Bayesian forests enjoy the general recipe of the posterior contraction theory (Ghosal et al., 2000; Ghosal and van der Vaart, 2007) which applies to density estimation or regression/classification with a random design.

Asymptotic minimaxity is often used to evaluate optimality of statistical procedures. Yang and Tokdar (2015) derived the minimax rates of sparse function estimation in high dimensions but their results are restricted to the isotropic cases. In fixed (low) dimensions, minimax rates over anisotropic function spaces have been extensively studied in the literature (Ibragimov and Hasminskii, 1981; Nussbaum, 1985; Birgé, 1986). If the true function only depends on a subset of coordinates, the minimax rate is improved and determined by smooth-
ness parameters of active coordinates (Hoffman and Lepski, 2002). However, to the best of our knowledge, there are no available studies on minimax rates over piecewise anisotropic function spaces like ours. While there exist results on piecewise isotropic classes (e.g., Imaizumi and Fukumizu, 2019), even the simpler fixed-dimensional setup without sparsity has not been studied for piecewise anisotropic classes. Focusing on Gaussian nonparametric regression, we derive the minimax rate for our piecewise heterogeneous anisotropic spaces under the high-dimensional scenario. This result verifies that our obtained contraction rates for Bayesian forests are indeed minimax-optimal, up to a logarithmic factor.

1.1 Our contribution

We summarize the contribution of this paper as follows.

- **Approximation theory**: The true function should be approximable by tree-based learners in order to establish the optimal rate of posterior contraction. Approximation theory for piecewise heterogeneous anisotropic classes is much more intricate when there are discontinuities and heterogeneity. We establish such approximation theory here under suitable regularity conditions (with smoothness up to 1 due to the limitation of piecewise constant learners).

- **Posterior contraction**: For functions belonging to piecewise heterogeneous anisotropic spaces, posterior contraction of Bayesian forests is established under the high-dimensional setup with sparse priors. The derived rates consist of the risk of variable selection uncertainty and the risk of function estimation, similar to isotropic cases (Yang and Tokdar, 2015; Ročková and van der Pas, 2017).

- **Minimax optimality**: Minimax rates in high-dimensional spaces have been unavailable even for simple anisotropic classes. For Gaussian nonparametric regression with high-dimensional inputs, we formally derive the minimax rate over piecewise heterogeneous anisotropic spaces. This certifies that our obtained contraction rate for Bayesian forests is optimal, up to a logarithmic factor.

- **Applications beyond regression**: Unlike traditional tree priors (Chipman et al., 1998; Denison et al., 1998) and their asymptotic studies (Ročková and van der Pas, 2017; Ročková and Saha, 2019), our findings show that splits for recursive partitioning do not necessarily have to be at observed covariate values. This implies that our proving technique extends beyond fixed-design regression to other estimation problems such as density estimation or regression/classification with a random design.

1.2 Outline

In Section 2, we describe the background of function spaces and Bayesian forests. In high-dimensional scenarios, the tree priors on functions are specified in Section 3. Section 4 sheds light on the approximation theory for our function spaces. In Section 5, we study posterior contraction of Bayesian forests and their minimax optimality in nonparametric regression with a fixed design. Posterior contraction properties in other statistical models such as density estimation and binary classification are investigated in Section 6. All technical proofs are collected in Appendix.
1.3 Notation and terminology

We work with a statistical experiment indexed by a measurable function $f : [0, 1]^p \mapsto \mathbb{R}$ for some $p > 0$. The statistical models we are dealing with will be specified for our examples in Sections 5–6. We observe $n$ observations with the true function denoted by $f_0$ and assume that $p$ is possibly increasing with the sample size $n$. The notation $\mathbb{E}_0$ and $\mathbb{P}_0$ denote the expectation and probability operators under the true model with $f_0$.

For a subspace $E$ of the Euclidean space, $C(E)$ denotes a class of continuous functions $f : E \mapsto \mathbb{R}$. For sequences $a_n$ and $b_n$, we write $a_n \lesssim b_n$ (or $b_n \gtrsim a_n$ equivalently) if $a_n \leq C b_n$ for some constant $C > 0$, and $a_n \asymp b_n$ implies $a_n \lesssim b_n \lesssim a_n$. For a given measure $\mu$ and a measurable function $f$, we denote by $\|f\|_{v, \mu} = (\int |f|^v d\mu)^{1/v}$ the $L_v(\mu)$-norm, $1 \leq v < \infty$. We also denote by $L_2(\mu)$ the linear space of real valued functions equipped with inner product $\langle f, g \rangle_\mu = \int fg d\mu$ and norm $\|f\|_2, \mu = (\int |f|^2 d\mu)^{1/2}$. The support of a measure $\mu$ is denoted by $\text{supp}(\mu)$. The supremum norm of a function $f$ is denoted by $\|f\|_{\infty}$. In particular, we write $\|f\|_v$ for the $L_v$-norm with the Lebesgue measure. For a given vector $u$, the notations $\|u\|_v$ and $\|u\|_{\infty}$ represent the $\ell_v$-norms, $1 \leq v < \infty$, and the maximum-norm, respectively. The minimal and maximal singular values of a matrix are denoted by $\sigma_{\text{min}}(\cdot)$ and $\sigma_{\text{max}}(\cdot)$. For a semimetric space $(X, d)$, the expressions $D(\epsilon, X, \rho)$ and $N(\epsilon, X, \rho)$ are $\epsilon$-packing and $\epsilon$-covering numbers of $X$, respectively. For a subset $S \subseteq \{1, \ldots, p\}$ and $x = (x_1, \ldots, x_p) \in \mathbb{R}^p$, let $x_S = (x_j, j \in S) \in \mathbb{R}^{|S|}$ be the indices chosen by $S$.

A hyper-rectangle $\Psi \subseteq [0, 1]^p$ with any $p > 0$ is often simply called a box. A partition $\mathcal{J} = (\Psi_1, \ldots, \Psi_J)$ of $[0, 1]^p$, consisting of disjoint boxes $\Psi_r \subseteq [0, 1]^p$, $r = 1, \ldots, J$, is called a box partition. For a given box $\Psi \subseteq [0, 1]^p$ with some $p > 0$, the length of interval formed by projecting $\Psi$ onto the $j$th coordinate is denoted by $|\Psi|_j, j = 1, \ldots, p$.

2 Modus operandi

2.1 Heterogeneous anisotropic function spaces with sparsity

In this subsection, we introduce our function spaces with heterogeneous smoothness and sparsity in high dimensions. The first assumption is that the true regression function $f_0 : [0, 1]^p \mapsto \mathbb{R}$ is $d$-sparse, i.e., it depends on a small subset of $d$ variables. This means that there exists a function $h_0 : [0, 1]^d \mapsto \mathbb{R}$ and a subset $S_0 \subseteq \{1, \ldots, p\}$ with $|S_0| = d$, such that $f_0(x) = h_0(x_{S_0})$ for any $x \in [0, 1]^p$. We assume that the lower-dimensional domain $[0, 1]^d$ of $h_0$ is partitioned into many boxes and $h_0$ is Hölder continuous with possibly different smoothness in each box. Moreover, the smoothness inside each box is anisotropic, i.e., different for each coordinate. Focusing on a single box, we first define an anisotropic Hölder space as follows.

**Definition 1** (Anisotropic Hölder space). For a smoothness parameter $\alpha = (\alpha_1, \ldots, \alpha_d)' \in (0, 1]^d$, a box $\Xi \subseteq [0, 1]^d$, and a Hölder coefficient $\lambda < \infty$, we denote by $H^\alpha_\lambda(\Xi)$ an anisotropic $\alpha$-Hölder space on $\Xi$, i.e.,

$$H^\alpha_\lambda(\Xi) = \left\{ h : \Xi \mapsto \mathbb{R}; \ |h(x) - h(y)| \leq \lambda \sum_{j=1}^{d} |x_j - y_j|^\alpha_j, \ x, y \in \Xi \right\}. $$

Note that the definition above imposes a restriction $\alpha \in (0, 1]^d$. Although one can generalize this definition to smoother classes (e.g. Bhattacharya et al., 2014), we do not
Figure 1: A graphical illustration of a piecewise heterogeneous anisotropic Hölder space with five boxes. Each piece has its own smoothness parameter, but the harmonic mean is assumed to be the same.

consider such extensions here since step function estimators cannot be optimal in classes smoother than Lipschitz.

As discussed above, our targeted function class is not necessarily globally anisotropic over the entire domain \([0,1]^d\). Instead, we assume that \(f_0\) has different anisotropic smoothness on several disjoint boxes of the domain with the same harmonic mean. The function space is formed by agglomerating anisotropic Hölder spaces for all boxes. We emphasize that the resulting function space is not necessarily continuous, which provides a lot more flexibility relative to the conventional Hölderian class. Considering that smoothness parameters can vary across boxes and functions can be discontinuous at their boundaries, we call this new class a \textit{piecewise heterogeneous anisotropic Hölder space}. We define these functions formally below.

**Definition 2** (Piecewise heterogeneous anisotropic Hölder space). Consider a box partition \(\mathcal{X} = (\Xi_1, \ldots, \Xi_R)\) of \([0,1]^d\) with boxes \(\Xi_r \subseteq [0,1]^d\) and smoothness parameters \(A = (\alpha_r)_{r=1}^R\) with \(\alpha_r = (\alpha_{r1}, \ldots, \alpha_{rd})' \in (0,1]^d\) such that \(\alpha^{-1}_r = d^{-1} \sum_{j=1}^d \alpha^{-1}_{rj}\) with some \(\alpha_* \in (0,1]\) for every \(r = 1, \ldots, R\). We define a piecewise heterogeneous anisotropic Hölder space as

\[
H^{A,d}_\lambda(\mathcal{X}; \alpha_*) = \left\{ h : [0,1]^d \mapsto \mathbb{R}; h|_{\Xi_r} \in H^{\alpha_{r},d}_\lambda(\Xi_r), \ r = 1, \ldots, R \right\}.
\]

A graphical illustration of the piecewise heterogeneous anisotropic Hölder spaces is given in Figure 1. Clearly, Definition 2 subsumes the anisotropic Hölder space in Definition 1. According to Definition 2, any \(h \in H^{A,d}_\lambda(\mathcal{X}; \alpha_*)\) is anisotropic on each \(\Xi_r\) with a smoothness parameter \(\alpha_r \in (0,1]^d\) and the same harmonic mean \(\alpha_*\) for all \(\Xi_r\) (an important assumption for obtaining the minimax rate). We again emphasize that discontinuities are allowed at the boundaries of boxes \(\Xi_r, \ r = 1, \ldots, R\). Definition 2 does not impose a specific structure on the partition \(\mathcal{X}\) other than a box partition. However, we will later see that depending on the approximation metric, our approximation theory will require it to be a tree-based recursive structure defined in the next section. Since any box partition can be extended to the required form by adding more splits, this discrepancy is not practically an issue. We refer the reader to Section 4.1.1 for more discussion.

**Remark 1.** We compare Definition 2 with piecewise smooth function spaces widely investigated in the literature. Approximation rates for piecewise smooth functions with smooth
jump curves/surfaces have been extensively studied in two dimensions (e.g., Candès and Donoho, 2000, 2004; Guo and Labate, 2007) as well as in higher dimensions (Chandrasekaran et al., 2008; Petersen and Voigtlaender, 2018; Imaizumi and Fukumizu, 2019). All these studies deal with smooth functions with smooth jump curves/surfaces under the isotropy assumption. On the other hand, our definition deals with different anisotropic smoothness parameters for the boxes in a box partition, and hence seems more flexible. Our jump surfaces, however, are restricted to hyper-planes parallel to the coordinates.

Note that Definition 2 is for mappings from a lower dimensional domain $[0,1]^d$ while the true function $f_0$ maps the entire $[0,1]^p$ to $\mathbb{R}$. We now characterize a sparse elaboration of Definition 2 for mappings $f_0 : [0,1]^p \mapsto \mathbb{R}$. For any $S \subseteq \{1, \ldots, p\}$, we denote with $W_S^p : C(\mathbb{R}^{|S|}) \mapsto C(\mathbb{R}^{|S|})$ the map that transmits $h \in C(\mathbb{R}^{|S|})$ onto $W_S^p h : x \mapsto h(x_S)$. Similarly to Yang and Tokdar (2015) for the isotropic cases, we now formalize $d$-sparse function spaces as follows.

**Definition 3** (Sparse function space). For a space $\mathcal{H}^{A,d}_\lambda(\mathcal{X}; \alpha_*)$ with required ingredients given in Definition 2, we define a $d$-sparse piecewise heterogeneous anisotropic Hölder space as

$$\Gamma^{A,d,p}_\lambda(\mathcal{X}; \alpha_*) = \bigcup_{S : |S| = d} W_S^p(\mathcal{H}^{A,d}_\lambda(\mathcal{X}; \alpha_*)).$$

Definition 3 incorporates $d$-sparse globally anisotropic spaces constructed by $\mathcal{H}^{\alpha,d}_\lambda([0,1]^d)$ in Definition 1 since it is encompassed by $\mathcal{H}^{A,d}_\lambda(\mathcal{X}; \alpha_*)$ according to Definition 2. Throughout this paper, we assume that the true function $f_0$ belongs to the class $\Gamma^{A,d,p}_\lambda(\mathcal{X}; \alpha_*)$, which allows for discontinuities, or its continuous variant $\Gamma^{A,d,p}_\lambda(\mathcal{X}; \alpha_*) \cap C([0,1]^p)$. This continuous variant achieves approximability under more relaxed assumptions (see Theorem 1 below). Going forward, it will be convenient to extend the box partition $\mathcal{X}$ of the $d$-dimensional cube $[0,1]^d$ to a partition of the $p$-dimensional cube $[0,1]^p$. To this end, we relate $\mathcal{X}$ to the corresponding box partition of $[0,1]^p$ by extending each $\Xi_r$ to a $p$-dimensional box $\Xi^*_r \subseteq [0,1]^p$ such that $\Xi^*_r = \{x \in [0,1]^p : x_{S_0} \in \Xi_r, x_{S_0} \in [0,1]^{p-d}\}$ for the true support $S_0$; that is, $\Xi_r$ is the projection of $\Xi^*_r$ onto the hyper-plane defined by $S_0$. The boxes $\Xi^*_r$ then constitute the box partition $\mathcal{X}^* = (\Xi^*_1, \ldots, \Xi^*_R)$. To determine sparsity of box partitions, we now make the following definition.

**Definition 4** (Sparse partition). Consider a box partition $\mathcal{Y} = (\Psi_1, \ldots, \Psi_J)$ of $[0,1]^p$ with boxes $\Psi_r \subseteq [0,1]^p$, $r = 1, \ldots, J$. For a subset $S \subseteq \{1, \ldots, p\}$, the partition $\mathcal{Y}$ is called $S$-sparse if $\max_{j \in S} |\Psi_r|_j < 1$ and $\min_{j \notin S} |\Psi_r|_j = 1$ for every $r = 1, \ldots, J$.

A graphical illustration of sparse partitions is provided in Figure 2. According to Definition 4, the box partition $\mathcal{X}^*$ is $S$-sparse for some $S \subseteq S_0$. In particular, $\mathcal{X}^*$ is $\emptyset$-sparse if $R = 1$. In what follows, we use the notation $S(\mathcal{X}^*) \subseteq S_0$ to denote sparsity of $\mathcal{X}^*$; that is, $\mathcal{X}^*$ is $S(\mathcal{X}^*)$-sparse.

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1We use the notation $\mathcal{Y} = (\Psi_r)$ to denote an arbitrary box partition of $[0,1]^p$ with boxes $\Psi_r \subseteq [0,1]^p$, $r = 1, 2, \ldots$, whereas we denote by $\mathcal{X} = (\Xi_1, \ldots, \Xi_S)$ and $\mathcal{X}^* = (\Xi^*_1, \ldots, \Xi^*_R)$ the box partitions associated with the true function $f_0$ through the piecewise heterogeneous anisotropic spaces in Definitions 2–3. The notation $\Psi \subseteq [0,1]^p$ is often used to denote an arbitrary $p$-dimensional box.

2Note that $\mathcal{Y}$ is $\emptyset$-sparse if $J = 1$. 7
Remark 2. The assumption $f_0 \in \Gamma^{A,d,p}_\lambda(\mathcal{X}; \alpha_*)$ means that there exists a subset $S_0 \subseteq \{1, \ldots, p\}$ with $|S_0| = d$ such that $f_0 \in W^p_{S_0}(\mathcal{H}^{A,d}_\lambda(\mathcal{X}; \alpha_*))$. We can opt for the latter style for the sake of simplicity, but the expression $\Gamma^{A,d,p}_\lambda(\mathcal{X}; \alpha_*)$ will be particularly useful in the minimax study in Section 5.2. A similar conclusion also holds for the continuous variant $\Gamma^{A,d,p}_\lambda(\mathcal{X}; \alpha_*) \cap C([0, 1]^p)$.

2.2 Tree-based partitions

In this work, for estimators of the true function $f_0$, we focus on piecewise constant learners, i.e., step functions that are constant on each piece of a box partition of $[0, 1]^p$. A precise description of piecewise constant learners requires an underlying partitioning rule that produces a partition for these step functions. In tree-structured models, the idea is based on recursively applying binary splitting rules to split the domain $[0, 1]^p$. Here we shed light on this mechanism to construct tree-based partitions, while deferring a complete description of the induced step functions to Section 2.3.

For a given box $\Psi \subseteq [0, 1]^p$ and its interior $\text{int}(\Psi)$, consider a split-point $\tau \in \text{int}(\Psi)$ and a splitting coordinate $j \in \{1, \ldots, p\}$. The pair $(\tau, j)$ then bisects $\Psi$ along the $j$th coordinate into two boxes: $\{x \in \Psi : x_j \leq \tau_j\}$ and $\{x \in \Psi : x_j > \tau_j\}$, where $x_j$ and $\tau_j$ are $j$th entries of $x$ and $\tau$, respectively. Starting from the root node $[0, 1]^p$, the procedure is iterated $K - 1$ times in a top-down manner by picking one box for a split each time. This generates $K$ disjoint boxes $(\Psi_k)_{k=1}^K$, called terminal nodes, which constitute a tree-shaped partition of $[0, 1]^p$, called a tree partition. We call this iterative procedure the binary tree partitioning.

We will further refer to our tree partitions as flexible tree partitions to emphasize that splits can occur everywhere in the domain $[0, 1]^p$ (not necessarily at dyadic midpoints or observed covariate values). According to Definition 4, we say that a flexible tree partition is $S$-sparse for some $S \subseteq \{1, \ldots, p\}$ if splitting coordinates $j$ are restricted to $S$. Note that while flexible tree partitions are always box partitions, the reverse is not generally true; see Figure 3.

Although tree-based partitioning allows splits to occur anywhere in the domain, it is often preferred to choose split-points from a discrete set. For example, in regression with continuous covariates, observed covariate values are typically used for splits (Chipman et al., 1998; Denison et al., 1998; Chipman et al., 2010). Following this manner, Ročková and van der Pas (2017) and Ročková and Saha (2019) investigated posterior contraction of BART.
in Gaussian nonparametric regression with fixed covariates. Here we relax this restriction. To this end, we define a discrete collection of locations where splits can occur, which we call a split-net.

**Definition 5 (split-net).** For an increasing integer sequence $b_n$ (i.e., $b_n \in \mathbb{N}$ and $b_n \to \infty$ as $n \to \infty$), a split-net $Z = \{z_i \in [0,1]^p, i = 1, \ldots, b_n\}$ is a discrete collection of $b_n$ points $z_i \in [0,1]^p$ at which possible splits occur along coordinates.

The number of split-points $b_n$ should grow sufficiently fast with $n$ to yield a fine approximation, but not too fast to overwhelm model complexity. As noted above, a typical example of $Z$ with $b_n = n$ is the observed covariate values in fixed-design nonparametric regression. This specific example will be discussed in Section 4.3.3. Our split-nets yield additional flexibility in situations when no deterministic covariate values are available, such as density estimation or in the analysis of nonparametric regression with random covariates. Another split-net example is the regular (equidistant) grid system, shown in Figure 4 and further discussed in Section 4.3.1.

We assume that the splits in the binary partitioning rule occur only at the points in $Z$; that is, for any given box $\Psi \subseteq [0,1]^p$, a split-point $\tau$ is chosen such that $\tau \in Z \cap \text{int}(\Psi)$. Clearly, a constructed tree partition based on $Z$ is an instance of flexible tree partitions, but the reverse is not the case. To distinguish the two more clearly, we make the following definition.

**Definition 6 (Z-tree partition).** For a given split-net $Z$, a flexible tree partition $T = (\Omega_1, \ldots, \Omega_K)^3$ of $[0,1]^p$ with boxes $\Omega_k \subseteq [0,1]^p$, $k = 1, \ldots, K$, is called a $Z$-tree partition if every split occurs at points $z_i \in Z$.

In summary, we have the following relationship among the three types of partitions: $\{Z$-tree partitions$\} \subseteq \{\text{Flexible tree partitions}\} \subseteq \{\text{Box partitions}\}$. Similar to flexible tree partitions, $Z$-tree partitions can be $S$-sparse for a subset $S \subseteq \{1, \ldots, p\}$ no matter what $Z$ is employed. Since we aim to do sparse estimation in high-dimensional setups, we are mostly interested in $S$-sparse $Z$-tree partitions for some low-dimensional $S$. It will later be shown that it is important to characterize the cardinality of $S$-sparse $Z$-tree partitions. This is partly because the complexity of tree topologies, which should be controlled to achieve optimality,

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**Figure 3:** Examples of non-tree box partitions and tree partitions.

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[^3]: The notation $T = (\Omega_k)_k$ is used only for Z-tree partitions with split-nets $Z$, with some suitable superscript and/or superscript if required. Note that we denote flexible tree partitions by $\mathcal{D}$ as general box partitions.
Figure 4: Examples of the split-net in two dimensions. For the regular grid in (a), some splits eliminate the possibility of other splits as the projected points are duplicated. The points of the split-net in (b) are unique in every coordinate, so splits can occur \( b_n \) times.

is directly related to the cardinality. Moreover, a prior may depend on the cardinality as well (see Section 3.2). The exact calculation of the cardinality may or may not be possible due to possible elimination of splits in a recursive procedure (see Figure 4). We thus provide a tractable upper bound of the cardinality in Lemma 4 in Appendix.

2.3 Bayesian trees and forests

We now describe our piecewise constant learners using \( Z \)-tree partitions. While single tree learners have received some attention (Chipman et al., 1998; Denison et al., 1998), it is widely accepted that additive aggregations of small trees are much more effective for prediction (Chipman et al., 2010). Noting that single trees are a special case of tree ensembles (forests), we will focus on forests throughout the rest of the paper.

