Optimal Bayesian estimation in random covariate design with a rescaled Gaussian process prior

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Abstract

In Bayesian nonparametric models, Gaussian processes provide a popular prior choice for regression function estimation. Existing literature on the theoretical investigation of the resulting posterior distribution almost exclusively assume a fixed design for covariates. The only random design result we are aware of (van der Vaart & van Zanten, 2011) assumes the assigned Gaussian process to be supported on the smoothness class specified by the true function with probability one. This is a fairly restrictive assumption as it essentially rules out the Gaussian process prior with a squared exponential kernel when modeling rougher functions. In this article, we show that an appropriate rescaling of the above Gaussian process leads to a rate-optimal posterior distribution even when the covariates are independently realized from a known density on a compact set. The proofs are based on deriving sharp concentration inequalities for frequentist kernel estimators; the results might be of independent interest.
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1 Introduction

Gaussian processes (Rasmussen, 2004; Seeger, 2004; Rasmussen & Williams, 2006) are widely used in the machine learning community as a principled probabilistic approach to function estimation. A mean-zero Gaussian process is completely specified by its covariance kernel; popular choices include the squared-exponential and Matérn families. Recently, there has been significant interest in frequentist convergence properties of Bayesian posteriors in Gaussian process models. Ghosal & Roy (2006); Choi & Schervish (2007); Tokdar & Ghosh (2007) established posterior consistency in a variety of settings including nonparametric regression, classification and density estimation. Seeger et al. (2008) used an information criterion to evaluate closeness of the posterior distribution to the truth; see also van der Vaart & van Zanten (2011). A major focus in the recent literature (van der Vaart & van Zanten, 2007, 2008a, 2009, 2011; Bhattacharya et al., 2014) has been on deriving the posterior convergence rate (Ghosal et al., 2000), which is defined as the minimum possible sequence \( \epsilon_n \to 0 \) such that for some constant \( M > 0 \),

\[
E_{\theta_0}\Pi(\|\theta - \theta_0\| < M\epsilon_n \mid \mathcal{D}_n) \to 1,
\]

where \( \mathcal{D}_n \) denotes the data, \( \theta \) is the parameter of interest with some known transformation \( \Psi(\theta) \) assigned a Gaussian process prior, \( \theta_0 \) is the true data generating parameter and \( \| \cdot \| \) is a distance measure relevant to the statistical problem. In the context of nonparametric regression, classification and density estimation, it has been established that the posterior convergence rate based on appropriate Gaussian process priors coincides with the minimax optimal rate \( n^{-\alpha/(2\alpha+d)} \) for \( d \)-variate \( \alpha \)-smooth functions up to a logarithmic factor (van der Vaart & van Zanten, 2007, 2008a), with rate-adaptivity to the unknown smoothness achieved in van der Vaart & van Zanten (2009); Bhattacharya et al. (2014).
In this paper, we focus on a non-parametric regression problem,

\[ Y_i = f(X_i) + \epsilon_i, \quad \epsilon_i \sim N(0, 1), \quad (2) \]

with \( f \) assigned a mean-zero Gaussian process prior. The above-mentioned literature on posterior convergence rates under (2) typically assume that the covariates \( X_i \)'s are fixed by design, in which the empirical \( L_2 \) norm \( \| f - f_0 \|_{2,n} = (1/n \sum_{i=1}^{n} |f(x_i) - f_0(x_i)|^2)^{1/2} \) is used as a discrepancy measure in (1). In this paper, we consider a random design setup where the covariates \( X_i \)'s are drawn independently from a known distribution \( q \), and derive the posterior convergence rates under an integrated \( L_1 \) metric:

\[ \| f - f_0 \|_{1,q} = \int |f(x) - f_0(x)|q(x)dx. \]

In the frequentist literature, existing results (Baraud, 2002; Brown et al., 2002; Birgé et al., 2004) on the convergence rates (with respect to an integrated metric) in random design regression require an appropriate lower bound on the smoothness of the underlying true function. For example, Brown et al. (2002); Birgé et al. (2004) assumed that the univariate function \( f_0 \) belongs to a Lipschitz class with smoothness index \( \alpha > 1/2 \). Moreover, Birgé et al. (2004) demonstrated the necessity of the \( \alpha > 1/2 \) condition by establishing a lower bound for the asymptotic risk for \( \alpha \leq 1/2 \). Similar lower bound condition will be assumed in our main Bayesian Theorem as well.

As far as we are aware, the only Bayesian literature considering the random design setting in (2) is van der Vaart & van Zanten (2011) who assigned Gaussian processes with Matérn or squared exponential kernels. Specifically, they obtained an optimal rate \( n^{-\alpha/(2\alpha+\delta)} \) (up to a logarithmic factor, with respect to \( L_2(q) \) norm) under a particularly strong assumption that the Gaussian process prior assigns probability one to the smoothness class containing the true function. Since the squared-exponential kernel has infinitely smooth sample paths, their result only delivers the optimal rate for analytic functions, but provides a highly suboptimal \( (\log n)^{-t} \) rate for \( \alpha \)-smooth functions. This significantly limits the applicability of their result in the sense that it rules out the use
of a squared-exponential kernel for less smooth (but more commonly used) functions. An influential idea developed in van der Vaart & van Zanten (2007, 2009) is to scale the sample paths of a Gaussian process with a squared-exponential kernel to enable better approximation of $\alpha$-smooth functions. However, the support of such a prior is the class of all continuous functions (van der Vaart & van Zanten, 2008b), and hence Theorem 2 of van der Vaart & van Zanten (2011) does not apply to such priors.