We consider a fixed number \( T \) of trees. For a given split-net \( Z \) and for each \( 1 \leq t \leq T \), we denote with \( T^t = (\Omega^t_1, \ldots, \Omega^t_{K^t}) \) a \( Z \)-tree partition of size \( K^t \) and with \( \beta^t = (\beta^t_1, \ldots, \beta^t_{K^t})' \in \mathbb{R}^{K^t} \) the heights of the step function, called the step-heights. An additive tree-based learner is then fully described by a tree ensemble \( E = (T^1, \ldots, T^T) \) and terminal node parameters \( B = (\beta^1', \ldots, \beta^T')' \in \mathbb{R}^{\sum_{t=1}^T K^t} \) through

\[
 f_{E,B}(x) = \sum_{t=1}^T \sum_{k=1}^{K^t} \beta^t_k 1(x \in \Omega^t_k). \tag{1}
\]

That is, \( f_{E,B} \) is constant on the boxes constructed by overlapping \( T \) \( Z \)-tree partitions (note that the resulting boxes are not the same as \( \Omega^t_k \)). Chipman et al. (2010) recommended the choice \( T = 200 \) which was seen to provide good empirical results. For a given ensemble \( E \), we henceforth define \( F_E = \{f_{E,B} : B \in \mathbb{R}^{\sum_{t=1}^T K^t}\} \) the set of functions (1). If \( E \) consists of a single tree \( T \), we instead write \( F_T \) to denote \( F_E \).

Our objective is to characterize the posterior asymptotic properties of the tree learners (1) in estimating the true function \( f_0 \) belonging to \( \Gamma_{\lambda, \delta, \beta}(\mathcal{X}; \alpha_*) \) or \( \Gamma_{\lambda, \delta, \beta}(\mathcal{X}; \alpha_*) \cap \mathcal{C}([0,1]^p) \). This goal requires two nice attributes of the procedure. First, appropriate prior distributions should be assigned to the tree learners \( f_{E,B} \) in (1) so that the induced posterior can achieve
the desired asymptotic properties. Second, there should exist a piecewise tree learner approximating \( f_0 \) with a suitable approximation error matched to our target rate. The following two sections aim to elucidate these in detail.

3 Tree and forest priors in high dimensions

3.1 Dimension reduction

Conventional tree priors (Chipman et al., 1998; Denison et al., 1998) are not necessarily designed for high-dimensional data with a sparse underlying structure. Prior modifications are thus required for trees to meet demands of high-dimensional applications (Linero, 2018; Linero and Yang, 2018). The prior should be adaptive to unknown sparsity levels and traditional Bayesian approaches for feature selection achieve this via hierarchical spike-and-slab priors (Castillo and van der Vaart, 2012; Castillo et al., 2015; Ročková, 2018). Ročková and van der Pas (2017) adapted this strategy for BART, introducing the so-called spike-and-tree priors. We deploy this prior construction here as well.

The prior is constructed in a hierarchical manner: a subset dimension \(|S|\) is first drawn from some prior \( \pi_{\text{dim}}(|S|) \) and, given the dimension, each subset \( S \) has an equal prior probability. The resulting prior on \( S \subseteq \{1, \ldots, p\} \) is formalized as

\[
\pi(S) = \left( \frac{p}{|S|} \right)^{-1} \pi_{\text{dim}}(|S|), \quad S \subseteq \{1, \ldots, p\}.
\]

We assume that \( \pi_{\text{dim}}(\cdot) \) satisfies

\[
a_1 p^{-a_3} \pi_{\text{dim}}(s - 1) \leq \pi_{\text{dim}}(s) \leq a_2 p^{-a_4} \pi_{\text{dim}}(s - 1), \quad s = 1, \ldots, p,
\]

for some constants \( a_1, a_2, a_3, a_4 > 0 \). This decaying property is crucial for obtaining optimal posterior contraction and variable selection consistency (Castillo et al., 2015). A typical example is the exponential decaying prior: \( \pi_{\text{dim}}(s) \propto c_1^{-s} p^{-c_2 s}, \quad s = 0, \ldots, p \), for some \( c_1, c_2 > 0 \), which is widely used in sparse estimation (e.g., Castillo and van der Vaart, 2012; Martin et al., 2017).

3.2 Priors over tree topologies

Once the subset of coordinates \( S \subseteq \{1, \ldots, p\} \) has been chosen from the prior in Section 3.1, the prior specification is completed by assigning a prior over the ensemble of tree-shaped partitions \( \mathcal{E} = (\mathcal{T}^1, \ldots, \mathcal{T}^T) \) and step-heights. We assume an independent product prior for \( \mathcal{T}^t \)'s, i.e., \( \pi(\mathcal{E}|S) = \prod_{t=1}^T \pi(\mathcal{T}^t|S) \). There are several ways to assign a prior on \( \mathcal{T}^t \). Throughout this study, we consider two conventional tree priors suggested by Chipman et al. (1998) and Denison et al. (1998). In the remainder of this subsection, we suppress the superscript \( t \) for \( \mathcal{T}^t \) and \( K^t \).

3.2.1 Galton-Watson process prior

In their pioneering work on Bayesian classification and regression trees, Chipman et al. (1998) proposed a prior over tree topologies through the heterogeneous Galton-Watson process (see Ročková and Saha (2019) for more discussion on this prior). Below we slightly modify the original form for theoretical purposes. In the statement, the notation \( \text{dep}(\Omega_k) \) denotes the depth of \( \Omega_k \), the number of nodes along the path from the root node down to \( \Omega_k \).
1. Start from the root node \([0, 1]^p\) and set \(\ell = 1\).
2. For the current partition \((\Omega_k)_k\), every node \(\Omega_k\) such that \(\text{dep}(\Omega_k) = \ell\) is split with a probability \(\nu^\ell\) for \(\nu \in (\nu_0, 1/2)\) with some \(\nu_0 > 0\), giving rise to two daughter nodes. For every \(\Omega_k\) that is chosen to be split, a split-point \(\tau \in \mathcal{Z} \cap \text{int}(\Omega_k)\) and a splitting coordinate \(j \in S\) are uniformly drawn.
3. Create a new partition \((\Omega_k)_k\) with the given boxes and increase \(\ell\) by 1.
4. Iterate 2–3 until there is no node chosen for split.

The number \(K\) of terminal nodes is solely determined by the number of splits, and hence by the parameter \(\nu\), but not by the given support \(S\). Its tail property is important to achieve optimal posterior contraction. The original prior proposed by Chipman et al. (1998) uses a splitting probability that decays polynomially. Ročková and Saha (2019) showed that this decay may not be fast enough, and suggested using an exponentially decaying probability as in our definition. This modification gives rise to the desirable exponential tail property of tree sizes.

### 3.2.2 Bayesian CART prior

Denison et al. (1998) proposed another Bayesian CART prior, which directly chooses the number of nodes \(K\) from a Poisson distribution. This guarantees the desirable tail properties by construction: \(\log \pi(K = k) \propto -k \log k\) for every \(k \in \mathbb{N}\). Given \(S\) and \(K\), a uniform prior is assigned over tree topologies; that is,

\[
\pi(\mathcal{T} | S, K) = \frac{1}{\#\mathcal{T}_{S,K}} 1(\mathcal{T} \in \mathcal{T}_{S,K}),
\]

where \(\mathcal{T}_{S,K}\) is the set of \(S\)-sparse \(\mathcal{Z}\)-tree partitions of size \(K\) and \(\#\mathcal{T}_{S,K}\) is its cardinality. To explore different \(S\) and \(K\) for the computation of the posterior, we hence need the exact evaluation of \(\#\mathcal{T}_{S,K}\). This requirement is not needed for the Galton-Watson process prior as it is free of \(\#\mathcal{T}_{S,K}\). We have an upper bound of \(\#\mathcal{T}_{S,K}\) in Lemma 4 in Appendix. This also gives the exact value of \(\#\mathcal{T}_{S,K}\) if any split does not preclude other splits (e.g., compare the two plots in Figure 4). This particular case (i.e., with no ties in the split-net) makes the prior in (3) actually computable in practice. If the exact value \(\#\mathcal{T}_{S,K}\) is not available due to duplications, one may slightly jitter the points in a split-net such that the exact expression for \(\#\mathcal{T}_{S,K}\) is available. See Remark 5 in Section 4.3.1 for more discussion.

Despite this drawback, the Bayesian CART prior has theoretical advantages over the Galton-Watson process prior. To be more specific, the same probability over tree topologies in (3) guarantees sufficient prior mass of the approximator to achieve a good prior concentration (the approximator will be specified in Section 4.2). On the other hand, this is not automatic for the Galton-Watson process prior as it penalizes the depth of trees. We will see that unless \(R = 1\), a mild additional condition is required for the Galton-Watson process prior. We refer the reader to Section 5.1 for more details.

### 3.3 Prior on step-heights

To complete the prior on the sparse function space, what remains to be specified is the prior on step-heights \(B\) in (1). Given \(K^1, \ldots, K^T\) induced by \(\mathcal{E}\), Chipman et al. (2010) suggested using an independent and identically distributed (i.i.d.) Gaussian prior on \(B\):
\[ \pi(B|K^1, \ldots, K^T) = \prod_{t=1}^T \prod_{k=1}^{K^t} \phi(\beta^k_t; 0, 1/T), \] where \( \phi \) is the standard Gaussian density. The variance \( 1/T \) shrinks step-heights toward zero, limiting the effect of individual components by keeping them small enough for large \( T \). Although this choice may be preferred in view of the practical performance, any zero-mean multivariate Gaussian prior on \( B \) gives rise to the same optimal properties as soon as the eigenvalues of the covariance matrix are bounded below and above. Throughout the paper, we put a Gaussian prior on the step-heights \( B \) in most cases. From the computational point of view, this choice is certainly appealing in Gaussian nonparametric regression due to its semi-conjugacy. In fact, Gaussian priors can easily be replaced by priors with thicker tails provided that they have exponentially decaying tail properties such as Laplace distributions. Although such a prior may loosen a restriction on \( \|f_0\|_\infty \) (Ročková, 2020), we mostly consider normal priors throughout the paper, even for non-Gaussian models for the sake of simplicity. We consider non-Gaussian priors only when required for theoretical purposes; see, for example, regression with a random design in Section 6.

4 Approximating the true function

Recall that tree learners \( f_{E,B} \) in (1) are piecewise constant, whereas the true function \( f_0 \) does not have to be. This will not be an issue as long as there exists a tree learner which can approximate \( f_0 \) sufficiently well. In this section, we establish the approximation theory for tree ensembles in the context of our targeted function spaces.

For isotropic classes, it is well-known that balanced \( k \)-d trees (Bentley, 1979) give rise to rate-optimal approximations under mild regularity conditions (Ročková and van der Pas, 2017). This is not necessarily the case for our general setup where smoothness may vary over the domain and where cycling repeatedly through the coordinates (as is done in the \( k \)-d tree) may not be enough to capture localized features of \( f_0 \). In this section, we generalize the notion of \( k \)-d trees and show that there exists a good partitioning scheme for piecewise heterogeneous anisotropic classes. Although our primary interest lies in additive tree aggregations in (1), we show that a single deep tree can approximate well. We thereby consider only single trees \( T \) and suppress the superscript \( t \) throughout this section.

4.1 Split-nets for approximation

Approximation properties of tree-based estimators are driven by the granularity and fineness of the underlying partition and are primarily determined by a chosen split-net. Roughly speaking, a good approximation requires that a split-net has two properties: (i) it should be dense enough so that the boundaries of the partition \( \mathcal{X}^* = (\Xi_1^*, \ldots, \Xi_R^*) \) can be detected with a minimal error; and (ii) it should be regular enough so that there exists a tree-based partition that captures local/global features of \( f_0 \) on each \( \Xi_r^* \). The next two subsections elucidate these properties.

4.1.1 Dense split-nets: Global approximability

Recall that the underlying partition \( \mathcal{X}^* = (\Xi_1^*, \ldots, \Xi_R^*) \) for the true function is unknown. From the sheer flexibility of tree partitioning, we expect that the boundaries can be detected

\[ \text{Recall that } \mathcal{X}^* = (\Xi_1^*, \ldots, \Xi_R^*) \text{ is the box partition of } [0, 1]^p \text{ extended from } \mathcal{X} = (\Xi_1, \ldots, \Xi_R). \]
\begin{figure}
\centering
\includegraphics[width=0.8\textwidth]{hausdorff_divergence.png}
\caption{A two-dimensional example of the Hausdorff-type divergence in Definition 7. The divergence is the maximum dependency of the boxes in the partitions.}
\end{figure}

'well enough' if \( \mathbf{X}^* \) is a tree-based partition as well. If the prior rewards partitions that are sufficiently close to \( \mathbf{X}^* \), Bayesian CART (BART) is expected to adapt to unknown \( \mathbf{X}^* \) without much loss of efficiency. We examine when this adaptivity can be achieved in more detail below.

The ability to detect \( \mathbf{X}^* \) is closely tied to the density of the split-net \( \mathbf{Z} \). The split-points should be dense enough so that a \( \mathbf{Z} \)-tree partition can be constructed that is 'sufficiently close' to \( \mathbf{X}^* \). We thus need a gadget to measure the closeness between two partitions. To this end, below we introduce a Hausdorff-type divergence; see Figure 5 for an illustration.

**Definition 7 (Hausdorff-type divergence).** For any two box partitions \( \mathcal{Y}_1 = (\Psi_1^1, \ldots, \Psi_J^1) \) and \( \mathcal{Y}_2 = (\Psi_1^2, \ldots, \Psi_J^2) \) with the same number \( J \) of boxes, we define a divergence between \( \mathcal{Y}_1 \) and \( \mathcal{Y}_2 \) as

\[
\Upsilon(\mathcal{Y}_1, \mathcal{Y}_2) = \inf_{\pi(1), \ldots, \pi(J) \in P_{\pi}[J]} \max_{1 \leq r \leq J} \text{Haus}(\Psi_{\pi(r)}^1, \Psi_{\pi(r)}^2),
\]

where \( P_{\pi}[J] \) denotes the set of all permutations of \( \{1, \ldots, J\} \) and \( \text{Haus}(\cdot, \cdot) \) is the Hausdorff distance.

The permutation in Definition 7 makes the specification immune to the ordering of boxes. We want the split-net \( \mathbf{Z} \) to produce a \( \mathbf{Z} \)-tree partition \( \mathcal{T} \) such that \( \Upsilon(\mathbf{X}^*, \mathcal{T}) \) is smaller than some threshold. Section 4.2 establishes how small these thresholds should be so that the tree learner is close to \( f_0 \) (for various approximation metrics). The following definition will be useful in characterizing the details.

**Definition 8 (Dense split-net).** For a subset \( S \subseteq \{1, \ldots, p\} \) and an integer \( J \geq 1 \), consider an \( S \)-sparse partition \( \mathcal{Y} = (\Psi_1, \ldots, \Psi_J) \) of \([0, 1]^p\) with boxes \( \Psi_r \subseteq [0, 1]^p, r = 1, \ldots, J \). A split-net \( \mathbf{Z} = \{z_i \in [0, 1]^p, i = 1, \ldots, b_n\} \) is said to be \((\mathcal{Y}, c_n)\)-dense for some \( c_n \geq 0 \) if for the same \( S \), there exists an \( S \)-sparse \( \mathbf{Z} \)-tree partition \( \mathcal{T} = (\Omega_1, \ldots, \Omega_J) \) of \([0, 1]^p\) such that \( \Upsilon(\mathcal{Y}, \mathcal{T}) \leq c_n \).

In Section 4.2, the approximation theory will require that \( \mathbf{Z} \) be \((\mathbf{X}^*, c_n)\)-dense for some \( c_n \geq 0 \). Note that the ideal case \( c_n = 0 \) can be achieved only when \( \mathbf{X}^* \) is a \( \mathbf{Z} \)-tree partition. This condition, while obviously satisfied in the case \( R = 1 \), is very restrictive in general situations. However, we will see in Theorem 1 that in many cases, it is sufficient that \( c_n \)

\[ \text{If } J = 1, \text{ i.e., } \mathcal{Y} = ([0, 1]^p), \text{ we have } \Upsilon(\mathcal{Y}, \mathcal{T}) = 0 \text{ for } \mathcal{T} = ([0, 1]^p). \text{ Hence, every split-net } \mathbf{Z} \text{ is } ([0, 1]^p, 0)\)-dense. \]
tends to zero at a suitable rate. This means that $X^*$ should be at least a flexible tree partition, but not necessarily a $Z$-tree partition. If $X^*$ is a box partition but not a flexible tree partition, we can redefine $X^*$ by adding more splits to make it a flexible tree partition. For example, the non-tree box partition in Figure 3 can be extended to a tree partition with a single extra split. In Section 4.3, we present some examples of dense split-nets.

### 4.1.2 Regular split-nets: Local approximability

Beyond closely tracking smoothness boundaries, good tree partitions should be able to capture local/global smoothness features of $f_0$. In other words, we require that there exists a $Z$-tree partition generated by a split-net $Z$ that gives rise to an optimal approximation error as determined by our target rate. In Section 4.1.1, we focused on more global approximability of underlying partitions which requires split-nets to be suitably dense. Now, we focus on local approximability which relies on how regular the split-net is.

Assume that $X^*$ can be approximated well (as discussed in the previous section) by an $S(X^*)$-sparse $Z$-tree partition $T^* = (\Omega^*_1, \ldots, \Omega^*_R)^6$. More specifically, for a $(X^*, c_n)$-dense split-net $Z$ with a given $c_n > 0$, $T^*$ is defined as $\argmin_{T \in T(S(X^*), R)} T(X^*, T)$. We now focus on local approximability inside each box $\Omega^*_s$. Ideally, one would like to construct a subtree partition of this local box that balances out approximation errors in every coordinate. Therefore, we first need to devise a splitting scheme to achieve this balancing condition. The regularity of split-nets can then be spelled out based on such a law.

We now zoom onto a single box $\Omega^*_s$. Intuitively, denser subdivisions are required for coordinates with less smoothness. Allowing splits to occur more often in certain directions, below we define the anisotropic $k$-d tree which achieves the desired approximation error for anisotropic smoothness.

**Definition 9 (Anisotropic $k$-d tree).** Consider a smoothness vector $\alpha = (\alpha_1, \ldots, \alpha_d)^t \in (0, 1]^d$, a box $\Psi \subseteq [0, 1]^p$, a split-net $Z = \{z_i \in [0, 1]^p, i = 1, \ldots, b_n\}$, an integer $L > 0$, and an index set $S = \{s_1, \ldots, s_d\} \subseteq \{1, \ldots, p\}$ with $|S| = d$. We define the anisotropic $k$-d tree $AKD(\Psi; Z, \alpha, L, S)$ as the iterative splitting procedure that partitions $\Psi$ into disjoint boxes as follows.

1. Start from the root domain $\Psi$ and $l_j = 0$ for every $j = 1, \ldots, d$.
2. For splits at iteration $1 + \sum_{j=1}^d l_j$, choose the coordinate $s_j$ corresponding to the smallest $l_j \alpha_j$. If the smallest $l_j \alpha_j$ is duplicated with multiple $j$, choose $s_j$ corresponding to the smallest $\alpha_j^7$.
3. For the chosen coordinate $s_j$, do midpoint-splits\(^8\) for all boxes at the current stage to give rise to new boxes, and increase $l_j$ by one.
4. Repeat 2–3 until $L = \sum_{j=1}^d l_j$ or the midpoint-split is no longer available.

Note that the anisotropic $k$-d tree construction depends on the smoothness that is unknown. Rather than a practical estimator, we use this construct in the proof to show that

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6The notation $T^* = (\Omega^*_1, \ldots, \Omega^*_R)$ with asterisks is only used to denote an $S(X^*)$-sparse $Z$-tree partition approximating $X^* = (\Xi^*_1, \ldots, \Xi^*_R)$.

7If the smallest $\alpha_j$ is also duplicated with multiple $j$, choose any $s_j$ corresponding to such $j$.

8A midpoint-split is a split that occurs at the $\lceil b/2 \rceil$th value for the number $b$ of split-points of a chosen box, such that the number of split-points in the resulting two offspring cells are $\lfloor (b - 1)/2 \rfloor$ and $\lceil b/2 \rceil$. 

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there exists a good tree approximator. One possible realization of the anisotropic $k$-d tree generating process is given in Figure 6. Note that $AKD(\Psi; \mathcal{Z}, \alpha, L, S)$ returns a partition $\mathcal{T}^\dagger := (\Omega_1^\dagger, \ldots, \Omega_{2^L}^\dagger)$ of $\Psi$ such that $\cup_{k=1}^{2^L} \Omega_k^\dagger = \Psi$ and a vector $L^\dagger := (l_1, \ldots, l_d)'$ such that $L \leq \sum_{j=1}^{d} l_j$. Although these returned items clearly depend on the inputs of the anisotropic $k$-d tree procedure, i.e., $\mathcal{T}^\dagger = \mathcal{T}^\dagger(\Psi; \mathcal{Z}, \alpha, L, S)$ and $L^\dagger = L^\dagger(\Psi; \mathcal{Z}, \alpha, L, S)$, we abbreviate them whenever there is no confusion throughout the paper. Each $l_j$ is a counter of how many times the $j$th coordinate has been used. The procedure is designed so that every $l_j$ is approximately proportional to $\alpha_j^{-1}$ after enough iterations. The total number of splits for the $j$th coordinate is thus close to $2^{C/\alpha_j}$ for some $C > 0$ and for every $j$. In the proof of Theorem 1 below, one can see that this matching is indeed optimal and minimizes the induced bias.

To play a role as a ‘sieve’ for approximation, $\Psi$ needs to be sufficiently finely subdivided to capture the global/local behavior of a function. The threshold $L$ determines the resolution of the returned tree partition $\mathcal{T}^\dagger = (\Omega_1^\dagger, \ldots, \Omega_{2^L}^\dagger)$. For a good approximation with that sieve, we are particularly interested in the situation when $L = \sum_{j=1}^{d} l_j$, i.e., the resulting tree has the desired depth. If $L < \sum_{j=1}^{d} l_j$, the resolution may not be good enough.

Now, we can define the regularity of a split-net on $\Psi \subseteq [0, 1]^p$ using $\mathcal{T}^\dagger$. The desirable situation is when all the splits occur nearly at the center of boxes such that for any given $j \in S$, all $|\Omega_k^\dagger|$, $k = 1, \ldots, 2^L$, are balanced well. The evenness of the returned partition is solely determined by the regularity of a split-net $\mathcal{Z}$. Intuitively, the split-points should be sufficiently regularly distributed to give rise to an appropriate partition, in which we say a split-net is regular. We make the definition technically precise below, which will be used as a basis for approximating the function classes. See Verma et al. (2012) for a related regularity condition.

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The notation $\mathcal{T}^\dagger = (\Omega_k^\dagger)_k$ with daggers is used only for tree partitions of some box $\Psi \subseteq [0, 1]^p$, returned by the anisotropic $k$-d trees, with some suitable subscript if required.
Definition 10 (Regular split-net). For a given box \( \Psi \subseteq [0,1]^p \), an integer \( L > 0 \), and an index set \( S = \{s_1, \ldots, s_d\} \subseteq \{1, \ldots, p\} \), we say that a split-net \( Z \) is \((\Psi, \alpha, L, S)\)-regular if \( T^\dagger = (\Omega^\dagger_1, \ldots, \Omega^\dagger_{2^d}) \) and \( L^\dagger = (l_1, \ldots, l_d) \) returned by \( AKD(\Psi; Z, \alpha, L, S) \) satisfy \( L = \sum_{j=1}^d l_j \) and \( \max_k |\Omega^\dagger_k|_{s_j} \lesssim |\Psi|_{s_j} 2^{-l_j} \) for every \( j = 1, \ldots, d \).

The condition \( \max_k |\Omega^\dagger_k|_{s_j} \lesssim |\Psi|_{s_j} 2^{-l_j} \) is the key to obtaining optimal approximation results. In the ideal case that all the splits occur exactly at the center, this condition is trivially satisfied as \( \max_k |\Omega^\dagger_k|_{s_j} = |\Psi|_{s_j} 2^{-l_j} \). The inequality provides a lot more flexibility where the condition can be satisfied in most cases except for very extreme situations. See Section 4.3 for examples of regular split-nets.

Remark 3. Since regular split-nets require the desired depth, i.e., \( L = \sum_{j=1}^d l_j \), it is of interest to see which \( L \) achieves this precondition. For a given box \( \Psi \subseteq [0,1]^p \) and a split-net \( Z = \{z_i \in [0,1]^p, \ i = 1, \ldots, b_n\} \), let us denote by \( b_n \) the number of split-points in \( Z \cap \text{int}(\Psi) \). If there are no ties in \( Z \) for any coordinate, it can be checked that any integer \( L \leq \lfloor \log_2(b_n + 1) \rfloor \) gives rise to \( L = \sum_{j=1}^d l_j \) with the anisotropic \( k \)-d tree. If there are ties, \( L \) may need to be much smaller than \( \lfloor \log_2(b_n + 1) \rfloor \), but the exact expression for an upper bound may not be available.

Remark 4. Regular split-nets have nested properties. More precisely, if a \( Z \) is \((\Psi, \alpha, L, S)\)-regular for some \( \Psi, \alpha, L, \) and \( S, \) then it is also \((\Psi, \alpha, L_s, S)\)-regular for any \( L_s \leq L \). This can be easily shown by noting that the latter property is determined only by a sub-tree of a blown tree for the former.

4.2 Approximation theory

Our goal is to establish asymptotic properties of the posterior distribution. This requires that tree learners can suitably approximate functions in the spaces \( \Gamma_{\alpha}^{A,d,p}(\mathcal{X}; \alpha) \) and \( \Gamma_{\alpha}^{A,d,p}(\mathcal{X}; \alpha*) \cap C([0,1]^p) \). Here, we establish the approximation properties for these sparse function spaces.

Recall that a split-net \( Z \) is required to be suitably dense and regular. First, a split-net \( Z \) should be \((\mathcal{X}^*, c_n)\)-dense for some suitable \( c_n \). The boundaries of \( \mathcal{X}^* = (\Xi_1^*, \ldots, \Xi_p^*) \) should thus be detected well by the binary tree partitioning rule. Since \( \mathcal{X}^* \) is approximated by a \( Z \)-tree partition with a given \( Z \), this implicitly requires that \( \mathcal{X}^* \) be at least a flexible tree partition, but a stronger result is obtained if it is a \( Z \)-tree partition (see Theorem 1 below). Denoting by \( T^* = (\Omega_1^*, \ldots, \Omega_R^*) \) the \( (\mathcal{X}^*)\)-sparse \( Z \)-tree partition approximating \( \mathcal{X}^* \), each box \( \Omega_r^* \) should be appropriately subdivided to capture the local/global nature of the true function on \( \Xi_r^* \). Hence, for smoothness parameters \( A = (\alpha_r)_{r=1}^d \) and \( L_0 \) specified below, \( Z \) should also be \((\Omega_r^*, \alpha_r, L_0, S_0)\)-regular, \( r = 1, \ldots, R \). The integer \( L_0 \) is chosen below such that the approximation error is balanced with our target rate. Let \( T^\dagger = (\Omega^\dagger_1, \ldots, \Omega^\dagger_{2^d}) \) be the tree partition of \( \Omega_r^* \) returned by \( AKD(\Omega_r^*; Z, \alpha_r, L_0, S_0) \), \( r = 1, \ldots, R \). Then, the approximating partition \( \hat{T} \) is formed by agglomerating all sub-tree partitions \( T^\dagger \), leading to an \( S_0 \)-sparse \( Z \)-tree partition \( \hat{T} = (T^\dagger_1, \ldots, T^\dagger_R) \). A graphical illustration of constructing \( \hat{T} \) is given in Figure 7.

The strongest approximation results relative to the supremum norm are of particular interest. Due to the possible discontinuity or heterogeneity at the unknown boundaries of \( \mathcal{X}^* \), however, this may require strong conditions on split-nets except for the case \( R = 1 \). As the following lemma shows, the conditions can be relaxed if we opt for weaker metrics, which often
The assertion (i) is given for the supremum norm, and hence is the most comprehensive and can be universally used in many statistical estimation problems. However, the condition \( c_n = 0 \) requires that the boundaries of the pieces be correctly detectable by the binary tree partitioning rule with a given split-net \( \mathcal{Z} \); that is, \( \mathcal{X}^* \) should be a \( \mathcal{Z} \)-tree partition. Except for the case \( R = 1 \), this limitation is quite restrictive and impractical as the locations of the boundaries are unknown. In contrast, the assertion (iv) requires a relaxed condition, which can be satisfied if \( c_n \) is decreasing sufficiently fast. Since \( c_n \) should tend to zero, this relaxed condition can be achieved even if \( \mathcal{X}^* \) is not a \( \mathcal{Z} \)-tree partition. The relief is due to the continuity of \( f_0 \) imposed for (iv). The assertions (ii) and (v) are with respect to the \( L_v \)-norm, \( v \geq 1 \), and are useful as many metrics are bounded by \( L_v \)-type norms; see Section 5.1 for example. In particular, unlike (i), the assertion (ii) can hold even if \( \mathcal{X}^* \) is not a \( \mathcal{Z} \)-tree

\[ \| f_0 - f_0^A \|_\infty \lesssim \bar{\epsilon}_n \text{ if } c_n = 0; \]
\[ \| f_0 - f_0^A \|_v \lesssim \bar{\epsilon}_n \text{ if } c_n \lesssim (\bar{\epsilon}_n/\| f_0 \|_\infty)^v \min_{r,j} | \Xi^*_r |/d, \text{ for any } v \geq 1; \]
\[ \| f_0 - f_0^A \|_{v,P_Z} \lesssim \bar{\epsilon}_n \text{ for any } v \geq 1, \text{ where } P_Z(\cdot) = b_n^{-1} \sum_{i=1}^{b_n} \delta_{z_i}(\cdot). \]

Furthermore, for any \( f_0 \in \Gamma^{A,d,p}_\lambda(\mathcal{X};\alpha_\ast) \cap C([0,1]^p) \), there exists \( f_0^A \in \mathcal{F}_T \) such that

\[ \| f_0 - f_0^A \|_\infty \lesssim \bar{\epsilon}_n \text{ if } c_n \lesssim (\bar{\epsilon}_n/(\lambda d) \rightleftharpoons \bar{\epsilon}_n/\sqrt{\log n}; \]
\[ \| f_0 - f_0^A \|_v \lesssim \bar{\epsilon}_n \text{ if } c_n \lesssim (\bar{\epsilon}_n/(\lambda d))^v \min_{r,j} | \Xi^*_r |/d, \text{ for any } v \geq 1. \]

Proof. See Section B.1 in Appendix. \qed
partition. The assertion (iii) is particularly useful in regression setups with $Z$ chosen by fixed covariates (see Section 4.3.3). Note that the condition of (iii) is free of $c_n$.

The conditions in Theorem 1 are oracle-type conditions since they depend on unknown attributes, e.g., $A = (\alpha_r)$, $\lambda$, and $d$. More practical bounds can be obtained by plugging in some reasonable upper and lower bounds of the unknown components. For example, we cannot hope for better than $\tilde{\epsilon}_n \gtrsim (\lambda d R (\log n) / n)^{1/3}$ due to the fundamental limitation of piecewise constant learners. The dimensionality $d$ should be assumed to be $o(\log n)$ for consistent estimation. We can also assume that $\lambda$ does not increase too fast and $\min_{r,j} |\Xi^*_r|_j$ is bounded away from zero or decreases sufficiently slowly. Putting everything together, the conditions in (ii), (iv), and (v) can be easily satisfied if $c_n$ decreases polynomially in $n$ with a suitable exponent.

There is no required upper bound of $b_n$ for Theorem 1; clearly, the approximation results are more easily achieved with larger values of $b_n$. However, values of $b_n$ increasing too fast may harm the contraction rate as they escalate the model complexity (see Lemma 4). In Section 5, we will see that our main results on the optimal posterior contraction require that $\log b_n \lesssim \log n$. Hence, we are ultimately interested in split-nets with $b_n$ balanced very well.

4.3 Examples of split-nets for approximation

Although the notion of dense and regular split-nets is crucial in characterizing the approximation theory in Section 4.2, it remains unclear whether one can obtain such good split-nets in practice. In this section, we provide examples of split-nets that are suitably dense and regular which can thereby fulfill the requirements of Theorem 1. Throughout this section, $\mathcal{T}^* = (\Omega^*_1, \ldots, \Omega^*_R)$ is defined as $\mathcal{T}^* = \arg\min_{\mathcal{T} \in \mathcal{Z}(\mathcal{X}^*), R} \mathcal{Y}(\mathcal{X}^*, \mathcal{T})$ for a given $Z$.

4.3.1 Regular grid

We first consider a regular grid $Z = \{(i - 1/2)/b_n^{1/p}, i = 1, \ldots, b_n^{1/p}\}^p$ for $b_n$ such that $b_n^{1/p}$ is an integer (see Figure 4). This simplest example is a split-net according to Definition 5. The following lemma shows that, for an appropriately chosen $b_n$, a regular grid is suitably dense and regular under mild conditions.

Lemma 1 (Complete grid). Consider a regular grid $Z$ with $b_n = n^{\alpha p}$ for some suitably large constant $c > 0$. If $\log \lambda + \log d \lesssim \log n$ and $\min_{r,j} |\Xi^*_r|_j \gtrsim -\log n$, then $Z$ is $(\mathcal{X}^*, c_n)$-dense and $(\Omega^*_r, \alpha_r, L_0, S_0)$-regular for $r = 1, \ldots, R$, where $c_n = b_n^{-1/p} \mathbb{I}(R > 1)$.

Proof. See Section B.2 in Appendix. 

We pay particular attention to the case $R = 1$, i.e., $\mathcal{X}^* = ([0, 1]^p)$, where the condition $\log \min_{r,j} |\Xi^*_r|_j \gtrsim -\log n$ is trivially satisfied. Since $Z$ is $(\mathcal{X}^*, 0)$-dense in this case, we obtain the strongest result in (i) of Theorem 1. For the case $R > 1$, note that $b_n^{-1/p}$ decreases polynomially in $n$ with this choice of $b_n$. Hence the assertions in (ii), (iv), and (v) of Theorem 1 hold if $c$ is sufficiently large. Note that (iii) of Theorem 1 also holds with this $Z$ as it is free of $c_n$.

While $b_n$ should be chosen such that $\log b_n \lesssim p \log n$ for Lemma 1, as mentioned previously, our main results on the optimal posterior contraction require that $\log b_n \lesssim \log n$, which is satisfied only when $p$ is bounded. This makes the regular grid system somewhat less attractive than other nontrivial split-nets, as we are also interested in high-dimensional
sets where \( p > n \). In Section 4.3.2, we will see that this drawback can be circumvented by considering another split-nets.

**Remark 5.** With a regular grid \( Z \), tied values eliminate the possibility of other splits, and hence make it difficult to calculate the exact value of \( \#T_{S,K} \) with given \( S \) and \( K \) (see Lemma 4 in Appendix). This is an obstacle to the use of the Bayesian CART prior in Section 3.2.2. To practically address this issue, we can slightly jitter all points in \( Z \) such that there are no ties in any coordinate. For example, every point \( z_i \) can be replaced by \( z_i + u_i \), where \( u_i \) is generated from a uniform distribution on \([−\xi_n, \xi_n] \) for some \( \xi_n > 0 \) decreasing faster than \( 1/b_n^{1/p} \). Note that the Galton-Watson process prior can be used without jittering as it is free of \( \#T_{S,K} \).

**Remark 6.** A regular grid can easily be extended to an irregular rectangular grid with boxes of different sizes. If every mesh-size of this irregular checkerboard is asymptotically proportional to \( 1/b_n^{1/p} \), the above results still hold with minor modification. This extension is particularly interesting in a regression setup where the distribution of covariates is explicitly available. For example, it allows us to use the quantiles for grid points, which is a natural way to generate a weakly balanced system (Castillo and Ročková, 2019).

### 4.3.2 Uniform generation

Although regular grids can be viewed as the archetype of split-nets, it is quite disappointing that it can only be used for low-dimensional problems. The limitation of a regular grid comes from the fact that there are only \( b_n^{1/p} \) points projected onto each coordinate, while there are \( b_n \) points in total on the entire domain. Motivated by this limitation, we consider a split-net that has no duplicated values in each coordinate. We want a split-net to be sufficiently evenly distributed such that it is dense and regular for some arbitrary partition and each box. Intuitively, the most promising pattern is a split-net generated by a uniform distribution on \([0, 1]^p \). In this section, we shall show that this choice is indeed very useful in high-dimensional setups.

Consider a split-net \( Z = \{z_i ∈ [0, 1]^p, i = 1, \ldots, b_n \} \) consisting of \( z_i, i = 1, \ldots, b_n \), drawn independently from a uniform distribution on the hypercube \([0, 1]^p \). For a sufficiently large \( b_n \), it is expected that the split-points are evenly distributed such that there exists \( z_i \) that is sufficiently close to each boundary of the tree partition \( X^* \). This would make the split-net \((X^*, c_n)\)-dense for some suitable \( c_n \geq 0 \). Moreover, since split-points are generated from a uniform distribution, midpoint-splits are likely to occur nearly at the center of the cells for a sufficiently large \( b_n \). This would make the split-net \((Ω_r^*, α_r, L_0, S_0)\)-regular for \( r = 1, \ldots, R \). The following lemma formally verifies this conjecture.

**Lemma 2** (Uniformly generated split-net). Consider a split-net \( Z \) uniformly generated on \([0, 1]^p \) with \( b_n = n^c \) for some suitably large constant \( c > 0 \). If \( \log λ + \log d \lesssim \log n \), \( \log \min_{r,j} |Ξ^*_r|_j \gtrsim −d^{-1} \log n \), and \( R = o(n) \), then \( Z \) is \((X^*, c_n)\)-dense and \((Ω_r^*, α_r, L_0, S_0)\)-regular with high probability for \( r = 1, \ldots, R \), where \( c_n = n^{-c/2}1(R > 1) \).

**Proof.** See Section B.3 in Appendix. \( \square \)

Based on the lemma above, we can assume that a generated \( Z \) is appropriately dense and regular. The implication is then similar to that of Lemma 1. That is, we obtain (i) of Theorem 1 if \( R = 1 \) (observe that the conditions \( \log \min_{r,j} |Ξ^*_r|_j \gtrsim −d^{-1} \log n \) and \( R = o(n) \)
are trivially satisfied in this case). If \( R > 1 \), the assertions in (ii), (iv), and (v) of Theorem 1 also hold with a sufficiently large \( c \), while (iii) always holds. Note that \( b_n \) should satisfy \( \log b_n \lesssim \log n \), which is also necessary for optimal posterior contraction. Hence, a uniformly generated split-net can be used for high-dimensional problems as well as low-dimensional models, which allows us to randomly generate a split-net in most situations for practical purposes.

**Remark 7.** One may generate split-points using other distributions rather than a uniform distribution. If the density of a chosen distribution is bounded away from zero on \([0, 1]^p\), the generated points should also be evenly distributed and we believe that the above results will also follow. Similar to Remark 6, this flexibility may be particularly useful in regression as the distribution of covariates can be used to generate a split-net if available.

### 4.3.3 Fixed design points

Now we focus on a fixed design regression setup, where observed covariate values are readily available. Although the above two split-nets can be used for regression, using fixed design points is particularly appealing in that (iii) of Theorem 1, coupled with this split-net, gives an approximation error relative to the empirical probability measure, no matter what \( c_n \) is. This strategy is a conventional technique in regression (Chipman et al., 1998; Denison et al., 1998; Chipman et al., 2010), and has some computational benefits as it ensures that every box contains at least one covariate value.

Suppose that a split-net \( \mathcal{Z} = \{z_i \in [0, 1]^p, i = 1, \ldots, n\} \) consists of the observed covariate values in a regression setup. We only assume that the design points are sufficiently evenly distributed such that for any box \( \Psi \subseteq [0, 1]^p \) and \( \alpha \in (0, 1]^d \), \( \mathcal{Z} \) is \((\Psi, \alpha, L, S_0)\)-regular for \( L = \lfloor \log_2 (n+1) \rfloor \), where \( n \) is the number of split-points in \( \mathcal{Z} \cap \text{int}(\Psi) \). Under this assumption, the following lemma can easily be obtained.

**Lemma 3 (Fixed design points).** Consider fixed design points \( \mathcal{Z} = \{z_i, i = 1, \ldots, n\} \) with the assumption above. If \( \lambda d \lesssim (n/R)^{\alpha_r/d} \sqrt{\log n} \) and \( \min_r P_\mathcal{Z}(\Xi^*_r) \gtrsim R^{-1} \), then \( \mathcal{Z} \) is \((\Omega^*_r, \alpha_r, L_0, S_0)\)-regular for \( r = 1, \ldots, R \).

**Proof.** See Section B.4 in Appendix.

Observe that \( n P_\mathcal{Z}(\Xi^*_r) \) is the number of split-points in \( \Xi^*_r \). Hence the condition \( \min_r P_\mathcal{Z}(\Xi^*_r) \gtrsim R^{-1} \) implies that the number of split-points should be balanced well. The condition \( \lambda d \lesssim (n/R)^{\alpha_r/d} \sqrt{\log n} \) slightly relaxes the condition \( \lambda d \lesssim \sqrt{\log n} \) of Theorem 4.1 in Ročková and van der Pas (2017). The two conditions are comparable if we take \( \alpha_r \to 0 \) from the practical perspective. We see that (iii) of Theorem 1 directly follows from this lemma. Since design points are used as \( \mathcal{Z} \), the term \( \|f_0 - f_0^\Lambda\|_{v, P_\mathcal{Z}} \) is translated into the approximation error relative the empirical probability measure. In regression setups, this fact makes fixed design points much more attractive than other split-nets in the previous sections. We also note that the requirement \( \log b_n \lesssim \log n \) for the optimal posterior contraction is trivially satisfied in this case.
5 Asymptotic results in nonparametric regression

5.1 Posterior contraction with Bayesian forests

Regression trees are an archetypal example of Bayesian forests (Chipman et al., 1998; Denison et al., 1998; Chipman et al., 2010). For a fixed design Gaussian nonparametric regression, Roˇckov´a and van der Pas (2017) and Roˇckov´a and Saha (2019) established $L_2$ rate-optimal posterior contraction of BART for high-dimensional isotropic regression functions. Our investigation goes beyond these studies in three aspects: (i) we treat the variance parameter $\sigma^2$ as unknown with a prior; (ii) we consider both fixed and random regression design; and, most importantly, (iii) the true function is assumed to be in the piecewise heterogeneous anisotropic space introduced earlier. The last point significantly enlarges the optimality scope of BART.

We separately deal with fixed and random designs. This section is focused on the fixed design case, while the random design case will be considered in Section 6 in Appendix. The fixed design regression model writes as

$$Y_i = f_0(x_i) + \varepsilon_i, \quad \varepsilon_i \sim N(0, \sigma^2_0), \quad i = 1, \ldots, n,$$

(4)

where $x_i = (x_{i1}, \ldots, x_{ip}) \in [0,1]^p, i = 1, \ldots, n$, are fixed. The model is independent but not identically distributed, and hence the asymptotic studies are established under the product measure for the $n$ observations. The general theory of posterior contraction requires an exponentially powerful test function of a semimetric under this product measure (Ghosal and van der Vaart, 2017). In nonparametric regression with a fixed design, such a good test function can be directly constructed for the empirical $L_2$-distance even when the noise error is unknown (Salomond, 2018). We also refer to Ning et al. (2020) and Jeong and Ghosal (2019) for the construction of relevant test functions with respect to the R´enyi divergence. The general theory also requires desirable properties of the prior. We show that the tree priors in Section 3 satisfy those conditions.

We impose the following assumptions on the true parameters.

(A1) The true function $f_0$ satisfies $f_0 \in \Gamma^{A,d,p}(\mathfrak{X}; \alpha_*)$ or $f_0 \in \Gamma^{A,d,p}(\mathfrak{X}; \alpha_*) \cap C([0,1]^p)$ for some $d > 0$, $\lambda > 0$, $\mathfrak{X} = (\Xi_1, \ldots, \Xi_R)$, and $A = (\alpha_r)_{r=1}^R$ with $\alpha_r = (\alpha_{rd})_{d=1}^d \in (0,1)^d$ such that $d^{-1} \sum_{j=1}^d \alpha_{rd, j}^{-1} = \alpha_*^{-1}$.

(A2) It is assumed that $d$, $p$, $\lambda$, $R$, and $A$ satisfy $d = o(\log n)$, $d \log p = o(n)$, $\lambda = o(n^{\alpha_*/d})$, and $R = o(n)$.

(A3) The true function $f_0$ satisfies $\|f_0\|_\infty \lesssim \sqrt{\log n}$.

(A4) The true variance parameter satisfies $\sigma^2_0 \in [c^{-1}, c]$ for some sufficiently large $c > 1$.

The assumption (A1) means that the true regression function $f_0$ lies on a sparse piecewise heterogeneous anisotropic space. If the continuity assumption is further imposed, the approximation results in Theorem 1 are obtained under milder conditions. The condition (A2) is required to make our rate tend zero (see the rate in (5) below). These two fundamental assumptions will also be required for other applications in Section 6. The boundedness condition in (A3) is made to guarantee a sufficient prior concentration under the normal prior on the step-heights specified in (P3) below. Although the Gaussian prior can be replaced with a ticker-tailed prior (e.g., Roˇckov´a, 2020), we only consider the Gaussian prior to leverage its semi-conjugacy. The assumption (A4) allows one to assign a standard prior to $\sigma^2$, e.g., an inverse gamma distribution.
A careful prior specification is required to obtain the optimal posterior contraction. We consider the following prior distributions.