In this article, we show that if $\alpha > d/2$, an appropriately rescaled Gaussian process prior with a squared-exponential covariance kernel leads to a rate-optimal posterior distribution (with respect to $L_1(q)$ norm) for any $\alpha$-smooth function $f_0$ in a random design setting. While van der Vaart & van Zanten (2011) conjecture (see pp. 2103 after Theorem 2) that their smoothness assumption on the prior is unavoidable for the $L_2(q)$ norm, our result shows that this situation turns out to be different under the $L_1(q)$ norm. Specifically, we develop exponentially consistent test functions under the $L_1(q)$ norm using concentration inequalities for the Nadaraya–Watson kernel estimator. Existence of such test functions plays a key role in Bayesian asymptotic theory (Ghosal et al., 2000). For example, the classical Birgé – Le Cam testing theory (Birgé, 1984; Le Cam, 1986) for the Hellinger metric provides appropriate tests in a wide variety of settings. Giné & Nickl (2011) proposed an alternative framework for constructing tests based on concentration inequalities of frequentist estimators which is particularly useful for stronger norms; see also Ray et al. (2013); Pati et al. (2014) for similar ideas in different contexts.

2 Posterior convergence in random design regression

2.1 Notations

Let $C[0,1]^d$ and $C^\alpha[0,1]^d$ denote the space of continuous functions and the Hölder space of $\alpha$-smooth functions $f : [0,1]^d \to \mathbb{R}$, respectively, endowed with the supremum norm $\|f\|_\infty = \sup_{t \in [0,1]^d} |f(t)|$. For $\alpha > 0$, the Hölder space $C^\alpha[0,1]^d$ consists of functions
\( f \in C[0,1]^d \) that have bounded mixed partial derivatives up to order \([\alpha]\), with the partial derivatives of order \([\alpha]\) being Lipschitz continuous of order \(\alpha - [\alpha]\). Let \(\| \cdot \|_1\) and \(\| \cdot \|_2\) respectively denote the \(L_1\) and \(L_2\) norm on \([0,1]^d\) with respect to the Lebesgue measure (i.e., the uniform distribution). To distinguish the \(L_2\) norm with respect to the Lebesgue measure on \(\mathbb{R}^d\), we use the notation \(\| \cdot \|_{2,d}\).

We write “\(~\)“ for inequality up to a constant multiple. Let \(\phi(t) = (2\pi)^{-1/2}\exp(-t^2/2)\) denote the standard normal density, and let \(\phi_n(x) = \prod_{i=1}^n \phi(x_i)\) for \(x \in \mathbb{R}^n\). Let a star denote a convolution, i.e., \(f_1 \ast f_2(y) = \int f_1(y-t)f_2(t)dt\). We denote the Fourier transform of \(f\), whenever defined, by \(\hat{f}\), with \(\hat{f}(\lambda) = (2\pi)^{-d}\int \exp(i \langle \lambda, t \rangle)f(t)dt\), where \(\langle \lambda, t \rangle\) denotes the complex inner product. Under this convention, the inverse Fourier transform \(f(t) = \int \exp(-i \langle \lambda, t \rangle)\hat{f}(\lambda)d\lambda\) and \(\hat{h} = (2\pi)^d \hat{f} \hat{g}\) when \(h = f \ast g\).

Throughout \(C,C',C_1,C_2,...\) are generically used to denote positive constants whose values might change from one line to another, but are independent from everything else. \(Z_{1:n}\) is used as a shorthand for \(Z_1,\ldots,Z_n\).

In the sequel, we consider a Gaussian process prior \(\Pi\) on the regression function \(f\) with \(\mathbb{E}f(x) = 0\) and covariance kernel \(c(x,x') = \text{cov}(f(x), f(x'))\). In particular, we focus on the squared-exponential kernel \(c_a(x,x') = \exp(-a^2\|x-x'\|^2)\) indexed by an “inverse-bandwidth” parameter \(a\). We next recall some important facts relevant to our setting from van der Vaart & van Zanten (2009) regarding the spectral measure and reproducing kernel Hilbert space of Gaussian process priors. For the squared-exponential kernel \(c_a\), the spectral measure \(\mu_a\) admits a density \(\omega_a\) with respect to Lebesgue measure, where \(\omega_a(\lambda) = a^{-d}\omega(\lambda/a)\), with \(\omega(\lambda) = \exp(-\|\lambda\|^2/4)/(2^d\pi^{d/2})\). The reproducing kernel Hilbert space \(\mathbb{H}^a\) associated with a Gaussian process prior \(\Pi\) consists of (real parts of) functions \(h(t) = \int \exp(i \langle \lambda, t \rangle)\xi(\lambda)\mu_a(\lambda)\), where \(\mu_a\) is the spectral measure of \(\Pi\) and \(\xi \in L_2(\mu_a)\). The squared Hilbert space norm of \(h\) above is given by \(\|h\|_{\mathbb{H}^a}^2 = \|\xi \omega_a^{1/2}\|_{2,d}^2 = \int \xi^2(\lambda)\omega_a(\lambda)d\lambda\); let \(\mathbb{H}_{1}^a\) denote the unit ball of the reproducing kernel Hilbert space \(\{h \in \mathbb{H}^a : \|h\|_{\mathbb{H}^a} \leq 1\}\). Finally, let \(B_1\) denote the unit ball of \(C[0,1]^d\) with respect to the supremum norm.
For a detailed review of reproducing kernel Hilbert space of Gaussian process priors and connections with posterior contraction rates, kindly refer to van der Vaart & van Zanten (2008b).

2.2 Main result

Consider the nonparametric regression model (2). We assume a random design setup, where given the regression function \( f : [0, 1]^d \to \mathbb{R} \), the data \((X_1, Y_1), \ldots, (X_n, Y_n)\) are independently generated, with \( X_i \) having a density \( q \) on \([0, 1]^d\) that is bounded away from zero and infinity. Let \( q(y, x) = q(y \mid x)q(x) \) denote the joint density of \((Y, X)\) given \( f \), where \( q(y \mid x) = \phi\{y - f(x)\} \). The joint data likelihood given \( f \) is therefore

\[
q(n)(Y_1, \ldots, Y_n, X_1, \ldots, X_n | f) = \prod_{i=1}^{n} q(Y_i, X_i) = \prod_{i=1}^{n} \phi(Y_i - f(X_i))q(X_i).
\]

Similarly, we define \( q(n)(Y_1, \ldots, Y_n, X_1, \ldots, X_n | X_1, \ldots, X_n, f) \) and \( q(n)(X_1, \ldots, X_n | f) \) as the density of \((Y, X)\) given \( f \) and \((X_1, \ldots, X_n)\) respectively. Let \( E_{Y,X}^f(\mathbb{P}_{Y,X}^f) \) denote an expectation (probability) with respect to \( q(n)(Y_1, \ldots, Y_n, X_1, \ldots, X_n | f) \). Similarly define \( E_{Y|X}^f(\mathbb{P}_{Y|X}^f) \) and \( E_{X}^f(\mathbb{P}_{X}^f) \). When \( f \) is clear from the context, we shall drop it from the superscript.