(P1) The subset index $S$ is endowed with a sparsity prior in $(2)$.

(P2) Given $S$, each tree $T^t$ for $t = 1, \ldots, T$ is independently assigned either the Galton-Watson process prior or the Bayesian CART prior.

(P3) The step-heights $B$ are assigned a normal prior with a zero-mean and a covariance matrix whose eigenvalues are suitably bounded below and above.

(P4) The variance parameter $\sigma^2$ is assigned an inverse gamma prior.

As explained in Section 3.2, the Galton-Watson process prior has no practical issue with implementation, and hence may be preferred to the Bayesian CART prior in terms of the actual computation. However, it requires an additional condition on a split-net $Z$ as seen in (A7) below, though the extra condition is certainly mild.

Lastly, it is important to choose a suitable split-net so that Theorem 1 can be deployed. We need an approximation result with respect to the empirical $L_2$-norm $\| \cdot \|_n$, where $\| f \|_n^2 = n^{-1} \sum_{i=1}^n |f(x_i)|^2$. We make the following assumptions on the split-net $Z$.

(A5) The number $b_n$ of split-points in $Z$ satisfies $\log b_n \lesssim \log n$.

(A6) The split-net $Z$ is suitably dense and regular to construct a $Z$-tree partition $\hat{T}$ such that there exists $f_0^* \in \mathcal{F}_T$ satisfying $\| f_0 - f_0^* \|_n \lesssim \varepsilon_n$ by Theorem 1.

(A7) If the Galton-Watson process prior is used for tree topologies, the $Z$-tree partition $T^* = (\Omega_1^*, \ldots, \Omega_R^*)$ approximating $X^*$, a sub-tree used to construct $\hat{T}$, satisfies $\max_r \text{dep}(\Omega_r^*) \lesssim \log n$.

As mentioned in Section 4, the assumption (A5) is required for a suitable bound of the entropy and a good prior concentration (see Lemmas 4 and 7). The assumption (A6) provides the desired approximation error with respect to the $\| \cdot \|_n$-distance. Due to Theorem 1 and Lemma 3, using fixed design points as $Z$ is of particular interest. The last assumption (A7) is required only when the Galton-Watson process prior is employed. An intuitive explanation is as follows. If $\max_r \text{dep}(\Omega_r^*)$ is too large, the depth of the terminal nodes of the entire approximator $\hat{T}$ is not controlled very well. Since the Galton-Watson process prior penalizes the depth of trees, this may give rise to insufficient prior mass for the approximator $\hat{T}$. On the other hand, the Bayesian CART prior does not require (A7) as it directly penalizes the total number of terminal nodes. One may scrutinize Lemma 7 in Appendix for more details. Nevertheless the condition (A7) is certainly mild. Note also that the condition is trivially satisfied if $R = 1$.

Under the above assumptions and priors, the following theorem formally investigates posterior contraction under the model (4).

**Theorem 2** (Nonparametric regression, fixed design). Consider the model (4) with the assumptions (A1)–(A7). The prior is assigned through (P1)–(P4). Then, there exists a constant $M > 0$ such that

$$
\mathbb{E}_0 \Pi \left\{ (f, \sigma^2) : \| f - f_0 \|_n + |\sigma^2 - \sigma_0^2| > M \epsilon_n \mid Y_1, \ldots, Y_n \right\} \to 0,
$$

where

$$
\epsilon_n = \sqrt{\frac{d \log p}{n}} + (\lambda d)^{d/(2\alpha + d)} \left( \frac{R \log n}{n} \right)^{\alpha(2\alpha + d)}.
$$

(5)
Proof. See Section B.5 in Appendix.

Intuitively, the rate in (5) resembles a near-minimax rate of estimation of high-dimensional anisotropic functions. The first part in (5) is the near-minimax risk of the penalty for not knowing the subset $S_0$ (Raskutti et al., 2011). The second part in (5) is incurred by anisotropic regression function estimation. Although $\lambda$ and $R$ can be an arbitrary polynomial in $n$ with a suitably small power to satisfy $\epsilon_n \to 0$, a particularly interesting case is when both are at most $\log c n$ for some $c > 0$. The second term then corresponds to the near-minimax rate of anisotropic function estimation (Hoffman and Lepski, 2002). Whether or not the rate (2) is in fact the actual (near) minimax rate remains to be established. The answer to this question is provided in the following subsection, where we formally derive the minimax rate with respect to the $L_2$-risk.

**Remark 8.** In isotropic regression using BART, Ročková and van der Pas (2017) assumed that the first part of the rate in (5) is dominated by the second part, whereby the resulting rate is simplified such that it only depends on the risk of function estimation. Since this restriction is not required, we keep the rate in its current form.

### 5.2 Minimax optimality

In Section 5.1, we established the posterior contraction rate of Bayesian forests in Gaussian nonparametric regression under relaxed smoothness assumptions. Although the rate (2) consists of two logical components (a penalty for variable selection uncertainty and a rate of anisotropic function estimation), it is not guaranteed that the whole rate is (near) minimax optimal. While minimax rates in high-dimensional isotropic function estimation were studied exhaustively in Yang and Tokdar (2015), extensions to (piecewise) anisotropic functions have not been obtained in the literature. We fill this gap by deriving the minimax rates in our general smoothness setup. These results will certify that the rates obtained in Section 5.1 are indeed minimax optimal (with respect to the $L_2$-risk), up to a logarithmic factor.

To deploy the conventional minimax theory, we consider the model with a random design given by

$$ Y_i = f_0(X_i) + \varepsilon_i, \quad X_i \sim Q, \quad \varepsilon_i \sim N(0, \sigma_0^2), \quad i = 1, \ldots, n, $$

where $X_i = (X_{i1}, \ldots, X_{ip}), \ i = 1, \ldots, n$, are $p$-dimensional random covariates and $Q$ is a probability measure such that $\text{supp}(Q) \subseteq [0,1]^p$. Specifically, we use the Le Cam equation (Birgé and Massart, 1993; Wong and Shen, 1995; Barron et al., 1999). Now the density $q$ of $Q$ is assumed to satisfy the following assumption.

\begin{align*}
(A8) \text{There exist constants } 0 < q \leq \overline{q} \leq \infty \text{ such that the density } q \text{ satisfies } q \leq \inf_x q(x) \leq \sup_x q(x) \leq \overline{q}.
\end{align*}

The $L_2(Q)$-norm is simply replaced by $L_2$-norm under this assumption. We define the minimax risk for any function space $\Sigma \in L_2(Q)$ as $r_n^2(\Sigma, Q) = \inf_{f \in A_n} \sup_{f_0 \in \Sigma} \mathbb{E}_{f_0,Q} \| \hat{f} - f_0 \|_{L_2,Q}^2$, where $A_n$ is the space of all $L_2(Q)$-measurable function estimators and $\mathbb{E}_{f,Q}$ is the expectation operator under the model with $f$ and $Q$.

Now, we formally investigate the minimax rates with respect to the $L_2$-risk. We first assume (without loss of generality) that $\sigma_0^2$ is fixed to 1. The function space is assumed to be
uniformly bounded for the Le Cam equation to be used. We thus define the bounded space \( \Gamma_{\lambda}^{A,d,p}(x; \alpha_*) = \{ f \in \Gamma_{\lambda}^{A,d,p}(x; \alpha_*) : \| f \|_\infty \leq \lambda \} \). For a given partition \( X = (\Xi_1, \ldots, \Xi_R) \) of \([0, 1]^d\), we also assume that the size of each box is bounded away from zero, i.e., \( \min_{r,j} |\Xi_r|_j \gtrsim 1 \). The following theorem provides the minimax rate over the space \( \Gamma_{\lambda}^{A,d,p}(x; \alpha_*) \cap C([0, 1]^p) \).

**Theorem 3** (Minimax rate). Consider the model (6) with the assumptions (A8) and \( \sigma_d^2 = 1 \).

Then, for any \( d \in \mathbb{N}, p \geq d, \lambda > 0, R \in \mathbb{N} \), a partition \( X = (\Xi_1, \ldots, \Xi_R) \) of \([0, 1]^d\) with \( \min_{r,j} |\Xi_r|_j \gtrsim 1 \), and smoothness parameters \( A = (\alpha_r)_{r=1}^R \) with \( \alpha_r = (\alpha_{r1}, \ldots, \alpha_{rd})' \in (0, 1]^d \) such that \( d^{-1} \sum_{j=1}^d \alpha_{rj}^{-1} = \alpha_*^{-1} \), \( r = 1, \ldots, R \), there exist constants \( M_{1,\alpha_*,d} > 1 \) (depending only on \( \alpha_* \) and \( d \)) and \( M_{2,\alpha_*,d,R} > 1 \) (depending only on \( \alpha_* \), \( d \), and \( R \)) such that

\[
M_{1,\alpha_*,d}^{-1} \gamma_n \leq \tau_n(\Gamma_{\lambda}^{A,d,p}(x; \alpha_*) \cap C([0, 1]^p), Q) \leq M_{1,\alpha_*,d} \gamma_n,
\]

\[
M_{2,\alpha_*,d,R}^{-1} \gamma_n \leq \tau_n(\Gamma_{\lambda}^{A,d,p}(x; \alpha_*), Q) \leq M_{2,\alpha_*,d,R} \gamma_n,
\]

for large enough \( n \), where \( \gamma_n = n^{-1/2} \log^{1/2}(p/d) + (\lambda^d/n^{\alpha_*})^{1/(2\alpha_* + d)} \).

Proof. See Section B.6 in Appendix. \( \square \)

Interestingly, \( M_{1,\alpha_*,d} \) is free of \( R \). Assuming that \( R \) is at most \( \log^c n \) for some \( c > 0 \), Theorem 3 justifies that our rate in (5) is near-minimax optimal. Note that the term involving \( \lambda \) in our rate is not an artifact as it also appears in the minimax risk \( \gamma_n \).

### 6 Further applications

Besides the fixed design nonparametric regression in Section 5.1, we also investigate posterior contraction in nonparametric regression with a random design. Our findings also generalize to setups beyond nonparametric regression. In other words, we have shown that the general theory of posterior contraction (Ghosal et al., 2000; Ghosal and van der Vaart, 2007) is attainable. This is partly because the approximation results in Theorem 1 are given with many interesting metrics. In addition to the random design regression model, here we investigate posterior contraction properties in two more practical applications of Bayesian forests: density estimation and nonparametric binary classification.

#### 6.1 Nonparametric regression with a random design

Theorem 2 quantifies the speed of posterior contraction under a fixed regression design. However, the fixed design assumption cannot be easily justified when there are measurement errors (Tuo and Wu, 2015). A random design is also useful in estimation of functionals in causal inference (Hahn et al., 2020; Ray and van der Vaart, 2018). Although there are no differences between fixed and random designs in practice, theoretical studies require different renderings for random designs (Xie et al., 2019). To complete the characterization, below we study posterior contraction in nonparametric regression with a random design.

A nonparametric regression model with a random design can be expressed as the model (6) for \( Q \) a probability measure such that \( \text{supp}(Q) \subseteq [0, 1]^p \) with a bounded density. Unlike the model (4), the model (6) is i.i.d. The well-known fact that exponentially powerful tests exist with respect to the Hellinger metric \( p_H(\cdot, \cdot) \) allows one to establish the contraction rate for the corresponding metric (Ghosal et al., 2000). However, in normal models, the
Hellinger distance is matched to the $L_2$-type metric only when $f$ and $\log \sigma^2$ are uniformly bounded in the entire parameter space, not only for the true values (e.g., Xie and Xu, 2018). Unlike in Theorem 2, this restriction requires that $f_0$ be uniformly bounded and a prior be appropriately truncated. Note also that we need a good approximation error with respect to an integrated $L_2$-type. Below we summarize the required modifications of (A3), (A6), (P3), and (P4).

(A3*) The true function $f_0$ satisfies $\|f_0\|_\infty \leq C$ for some sufficiently large $C > 0$. 

(A6*) The split-net $Z$ is suitably dense and regular to construct a $Z$-tree partition $\hat{T}$ such that there exists $f^0_\Lambda \in \mathcal{F}_{\hat{T}}$ satisfying $\|f_0 - f^0_\Lambda\|_2 \lesssim \bar{\epsilon}_n$ by Theorem 1.

(P3*) A prior on the compact support $[-\bar{C}, \bar{C}]$ is assigned to the step-heights $B$ for some $\bar{C} > C$.

(P4*) A prior on the compact support $[\bar{c}^{-1}, \bar{c}]$ is assigned to $\sigma^2$ for some $\bar{c} > c$.

Note that (A6*) requires good approximability with respect to the $L_2$-norm. Due to Theorem 1, a complete grid and a uniformly generated split-net in Sections 4.3.1–4.3.2 are useful to meet this requirement. We wrap up this section with a theorem that formalizes posterior contraction of Bayesian forests under the model (6).

**Theorem 4** (Nonparametric regression, random design). Consider the model (6) with the assumptions (A1), (A2), (A3*), (A4), (A5), (A6*), and (A7). The prior is assigned through (P1), (P2), (P3*), and (P4*). Then, there exists a constant $M > 0$ such that for $\epsilon_n$ in (5),

$$\mathbb{E}_0 \Pi \left\{ (f, \sigma^2) : \|f - f_0\|_{2,Q} + |\sigma^2 - \sigma^2_0| > M\epsilon_n \mid (X_1, Y_1), \ldots, (X_n, Y_n) \right\} \to 0.$$

*Proof.* See Section B.5.

### 6.2 Density estimation

For some probability measure $P$ such that $\text{supp}(P) \subseteq [0, 1]^p$, suppose $n$ independent observations $X_i$, $i = 1, \ldots, n$, are drawn from $P$, i.e.,

$$X_i \sim P, \quad i = 1, \ldots, n. \quad (7)$$

Assume that $P$ is absolutely continuous with respect to the Lebesgue measure with the true density $p_0$. We assign a prior on $p_f$ indexed by $f$ such that $p_f = \exp(f) / \int_{[0,1]^p} \exp(f(x)) \, dx$ with $f$ assigned the forest priors in Section 3. We write $f_0 = \log p_0$ while assuming (A1)–(A3). We leverage the existence of an exponentially powerful test for the Hellinger metric $\rho_H(\cdot, \cdot)$. Due to the relationship between Hellinger balls and supremum-norm balls in density estimation with the exponential link, we need the approximation results with respect to the supremum-norm. These are obtained by (i) or (iv) of Theorem 1, requiring the following assumption on a split-net.

(A6†) The split-net $Z$ is suitably dense and regular to construct a $Z$-tree partition $\hat{T}$ such that there exists $f^0_\Lambda \in \mathcal{F}_{\hat{T}}$ satisfying $\|f_0 - f^0_\Lambda\|_\infty \lesssim \bar{\epsilon}_n$ by Theorem 1.
As mentioned above, if \( f_0 \in \Gamma_{\lambda}^{A,d,p}(\mathcal{X}; \alpha_*) \), this assumption may be restrictive unless \( f_0 \) has globally anisotropic smoothness over the entire domain, i.e., \( R = 1 \). If \( f_0 \in \Gamma_{\lambda}^{A,d,p}(\mathcal{X}; \alpha_*) \cap \mathcal{C}([0,1]^p) \), the assumption is relatively easily satisfied as we only need to verify (iv) of Theorem 1. If \( f_0 \in \Gamma_{\lambda}^{A,d,p}(\mathcal{X}; \alpha_*) \) and \( R > 1 \), the underlying partition \( \mathcal{X}^* \) should be a Z-tree partition, and thus the split-net should be very nicely distributed to exactly detect the boundaries in \( \mathcal{X}^* \). This limitation makes the latter case far less practical. Under suitable assumptions, the following theorem provides the posterior contraction rate of \( p_f \) with respect to the Hellinger distance.

**Theorem 5** (Density estimation). Consider the model (7) with the assumptions (A1)–(A3), (A5), (A6†), and (A7). The prior is assigned through (P1)–(P3). Then, there exists a constant \( M > 0 \) such that for \( \epsilon_n \) in (5),

\[
\mathbb{E}_0 \Pi \left\{ f : \rho_H(p_f, p_0) > M \epsilon_n \mid X_1, \ldots, X_n \right\} \to 0.
\]

**Proof.** See Section B.7.

It should be noted that we have again used the normal prior in (P3). As mentioned in Section 5.1, this is not necessary and a heavy-tailed prior can relax the assumption on \( \|f\|_0 \). Unlike Theorem 2, there is no advantage of a normal prior as it is not conjugate in the density estimation example. This is also the case in the example of binary classification given in the next subsection. Nevertheless, we employ (P3) for the sake of simplicity.

### 6.3 Nonparametric binary classification

For a binary response \( Y_i \in \{0, 1\} \) and a random covariate \( X_i \in \mathbb{R}^p \), assume that we have \( n \) independent observations \( (X_1, Y_1), \ldots, (X_n, Y_n) \) from the binary classification model:

\[
\mathbb{P}_0(Y_i = 1 \mid X_i = x) = \varphi_0(x), \quad X_i \sim Q, \quad i = 1, \ldots, n,
\]

for some \( \varphi_0 : [0,1]^p \mapsto [0,1] \) and some probability measure \( Q \) such that \( \text{supp}(Q) \subseteq [0,1]^p \) with a bounded density. We parameterize the probability function using the logistic link function \( H : \mathbb{R} \mapsto [0,1] \) such that \( \varphi_f = H(f) \) for \( f \) on which the forest priors in Section 3 are assigned. For true function \( \varphi_0 \), we write \( f_0 = H^{-1}(\varphi_0) \) while assuming (A1)–(A3) as in the density estimation problem. In the proof, it will be shown that the Hellinger metric is bounded by the \( L_2(Q) \)-distance in this example, and hence (A6*) is assumed. This means that the required assumption on the split-net is weaker than density estimation. The following theorem formalizes the posterior contraction rate of \( \varphi \) with respect to the \( L_2(Q) \)-distance.

**Theorem 6** (Binary classification). Consider the model (8) with the assumptions (A1)–(A3), (A5), (A6*), and (A7). The prior is assigned through (P1)–(P3). Then, there exists a constant \( M > 0 \) such that for \( \epsilon_n \) in (5),

\[
\mathbb{E}_0 \Pi \left\{ f : \|H(f) - H(f_0)\|_{2,Q} > M \epsilon_n \mid (X_1, Y_1), \ldots, (X_n, Y_n) \right\} \to 0.
\]

**Proof.** See Section B.7.
7 Discussion

In this paper, we have enlarged the scope of theoretical understanding of Bayesian forests in the context of function estimation by considering relaxed smoothness assumptions. We introduced a new class of piecewise anisotropic sparse functions, which form a blend of anisotropy and spatial inhomogeneity. We have derived the minimax rate of estimation of these functions in high-dimensional regression setups, extending existing results obtained earlier only for isotropic functions. Next, we have formalized that Bayesian forests attain the near-optimal posterior concentration rate for these general function classes without any need for prior modification. Our results apply to a general class of estimation problems including nonparametric regression with a fixed and random design, binary classification, and density estimation.

Appendix

A Cardinality of tree topologies

Here we provide a lemma that gives an upper bound of the cardinality of tree topologies. The lemma plays an important role in both computational and theoretical aspects. The results can be viewed as a generalization of Lemma 3.1 of Ročková and van der Pas (2017).

Lemma 4 (Cardinality of tree topologies). For a given $S \subseteq \{1, \ldots, p\}$ and $Z = \{z_i \in [0,1]^p, i = 1, \ldots, b_n\}$, let $\mathbb{T}_{S,K}$ be the set of $S$-sparse $Z$-tree partitions of size $K$. Then, the cardinality $\#\mathbb{T}_{S,K}$ of $\mathbb{T}_{S,K}$ satisfies

$$\#\mathbb{T}_{S,K} \leq \frac{|S|^K - 1}{b_n - K + 1}.$$  \hfill (9)

In particular, the equality holds if the points $z_i$ in $Z$ projected onto each coordinate in $S$ are not duplicated such that no split eliminates the possibility of other splits.

Proof. Given $S$ and $K$, the cardinality is maximized when no split eliminates the possibility of other splits. In this case, it is easily shown that the cardinality is the same as the right-hand side of (9), following the proof of Lemma 3.1 of Ročková and van der Pas (2017). The proof of the assertion is thus complete.

Note that the equality in (9) holds if there are no ties in $Z$ for every coordinate, which gives the exact evaluation of $\#\mathbb{T}_{S,K}$. We believe that there is no simple expression for $\#\mathbb{T}_{S,K}$ in general situations with possible ties.

B Proofs

B.1 Proof of Theorem 1

Proof of Theorem 1. We let $f_0^N(x) = \sum_{r,k} \mathbb{1}_{\Omega_r^+} (x)\beta_{r,k,0}$, where $\beta_{r,k,0} = f_0(y_{rk})$ for some $y_{rk} \in \Omega_r^+ \cap \Xi_r^*$, such that we have

$$f_0(x) - f_0^N(x) = \sum_{r=1}^{R} \sum_{k=1}^{2^{q_0}} \mathbb{1}_{\Omega_r^+} (x)(f_0(x) - f_0(y_{rk})).$$
For any \( x \in \Omega^\dagger_{rk} \), define \( x^* = \arg\min_{z \in \Omega^\dagger_{rk} \cap \Xi_r^c} \| x - z \|_1 \), i.e., \( x^* = x \) if \( x \in \Omega^\dagger_{rk} \cap \Xi_r^c \). Below, we verify the assertions for each of the given metrics.

**Verification of (i) and (iv):** We first prove (iv). In what follows, we write \( S_0 = \{ s_{0,1}, \ldots, s_{0,d} \} \).