We assume a mean zero Gaussian process prior \( \pi \) on \( f \) with a squared exponential kernel

\[
\exp(-a_n^2 \|x - x'\|^2)
\]

and denote the corresponding posterior measure by \( \pi(\cdot | Y_1, \ldots, Y_n) \), so that

\[
\pi(f | Y_1, \ldots, Y_n) \propto q(n)(Y_1, \ldots, Y_n | X_1, \ldots, X_n, f) \pi(f).
\]

Assuming the true regression function is \( f_0 \), we study concentration of the posterior \( \pi(\cdot | Y_1, \ldots, Y_n) \) in an \( L_1(q) \) neighborhood of \( f_0 \).

**Theorem 2.1.** Assume that \( f_0 \in C^\alpha[0,1]^d \) with \( \alpha > d/2 \) and \( \pi \) is a mean-zero Gaussian process prior with a squared exponential covariance kernel \( c(x, x') = \exp(-a_n^2 \|x - x'\|^2) \). Set \( a_n = n^{1/(2\alpha + d)} \). Then with \( \epsilon_n = n^{-\alpha/(2\alpha + d)} \log^{t_1} n \) for \( t_1 \geq d/4 \), and some fixed constant \( M > 0 \),

\[
E_{Y,X}^f(\|f - f_0\|_{L_1(q)} > M \epsilon_n | Y_1, \ldots, Y_n) \to 0.
\]

(3)
As stated in Introduction, the condition $\alpha > d/2$ is necessary to obtain the optimal rate.

2.3 Contributions relative to earlier work

The proof of Theorem 2.1 follows from a general set on sufficient conditions for posterior concentration in model (2); kindly refer to Theorem 3.1 stated in the next Section. In particular, we exploit concentration inequalities for suitable kernel estimators to construct the aforementioned exponentially consistent sequence of test functions. Such techniques have been used previously to show convergence rates in density estimation (Giné & Nickl, 2011) and in linear inverse problems (Ray et al., 2013). Their techniques do not directly apply to our case partly due to the lack of concentration bounds for kernel based estimators. Giné & Nickl (2011); Ray et al. (2013) construct estimators based on truncated spectral representations which are well suited to sieve priors. However, to deal with a Gaussian process prior with a squared-exponential covariance kernel, we need to construct test functions based on the Nadaraya–Watson kernel estimator and derive sharp concentration bounds for this class of estimators in Lemma 3.2 and 3.3.

The effect of scaling the prior using the “inverse bandwidth” $a$ to yield the optimal posterior concentration was noted in van der Vaart & van Zanten (2007), who showed (for $d = 1$) that a deterministic scaling $a_n = n^{1/(2\alpha+1)}$ produces priors that are suitable for modeling $\alpha$-regular functions. van der Vaart & van Zanten (2009) extended this idea by showing that an appropriate prior on $a$, for example $a^d \sim \text{Ga}(c_0, d_0)$, leads to the optimal posterior concentration in the model (2) adaptively over $f_0 \in C^\alpha[0,1]^d$ for any $\alpha > 0$. Both papers focus on the empirical $L_2$ norm to derive posterior concentration rates for the model (2). Using the same rescaled prior as in van der Vaart & van Zanten (2007), Theorem 2.1 establishes the optimal posterior concentration with respect to an integrated $L_1(q)$ norm.

The choice of the norm dictating the neighborhood around the true parameter plays a critical role in Bayesian asymptotics. A fundamental tool for relating the likelihood ra-
tio with the neighborhood in consideration is a sequence of exponentially consistent test functions (Ghosal et al., 2000). In a regression setting, such test functions are guaranteed to exist for the empirical $L_2$ norm by exploiting a direct relation between the empirical $L_2$ norm and the likelihood ratio of the multivariate Gaussian densities involved; refer to Section 4 of van der Vaart & van Zanten (2011). However, the integrated norm involves covariate points different from the observations, which makes the problem more challenging. van der Vaart & van Zanten (2011) applied Bernstein’s inequality to extrapolate to the $L_2(q)$ norm from the empirical $L_2$ norm. However, as stated in the Introduction, their approach only works for priors that are supported on the true smoothness class with probability one.

Among other related work, Section 4 of Kleijn & van der Vaart (2006) considers random design regression, where a correspondence between the Kullback–Leibler and $L_2(q)$ neighborhood is established to derive the test function, assuming the prior support consists of uniformly bounded functions. However, this assumption does not hold for the rescaled Gaussian process prior in Theorem 2.1. In particular, the sieves constructed in van der Vaart & van Zanten (2007) of the form $M_n\mathbb{H}_1 + \epsilon_n\mathbb{B}_1$ with $M_n \to \infty$ do not correspond to sup-norm bounded subsets of $C[0,1]^d$.

We comment here that convergence in the integrated metric has been settled in the binary regression setting. Using a logistic link function, a direct agreement can be established between the integrated $L_1$ metric on the function space and the Hellinger distance between the resulting densities arising from the Bernoulli likelihood; see for example, Section 3.2 of van der Vaart & van Zanten (2008a). Second, in this paper we implicitly refer to Gaussian processes which are specified by a kernel function; specifically, kernel functions which do not admit a finite series representation, such as the squared-exponential kernel. If a Gaussian process is specified via a truncated orthogonal series representation with independent Gaussian priors on the coefficients, the integrated metric can be related to the $l_2$ norm of the coefficient vector (Bontemps, 2011).
3 Auxiliary results

We now state a general theorem which presents a set of sufficient conditions for proving Theorem 2.1. From now onwards, we shall assume the covariate distribution \( q \) to be a uniform distribution on \([0,1]^d\) for notational simplicity; modifying our construction to a general \( q \), which is bounded from above and below, is straightforward. The \( L_1(q) \) norm \( \| \cdot \|_{1,q} \) with \( q \) the uniform distribution on \([0,1]^d\) shall be simply denoted by \( \| \cdot \|_1 \) following our convention in Section 2.1. A proof of Theorem 3.1 can be found in the Appendix.