For any \( x \in \Omega^\dagger_{rk} \) with given \( r, k \), note that \( |f_0(x) - f_0(x^*)| \leq \lambda \sum_{j=1}^d |x_{s_{0,j}} - x^*_{s_{0,j}}|^{\min_{r,j} \alpha_{r,j}} \) since \( f_0 \) is continuous. This is further bounded by \( \lambda d c_n^{\min_{r,j} \alpha_{r,j}} \) since \( \| x - x^* \|_\infty \leq c_n \). Hence, by the triangle inequality, for any \( r, k \),

\[
1_{\Omega^\dagger_{rk}}(x)|f_0(x) - f_0(y_{rk})| \leq 1_{\Omega^\dagger_{rk}}(x) \lambda d c_n^{\min_{r,j} \alpha_{r,j}} + 1_{\Omega^\dagger_{rk}}(x)|f_0(x^*) - f_0(y_{rk})|. \tag{10}
\]

For \( l_{rj} \) returned by \( AKD(\Omega^\dagger_r; \mathcal{Z}, \alpha, L_0, S_0) \) such that \( L_0 = \sum_{j=1}^d l_{rj}, r = 1, \ldots, R \), observe that

\[
1_{\Omega^\dagger_{rk}}(x)|f_0(x^*) - f_0(y_{rk})| \leq 1_{\Omega^\dagger_{rk}}(x) \lambda \sum_{j=1}^d |\Omega^\dagger_{rk}s_{0,j}|^{\alpha_{r,j}} \leq 1_{\Omega^\dagger_{rk}}(x) \lambda \sum_{j=1}^d 2^{-\alpha_{r,j}l_{rj}} \tag{11}
\]

since \( x^*, y_{rk} \in \Omega^\dagger_{rk} \cap \Xi_r^c \subseteq \Xi^c_r \). Let \( \tilde{l}_{rj} = L_0 \alpha_{r,j} / (d \alpha_{r,j}) \) for \( r = 1, \ldots, R, j = 1, \ldots, d \), such that \( \alpha_{r,1} \tilde{l}_{r1} = \cdots = \alpha_{r,d} \tilde{l}_{rd} \) and \( L_0 = \sum_{j=1}^d \tilde{l}_{rj} \) for every \( r \) (note that \( \tilde{l}_{rj} \) are not integers). Then it can be seen that \( l_{rj} > \tilde{l}_{rj} - 1 \) for every \( r, j \), and hence

\[
\lambda \sum_{j=1}^d 2^{-\alpha_{r,j}l_{rj}} \leq 2\lambda \sum_{j=1}^d 2^{-\alpha_{r,j}\tilde{l}_{rj}} \leq 2\lambda d 2^{-\alpha_r} L_0 / d. \tag{12}
\]

Putting the bounds together, we obtain

\[
\| f_0 - f_0^\Lambda \|_\infty \lesssim \lambda d \left( c_n^{\min_{r,j} \alpha_{r,j}} + 2^{-\alpha_r} L_0 / d \right),
\]

which verifies (iv). To prove (i), note that if \( x \in \Omega^\dagger_{rk} \cap \Xi^c_r, |f_0(x) - f_0(x^*)| \) is not well-bounded as before due to the possible discontinuity of \( f_0 \). However, if \( \Omega^\dagger_{rk} \cap \Xi^c_r = \Omega^\dagger_{rk} \) for every \( r, k \) (i.e., \( c_n = 0 \)), we always have

\[
1_{\Omega^\dagger_{rk}}(x)|f_0(x) - f_0(y_{rk})| = 1_{\Omega^\dagger_{rk}}(x)|f_0(x^*) - f_0(y_{rk})|,
\]

in place of (10). The rest of the proof can easily be completed by following that of the assertion (iv).

**Verification of (ii) and (iii):** To verify these assertions, we first show that when \( f_0 \in \Gamma^A_{\alpha, \mu}(\mathcal{X}; \alpha, \mu) \), for any finite measure \( \mu \) and any \( v \geq 1 \), we have that \( \| f_0 - f_0^\Lambda \|_{v,\mu} \lesssim \tilde{c}_n \) if \( \sum_{r=1}^R \mu(\Omega^c_r \cap \Xi^c_r) \lesssim (\tilde{c}_n / \| f_0 \|_\infty)^v \). Observe that

\[
\int |f_0(x) - f_0^\Lambda(x)|^v d\mu(x) = \sum_{r=1}^R \sum_{k=1}^{2^{k_0}} \int_{\Omega^\dagger_{rk}} |f_0(x) - f_0(y_{rk})|^v d\mu(x). \tag{13}
\]

The integral term in each summand is bounded by

\[
\int_{\Omega^\dagger_{rk} \cap \Xi^c_r} |f_0(x) - f_0(y_{rk})|^v d\mu(x) + \mu(\Omega^\dagger_{rk} \cap \Xi^c_r)(2\| f_0 \|_\infty)^v.
\]
Using (11)–(12) again, we see that the first term is bounded by
\[ \mu(\Omega^\dagger_{r_k} \cap \Xi^*_r) \left( \lambda \sum_{j=1}^d |\Omega^\dagger_{r_k}|_{\alpha_{r_j}} \right)^v \lesssim \mu(\Omega^\dagger_{r_k} \cap \Xi^*_r) \left( \lambda d 2^{-\alpha^* L_0/d} \right)^v. \]

Note also that \( \sum_k \mu(\Omega^\dagger_{r_k} \cap \Xi^* c) = \mu(\Omega^*_r \cap \Xi^* c). \) Therefore,
\[ \|f_0 - f_0^\Lambda\|_{v, \mu} \lesssim \sum_{r=1}^R \sum_{k=1}^{2L_0} \left\{ \mu(\Omega^\dagger_{r_k} \cap \Xi^*_r) \left( \lambda d 2^{-\alpha^* L_0/d} \right)^v + \mu(\Omega^\dagger_{r_k} \cap \Xi^*_r c) \right\} \|f_0\|_{\infty}^v \]
\[ \leq \mu([0, 1]^p) \left( \lambda d 2^{-\alpha^* L_0/d} \right)^v + \|f_0\|_{\infty}^v \sum_{r=1}^R \mu(\Omega^*_r \cap \Xi^* c). \]

This leads to the desired assertion. Now, to verify (ii), take the Lebesgue measure for \( \mu. \) Observe that
\[ \mu(\Omega^*_r \cap \Xi^* c) = \prod_{j=1}^d |\Omega^*_r \cap \Xi^*_{r_j}|_{s_{0,j}} \leq \sum_{j=1}^d |\Omega^*_r \cap \Xi^*_{r_j}|_{s_{0,j}} \prod_{k \neq j} |\Omega^*_r \cap \Xi^*_{r_k} |_{s_{0,k}} \leq \frac{dc_n \text{vol}(\Omega^*_r)}{\min_j |\Omega^*_r|_j}. \]

Since \( |\Omega^*_r|^j \geq |\Xi^*|^j - 2c_n, \)
\[ \sum_{r=1}^R \mu(\Omega^*_r \cap \Xi^* c) \leq \frac{dc_n}{\min_j |\Xi^*|^j - 2c_n} \leq \frac{2dc_n}{\min_j |\Xi^*|^j}. \]

Plugging in this, we see that \( \sum_{r=1}^R \mu(\Omega^*_r \cap \Xi^* c) \lesssim (\epsilon_n/\|f_0\|_{\infty})^v \) if \( c_n \lesssim (\epsilon_n/\|f_0\|_{\infty})^{v \min_{r,j} |\Xi^*|^j/d}. \)
Hence (ii) is verified. To verify (iii), now take \( P_\Xi \) for \( \mu. \) Then, it can be seen that split-points can be picked up such that there are no \( z_i \) on \( \cup_r (\Omega^*_r \cap \Xi^* c) \) by choosing the points closest to the boundaries. Since we have \( \sum_{r=1}^R \mu(\Omega^*_r \cap \Xi^* c) = 0 \) in this case, (iii) is verified.

Verification of (v): Similar to the above, we first show that when \( f_0 \in \Gamma^{A, d, p}(\Xi; \alpha_s) \cap C([0, 1]^p), \) for an any finite measure \( \mu \) and any \( v \geq 1, \) we have that \( \|f_0 - f_0^\Lambda\|_{v, \mu} \lesssim \epsilon_n \) if \( c_n^{v \min_{r,j} \alpha_{r,j}} \sum_{r=1}^R \mu(\Omega^*_r \cap \Xi^*_c) \lesssim (\epsilon_n/\lambda)^v. \) We start from the identity in (13). Observe that the integral term in (13) is bounded by
\[ \mu(\Omega^\dagger_{r_k} \cap \Xi^*_r) \left( \lambda \sum_{j=1}^d |\Omega^\dagger_{r_k}|_{\alpha_{r_j}} \right)^v + \int_{\Omega^\dagger_{r_k} \cap \Xi^*_c} |f_0(x) - f_0(y_{rk})|^v \, d\mu(x). \]  

For any \( v \geq 1, \) the second term of the last display is bounded by
\[ 2^{v-1} \int_{\Omega^\dagger_{r_k} \cap \Xi^*_c} \left( |f_0(x) - f_0(x^*)|^v + |f_0(x^*) - f_0(y_{rk})|^v \right) \, d\mu(x) \]
\[ \leq 2^{v-1} \mu(\Omega^\dagger_{r_k} \cap \Xi^*_c) \left\{ \left( \lambda d c_n^{v \min_{r,j} \alpha_{r_j}} \right)^v + \left( \lambda \sum_{j=1}^d |\Omega^\dagger_{r_k}|_{\alpha_{r_j}} \right)^v \right\}, \]
where the inequality holds since \( |f_0(x) - f_0(x^*)| \leq \lambda d c_n^{v \min_{r,j} \alpha_{r_j}} \) by the argument used to verify (iv). Hence, (15) is further bounded by a constant multiple of
\[ \mu(\Omega^\dagger_{r_k}) \left( \lambda d 2^{-\alpha^* L_0/d} \right)^v + \mu(\Omega^\dagger_{r_k} \cap \Xi^*_c) \left( \lambda d c_n^{v \min_{r,j} \alpha_{r_j}} \right)^v, \]
and we have that
\[ \|f_0 - f_0^h\|_\nu \lesssim \sum_{r=1}^{R} \sum_{k=1}^{G} \left\{ \mu(\Omega_{rk}^*) \left( \lambda 2^{-\alpha_* L_0/d} \right)^v + \mu(\Omega_{rk}^* \cap \Xi^*) \left( \lambda d n^{-\alpha_{\min} j} \alpha_{\min} j \right)^v \right\} \]
\[ \lesssim \mu([0,1]^p) \left( \lambda 2^{-\alpha_* L_0/d} \right)^v + \left( \lambda d n^{-\alpha_{\min} j} \alpha_{\min} j \right)^v \sum_{r=1}^{R} \mu(\Omega_{r}^* \cap \Xi^*). \]

This leads to the desired assertion. Now, we take the Lebesgue measure for \( \mu \) to verify (v). Then similarly as before, we have that \( (\lambda d n^{-\alpha_{\min} j} \alpha_{\min} j) \sum_{r=1}^{R} \mu(\Omega_{r}^* \cap \Xi^*) \lesssim \epsilon_n^v \) if \( \epsilon_n^v \min_{r,j} |\Xi^*|_j / d \). This verifies (v).

### B.2 Proof of Lemma 1

To prove Lemma 1, we first give the following lemma which shows that a regular grid is dense and regular for arbitrary inputs under suitable conditions.

**Lemma 5** (Complete grid, general case). For a regular grid \( Z \), we have the following assertions.

(i) For any \( S \subseteq \{1, \ldots, p\} \) and any \( S \)-sparse flexible tree partition \( \mathcal{T} = (\Psi_1, \ldots, \Psi_J) \) with \( J \geq 2 \), \( Z \) is \( (\mathcal{Q}, 1/b_n^{1/p}) \)-dense if \( b_n^{1/p} \min_{r,j} |\Psi_{r,j}| \geq 1 \).

(ii) For any \( S \subseteq \{1, \ldots, p\} \), \( \alpha \in (0,1]^d \), \( \Psi \subseteq [0,1]^p \), and \( L = [\log_2(\lfloor b_n^{1/p} \min_j |\Psi_{j}| + 1\rfloor) \]

### Proof of (i): Note that each point \( z_i \) in \( Z \) is located at the center of each box of the \( p \)-dimensional checkerboard. Since the mesh-size of the checkerboard is \( 1/b_n^{1/p} \), there exists an \( S \)-sparse \( Z \)-tree partition \( \mathcal{T} \) such that \( \mathcal{Y}(\mathcal{Q}, \mathcal{T}) \leq 1/b_n^{1/p} \) if \( \min_{r,j} |\Psi_{r,j}| \geq 1/b_n^{1/p} \). The assertion easily follows.

### Proof of (ii): For any given \( \Psi \subseteq [0,1]^p \), the interval formed by projecting \( \Psi \) onto the \( j \)th coordinate contains at least \( \lfloor b_n^{1/p} |\Psi_{j}| \rfloor \) non-duplicated points projected onto the \( j \)th coordinate. We consider the worst case that all splits occur in the same direction. In this worst scenario, it can be seen that midpoint-splits can occur up to depth \( L \) such that \( 2L \leq [b_n^{1/p} \min_j |\Psi_{j}| + 1] \). The resulting boxes are naturally balanced due to the equispaced points in the complete grid. This leads to the assertion.

Now, we prove Lemma 1 below.

**Proof of Lemma 1.** If \( R = 1 \), it is obvious that \( Z \) is \((X^*, 0,0)^p \)-dense. If \( R > 1 \), by (i) of Lemma 5, \( Z \) is \((X^*, 1/b_n^{1/p}) \)-dense if \( b_n^{1/p} \min_{r,j} |\Xi^*|_j \geq 1 \). Then, there exists an \( S_0 \)-sparse \( Z \)-tree partition approximating \( X^* \), denoted by \( \mathcal{T}^* = (\Omega^*_1, \ldots, \Omega^*_R) \), such that \( \mathcal{Y}(X^*, \mathcal{T}^*) \leq 1/b_n^{1/p} \). Note that by (ii) of Lemma 5, \( Z \) is \((\Omega^*_r, \alpha_r, L_r, S_0)^p \)-regular for \( L_r = [\log_2(\lfloor b_n^{1/p} \min_j |\Omega^*_r|_j + 1\rfloor) \]

for a large enough \( C > 0 \). Due to the condition \( \log \min_{r,j} |\Xi^*|_j \geq -\log n \), this is trivially satisfied if \( c > 0 \) is chosen to be much larger than \( C \).
B.3 Proof of Lemma 2

Similarly as above, we first provide the following lemma for general cases.

Lemma 6 (Uniformly generated split-net, general case). For a split-net \( \mathcal{Z} \) uniformly generated on \([0,1]^p\), we have the following assertions.

(i) For any \( S \subseteq \{1, \ldots, p\} \) and \( S \)-sparse partition \( \Psi = (\Psi_1, \ldots, \Psi_J) \) with \( J \geq 2 \), \( \mathcal{Z} \) is \((\Psi, c_n)\)-dense with high probability for any \( c_n \geq 0 \) such that \( c_n b_n \min_{1 \leq r \leq J} \text{vol}(\Psi_r)/\log J \to \infty \).

(ii) For any \( S \subseteq \{1, \ldots, p\} \), \( \alpha \in (0,1]^d \), \( \Psi \subseteq [0,1]^p \), and \( L = [k \log_2(b_n \text{vol}(\Psi))] \) with \( 0 < k < 1/2 \), \( \mathcal{Z} \) is \((\Psi, \alpha, L, S)\)-regular with high probability if \( b_n \text{vol}(\Psi) \to \infty \).

(iii) For any \( S \subseteq \{1, \ldots, p\} \), any \( S \)-sparse partition \( \Psi = (\Psi_1, \ldots, \Psi_J) \) with \( J \geq 2 \), and \( L_r = [k \log_2(b_n \text{vol}(\Psi_r))] \) with \( 0 < k < 1/2 \), \( \mathcal{Z} \) is \((\Psi_r, \alpha, L_r, S)\)-regular with high probability for every \( r = 1, \ldots, J \) if \( b_n \min_{1 \leq r \leq J} \text{vol}(\Psi_r)/J \to \infty \).

Proof. Verification of (i): Consider the iterative procedure that generates the given flexible tree partition \( \Psi = (\Psi_1, \ldots, \Psi_J) \) via the binary tree partitioning rule with \( J - 1 \) splits. Starting from \([0,1]^p\), for every \( r = 1, \ldots, J - 1 \), we denote by \( \bar{\Psi}_r \) the interim box chosen for the \( r \)th split in a top-down manner. For example, in two dimension, a possible sequence could be \( \bar{\Psi}_1 = [0,1]^2 \), \( \bar{\Psi}_2 = [0,1] \times [0,1/2] \), \( \bar{\Psi}_3 = [1/3,1] \times [0,1/2] \), etc. For every \( r = 1, \ldots, J - 1 \), we let \( a_r \) be the split-point in the coordinate chosen for the split in \( \bar{\Psi}_r \). For example, in the two-dimensional example above, \( a_1 = 1/2 \), \( a_2 = 1/3 \), etc. We also write \( j_r \) for the coordinate for the \( r \)th split, i.e. for the above example, \( j_1 = 1 \), \( j_2 = 1 \), etc. We now define \( B_r = \{ x \in \bar{\Psi}_r \cap B_{r-1} : |x_{j_r} - a_r| \leq c_n \} \), a band around the \( r \)th split with radius \( 2c_n \). It suffices to show that with high probability, there exists at least one \( z_i \in \mathcal{Z} \) in each of \( B_r \). Writing \( U_i \) for a random variable having a uniform distribution on \([0,1]^p\), observe that

\[
\mathbb{P}(\text{at least one } z_i \text{ exists in each of } B_r) = 1 - \mathbb{P}\left( \bigcup_{i=1}^{b_n} \{ U_i \notin B_r, \ i = 1, \ldots, b_n \} \right) \\
\geq 1 - \sum_{r=1}^{J-1} \mathbb{P}(U_i \notin B_r, i = 1, \ldots, b_n).
\]

It is trivial to see that \( \mathbb{P}(U_i \notin B_r, i = 1, \ldots, b_n) = (1 - \text{vol}(B_r))^{b_n} \). Using the fact that \( B_{r-1} \) is excluded in the definition of \( B_r \), observe that \( \text{vol}(B_r) \geq 2c_n \text{vol}(\bar{\Psi}_r)/\text{vol}(\bar{\Psi}_r)_{j(r)} \geq 2c_n \text{vol}(\bar{\Psi}_r) \).

Since \( \min_{\Psi_r} \text{vol}(\bar{\Psi}_r) = \min_{\Psi_r} \text{vol}(\Psi_r) \), it follows that \( \min_{\Psi_r} \text{vol}(B_r) \geq 2c_n \min_{\Psi_r} \text{vol}(\Psi_r) \). Therefore, the last display is equal to

\[
1 - \sum_{r=1}^{J-1} (1 - \text{vol}(B_r))^{b_n} \geq 1 - (J - 1) \left( 1 - 2c_n \min_{1 \leq r \leq J} \text{vol}(\Psi_r) \right)^{b_n}.
\]

Observe that

\[
\log(J - 1) + b_n \log \left( 1 - 2c_n \min_{1 \leq r \leq J} \text{vol}(\Psi_r) \right) \leq \log J - 2c_nb_n \min_{1 \leq r \leq J} \text{vol}(\Psi_r)
\]

since \( \log(1-2x) \leq -2x \) for every \( x > 0 \). Therefore, (17) tends to one if \( c_n b_n \min_{\Psi_r} \text{vol}(\Psi_r)/\log J \to \infty \), which verifies the assertion.
Verification of (ii): We split $\Psi$ into $2^L$ pieces via $AKD(\Psi; Z, \alpha, L, S)$. Let $\bar{\Omega}_\ell$ be the box where the $\ell$th split occurs in a top-down manner, i.e., $\Omega_1 = \Psi$, $\bar{\Omega}_2 \cup \bar{\Omega}_3 = \Omega_1$, $\bar{\Omega}_4 \cup \bar{\Omega}_5 = \Omega_2$, $\bar{\Omega}_6 \cup \bar{\Omega}_7 = \Omega_3$, etc. For a given box $\bar{\Omega}_\ell \subset \Psi$ and the corresponding splitting coordinate $j_\ell$, denote by $[I_{j_\ell, L}^L, I_{j_\ell, U}^U]$ the interval generated by projecting $\bar{\Omega}_\ell$ onto the $j_\ell$th coordinate, i.e., $[\bar{\Omega}_\ell|_{j_\ell}] = I_{j_\ell, L}^L - I_{j_\ell, U}^U$. If a split occurs in $((I_{j_\ell, L}^L + I_{j_\ell, U}^U)/2 \pm c_1|\bar{\Omega}_\ell|_{j_\ell}[b_n \log(\Psi)]^{c_2})$ for some $c_1, c_2 > 0$, i.e., the interval centered at $(I_{j_\ell, L}^L + I_{j_\ell, U}^U)/2$ with length $2c_1|\bar{\Omega}_\ell|_{j_\ell}[b_n \log(\Psi)]^{c_2}$, then the split-point is $[\bar{\Omega}_\ell|_{j_\ell}(1/2 + c_1[b_n \log(\Psi)]^{c_2})]$-separated from $I_{j_\ell, L}^L$ and $I_{j_\ell, U}^U$ and gives rise to two children whose lengths are at most $|\bar{\Omega}_\ell|_{j_\ell}(1/2 + c_1[b_n \log(\Psi)]^{c_2})$. Let us suppose for now that this happens for all $\ell$ in the iterative procedure with $AKD(\Psi; Z, \alpha, L, S)$. For $T_n$ returned by $AKD(\Psi; Z, \alpha, L, S)$, the maximum box size in the $j$th coordinate will be at most $|\Psi|_{j}(1/2 + c_1[b_n \log(\Psi)]^{c_2})$.

Using that $l_j \leq L \leq [k \log(b_n \log(\Psi))] \lesssim \log(b_n \log(\Psi))$, we obtain $l_j \log((1/2 + c_1[b_n \log(\Psi)]^{c_2}) \leq l_j \log(1/2 + c_1[b_n \log(\Psi)]) \log(1 + 2c_1[b_n \log(\Psi)]^{c_2})$ for some $C_1 > 0$. Since the second term is bounded, it follows that $|\Psi|_{j}(1/2 + c_1[b_n \log(\Psi)]^{c_2}) \lesssim |\Psi|_{j}2^{-l_j}$ for every $j = 1, \ldots, d$, which leads to the desired assertion.

It only remains to show that for some $c_1, c_2 > 0$, the splits occur on the interval $((I_{j_\ell, L}^L + I_{j_\ell, U}^U)/2 \pm c_1|\bar{\Omega}_\ell|_{j_\ell}[b_n \log(\Psi)]^{c_2})$ for all $\ell$ with high probability. For a given box $\Psi \in [0, 1]^d$, we write $b_n(\Psi)$ for the number of split-points in $Z \cap \text{int}(\Psi)$. Denoting by $Z_{j_\ell, L}$ the $[b_n(\Omega_\ell)/2]$ th split-point for the midpoint-split of $\bar{\Omega}_\ell$, this can be written formally as $P(\cap_{\ell=1}^{2^L} \mathcal{G}_\ell(c_1, c_2)) \to 1$, for

$$\mathcal{G}_\ell(c_1, c_2) := \left\{ \left| Z_{j_\ell, L} - \frac{I_{j_\ell, L}^L + I_{j_\ell, U}^U}{2} \right| \leq c_1|\bar{\Omega}_\ell|_{j_\ell}[b_n \log(\Psi)]^{c_2}, \text{with } I_{j_\ell, L}^L, I_{j_\ell, U}^U \text{ being given} \right\}.$$

Given $b_n(\Psi)$, it is easy to see that $U_i(U_i \in \Psi), i = 1, \ldots, b_n(\Psi)$, are still uniformly distributed on $\Psi$. Note also that $b_n(\Omega_\ell)$ is deterministic for every $\ell$ if $b_n(\Psi)$ is given, as it is determined by the midpoint-split rule.