**Theorem 3.1.** Let \( \epsilon_n \) be a sequence such that \( \epsilon_n \to 0 \) and \( n\epsilon_n^2 \to \infty \). Let \( U_n = \{ f : \| f - f_0 \|_1 > M\epsilon_n \} \) for some fixed \( M > 0 \). Suppose that there exists a sequence of estimators \( \tilde{f}_n \) for \( f \) based on \((Y_{1:n}, X_{1:n})\) and a sequence of subsets/sieves \( P_n \) of \( C[0,1]^d \) such that

\[
\Pi(P_n^c) \leq \exp\{-(C + 4)n\epsilon_n^2\}, \quad \text{(PCS)}
\]
\[
\|\mathbb{E}_{Y,X}^{f_0} \tilde{f}_n - f_0\|_1 < \epsilon_n, \quad \text{(BT)}
\]
\[
\mathbb{P}_{Y,X}^{f_0}\left(\|\tilde{f}_n - \mathbb{E}_{Y,X}^{f_0} \tilde{f}_n\|_1 > \epsilon_n\right) \leq \exp\{-(C + 4)n\epsilon_n^2\}, \quad \text{(DT)}
\]
\[
\sup_{f \in P_n \cap U_n} \|\mathbb{E}_{Y,X}^{f} \tilde{f}_n - f\|_1 < \epsilon_n, \quad \text{(BS)}
\]
\[
\sup_{f \in P_n \cap U_n} \mathbb{P}_{Y,X}^{f}\left(\|\tilde{f}_n - \mathbb{E}_{Y,X}^{f} \tilde{f}_n\|_1 > \epsilon_n\right) \leq \exp\{-(C + 4)n\epsilon_n^2\}, \quad \text{(DS)}
\]
\[
\Pi\left(\| f - f_0\|_\infty \leq \epsilon_n\right) \geq \exp\{-n\epsilon_n^2\}. \quad \text{(PCN)}
\]

Then, \( \mathbb{E}_{Y,X}^{f_0}\Pi(U_n \mid Y_{1:n}, X_{1:n}) \to 0. \)

Condition (PCS) implies that the prior probability of the complement of the sieve \( P_n \) is exponentially small. Condition (BT) assumes a sufficiently accurate estimator \( \tilde{f}_n \) with bias smaller than \( \epsilon_n \) at \( f_0 \) while (DT) assumes an exponential concentration bound of \( \tilde{f}_n \) from its expectation under \( q^{(n)}(\cdot \mid f_0) \). (BS) and (DS) assume similar conditions as (BT) and (DT) under \( q^{(n)}(\cdot \mid f) \) for any \( f \in P_n \cap U_n \). The conditions (BT), (DT); (BS), (DS) jointly guarantee the existence of exponentially consistent test functions; see Lemma [2] in
the Appendix. Condition (PCN) assumes that the prior II places “enough” mass in an \( \epsilon_n \)-neighborhood of the truth \( f_0 \) in terms of the sup-norm.

### 3.1 Verifying the conditions of Theorem 3.1 to prove Theorem 2.1

We now proceed to construct \( P_n \) and \( \tilde{f}_n \) that satisfy the conditions of Theorem 3.1. While we choose the same sieve as in van der Vaart & van Zanten (2007), part of the technical challenge lies in the fact that the concentration bounds need to be derived not just for the truth, but rather for every function in the sieve. This requires precise control on the size of the functions in the sieve \( P_n \). We show in Proposition 3.5 below that the functions in the chosen sieve are uniformly bounded in \( L_2 \) norm, although they are unbounded in the supremum norm.

Let \( \psi : \mathbb{R}^d \to \mathbb{C} \) be a function such that \( \int \psi(t)dt = 1 \), \( \int t^k \psi(t)dt = 0 \) for any non-zero multi-index \( k = (k_1, \ldots, k_d) \) of non-zero integers, \( \int |t|^{\max\{\alpha,2\}} |\psi(t)| dt < \infty \), and the functions \( \hat{\psi}/\omega \) and \( |\hat{\psi}|^2/\omega \) are uniformly bounded; see proof of Lemma 4.3 in van der Vaart & van Zanten (2009). Define,

\[
\tilde{f}_n(x) = \frac{1}{n} \sum_{i=1}^{n} \psi_{\sigma_n}(x - X_i) Y_i,
\]

where \( \psi_{\sigma}(t) = \sigma^{-d} \psi(t/\sigma) \) for \( \sigma > 0 \) and set \( \sigma_n = n^{-1/(2\alpha+d)} \log^{-t_2} n \) for some constant \( t_2 \geq 1/2 \). Next, with \( M_n = a_n^{d/2} \), set

\[
P_n = M_n B_{1}^{\alpha n} + \epsilon_n B_1.
\]

Assume \( f_0 \in C^{\alpha}[0,1]^d \). Let \( \tilde{f}_n \) and \( P_n \) be as in (4) and (5) respectively. We show below that the conditions of Theorem 3.1 are satisfied with \( \epsilon_n = n^{-\alpha/(2\alpha+d)} \log_t n \) for \( t_1 \geq t_2d/2 \), provided \( \alpha > d/2 \). (PCS) & (PCN) follow from the proof of Theorem 3.1 in van der Vaart & van Zanten (2009). We verify (BS) and (DS); the verifications of (BT) and (DT) follow along similar lines.

**We first show that (DS) holds.** Fix \( f \in P_n \cap U_n \). We drop the superscript \( f \) from \( \mathbb{E}^f \) in the sequel. Let \( f_n(x) = \psi_{\sigma_n} \ast f(x) = \int \psi_{\sigma_n}(x-t)f(t) dt \) and \( f_n^X(x) = n^{-1} \sum_{i=1}^{n} \psi_{\sigma_n}(x - \)
$X_i)f(X_i)$. Observe that $E_{Y,X}\tilde{f}_n = f_n$ and $E_{Y|X}\tilde{f}_n = f_n^X$. Then,

$$P_{Y,X}\left(\|\tilde{f}_n - E_{Y,X}\tilde{f}_n\|_1 > \epsilon_n\right) = P_{Y,X}\left(\|\tilde{f}_n - f_n\|_1 > \epsilon_n\right)$$

$$\leq P_{Y,X}\left(\|\tilde{f}_n - f_n\|_1 > \epsilon_n, \|f_n^X - f_n\|_1 \leq \epsilon_n/2\right) + P_X\left(\|f_n^X - f_n\|_1 \geq \epsilon_n/2\right)$$

$$\leq E_XP_{Y|X}\left(\|\tilde{f}_n - f_n^X\|_1 > \epsilon_n/2 \mid X_{1:n}\right) + P_X\left(\|f_n^X - f_n\|_1 \geq \epsilon_n/2\right).$$

(6)

Lemmas 3.2 and 3.3 below deliver the desired bounds for the two terms appearing in (6).

**Lemma 3.2.** Under conditions of Theorem 2.1,

$$P_{Y|X}\left(\|\tilde{f}_n - f_n^X\|_1 \geq \epsilon_n/2 \mid X_{1:n}\right) \leq \exp(-Cn\epsilon_n^2) \text{ a.s.}$$

for some constant $C > 0$.

**Proof.** For simplicity of notation, we suppress the term “a.s.” in the displays that follow.

Let $T(x) = n(\tilde{f}_n - f_n^X)(x) = \sum_{i=1}^n \psi\sigma_i(x - X_i)Z_i$, where $Z_i = Y_i - f(X_i)$ with $Z_{1:n} \mid X_{1:n}, f \sim N_n(0, 1)$. Given $X_{1:n}$, $T$ is a random element of $L_1[0, 1]^d$ and $\|T\|_1$ is a non-negative random variable. By the Hahn–Banach theorem, there exists a bounded linear functional $G$ on $L_\infty[0, 1]^d$ such that $G(h) = \int T(x)h(x)dx$ for all $h \in L_\infty[0, 1]^d$ and $\|T\|_1 = \|G\|_F$, where $\|G\|_F = \sup_{h \in F}\{|G(h)|\}$ and $F$ is a countable dense subset of $\{h \in L_\infty[0, 1]^d : \|h\|_\infty \leq 1\}$.

By definition, $G(h) = \sum_{i=1}^n a_i Z_i$, where $a_i = \int \psi\sigma_i(x - X_i)h(x)dx$. Thus, given $X_{1:n}$, \{G(h) : h \in F\} is a Gaussian process and

$$P_{Y|X}\left(\|\tilde{f}_n - f_n^X\|_1 \geq \epsilon_n/2 \mid X_{1:n}\right) = P_{Y|X}\left(\|G\|_F \geq n\epsilon_n/2 \mid X_{1:n}\right).$$

(7)

By Borell’s inequality (Adler, 1990),

$$P_{Y|X}\left(\|G\|_F - E_{Y|X}\|G\|_F \geq t \mid X_{1:n}\right) \leq 2\exp\{-t^2/(2\sigma_F^2)\},$$

(8)

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where $\sigma_F^2 = \sup_{h \in \mathcal{F}} \mathbb{E}_Y|X|G(h)^2$. We now proceed to estimate $\sigma_F^2$ and $\mathbb{E}_Y|X|\|G\|_F$. For any $h \in \mathcal{F}$,

$$
\mathbb{E}_Y|X|G(h)^2 = \sum_{i=1}^{n} \left\{ \int_{[0,1]^d} \psi_{\sigma_n}(x - X_i)h(x) dx \right\}^2 \\
\leq \|h\|_F^2 \sum_{i=1}^{n} \left\{ \int_{[0,1]^d} |\psi_{\sigma_n}(x - X_i)| dx \right\}^2 \leq C_1 n, \tag{9}
$$

where $C_1 = \int |\psi(t)| dt$. Hence, $\sigma_F^2 \leq C_1 n$.

We next bound $\mathbb{E}_Y|X|\|G\|_F = \mathbb{E}_Y|X|T_1$. By Jensen’s inequality, $\mathbb{E}_Y|X|T_1 \leq (\mathbb{E}_Y|X|T_1^2)^{1/2}$. Further,

$$
(\mathbb{E}_Y|X|T_1^2)^{1/2} = \left[ \int \left\{ \int |T(x)|dx \right\}^2 \phi_n(t) dt \right]^{1/2} \leq \int \left\{ \int T(x)^2 \phi_n(t) dt \right\} dx,
$$

where the above inequality follows from an integral version of Minkowski’s inequality. Recalling $T(x) = \sum_{i=1}^{n} \psi_{\sigma_n}(x - X_i)Z_i$, $\int T(x)^2 \phi_n(t) dt = \mathbb{E}[T(x)^2 | X_{1:n}] = \sum_{i=1}^{n} \psi_{\sigma_n}(x - X_i)^2$. Substituting this in the above display and using Jensen’s inequality one more time, we get

$$
\mathbb{E}_Y|X|T_1 \leq \int \left\{ \sum_{i=1}^{n} \psi_{\sigma_n}(x - X_i)^2 \right\}^{1/2} dx \\
\leq \left\{ \sum_{i=1}^{n} \int \psi_{\sigma_n}(x - X_i)^2 dx \right\}^{1/2} \leq C_2(n/\sigma_n^d)^{1/2}, \tag{10}
$$

where $C_2 = \int |\psi(t)|^2 dt^{1/2}$. In [8], set $t = n\epsilon_n/4$. From the above calculations, $\mathbb{E}_Y|X|\|G\|_F \leq C_2(n/\sigma_n^d)^{1/2} \leq n\epsilon_n/4$ since $t_1 \geq t_2d/2$. Using $\sigma_F^2 \leq C_1 n$, we finally obtain $\mathbb{P}_Y|X|\|G\|_F \geq n\epsilon_n/2 | X_{1:n} \leq 2 \exp(-C n\epsilon_n^2)$.