Using the distribution of $U_i(U_i \in \Psi)$ and the theory of conditional distributions of order statistics (e.g., Theorems 2.4.1 and 2.4.2 of Arnold et al. (1992)), one can see that $Z_{j_\ell, L}$ has $Beta([b_n(\Omega_\ell)/2], [(b_n(\Omega_\ell) + 1)/2]; I_{j_\ell, L}, I_{j_\ell, U})$ when $I_{j_\ell, L}, I_{j_\ell, U}$ and $b_n(\Psi)$ are given, where $Beta(\alpha; \beta; a, b)$ stands for a beta distribution with $(\alpha, \beta)$ shifted and scaled to the interval $(a, b)$. We use the fact that mean and variance of $Beta(\alpha; \beta; a, b)$ are $(ab + \beta a)/(\alpha + \beta)$ and $[\alpha(b - a)^2]/[\alpha(\alpha + \beta)^2(\alpha + \beta + 1)]$, respectively. Note further that

$$\left| \frac{ab + \beta a}{\alpha + \beta} \right| = \frac{|a - b||\alpha - \beta|}{2(\alpha + \beta)}.$$

Observe also that the number $b_n(\bar{\Omega}_\ell)$ of split-points in $\bar{\Omega}_\ell$ satisfies $[(b_n(\Psi) + 1)/2^{\text{dep}(\Omega_\ell)} - 1] \leq b_n(\bar{\Omega}_\ell) \leq [(b_n(\Psi) + 1)/2^{\text{dep}(\Omega_\ell)} - 1]$ for any $\ell$. Putting everything together, it is easy to see that the (conditional) mean $\bar{\mu}_{j_\ell, L}$ and variance $\sigma^2_{j_\ell, L}$ of $Z_{j_\ell, L}$ satisfy

$$\left| \bar{\mu}_{j_\ell, L} - \frac{I_{j_\ell, L}^L + I_{j_\ell, U}^U}{2} \right| \leq \frac{\bar{\Omega}_{|j_\ell}|_{j_\ell}}{b_n(\Omega_\ell)} \leq \frac{2^{\text{dep}(\Omega_\ell)}|\bar{\Omega}_{|j_\ell}|_{j_\ell}}{b_n(\Psi)} \leq \frac{|b_n \log(\Psi)|^{c_2}|\bar{\Omega}_{|j_\ell}|_{j_\ell}}{b_n(\Psi)}.$$

for large enough $n$, since $2^{\text{dep}(\Omega_\ell)} \leq 2^L \leq [b_n \log(\Psi)]^k$ due to the range of $L$. By Chebyshev’s
inequality coupled with the first relation of (18), we have that

\[ \mathbb{P}\left( Z_{\ell,j} - \frac{I_{\ell,j}^L + I_{\ell,j}^U}{2} \leq C_2 \frac{[b_n \text{vol}(\Psi)]^{(k+j')/2} |\Omega_{\ell,j}|_{j_k}}{\sqrt{b_n(\Psi)}} \right) \geq 1 - \frac{1}{[b_n \text{vol}(\Psi)]^{k'}} \]

for some \( C_2 > 0 \) and any \( k' > k \). We define

\[ \tilde{G}_{\ell} := \left\{ Z_{\ell,j} - \frac{I_{\ell,j}^L + I_{\ell,j}^U}{2} \leq C_2 \frac{[b_n \text{vol}(\Psi)]^{(k+j')/2} |\Omega_{\ell,j}|_{j_k}}{\sqrt{b_n(\Psi)}}, \text{with } I_{\ell,j}^L, I_{\ell,j}^U \text{ being given} \right\} \]

for given \( C_2 > 0 \) and \( k' > k \). Using (19), we see that

\[ \mathbb{P}\left( \bigcap_{\ell=1}^{2^L} \tilde{G}_{\ell} | b_n(\Psi) \right) \geq \left( 1 - \frac{1}{[b_n \text{vol}(\Psi)]^{k'}} \right)^{2^L} \]

Since the number \( b_n(\Psi) \) has a binomial distribution with \((b_n, \text{vol}(\Psi))\), Chebyshev’s inequality gives that

\[ \mathbb{P}\left( \frac{1}{2} b_n \text{vol}(\Psi) \leq b_n(\Psi) \leq \frac{3}{2} b_n \text{vol}(\Psi) \right) \geq 1 - \frac{4(1 - \text{vol}(\Psi))}{b_n(\Psi)} \geq 1 - \frac{4}{b_n(\Psi)} \]

which tends to one if \( b_n(\Psi) \to \infty \). Hence,

\[ \mathbb{P}\left( \bigcap_{\ell=1}^{2^L} \tilde{G}_{\ell}, \frac{1}{2} b_n \text{vol}(\Psi) \leq b_n(\Psi) \leq \frac{3}{2} b_n \text{vol}(\Psi) \right) \geq \mathbb{P}\left( \frac{1}{2} b_n \text{vol}(\Psi) \leq b_n(\Psi) \leq \frac{3}{2} b_n \text{vol}(\Psi) \right) \inf_{b_n(\Psi)} \mathbb{P}\left( \bigcap_{\ell=1}^{2^L} \tilde{G}_{\ell} | b_n(\Psi) \right) \]

\[ \geq (1 + o(1)) \left( 1 - \frac{1}{[b_n \text{vol}(\Psi)]^{k'}} \right)^{[b_n \text{vol}(\Psi)]^k} \]

since \( 2^L \leq b_n^k \text{vol}(\Psi)^k \). The leftmost side of (21) is bounded by \( \mathbb{P}(\bigcap_{\ell=1}^{2^L} G_{\ell}(C_2, (k + k' - 1)/2)) \). The rightmost side tends to one if \( b_n(\Psi) \to \infty \) and \( k' > k \). We take \( k < 1/2 \) and \( k' = k + \delta \) for some \( \delta > 0 \), and then take \( \delta \) sufficiently close to zero such that \( k + k' - 1 < 0 \). The assertion is then verified.

**Verification of (iii):** Note that \((b_n(\Psi_1), \ldots, b_n(\Psi_J))\) has a multinomial distribution with a probability vector \((\text{vol}(\Psi_1), \ldots, \text{vol}(\Psi_J))'\) such that \( \sum_{r=1}^{J} b_n(\Psi_r) = b_n \). Using (20) and Boole’s inequality,

\[ \mathbb{P}\left( \frac{1}{2} b_n \text{vol}(\Psi_r) \leq b_n(\Psi_r) \leq \frac{3}{2} b_n \text{vol}(\Psi_r), \ r = 1, \ldots, J \right) \geq 1 - \frac{4J}{b_n \min_r \text{vol}(\Psi_r)} \]

This tends to one if \( b_n \min_r \text{vol}(\Psi_r)/J \to \infty \). Similar to the verification of (ii), it only remains to show that all midpoint-splits occur near the center of the cells with high probability. Given \((b_n(\Psi_1), \ldots, b_n(\Psi_J))\), splits occur independently across the cells, so we can simply follow the calculations used to verify (ii) for every \( \Psi_r, \ r = 1, \ldots, J \). The assertion then easily follows. \(\square\)
Now, we prove Lemma 2 below.

**Proof of Lemma 2.** It is obvious that \( Z \) is \((X^*,0)\)-dense if \( R = 1 \). For the case \( R > 1 \), note that by (i) of Lemma 6, \( Z \) is \((X^*,c_n)\)-dense with high probability for any \( c_n > 0 \) such that \( c_n b_n \min_{1 \leq r \leq R} \text{vol}(\Omega_r^*)/\log R \rightarrow \infty \). Since \( \log \min_r \text{vol}(\Omega_r^*) \geq \log \min_{r,j} |\Xi_r^*|_j \gtrsim -\log n \) and \( R = o(n) \), this condition is satisfied with \( b_n = n^c \) and \( c_n = n^{-c/2} \) if \( c \) is sufficiently large. Next, by (iii) of Lemma 6, we see that for \( L_r = [k \log_2 (b_n \text{vol}(\Omega_r^*))] \) with \( 0 < k < 1/2 \), \( Z \) is \((\Omega_r^*,\alpha_r,L_r,S_r)\)-regular with high probability for every \( r = 1, \ldots, R \) if \( b_n \min_{1 \leq r \leq R} \text{vol}(\Omega_r^*)/R \rightarrow \infty \). Since \( \text{vol}(\Omega_r^*) \geq (\min_j |\Omega_r^*|_j)^d \geq (\min_j |\Xi_r^*|_j - 2c_n)^d \), we have that \( \min_r \text{vol}(\Omega_r^*) \gtrsim \min_j |\Xi_r^*|_j^d \) for every \( r \) if \( c_n = o(\min_{r,j} |\Xi_r^*|_j \) \). The latter condition is easily achieved with \( c_n = n^{-c/2} \) since \( \min_{r,j} |\Xi_r^*|_j \gtrsim -d^{-1} \log n \). Therefore, the requirement \( b_n \min_{1 \leq r \leq R} \text{vol}(\Omega_r^*)/R \rightarrow \infty \) is easily satisfied with \( b_n = n^c \) since \( R = o(n) \). It only remains to show that \( L_0 \leq [k \log_2 (b_n \text{vol}(\Omega_r^*))] \) for some \( k \leq 1/2 \). Since \( 2^{L_0} \leq n(\lambda d)^2/(R \log n) \) taking \( \alpha_r \rightarrow 0 \), it suffices to show that \( n(\lambda d)^2/(R \log n) \lesssim b_n^k \text{vol}(\Omega_r^*)^k \) for some \( k \leq 1/2 \) (since \( x/2 \leq 2^{[\log_2 x]} \) for any \( x > 0 \)). This is easily satisfied with \( b_n = n^c \) if \( c \) is sufficiently large. □

**B.4 Proof of Lemma 3**

**Proof of Lemma 3.** The assumption implies that a fixed design \( Z \) is \((\Omega_r^*,\alpha_r,L_r,S_r)\)-regular for \( L_r = [\log_2 (\tilde{n}_r + 1)] \), \( r = 1, \ldots, R \), where \( \tilde{n}_r = n P_Z(\Omega_r^*) \) is the number of split-points in \( \Omega_r^* \cap Z \). We only need to show that \( L_0 \leq \min_r L_r \). Since \( 2^{L_0} \asymp (n(\lambda d)^2/(R \log n))^{d/(2\alpha_r + d)} \), it suffices to show that \( (n(\lambda d)^2/(R \log n))^{d/(2\alpha_r + d)} \lesssim \tilde{n}_r \). Since \( P_Z(\Xi^*_r) = P_Z(\Omega_r^*) \gtrsim R^{-1} \), the inequality is translated into \( \lambda d \lesssim (n/R)^{\alpha_r/d} \sqrt{\log n} \). □

**B.5 Proof of Theorem 2 and Theorem 4**

We first make the following two definitions excerpted from Ročková and van der Pas (2017). For clearer explanations for the following definitions, we refer the reader to the graphical illustrations in Figure 1 and Figure 2 of Ročková and van der Pas (2017).

**Definition 11** (Definition 5.1 of Ročková and van der Pas (2017)). For an ensemble \( \mathcal{E} = (\mathcal{T}^1, \ldots, \mathcal{T}^T) \), we define the global partition \( \mathcal{F}(\mathcal{E}) = (\tilde{\Omega}_k)_{k=1}^K \) as the partition obtained by merging all cuts in \( \mathcal{T}^1, \ldots, \mathcal{T}^T \), where \( \tilde{\Omega}_k \) are the induced cells and \( K(\mathcal{E}) \) is their total number.

**Definition 12** (Definition 5.2 of Ročková and van der Pas (2017)). For an ensemble \( \mathcal{E} = (\mathcal{T}^1, \ldots, \mathcal{T}^T) \), we define the stretching matrix \( A_\mathcal{E} = (a_{ij}) \) for \( 1 \leq i \leq K(\mathcal{E}) \) and \( 1 \leq j \leq \sum_{t=1}^T K_t \), where \( a_{ij} = 1(\tilde{\Omega}_i \cap \Omega^t_k \neq \emptyset) \) for \( 1 \leq t \leq T \) and \( 1 \leq k \leq K_t \) such that \( j = \sum_{t=1}^T K_t + m \).

We deploy the standard theory on posterior contraction to prove Theorem 2 (Ghosal et al., 2000; Ghosal and van der Vaart, 2007). The general theory requires enough prior mass around the true parameters. To be in line with this, we first show that the approximating tree partition is supported with sufficient prior mass, for both Galton-Watson process prior and Bayesian CART prior.

**Lemma 7** (Prior concentration). Let \( \mathcal{F} \) be the \( Z \)-tree partition defined in Section 4.2. Assume that (A5) is satisfied. Then the Bayesian CART prior gives \( \log \pi(\mathcal{F}|S_0) \gtrsim -K \log n \). The Galton-Watson process prior also gives the same conclusion under (A7).
Proof. For the Bayesian CART prior, it is easy to see that using (9),
\[
\log \pi(\hat{T} | S_0) = \log \pi(\hat{K}) - \log(\# T_{S_0, \hat{K}}) \gtrsim -\hat{K} \log n - \hat{K} \log (b_n d).
\]
Since \(\log(b_n d) \lesssim \log n\), this leads to the desired assertion.

Next, we prove the assertion for the Galton-Watson process prior. Recall that \(T^* = (\Omega_1^*, \ldots, \Omega_k^*)\) is the approximating tree partition of \(X^*\) and \(T_r^\dagger\) is the tree partition of \(\Omega_r^*\) constructed by an anisotropic \(k\)-d tree. Hence, we can write
\[
\pi(\hat{T} | S_0) = \pi(\hat{T} \text{ contains the subtree } T^* | S_0) \prod_{r=1}^R \pi(\hat{T}_r^\dagger | \Omega_r^*, S_0).
\]
We first focus on the prior probability \(\pi(\hat{T} \text{ contains the subtree } T^* | S_0)\). To generate \(\hat{T}\), the root node is subdivided \(R - 1\) times in a top-down manner. Clearly, this happens with probability at least \(\prod_{r=1}^{R-1} \log(\# T_{S_0, \hat{K}})\) no matter what the partition is. Note also that \(T^*\) has \(R - 1\) splits, where each step has at most \(b_n d\) ways for splits (\(d\) variables and no more than \(b_n\) split-points). Therefore,
\[
\pi(\hat{T} \text{ contains the subtree } T^* | S_0) \geq \prod_{r=1}^{R-1} \log(\# T_{S_0, \hat{K}}) \geq \frac{\nu \log(\# T_{S_0, \hat{K}})}{(b_n d)^{R-1}},
\]
which gives that \(\log \pi(T^* | S_0) \gtrsim R \max_r \log(\# T_{S_0, \hat{K}}) - \log(b_n d) \gtrsim -\log n\). Now, observe that in splitting each \(\Omega_r^*\), there are \(2^k\) cells at depth \(k\) and each cell splits with probability \(\nu \log(\# T_{S_0, \hat{K}})\). Note also that closing each of the terminal nodes is of probability at least \(1 - \nu\), as the depth of every terminal node is at least 1. Hence, similar to above,
\[
\pi(T_r^\dagger | \Omega_r^*, S_0) \geq \frac{(1 - \nu)^{2L_0}}{(b_n d)^{2L_0 - 1}} \frac{\nu \log(\# T_{S_0, \hat{K}})_{1+k}^{2k}}{(b_n d)^{2L_0 - 1}}
\]
using the formulae \(\sum_{k=0}^{L_0} 2^k = 2^{L_0 + 1} - 1\) and \(\sum_{k=0}^{L_0} k 2^k = (L - 1)2^{L_0 + 1} + 2\). This gives that \(\sum_{r=1}^R \pi(T_r^\dagger | \Omega_r^*, S_0) \gtrsim -R2^{L_0} \log(b_n d) - R2^{L_0} \max_r \log(\# T_{S_0, \hat{K}}) - R L_0 2^{L_0} \gtrsim -R2^{L_0} \log n\) since \(L_0 \lesssim \log n\). Putting everything together, we thus have log \(\pi(\hat{T} | S_0) \gtrsim -R2^{L_0} \log n\). Since \(\hat{K} = R2^{L_0}\), this verifies the assertion. \(\square\)

Now we prove Theorems 2 and 4 below.

Proof of Theorem 2. We write \(\rho_n^2((f_1, \sigma_1^2), (f_2, \sigma_2^2)) = \|f_1 - f_2\|^2_n + |\sigma_1^2 - \sigma_2^2|^2\) for any \(f_1, f_2 : \mathbb{R}^p \mapsto \mathbb{R}\) and any \(\sigma_1^2, \sigma_2^2 \in (0, \infty)\). By Lemma 1 in the supplementary material of Salomond (2018), if the \(\epsilon_n\)-covering number of \(\Theta_{j,n} = \{(f, \sigma^2) : j^2 \epsilon_n^2 \leq \rho_n^2((f, \sigma^2), (f_0, \sigma_0^2)) \leq (j + 1)^2 \epsilon_n^2\}\) is bounded by \(e^{Cn\epsilon_n^2j^2}\) for some \(C > 0\), there exists a test function \(\phi_n\) such that for some \(K_1 > 0\) and every large \(j\),
\[
\mathbb{E}_0 \phi_n \to 0, \quad \sup_{(f, \sigma^2) \in \Theta_{j,n}} \mathbb{E}_{f, \sigma^2} (1 - \phi_n) \leq e^{-K_1 \nu \epsilon_n^2 j^2}.
\]

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We write $\mathcal{F} = \cup_{\mathcal{E}} \mathcal{F}_{\mathcal{E}}$, where the union is taken over all $\mathcal{E}$ generated by a given $\mathcal{Z}$. By Theorem 8.12 of Ghosal and van der Vaart (2017), we only need to verify that there exists a sieve $\Theta_n \subset \mathcal{F} \times (0, \infty)$ such that for some $\tilde{c} > 0$,

$$
\Pi(B_n) \geq e^{-\tilde{c}n\epsilon_n^2},
$$
(22)

$$
\log N(\epsilon_n, \Theta_n, \rho_n) \lesssim n\epsilon_n^2,
$$
(23)

$$
\Pi((f, \sigma^2) \notin \Theta_n) = o(e^{-\alpha n\epsilon_n^2}),
$$
(24)

where $B_n = \{(f, \sigma^2) : \sum_{i=1}^{n} K(p_{0,i}^*, p) \sigma^2 \leq n\epsilon_n^2, \sum_{i=1}^{n} V(p_{0,i}^*, p) \sigma^2 \leq n\epsilon_n^2\}$.

We first verify (22). By direct calculations,

$$
\frac{1}{n} \sum_{i=1}^{n} K(p_{0,i}, p_i) = \frac{1}{2} \log \left(\frac{\sigma^2}{\sigma_0^2}\right) - \frac{1}{2} \left(1 - \frac{\sigma_0^2}{\sigma^2}\right) + \frac{\|f-f_0\|^2}{2\sigma^2},
$$

$$
\frac{1}{n} \sum_{i=1}^{n} V(p_{0,i}, p_i) = \frac{1}{2} \left(1 - \frac{\sigma_0^2}{\sigma^2}\right)^2 + \frac{\sigma_0^2\|f-f_0\|^2}{\sigma^2}.
$$

Using the Taylor expansion, it is easy to see that for any $\epsilon_n \to 0$, there exists a constant $C_1 > 0$ such that

$$
B_n \supset \{(f, \sigma^2) : \|f-f_0\|_n \leq C_1\epsilon_n, |\sigma^2 - \sigma_0^2| \leq C_1\epsilon_n\}.
$$

First, note that $\log \Pi(\sigma^2 : |\sigma^2 - \sigma_0^2| \leq C_1\epsilon_n) \gtrsim -\log n$ if $\sigma_0^2$ lies on a compact subset of $(0, \infty)$. Assume for now that there exists a good approximating ensemble, denoted by $\hat{\mathcal{E}} = (\hat{T}^1, \ldots, \hat{T}^T)$. By restricting the function space to the one constructed by $\hat{\mathcal{E}}$, it is easy to see that using the sparse prior,

$$
\Pi(f \in \mathcal{F} : \|f-f_0\|_n \leq C_1\epsilon_n)
\geq \left(\frac{p}{d}\right)^{-1} \pi_{\text{dim}}(d) \pi(\hat{\mathcal{E}}|S_0) \Pi(f \in \mathcal{F}_{\hat{\mathcal{E}}} : \|f-f_0\|_n \leq C_1\epsilon_n).
$$
(25)

Note that by Theorem 1, there exists an approximating single tree partition $\hat{T}$ with size $\hat{K} = R^{2L_0}$ terminal nodes. An approximating ensemble $\hat{\mathcal{E}} = (\hat{T}^1, \ldots, \hat{T}^T)$ can be constructed by chopping the branches of $\hat{T}$ such that $\hat{\mathcal{E}}(\hat{T}) = \hat{T}$ (Lemma 10.1 of Ročková and van der Pas (2017)). Since $T$ is fixed, the pruned trees $\hat{T}^t$ do not much overlap for large $n$ and the tree sizes $\hat{K}^t$ satisfy $\log_2 \hat{K} + 1 \leq \hat{K}^t \leq \hat{K}$. We refer the reader to Section 10.2 of Ročková and van der Pas (2017) and Section 6 of Ročková and Saha (2019) for more details. Note that by Lemma 7, we have $\log \pi(\hat{T}^t|S_0) \gtrsim -\hat{K} \log n$ for both Galton-Watson process prior and Bayesian CART prior. Since $\pi(\hat{T}^t|S_0) \geq \pi(\hat{T}|S_0)$ for every $1 \leq t \leq T$, for both the tree priors, $\sum_{t=1}^{T} \log \pi(\hat{\mathcal{E}}|S_0) = \sum_{t=1}^{T} \log \pi(\hat{T}^t|S_0) \gtrsim -\hat{K} \log n \gtrsim -n\epsilon_n^2$. Note also that $\log \left(\frac{p}{d}\right) - \log \pi_{\text{dim}}(d) \lesssim d \log p \lesssim n\epsilon_n^2$. It only remains to establish a lower bound for the prior probability on the right-hand side of (25). By (A6), observe that there exists $f_0^\Lambda \in \mathcal{F}_{\hat{\mathcal{E}}}$ such that $\|f-f_0\|_n \lesssim \|f-f_0^\Lambda\|_n + \epsilon_n$. We denote this $f_0^\Lambda$ by $f^{\Lambda}_{0,\hat{T},\beta}$, where $\beta$ is its step-heights. Since $\hat{T}(\hat{\mathcal{E}}) = \hat{T}$, there exists $\hat{B}$ such that $f^{\Lambda}_{0,\hat{T},\beta} = f^{\Lambda}_{0,\hat{T},\hat{B}}$. Hence, for some $C_2 > 0$,

$$
\Pi(f \in \mathcal{F}_{\hat{\mathcal{E}}} : \|f-f_0\|_\infty \leq C_1\epsilon_n) \geq \Pi \left(f \in \mathcal{F}_{\hat{\mathcal{E}}} : \|f-f^{\Lambda}_{0,\hat{T},\hat{B}}\|_\infty \leq C_2\epsilon_n\right).
$$
(26)
For any $B_1, B_2 \in \mathbb{R}^{\sum_{t=1}^{T} K^t}$ with given $\mathcal{E}$, we write $f_{\mathcal{E}, B_1}, f_{\mathcal{E}, B_2} \in \mathcal{F}_{\mathcal{E}}$ for two additive tree functions that lie on the same partition ensemble $\mathcal{E}$. Let $\tilde{\beta}_1 = A_\mathcal{E} B_1$ and $\tilde{\beta}_2 = A_\mathcal{E} B_2$ be the aggregated step sizes with the stretching mating $A_\mathcal{E}$. Then,

$$\|f_{\mathcal{E}, B_1} - f_{\mathcal{E}, B_2}\|_\infty = \|\tilde{\beta}_1 - \tilde{\beta}_2\|_\infty \leq \|A_\mathcal{E}(B_1 - B_2)\|_2 \leq \sigma_{\text{max}}(A_\mathcal{E})\|B_1 - B_2\|_2.$$ 