Lemma 3.3. Under conditions of Theorem 2.1

$$
\mathbb{P}_X \left( \|f_n^X - f_n\|_1 \geq \epsilon_n/2 \right) \leq \exp(-n\epsilon_n^2).
$$

Proof. As in Lemma 3.2, we express the desired probability in terms of a tail bound for the supremum of a stochastic process. However, the stochastic process in this case is no longer
a Gaussian process and we cannot use Borell's inequality here. We instead use Bosquet’s version of Talagrand’s inequality for the supremum of a centered empirical process. The following Proposition 3.4 is adapted from Bousquet (2003) which also appears in Section 3.1 of Giné & Nickl (2011).

**Proposition 3.4.** Assume $X_1, \ldots, X_n$ are independent and identically distributed as $P$. Let $\mathcal{G}$ be a countable set of real valued functions and assume all functions $g \in \mathcal{G}$ are $P$-measurable, square integrable and satisfy Tonelli’s theorem as in the proof of Lemma 3.2, and let $W = \sup_{g \in \mathcal{G}} |\sum_{i=1}^n g(X_i)|$. Further, let $\sigma^2_\mathcal{G} = \sup_{g \in \mathcal{G}} \mathbb{E}_P[g(X_1)^2]$ and $K_2 = n\sigma^2_\mathcal{G} + K_1\mathbb{E}_P[W]$. Then, for any $t > 0$,

$$\mathbb{P}\left\{W \geq \mathbb{E}_P W + (2K_2t)^{1/2} + \frac{K_1 t}{3}\right\} \leq \exp(-t).$$

Let $L_x(t) = \psi_{\sigma_n}(x-t)f(t) - \psi_{\sigma_n} \ast f(x)$ for $x, t \in [0,1]^d$ and $W = \int_{[0,1]^d} |\sum_{i=1}^n L_x(X_i)| dx$. Clearly, $\mathbb{P}_X(\|f_n^X - f_n\|_1 > \epsilon_n/2) = \mathbb{P}_X(W > n\epsilon_n/2)$. By an application of Hahn–Banach theorem as in the proof of Lemma 3.2, $W = \|G\|_\mathcal{F}$, where $\mathcal{F}$ is a countable dense subset of the unit ball of $L_\infty[0,1]^d$, $G(h) = \sum_{i=1}^n g(X_i)$, and $g(t) = \int_{[0,1]^d} L_x(t)h(x)dx$. Letting $\mathcal{G}$ denote the class of functions $\{g(t) = \int_{[0,1]^d} L_x(t)h(x)dx, h \in \mathcal{F}\}$, one has $\|G\|_\mathcal{F} = \sup_{g \in \mathcal{G}} |\sum_{i=1}^n g(X_i)|$. Putting together, $W = \sup_{g \in \mathcal{G}} |\sum_{i=1}^n g(X_i)|$ and $\mathbb{E}_X g(X_1) = 0$ by Tonelli’s theorem. We now aim to apply Proposition 3.4 to bound $\mathbb{P}_X(W > n\epsilon_n/2)$. In order to apply Proposition 3.4 we need to estimate $K_1, \sigma^2_\mathcal{G}, K_2$ and $\mathbb{E}_P(W)$ which is carried out below.

Fix $g \in \mathcal{G}$. Then, there exists $h \in \mathcal{F}$ such that $g(t) = \int_{[0,1]^d} L_x(t)h(x)dx = f(t) \int_{[0,1]^d} \psi_{\sigma_n}(t-x)h(x)dx - \int \psi_{\sigma_n} \ast f(x) h(x)dx$. Using the triangle inequality,

$$|g(t)| \leq |f(t)| \int_{[0,1]^d} |\psi_{\sigma_n}(t-x)h(x)|dx + \int_{[0,1]^d} |\psi_{\sigma_n} \ast f(x)||h(x)||dx.$$ 

Using $\|h\|_\infty \leq 1$, the first term in the above display can be bounded above by $C_1\|f\|_\infty$ where $C_1 = \int |\psi(t)||dt$. Similarly, the second term can be bounded above by $\|\psi_{\sigma_n} \ast f\|_1 \leq \|\psi_{\sigma_n} \ast f\|_\infty \leq \|f\|_\infty + \epsilon_n$, where the final inequality follows from (BS). Noting that for any
Since \( f \in \mathcal{P}_n \), \( \|f\|_{\infty} \leq 2M_n \) (since the Hilbert space norm is stronger than the \( \| \cdot \|_{\infty} \) norm), we have \( K_1 \leq CM_n \).

Next we bound \( \sigma_2^2 = \sup_{g \in \mathcal{G}} \int_{[0,1]^d} g(t)^2 dt \). Fix \( g \in \mathcal{G} \). Using the expression for \( g(t) \) in the previous paragraph, \( |g(t)| \leq |f(t)| \int |\psi_{\sigma_n}(x-t)| dx + \int |\psi_{\sigma_n} \ast f(x)| dx \). As before, we can bound \( \int |\psi_{\sigma_n}(x-t)| dx \) from above by \( C_1 \) and also \( \int |\psi_{\sigma_n} \ast f(x)| dx \leq C_1 \int_{s \in [0,1]^d} |f(s)| ds \). Using \( (|a| + |b|)^2 \leq 2(|a|^2 + |b|^2) \) and the Cauchy–Schwarz inequality, \( |g(t)|^2 \leq C \|f(t)\|^2 + C \{ \int_{s \in [0,1]^d} |f(s)| ds \}^2 \leq C \{ |f(t)|^2 + \|f\|_2^2 \} \). Thus, we have \( \sigma_2^2 \leq C \|f\|_2^2 \) for some absolute constant \( C \). Using the bound for \( \sup_{f \in \mathcal{P}_n} \|f\|_2^2 \) in the following Proposition 3.5, we conclude that \( \sigma_2^2 \leq C \) for some absolute constant \( C > 0 \).