Since $\sigma_{\text{max}}^2(A_\mathcal{E}) \leq \tilde{K}(\mathcal{E})\sum_{t=1}^{T} K^t$ for any $\mathcal{E}$ by Lemma 12.1 of Ročková and van der Pas (2017), (26) is bounded below by

$$\Pi \left( B \in \mathbb{R}^{K^*} : \|B - \tilde{B}\|_2 \leq C_2\epsilon_n/\sqrt{\tilde{K}(\mathcal{E})K^*} \right),$$

where $K^* = \sum_{t=1}^{T} \tilde{K}^t$. For a matrix $D \in \mathbb{R}^{K^* \times K^*}$ such that $DB$ has a product of independent standard normal priors, the last display is further bounded below by

$$\Pi \left( B \in \mathbb{R}^{K^*} : \|DB\|_2 \leq C_2\epsilon_n\sigma_{\text{max}}^{-1}(D^{-1})/\sqrt{\tilde{K}(\mathcal{E})K^*} \right) \geq 2^{-K^*/2}e^{-\|DB\|_2^2/2}\Pi \left( B \in \mathbb{R}^{K^*} : \|DB\|_2 \leq C_2\epsilon_n\sigma_{\text{max}}^{-1}(D^{-1})/\sqrt{2\tilde{K}(\mathcal{E})K^*} \right) \geq 2^{-K^*/2}e^{-\|DB\|_2^2/2}(C_2\epsilon_n)^{K^*} e^{-C_2^2\epsilon_n^2/4},$$

following the computations in page 216 of Ghosal and van der Vaart (2007). Since the induced prior for $\|DB\|_2^2$ is a chi-squared distribution with degree of freedom $K^*$, we obtain that for $\tilde{\epsilon}_n = \epsilon_n\sigma_{\text{max}}^{-1}(D^{-1})/\sqrt{\tilde{K}(\mathcal{E})K^*} \lesssim \epsilon_n$,

$$\Pi(B \in \mathbb{R}^{K^*} : \|DB\|_2 \leq C_2\tilde{\epsilon}_n/\sqrt{2}) \geq \frac{2/K^*}{2\tilde{K}(K^*/2)}(C_2\tilde{\epsilon}_n)^{K^*} e^{-C_2^2\tilde{\epsilon}_n^2/4}.$$ 

The logarithm of the right-hand side is bounded below by a constant multiple of $-K^* \log n - \tilde{\epsilon}_n^2 \gtrsim -n\epsilon_n^2$. It only remains to bound $e^{-\|DB\|_2^2}$ in (27). Note that for $\tilde{\beta} = A_\mathcal{E}\tilde{B}$,

$$\|\tilde{\beta}\|_2 \leq \sqrt{K^*}\|\tilde{\beta}\|_\infty = \sqrt{K^*}\|f_{\tilde{\mathcal{E}}, \tilde{B}}\|_\infty \leq \sqrt{\tilde{K}}\|f_0\|_\infty,$$

since $\|f_{\tilde{\mathcal{E}}, \tilde{B}}\|_\infty \leq \|f_0\|_\infty$ by the definition of $\|f_{\tilde{\mathcal{E}}, \tilde{B}}\|_\infty$ (see the proof of Theorem 1). The last display gives that

$$\|DB\|_2^2 \lesssim \|\tilde{\beta}\|_2^2 \leq \sigma_{\text{min}}^{-2}(A_\mathcal{E})\|\tilde{\beta}\|_2^2 \lesssim \sigma_{\text{min}}^{-2}(A_\mathcal{E})\tilde{K}\log n,$$

as soon as $\|f_0\|_\infty \lesssim \sqrt{\log n}$. Observe that with a suitable permutation of the columns, $A_\mathcal{E}$ can be expressed as $A_\mathcal{E} = [I_{\tilde{K}}, A_0]$ for the $\tilde{K} \times \tilde{K}$ identity matrix $I_{\tilde{K}}$ and some binary matrix $A_0$. Using Lemma 1(g) of Govaerts and Pryce (1989), we see that $\sigma_{\text{min}}(A_\mathcal{E}) = 1 + \sigma_{\text{min}}(A_0) \geq 1$. It follows that (28) is further bounded by a constant multiple of $\tilde{K}\log n$. Putting everything together, we conclude that there exists a constant $\tilde{c}$ such that $\Pi(B_n) \geq e^{-\tilde{c}\epsilon_n^2\log n}$.

Next we verify the entropy condition (23). We denote by $\tilde{\mathcal{E}}_{S,K^1,\ldots,K^T}$ the collection of $\mathcal{E} = (T^1, \ldots, T^T)$ with given $S, K^1, \ldots, K^T$; that is, each $T^t$ is an $S$-sparse $Z$-tree partition of size $K^t$. We define the function space

$$\mathcal{F}_{\tilde{\mathcal{E}}_{S,K^1,\ldots,K^T}; |S| \leq \tilde{s}_n, K^t \leq K^t_{n,t=1,\ldots,T}} := \bigcup_{\mathcal{E} \in \tilde{\mathcal{E}}_{S,K^1,\ldots,K^T}; |S| \leq \tilde{s}_n, K^t \leq K^t_{n,t=1,\ldots,T}} \mathcal{F}_{\mathcal{E}^t};$$

$$\mathcal{F}_{\tilde{\mathcal{E}}_{S,K^1,\ldots,K^T}; |S| = \tilde{s}_n} := \bigcup_{\mathcal{E} \in \tilde{\mathcal{E}}_{S,K^1,\ldots,K^T}; |S| = \tilde{s}_n} \mathcal{F}_{\mathcal{E}}.$$
for $\tilde{K}_n \times n\epsilon_n^2 / \log n$ and $\tilde{s}_n \times n\epsilon_n^2 / \log p$. That is, $F_{\tilde{s}_n, \tilde{K}_n}$ is the collection of all $F_{\mathcal{E}}$ such that $K^t \leq \tilde{K}_n$ and $|S| \leq \tilde{s}_n$. We take $\Theta_n = \{ f \in F_{\tilde{s}_n, \tilde{K}_n} : \|B\|_\infty \leq nM_1 \} \times (n^{-M_2}, e^{M_2n\epsilon_n^2})$ for large $M_1, M_2 > 0$. First it is easy to see that $\log N(\epsilon_n, (n^{-M_2}, e^{M_2n\epsilon_n^2}), \cdot) \lesssim n\epsilon_n^2$. We also obtain that

$$N(\epsilon_n, \{ f_{\mathcal{E}, \mathcal{B}} \in F_{\tilde{s}_n, \tilde{K}_n} : \|B\|_\infty \leq nM_1 \}, \|\cdot\|_\infty) \leq \sum_{S: |S| = \tilde{s}_n} \sum_{\tilde{E} \in \tilde{F}_{\tilde{s}_n, \tilde{K}_n} \ldots \tilde{s}_n} N(\epsilon_n, \{ f_{\mathcal{E}, \mathcal{B}} \in F_{\mathcal{E}} : \|B\|_\infty \leq nM_1 \}, \|\cdot\|_\infty).$$

For any given $\mathcal{E}$ and $B_1, B_2 \in \mathbb{R}^{\sum_{t=1}^T K^t}$, $\|f_{\mathcal{E}, B_1} - f_{\mathcal{E}, B_2}\|_\infty \leq \lambda_{\max}(A_{\mathcal{E}})\|B_1 - B_2\|_2 \leq \lambda_{\max}(A_{\mathcal{E}})\sqrt{\sum_{t=1}^T K^t}\|B_1 - B_2\|_\infty$. Observe that $\lambda_{\max}(A_{\mathcal{E}}) \leq K(\mathcal{E})\sum_{t=1}^T K^t \leq (\prod_{t=1}^T K^t)(\sum_{t=1}^T K^t)$ and the cardinality of the set $\tilde{F}_{\tilde{s}_n, \tilde{K}_n}$ is at most $(\# \mathcal{T}_{\tilde{s}_n, \tilde{K}_n})^T$. Hence, the last display is further bounded by

$$N\left(\epsilon_n, \left\{ B \in \mathbb{R}^{TK_n} : \|B\|_\infty \leq nM_1 \right\}, \|\cdot\|_\infty \right) \sum_{S: |S| = \tilde{s}_n} (\# \mathcal{T}_{\tilde{s}_n, \tilde{K}_n})^T.$$

Since $\sum_{S: |S| = \tilde{s}_n} (\# \mathcal{T}_{\tilde{s}_n, \tilde{K}_n})^T \leq (p_{\tilde{s}_n})^T\tilde{s}_n b_n^{TK_{\tilde{n}}} n^{M_1}/\epsilon_n K_n$ for some $C_3 > 0$. Hence the entropy, the logarithm of the covering number, is bounded by a constant multiple of $\tilde{s}_n \log p + \tilde{K}_n \log n \lesssim n\epsilon_n^2$ as soon as $\log b_n \lesssim \log n$. This verifies (23).

Next, we verify (24). First, it is easy to see that $\Pi(\sigma^2 \notin (n^{-M_2}, e^{M_2n\epsilon_n^2})) e^{c_n \epsilon_n^2} \to 0$ if $M_2$ is large enough, using the tail probabilities of inverse gamma distributions. Now we show that $\Pi(F \setminus \{ f_{\mathcal{E}, \mathcal{B}} \in F_{\tilde{s}_n, \tilde{K}_n} : \|B\|_\infty \leq nM_1 \}) e^{c_n \epsilon_n^2} \to 0$. Note first that using the tail probability of normal distributions,

$$\Pi\left( f_{\mathcal{E}, \mathcal{B}} \in F_{\tilde{s}_n, \tilde{K}_n} : \|B\|_\infty > nM_1 \right) \leq \sum_{S: |S| = \tilde{s}_n} \sum_{\tilde{E} \in \tilde{F}_{\tilde{s}_n, \tilde{K}_n} \ldots \tilde{s}_n} \Pi\left( f_{\mathcal{E}, \mathcal{B}} \in F_{\mathcal{E}} : \|B\|_\infty > nM_1 \right) \leq \left( p_{\tilde{s}_n} \right)^T \tilde{s}_n b_n^{TK_n} 2T \tilde{K}_n e^{-n^2M_1/2}.$$

Hence the right most side is $o(e^{-n^{2\epsilon_n^2}})$ as soon as $\log b_n \lesssim \log n$ and $M_1 > 1/2$. Now observe that $\Pi(F \setminus \{ F_{\tilde{s}_n, \tilde{K}_n} \} \leq \sum_{t=1}^T \Pi(K^t > \tilde{K}_n) + \Pi(S : s \geq \tilde{s}_n).$ The prior satisfies $\log \Pi(K^t > \tilde{K}_n) \lesssim -\tilde{K}_n \log \tilde{K}_n$ for every $t = 1, \ldots, T$. Using that $\tilde{K}_n \times n\epsilon_n^2 / \log n$ and $\epsilon_n \gtrsim n^{-\alpha_0/(2\alpha_0 + d)}$, we obtain $\tilde{K}_n \log \tilde{K}_n \gtrsim (d/(2\alpha_0 + d)) n\epsilon_n^2 \gtrsim n\epsilon_n^2$. Note also that

$$\Pi(S : s \geq \tilde{s}_n) = \sum_{m=\tilde{s}_n+1}^{p} \pi_p(s) \leq \pi_p(0) \sum_{m=\tilde{s}_n+1}^{p} (A_2p^{-A_1})^m \lesssim (A_2p^{-A_1})^{\tilde{s}_n+1}. $$

Therefore, choosing $\tilde{K}_n = [M_3n\epsilon_n^2 / \log n]$ and $\tilde{s}_n = [M_3n\epsilon_n^2 / \log p]$ for a sufficiently large $M_3 > 0$, we have $(\sum_{t=1}^T \Pi(K > \tilde{K}_n) + \Pi(S : s \geq \tilde{s}_n)) e^{c_n \epsilon_n^2} \to 0.$

**Proof of Theorem 4.** Let $p_{f, \sigma^2}$ be the density of the model 6 with $f$ and $\sigma^2$. By Lemma B.1 of Xie and Xu (2018), the Hellinger distance $p_n$ satisfies

$$\|f_1 - f_2\|_{2,Q} + |\sigma_1^2 - \sigma_2^2|^{1/2} \lesssim \rho_H(p_{f_1, \sigma_1^2}, p_{f_2, \sigma_2^2}) \lesssim \|f_1 - f_2\|_{1,Q} + |\sigma_1^2 - \sigma_2^2|^{1/2}. $$

(29)
if \( f_1, f_2, \log \sigma_1, \log \sigma_2 \) are uniformly bounded (we use variance parameters in place of standard deviations; both are identical up to constants under the boundedness assumption). Hence, it suffices to show the assertion with respect to the Hellinger distance.

By the well-known theory of posterior contraction (e.g., Theorem 2.1 of Ghosal et al. (2000)), we need to verify that there exists \( \Theta_n \subset \mathcal{F} \times [\bar{c}^{-1}, \bar{c}] \) such that for some \( \bar{c} > 0 \),

\[
\Pi(B_n) \geq e^{-c_n \epsilon_n^2}, \tag{30}
\]
\[
\log N(\epsilon, \Theta_n, \rho_H) \leq n \epsilon_n^2, \tag{31}
\]
\[
\Pi((f, \sigma^2) \notin \Theta_n) = o(e^{-c_n \epsilon_n^2}), \tag{32}
\]

similar to (22)–(24), where \( B_n = \{ f : K(p_0, p_{f, \sigma^2}) \leq \epsilon_n^2, V(p_0, p_{f, \sigma^2}) \leq \epsilon_n^2 \} \). Using (29), the conditions (31) and (32) can be similarly verified as in the proof of Theorem 2; only difference is that we use truncated priors, so (32) is even more easily satisfied. For (30), note that by Lemma B.2 of Xie and Xu (2018),

\[
\max \{ K(p_0, p_{f, \sigma^2}), V(p_0, p_{f, \sigma^2}) \} \lesssim \| f - f_0 \|_{2,Q}^2 + |\sigma^2 - \sigma_0^2|,
\]

since \( f_0 \) and \( \log \sigma_0 \) are uniformly bounded and the priors are truncated. Hence, there exists a constant \( C_1 > 0 \) such that

\[
B_n \supseteq \{ (f, \sigma^2) : \| f - f_0 \|_{2,Q} \leq C_1 \epsilon_n, |\sigma^2 - \sigma_0^2| \leq C_1 \epsilon_n^2 \}.
\]

Note that \( \| f - f_0 \|_{2,Q} \lesssim \| f - f_0 \|_2 \) if the density \( q \) is bounded. The rest of the proof follows similarly to that of Theorem 2. \( \square \)

### B.6 Proof of Theorem 3

Our proof is similar to the proofs of Lemma 5.1 and Theorem 3.1 in Yang and Tokdar (2015), which uses the Le Cam equation (Birgé and Massart, 1993; Wong and Shen, 1995; Barron et al., 1999). More specifically, the minimax rate of nonparametric regression can be obtained by solving the Le Cam equation with the metric entropy of the target function space. While an upper bound of the metric entropy is well known for isotropic classes (e.g., Theorem 2.7.1 of van der Vaart and Wellner (1996)), we believe that there is no available result on more complicated function space in the literature, even for the simple anisotropic classes in Definition 1. We hence first formalize this in the following lemma. Below we write \( \mathcal{H}_\lambda^{A,d}(x; \alpha_\ast) = \{ h \in \mathcal{H}_\lambda^{A,d}(x; \alpha_\ast) : \| h \|_\infty \leq \lambda \} \).

**Lemma 8.** For any \( d \in \mathbb{N}, R \in \mathbb{N}, \) a partition \( X = (\Xi_1, \ldots, \Xi_R) \) with \( \min_{r,j} |\Xi_r| \geq 1 \), and smoothness parameters \( A = (\alpha_r)_{r=1}^R \) with \( \alpha_r = (\alpha_{r,1}, \ldots, \alpha_{r,d}) \in (0,1]^d \) such that \( \alpha_r^{-1} = d^{-1} \sum_{j=1}^d \alpha_{r,j}^{-1}, r = 1, \ldots, R \), there exist \( \epsilon_0 > 0 \) and \( M_0 > 0 \) depending only on \( d \) and \( \alpha_\ast \), such that for any \( \epsilon < \epsilon_0 \),

\[
\log N(\epsilon, \mathcal{H}_1^{A,d}(x; \alpha_\ast) \cap \mathcal{C}([0,1]^d), \| \cdot \|_\infty) \leq M_0(1/\epsilon)^{d/\alpha_\ast}, \tag{33}
\]
\[
\log N(\epsilon, \mathcal{H}_1^{A,d}(x; \alpha_\ast), \| \cdot \|_\infty) \leq M_0 R(1/\epsilon)^{d/\alpha_\ast}. \tag{34}
\]
Proof. We fix a sufficiently small $\delta > 0$ such that $\min_{r,j} |\Xi_r| j^{-1/\alpha r} > 1$. For $\tilde{m}_r = \prod_{j=1}^d (1 + \lfloor |\Xi_r| j^{-1/\alpha r} \rfloor)$, consider a rectangular grid \( \{x^\ell_r, \ell = 1, \ldots, \tilde{m}_r \} \) on each $\Xi_r$ with mesh-width $w^r := |\Xi_r| / |\Xi_r| j^{-1/\alpha r}$ for the $j$th coordinate such that the grid is a Cartesian product $\prod_{j=1}^d \{ I^r_{x,j}, I^r_{x,j} + w^r, I^r_{x,j} + 2w^r, \ldots, |\Xi_r| j \}$, where $I^r_{x,j}$ is the left-boundary of $\Xi_r$ in the $j$th coordinate. Note that $\tilde{m}_r \leq \prod_{j=1}^d (2 + |\Xi_r| j^{-1/\alpha r}) \leq \text{vol}(\Xi_r) 3^d d^{-\alpha \star}$. Combining all $x^\ell_r$ on $[0,1]^d$, we index the full grid by $\{x^\ell, \ell = 1, \ldots, \tilde{m} \}$ with $\tilde{m} = \sum_{r=1}^R m_r \leq 3^d d^{-\alpha \star}$.

We first verify (33). For each $h \in \overline{\mathcal{H}}_1^{A,d}(\Xi; \alpha_\star) \cap C([0,1]^d)$, we define the vector $G h = (|h(x^1)/\delta|, \ldots, |h(x^\tilde{m})/\delta|)$. Note that for every $x \in \Xi_r$ there exists $x^\ell \in \Xi_r$ such that $\sum_{j=1}^d |x_j - x_j^\ell|^{\alpha r} \leq \delta$ since $u_{r j} \leq \delta^{1/\alpha r}$. Hence for such $x$ and $x^\ell$, every pair $h_1, h_2 \in \overline{\mathcal{H}}_1^{A,d}(\Xi; \alpha_\star) \cap C([0,1]^d)$ such that $G h_1 = G h_2$ satisfies

\[
|h(x) - h(2)| \leq |h(x^\ell) - h(2)| + 2 \sum_{j=1}^d |x_j - x_j^\ell|^{\alpha r} \leq \delta + 2d \delta.
\]

Since this holds for every $x \in [0,1]^p$, it follows that $\|h_1 - h_2\|_\infty \leq 3d \delta$ for any $h_1, h_2$ such that $G h_1 = G h_2$. This means that the covering number $N(3d \delta, \overline{\mathcal{H}}_1^{A,d}(\Xi; \alpha_\star) \cap C([0,1]^d), \|\cdot\|_\infty)$ is bounded by the number of possible vectors $G h$ for $h$ that ranges over $\overline{\mathcal{H}}_1^{A,d}(\Xi; \alpha_\star) \cap C([0,1]^d)$. For the enumeration, we begin with the first entry of $G h$. Since $\|h\|_\infty \leq 1$, it is easy to see that the number of possible values of the first entry does not exceed $2 \delta + 1$. For the remainder, we assume without loss of generality that $(x^\ell)$ is appropriately sorted such that for every $\ell > 1$, there exists $\ell' < \ell$ such that $\sum_{j=1}^d |x_j^\ell - x_j^{\ell'}|^{\alpha r} \leq \delta$. This holds since all $\Xi_r$ are connected well through the points lying on the boundaries. Therefore, for every $\ell > 1$, there exists $\ell' < \ell$ such that

\[
|h(x^\ell)/\delta| - |h(x^{\ell'})/\delta| \\
\leq \delta^{-1} |h(x^\ell)/\delta| + |h(x^{\ell'})/\delta| - |h(x^\ell)/\delta| + |h(x^{\ell'})/\delta| \\
\leq \delta^{-1} \sum_{j=1}^d |x_j^\ell - x_j^{\ell'}|^{\alpha r} + 2 \leq 3.
\]

It follows that for a given $|h(x^\ell)/\delta|$, the number of possible values of $|h(x^{\ell'})/\delta|$ is at most 7, which is the case for every $\ell > 1$. Putting the bounds together, the number of possible vectors $G h$ is bounded by $(2/\delta + 1)^7^{\tilde{m}^{-1}}$. Taking $\epsilon = 3d \delta$,

\[
\log N(\epsilon, \overline{\mathcal{H}}_1^{A,d}(\Xi; \alpha_\star) \cap C([0,1]^d), \|\cdot\|_\infty) \leq \log(6d/\epsilon + 1) + 3d(3d/\epsilon)^{d/\alpha \star} \log 7.
\]

Since $\log(6d/\epsilon + 1) \lesssim (6d/\epsilon)^{d/\alpha \star}$, the last display leads to the desired assertion.

For (34), similarly as above, observe that every pair $h_1, h_2 \in \overline{\mathcal{H}}_1^{A,d}(\Xi; \alpha_\star)$ such that $G h_1 = G h_2$ also satisfies $\|h_1 - h_2\|_\infty \leq 3d \delta$. Hence, $N(3d \delta, \overline{\mathcal{H}}_1^{A,d}(\Xi; \alpha_\star), \|\cdot\|_\infty)$ is bounded by the number of possible vectors $G h$ for $h$ that ranges over $\overline{\mathcal{H}}_1^{A,d}(\Xi; \alpha_\star)$. We use the similar technique as above, but now points in different boxes $\Xi_r$ can behave freely. Then one can see that the number of possible vectors $G h$ is bounded by $\prod_{r=1}^R (2/\delta + 1)^7^{\tilde{m}^{-1} - R} = (2/\delta + 1)^R 7^{\tilde{m} - R}$. Taking $\epsilon = 3d \delta$, we have that

\[
\log N(\epsilon, \overline{\mathcal{H}}_1^{A,d}(\Xi; \alpha_\star), \|\cdot\|_\infty) \leq R \log(6d/\epsilon + 1) + 3d(Rd/\epsilon)^{d/\alpha \star} \log 7 \\
\lesssim R(6d/\epsilon)^{d/\alpha \star} + 3d(Rd/\epsilon)^{d/\alpha \star}.
\]
which verifies the assertion. □

The following two lemmas are useful in solving the Le Cam equation, as in Yang and Tokdar (2015). Lemma 9 contributes the packing number of the space \( \mathcal{H}_1^{d,1}(\mathcal{X},\alpha_*) \cap \mathcal{C}([0,1]^d) \). Combined with Lemma 8, this builds an estimate of the entropy given in Lemma 10, which will be the key to using the Le Cam equation to prove Theorem 3.

**Lemma 9.** For any \( d \in \mathbb{N}, R \in \mathbb{N}, \) a partition \( \mathcal{X} = (\Xi_1, \ldots, \Xi_R) \) with \( \min_{r,j} |\Xi_r| \geq 1 \), and smoothness parameters \( A = (\alpha_r)_{r=1}^R \) with \( \alpha_r = (\alpha_{r1}, \ldots, \alpha_{rd})^t \in (0,1]^d \) such that \( \alpha_*^1 = d^{-1} \sum_{j=1}^d \alpha_{rj}^{-1}, r = 1, \ldots, R, \) there exist \( \epsilon_1 > 0 \) and \( M_1 > 0 \) depending only on \( d \) and \( \alpha_* \), such that for any \( \epsilon < \epsilon_1 \), there are \( N \geq \exp(M_1(1/\epsilon)^{d/\alpha_*}) \) functions \( h_i \in \mathcal{H}_1^{A,d}(\mathcal{X};\alpha_*) \cap \mathcal{C}([0,1]^d), 1 \leq i \leq N, \) and \( h_0 = 0 \) satisfying

\[
\int_{[0,1]^d} h_i(x)dx_j = 0, \quad 0 \leq i \leq N, \quad 1 \leq j \leq d, \quad (35)
\]

\[
\|h_i - h_k\|_2 \geq \epsilon, \quad 0 \leq i \leq k \leq N. \quad (36)
\]

**Proof.** We take the kernel \( K(t) = t \mathbb{1}(|t| \leq 1/2) + (\text{sgn}(t)-t) \mathbb{1}(1/2 < |t| \leq 1), t \in \mathbb{R}, \) supported on \([-1,1]\). Clearly, \( K \) is 1-Lipschitz and satisfies \( \int K(t)dt = 0 \). Fix a sufficiently small \( \delta > 0 \) such that \( \min_{r,j} \delta^{-1/\alpha_{rj}} > 2 \). For \( m_r = \prod_{j=1}^d |\Xi_r|^{\delta^{-1/\alpha_{rj}}}, \) consider a rectangular grid \( \{x_{\ell}^r, \ell = 1, \ldots, m_r\} \) on \( \Xi_r \) with mesh-width \( u_{rj} = |\Xi_r|^{1/|\Xi_r|} \delta^{-1/\alpha_{rj}} \) for the \( j \)th coordinate such that the grid is a Cartesian product \( \prod_{j=1}^d \{I_{j,r} + u_{rj}/2, I_{j,r}^L + 3u_{rj}/2, I_{j,r}^L + |\Xi_r| - u_{rj}/2\} \), where \( I_{j,r}^L \) is the left-boundary of \( \Xi_r^j \) in the \( j \)th coordinate (cf. the grid used in the proof of Lemma 8). Observe that \( m_r \geq \text{vol}(\Xi_r)\delta^{-d/\alpha_*} \).

For each \( 1 \leq \ell \leq m_r \) and \( 1 \leq r \leq R \), we define the function

\[
\phi_{\ell}^r(x) = \delta \prod_{j=1}^d \frac{1}{2} K \left( \frac{x_j - x_{\ell}^r_j}{u_{rj}/2} \right),
\]

which is supported on \( \mathcal{X}_{\ell}^r := \prod_{j=1}^d \left[ x_{\ell}^r_j - u_{rj}/2, x_{\ell}^r_j + u_{rj}/2 \right] \). Since \( \|K\|_\infty = 1/2 \), we can assume that \( \delta \) is chosen small such that \( \|\phi_{\ell}^r\|_\infty \leq 1 \). Using the Lipschitz continuity of \( K \) and the inequality \( |\prod_j a_j - \prod_j b_j| \leq \sum_j |a_j - b_j| \) for any \( a_j, b_j \in [-1,1] \), we have that for any \( x, y \) on the support \( \mathcal{X}_{\ell}^r \),

\[
|\phi_{\ell}^r(x) - \phi_{\ell}^r(y)| \leq \frac{\delta}{2} \sum_{j=1}^d \left| \frac{x_j - y_j}{u_{rj}} \right|. \]

To further bound this, we use the inequality \( x \leq x^a \) for any \( x \in [0,1] \) and \( a \in [0,1] \). Then, the last display is bounded by

\[
\frac{\delta}{2} \sum_{j=1}^d \left| \frac{x_j - y_j}{u_{rj}} \right|^{\alpha_{rj}} \leq \sum_{j=1}^d |x_j - y_j|^{\alpha_{rj}},
\]

since \( u_{rj} \geq 1/(2\delta^{-1/\alpha_{rj}}) \) for any \( \delta \) such that \( |\Xi_r|^{\delta^{-1/\alpha_{rj}}} \geq 1/2 \). This implies that \( \phi_{\ell}^r \in \mathcal{H}_1^{A_r,d}(\mathcal{X}_{\ell}^r) \) for every \( 1 \leq \ell \leq m_r \) and \( 1 \leq r \leq R \). For each binary vector \( \omega_r = (\omega_{r1}, \ldots, \omega_{rm_r})^t \in \mathbb{R}^{m_r} \),

\[
\sum_{\ell=1}^{m_r} \phi_{\ell}^r \in \mathcal{H}_1^{A_r,d}(\mathcal{X}_{\ell}^r) \quad \text{for every} \quad 1 \leq \ell \leq m_r
\]

\[
\sum_{\ell=1}^{m_r} \phi_{\ell}^r \in \mathcal{H}_1^{A_r,d}(\mathcal{X}_{\ell}^r) \quad \text{for every} \quad 1 \leq \ell \leq m_r
\]
\{0,1\}^{m_r}$, define $h_{\omega_r} = \sum_{j=1}^{m_r} \omega'_j \phi'_{j}$ a continuous function supported on $\Xi$. Since $\int \phi'_{j}(x) dx_{j} = 0$ for every $j$ and each $\phi'_j$ is a shifted copy of another, $h_{\omega_r}$ satisfies $\int h_{\omega_r}(x) dx_{j} = 0$ for every $j$ and $h_{\omega_r} \in \mathcal{H}_{1}^{\alpha,d}(\Xi)$. For $m := \sum_{j=1}^{R} m_r \geq \delta^{-d/\alpha}$, we write $\bar{\omega} = (\bar{\omega}_1, \ldots, \bar{\omega}_m)' \in \{0,1\}^m$ and define $h_{\bar{\omega}} = \sum_{j=1}^{R} h_{\omega_r}$. Then, since each $h_{\omega_r}$ is zero at every point in the boundaries of $X$, it is easy to see that $h_{\bar{\omega}} \in \mathcal{P}_1^{A,d}(X,\alpha_*) \cap C([0,1]^d)$ and $\int h_{\bar{\omega}}(x) dx_{j} = 0$. We also have that for any $\omega, \omega' \in \{0,1\}^m$,

$$\|h_{\omega} - h_{\omega'}\|_2^2 \geq \sum_{\ell=1}^{m} (\omega_\ell - \omega'_\ell)^2 \min_{1 \leq r \leq R} \int \phi'_{\ell}(x)^2 dx = \rho(\bar{\omega}, \bar{\omega}') \left( \frac{\|K\|_2}{8} \right)^d \omega,$$

(37)

where $\omega = \min_{1 \leq r \leq R} \prod_{j=1}^{d} u_{r,j} \geq 1/(2\delta^{-d/\alpha_+})$ and $\rho(\bar{\omega}, \bar{\omega}') = \sum_{\ell=1}^{m} \min \{1(\bar{\omega}_\ell \neq \bar{\omega}'_\ell)\}$ is the Hamming distance between $\bar{\omega}$ and $\bar{\omega}'$. We assume that $\delta$ is chosen sufficiently small such that $m \geq 8$. By the Gilbert-Varshamov bound (Lemma 2.9 of Tsybakov (2008)), there exist $N \geq 2^{m/8}$ binary strings $\bar{\omega}_1^{(1)}, \ldots, \bar{\omega}_m^{(N)} \in \{0,1\}^m$ such that $\rho(\bar{\omega}_\ell^{(i)}, \bar{\omega}_\ell^{(j)}) \geq 0, 0 \leq \ell \leq \ell' \leq N$, with $\bar{\omega}_0^{(0)} = 0$. Since $m \omega u \geq 1/2$ and $\|K\|_2 = 1/\sqrt{6}$, we obtain from (37) that $\|h_{\bar{\omega}_\ell^{(i)}} - h_{\bar{\omega}_\ell^{(j)}}\|_2 \geq 48^{-d}/64$ while $N \geq 2^{m/8} \geq \exp(\delta^{-d/\alpha_+}(\log 2)/8)$. Taking $\epsilon = 48^{-d/2}/8$, the assertion is achieved.

**Lemma 10.** For any $d \in \mathbb{N}$, $p \geq 1$, $\lambda > 0$, $R \in \mathbb{N}$, a partition $X = (\Xi_1, \ldots, \Xi_R)$ with $\min_{r \in [R]} |\Xi_r| \geq 1$, and smoothness parameters $A = (\alpha_r)^{R_1}_{r=1}$ with $\alpha_r = (\alpha_1, \ldots, \alpha_{rd}) \in (0,1]^d$ such that $\alpha^{-1}_+ = d^{-1} \sum_{j=1}^{d} \alpha^{-1}_{r,j}$, $r = 1, \ldots, R$, there exist $\epsilon_2, M_2, M_2 > 0$ depending only on $d$ and $\alpha_*$ such that for any $\epsilon < \epsilon_2$,

$$\log D(\epsilon, \mathcal{P}_1^{A,d,p}(X,\alpha_*)) \cap C([0,1]^p), \|\cdot\|_2) \geq M_2\left( \frac{\lambda}{\epsilon} \right)^{d/\alpha_*} + \log \left( \frac{p}{d} \right),$$

(38)

$$\log D(\epsilon, \mathcal{P}_1^{A,d,p}(X,\alpha_*)) \cap C([0,1]^p), \|\cdot\|_2) \leq M_2\left( \frac{\lambda}{\epsilon} \right)^{d/\alpha_*} + \log \left( \frac{p}{d} \right),$$

(39)

$$\log D(\epsilon, \mathcal{P}_1^{A,d,p}(X,\alpha_*)) \cap C([0,1]^p), \|\cdot\|_2) \leq M_2R\left( \frac{\lambda}{\epsilon} \right)^{d/\alpha_*} + \log \left( \frac{p}{d} \right).$$

(40)

**Proof.** We only need to verify the assertion for $\lambda = 1$ since $D(\epsilon, \lambda F, \|\cdot\|_2) = D(\epsilon, \lambda F, \|\cdot\|_2)$ for any set $F$. We first verify the lower bound (38). By Lemma 9, there exist $\epsilon_1$ and $M_1$ such that for any $\epsilon < \epsilon_1$, there are functions $h_0 = 0, h_i \in \mathcal{P}_1^{A,d}(X,\alpha_*) \cap C([0,1]^d), 1 \leq i \leq N$ satisfying (35)–(36), with $N \geq \exp(M_1(1/\epsilon)\delta/d)$. This means that for any $S \subseteq \{1, \ldots, p\}$ such that $|S| = d$, we have that $W_{S}^p h_i \in \mathcal{P}_1^{A,d,p}(X,\alpha_*) \cap C([0,1]^p)$ for any such $h_i$, $0 \leq i \leq N$. Therefore,

$$\mathcal{W}_{\alpha,d}(\epsilon) \coloneqq \bigcup_{S \subseteq \{1, \ldots, p\}, |S| = d} \{W_{S}^p h_i : 1 \leq i \leq N\} \subseteq \mathcal{P}_1^{A,d,p}(X,\alpha_*) \cap C([0,1]^p).$$

Now, observe that for any $S \neq S' \subseteq \{1, \ldots, p\}$ and $1 \leq i \leq k \leq N$, since $\langle W_{S}^p h_i, W_{S'}^p h_k \rangle = 0$ by (35), $\|W_{S}^p h_i - W_{S'}^p h_k\|_2 = (\|h_i\|_2^2 + \|h_k\|_2^2)^{1/2} \geq \epsilon$ by (36), where we used $h_0 = 0$. Also for any $S \subseteq \{1, \ldots, p\}$, it is easy to see that $\|W_{S}^p h_i - \bar{W}_{S}^p h_k\|_2 = \|h_i - h_k\|_2 \geq \epsilon$ by (36). These imply that $\mathcal{W}_{\alpha,d}(\epsilon)$ is c-separated, and hence the packing number $D(\epsilon, \mathcal{P}_1^{A,d,p}(X,\alpha_*) \cap C([0,1]^p), \|\cdot\|_2)$ is bounded below by the cardinality of $\mathcal{W}_{\alpha,d}(\epsilon)$, which is $(p/d)^d N$. This leads to the assertion.
For (39), note that $\Gamma_{1}^{A,d,p}(x;\alpha_{*})\cap C([0,1]^{p})$ is a union of $(\binom{n}{0})$ many $\mathcal{H}_{1}^{A,d}(x;\alpha_{*})\cap C([0,1]^{d})$. By (33) of Lemma 8, each $\mathcal{H}_{1}^{A,d}(x;\alpha_{*})\cap C([0,1]^{d})$ satisfies $\log D(\epsilon,\mathcal{H}_{1}^{A,d}(x;\alpha_{*})\cap C([0,1]^{d}),\|\cdot\|_{2}) \leq \log N(\epsilon/2,\mathcal{H}_{1}^{A,d}(x;\alpha_{*})\cap C([0,1]^{d}),\|\cdot\|_{2}) \leq M_{0}2^{d/\alpha_{*}}(1/\epsilon)^{d/\alpha_{*}}$. Choosing $M_{2} = M_{0}2^{d/\alpha_{*}}$, the second inequality of the assertion easily follows.

Following the same manner, the assertion (40) can easily be verified using (34) of Lemma 8.

Now we prove Theorem 3 below.

Proof of Theorem 3. We first show the minimax rate over $\Gamma_{\lambda}^{A,d,p}(x;\alpha_{*})\cap C([0,1]^{p})$. By Theorem 6 of Yang and Barron (1999), the minimax rate $\tilde{\gamma}_{n}$ is the solution to $\log D(\tilde{\gamma}_{n},\Gamma_{\lambda}^{A,d,p}(x;\alpha_{*})\cap C([0,1]^{p}),\|\cdot\|_{2,Q}) = n^{\gamma_{n}^{2}}$. We use $\gamma_{n}$ defined in Theorem 3. Using $\|\cdot\|_{2,Q} \leq \sqrt{\|\cdot\|_{2}}$ and the relation $N(\epsilon,A,d) \leq D(\epsilon,A,d) \leq N(\epsilon/2,A,d)$ between packing and covering numbers for a metric space $(A,d)$,

$$
\log D \left( 2\sqrt{q}\gamma_{n},\Gamma_{\lambda}^{A,d,p}(x;\alpha_{*})\cap C([0,1]^{p}),\|\cdot\|_{2,Q} \right) \\
\leq \log N \left( \gamma_{n},\Gamma_{\lambda}^{A,d,p}(x;\alpha_{*})\cap C([0,1]^{p}),\|\cdot\|_{2} \right) \\
\leq \log D \left( \lambda(\sqrt{n}\lambda)^{-2\alpha_{*}/(2\alpha_{*}+d)},\Gamma_{\lambda}^{A,d,p}(x;\alpha_{*})\cap C([0,1]^{p}),\|\cdot\|_{2} \right).
$$

It is easy to see that using Lemma 10, the rightmost side is further bounded by a constant multiple of $n^{\gamma_{n}^{2}}$. For the other direction, let

$$\kappa_{n} = \max \left\{ \lambda(\sqrt{n}\lambda)^{-2\alpha_{*}/(2\alpha_{*}+d)}, \frac{1}{\sqrt{n}} \log^{1/2} \left( \frac{p}{d} \right) \right\} \geq \gamma_{n}/2.$$

Since $\|\cdot\|_{2,Q} \geq \sqrt{\|\cdot\|_{2}}$, we obtain that

$$\log D \left( \sqrt{q}k_{n}/2,\Gamma_{\lambda}^{A,d,p}(x;\alpha_{*})\cap C([0,1]^{p}),\|\cdot\|_{2,Q} \right) \\
\geq \log D \left( \kappa_{n},\Gamma_{\lambda}^{A,d,p}(x;\alpha_{*})\cap C([0,1]^{p}),\|\cdot\|_{2} \right).$$

By Lemma 10 again, the right-hand side is bounded below by a constant multiple of $n^{\gamma_{n}^{2}}$. These two bounds imply that $\tilde{\gamma}_{n}$ solving $\log D(\tilde{\gamma}_{n},\Gamma_{\lambda}^{A,d,p}(x;\alpha_{*})\cap C([0,1]^{p}),\|\cdot\|_{2,Q}) = n^{\gamma_{n}^{2}}$ satisfies $\tilde{\gamma}_{n} \propto \gamma_{n}$.

Similarly, the minimax rate over $\Gamma_{\lambda}^{A,d,p}(x;\alpha_{*})$ can also be obtained, but the constant depends on $R$ due to in view of (40).

B.7 Proof of Theorems 5–6

Proof of Theorem 5. It is well known that the Hellinger distance possesses an exponentially powerful local test with respect to both the type-I and type-II errors (e.g., Section 7 of Ghosal et al. (2000) or Lemma 2 of Ghosal and van der Vaart (2007)). Therefore by the general posterior contraction theory, it suffices to show that there exists $\Theta_{n} \subset \mathcal{F}$ such that for some $\tilde{\epsilon} > 0$,

$$\Pi(B_{n}) \geq e^{-\tilde{\epsilon}n\epsilon_{n}^{2}},$$

$$\log N(\epsilon_{n}/36,\Theta_{n},\rho_{1}) \lesssim n\epsilon_{n}^{2},$$

$$\Pi(f \notin \Theta_{n}) = o(e^{-\tilde{\epsilon}n\epsilon_{n}^{2}}).$$
where $B_n = \{ f : K(p_0, p_f) \leq \epsilon_n^2, V(p_0, p_f) \leq \epsilon_n^2 \}$. The last condition (43) follows directly from the proof of Theorem 2, so we only need to verify (41) and (42).

By Lemma 3.1 of van der Vaart and van Zanten (2008), for any measurable $f, g$,

$$
K(p_f, p_g) \lesssim \| f - g \|_\infty e^{\| f - g \|_\infty (1 + \| f - g \|_\infty)}.
$$

By Lemma 3.2 of van der Vaart and van Zanten (2008), for any measurable $f, g$,

$$
V(p_f, p_g) \lesssim \| f - g \|_\infty e^{\| f - g \|_\infty (1 + \| f - g \|_\infty)^2},
$$

The first two assertions imply that there exists $C_1 > 0$ such that $B_n \supseteq \{ f : \| f - f_0 \|_\infty \leq C_1 \epsilon_n \}$ if $\epsilon_n \to 0$. Hence we follow the calculation in the proof of Theorem 2 to conclude that there exists a constant $\bar{c} > 0$ such that $\Pi(B_n) \geq e^{-\bar{c} \epsilon_n^2}$. The last assertion of (44) enables us to work with the supremum norm in the calculation of the Hellinger covering number. The entropy calculation in Theorem 2 also verifies (42), completing the proof. \qed

Proof of Theorem 6. Denote by $p_f(x, y)$ the density of the model (8) and by $p_0(x, y)$ the true density. We also write $f_0 = H^{-1}(\varphi_0)$. It follows from $|p_f(0|x) - p_0(0|x)| = |p_f(1|x) - p_0(1|x)| = |H(f(x)) - H(f_0(x))|$ that $\| p_f - p_0 \|_2 = \sqrt{2} \| H(f) - H(f_0) \|_{2,Q}$. The $L_2$-norm is bounded by a multiple of the Hellinger distance as $p_f$ and $p_0$ are uniformly bounded, (see, for example, Lemma B.1 of Ghosal and van der Vaart (2017)). Hence, it suffices to show the contraction rate results with respect to the Hellinger distance. This means that the assertion can be verified if there exists $\Theta_n \subset \mathcal{F}$ satisfying (41)–(43) for some $\bar{c} > 0$. By Lemma 2.8 of Ghosal and van der Vaart (2017), $K(p_0, p_f) \lesssim \| f - f_0 \|_{2,Q}$ and $V(p_0, p_f) \lesssim \| f - f_0 \|_{2,Q}$. We also have that $\rho_H(p_f, p_g) \lesssim \| f - g \|_{2,Q}$ for every measurable $f, g$ by the same lemma. Similar to the proof of Theorem 5, the proof is completed by following that of Theorem 2. \qed

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