**Proposition 3.5.** Recall \( \mathcal{P}_n \) from (5). Then, \( \sup_{f \in \mathcal{P}_n} \|f\|_2^2 \leq C \) for some absolute constant \( C > 0 \).

**Proof.** Let \( f \in \mathcal{P}_n \). Then, there exists \( h \in \mathbb{H}^d \) with \( \|h\|_{\mathbb{H}^d} \leq M_n \) such that \( \|f - h\|_{\infty} \leq \epsilon_n \). Hence, \( \|f\|_2^2 \leq 2(\|h\|_2^2 + \epsilon_n^2) \) and it is enough to bound \( \|h\|_2^2 \). Recalling that \( \| \cdot \|_{2,d} \) denotes the \( L_2 \) norm of \( \mathbb{R}^d \), we have \( \|h\|_2^2 \leq \|h\|_{2,d}^2 \). We provide a bound for \( \|h\|_{2,d}^2 \) below.

There exists \( \psi \in L_2(\mu_{a_n}) \) such that \( h(t) = \int \exp(i \langle \lambda, t \rangle) \xi(\lambda) \omega_{a_n}(\lambda) d\lambda \). Letting \( \hat{h} \) denote the Fourier transform of \( h \), one has from the Fourier inversion theorem that \( \hat{h}(\lambda) = \xi(-\lambda) \omega_{a_n}(\lambda) \). By Parseval’s theorem, \( \|h\|_{2,d}^2 = \|\hat{h}\|_{2,d}^2 = \int \xi^2(\lambda) \omega_{a_n}^2(\lambda) d\lambda \). Observe that \( \omega_{a_n}^2(\lambda) = a_n^{-2d} \exp\{-\|\lambda\|^2/(2a_n^2)\} \). Hence, \( \|h\|_{2,d}^2 = a_n^{-2d} \frac{C}{\xi^2(\lambda)} \int \xi^2(\lambda) \exp\{-\|\lambda\|^2/(2a_n^2)\} d\lambda \leq a_n^{-2d} \frac{C}{\xi^2(\lambda)} \int \xi^2(\lambda) \exp\{-\|\lambda\|^2/(4a_n^2)\} d\lambda \)

\[ = \frac{a_n^{-d}}{C} \int \xi^2(\lambda) \omega_{a_n}(\lambda) d\lambda = \frac{\|h\|_{\mathbb{H}^d}^2}{C a_n^d} \leq \frac{M_n^2}{C a_n^d} = \frac{1}{C}, \]

since \( \|h\|_{\mathbb{H}^d}^2 = \|\xi \omega_{a_n}^{1/2}\|_{2,d}^2 \) and \( M_n = a_n^{d/2} \). \( \square \)

Finally, we proceed to bound \( \mathbb{E}_X W \), where \( W = \int_{[0,1]^d} \sum_{i=1}^n L_2(X_i) dx \). Using Jensen’s

\(^1\omega_{a_n} \) is symmetric about zero.
inequality and the integral version of Minkowski’s inequality, one has
\[
\mathbb{E}XW \leq (\mathbb{E}W^2)^{1/2} = \left[ \int_{\prod_{i=1}^n [0,1]^d} \left\{ \int_{[0,1]^d} |\sum_{i=1}^n L_x(t_i)dx| \right\}^2 dt_1 \ldots dt_n \right]^{1/2}
\]
\[
\leq \int_{[0,1]^d} \left\{ \int_{\prod_{i=1}^n [0,1]^d} |\sum_{i=1}^n L_x(t_i)|^2 dt_1 \ldots dt_n \right\}^{1/2} dx.
\]

Clearly, \( \int_{\prod_{i=1}^n [0,1]^d} |\sum_{i=1}^n L_x(t_i)|^2 dt_1 \ldots dt_n = \text{Var}_X \left\{ \sum_{i=1}^n L_x(X_i) \right\} = n \text{Var}_X \{L_x(X_1)\}, \) since \( \mathbb{E}_X L_x(X_1) = 0. \) Further, \( \text{Var}_X \{L_x(X_1)\} \leq \mathbb{E}_X \left\{ \psi_{\sigma_n}(x-X_1)f(X_1) \right\}^2 = \int_{[0,1]^d} \psi_{\sigma_n}(x-t)^2 f(t)^2 dt \leq \frac{1}{\sigma_n^2} \psi_{\sigma_n} \ast f^2. \) Substituting this in the above display
\[
\mathbb{E}_X W \leq \left( \frac{n}{\sigma_n^2} \right)^{1/2} \int_{[0,1]^d} \left\{ \psi_{\sigma_n} \ast f^2(x) \right\}^{1/2} dx
\]
\[
\leq \left( \frac{n}{\sigma_n^2} \right)^{1/2} \left\{ \int_{[0,1]^d} |\psi_{\sigma_n} \ast f^2(x)dx| \right\}^{1/2}
\]
\[
\leq \left( \frac{n}{\sigma_n^2} \right)^{1/2} \left\{ \int_{[0,1]^d} \int_{[0,1]^d} |\psi_{\sigma_n}(x-t)| f^2(t)dt dx \right\}^{1/2}
\]
\[
\leq \left( \frac{n}{\sigma_n^2} \right)^{1/2} \left[ \int_{[0,1]^d} f^2(t) \left\{ \int_{\mathbb{R}^d} |\psi_{\sigma_n}(x-t)| dx \right\} dt \right]^{1/2}
\]
\[
\leq C \left( \frac{n}{\sigma_n^2} \right)^{1/2} = C n^{\frac{d+\alpha}{4d}} \log^{1/2} n \leq C n \epsilon_n.
\]

From the penultimate line to the last line of the above display, we invoked Proposition 3.4 to bound \( \|f\|_2 \) by a constant. We have thus obtained \( K_1 \leq CM_n \) and \( K_2 \leq Cn. \) In Proposition 3.3, set \( t = n \epsilon_n^2. \) We have \( K_1 t \leq C(n \epsilon_n M_n) \epsilon_n \leq n \epsilon_n \) for sufficiently large \( n \) provided \( \alpha > d/2. \) Further, \( K_2 t \leq n^2 \epsilon_n^2 + K_1 \mathbb{E}(W) t = n^{\frac{d+\alpha}{2d}} \log^{2t_1} n \left\{ n^{\frac{d+\alpha}{2d}} \log^{2t_1} n \right\} \leq 2n \frac{2d+\alpha}{2d} \log^{2t_1} n \) for sufficiently large \( n \) if \( \alpha > d/2. \) Therefore, \( (K_2 t)^{1/2} \leq n \epsilon_n. \)

We next show that (BS) holds. Fix \( f \in \mathcal{P}_n \cap U_n. \) Since \( f \in \mathcal{P}_n, \) there exists \( h \in \mathbb{H}^n \) with \( \|h\|_{\mathbb{H}^n} \leq M_n \) such that \( \|f - h\|_{\infty} \leq \epsilon_n. \) By the triangle inequality, \( \|\psi_{\sigma_n} \ast f - f\|_1 \leq \|\psi_{\sigma_n} \ast f - \psi_{\sigma_n} \ast h\|_1 + \|\psi_{\sigma_n} \ast h - h\|_1 + \|h - f\|_1. \) Using \( \|\psi_{\sigma_n} \ast g\|_1 \leq \|g\|_1 \) for any \( L_1 \) function \( g, \) we can further bound \( \|\psi_{\sigma_n} \ast f - f\|_1 \) from above by \( 2\epsilon_n + \|\psi_{\sigma_n} \ast h - h\|_{\infty}. \) It thus remains to show that \( \|\psi_{\sigma_n} \ast h - h\|_{\infty} \leq \epsilon_n. \)
There exists $\xi \in L_2(\mu_{a_n})$ such that $h(t) = \int \exp(i \langle \lambda, t \rangle)\xi(\lambda)\omega_{a_n}(\lambda)d\lambda$. Clearly, $\hat{h}(\lambda) = \xi(-\lambda)\omega_a(\lambda)$. Since the Fourier transform of $(\psi_{\sigma_n} \ast h)$ is $(2\pi)^d \hat{\psi}_{\sigma_n} \hat{h}$ and $\hat{\psi}_{\sigma_n}(\lambda) = \hat{\psi}(\sigma_n \lambda)$, we have $\psi_{\sigma_n} \ast h(t) = (2\pi)^d \int \exp(-i \langle \lambda, t \rangle)\hat{\psi}(\sigma_n \lambda)\hat{h}(\lambda)d\lambda$. We can choose $\psi$ in a manner such that $\hat{\psi}$ is compactly supported, equals $(2\pi)^{-d}$ on $[-1, 1]^d$ and is bounded above by this constant everywhere; see proof of Lemma 4.3 in van der Vaart & van Zanten (2009). Putting together,

$$
|\psi_{\sigma_n} \ast f(t) - f(t)|^2 \leq \left\{ \int_{\|\lambda\|>\sigma_n^{-1}} |\hat{h}(\lambda)| \right\}^2 \leq \left\{ \int \xi(\lambda)^2\omega_{a_n}(\lambda)d\lambda \right\} \int_{\|\lambda\|>\sigma_n^{-1}} \omega_{a_n}(\lambda)d\lambda
\leq C\|h\|_{H_n}^2 \exp\{-\sigma_n^{-2}/(4a_n^2)\} \leq CM_n^2 \exp\{-\sigma_n^{-2}/(4a_n^2)\} = Ca_n^d \exp\{-\log^{2t_2} n/4\},
$$

where $C$ is an absolute constant. The proof follows by noting that $Ca_n^d \exp\{-\log^{2t_2} n/4\} \leq \epsilon_n^2$ whenever $t_2 \geq 1/2$.

4 Discussion

The article extends upon previous results on random design regression using Gaussian process priors. A limitation of the current exposition is the requirement of the knowledge of the smoothness parameter to construct the rescaling sequence. A natural question is whether one can find a suitable prior on the bandwidth parameter which adapts to the unknown smoothness level as in the fixed design case in van der Vaart & van Zanten (2009). We leave this as a topic for future research.

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Appendix

Proof of Theorem 3.1

Let \( \|f\|_{2,n} \) denote the empirical \( L_2 \) norm of \( f \), so that \( \|f\|_{2,n}^2 = n^{-1} \sum_{i=1}^{n} f^2(X_i) \). Also, define

\[
L_n(f, f_0) = \frac{q^{(n)}(Y_{1:n}, X_{1:n} \mid f)}{q^{(n)}(Y_{1:n}, X_{1:n} \mid f_0)}.
\]

**Lemma 1.** Let \( A_n \) denote the following event in the sigma-field generated by \( (Y_{1:n}, X_{1:n}) \):

\[
A_n = \left\{ (Y_{1:n}, X_{1:n}) : \int L_n(f, f_0) \Pi(df) \geq e^{-n\epsilon_0^2/2} (\|f - f_0\|_\infty \leq \epsilon_n) \right\}. \tag{11}
\]

Then, \( \mathbb{P}_{Y,X}^0(A_n) \geq 1 - e^{-Cn\epsilon_0^2/2} \).

**Proof.** Clearly, \( \mathbb{P}_{Y,X}^0(A_n) = \mathbb{E}_{Y,X}^0[\mathbb{P}_{Y|X}^0(A_n)] \). By Lemma 14 of van der Vaart & van Zanten [2011], \( \mathbb{P}_{Y|X}^0 \{ \int L_n(f, f_0) \Pi(df) \geq e^{-n\epsilon_0^2/2} (\|f - f_0\|_{2,n} \leq \epsilon_n) \} \geq 1 - e^{-n\epsilon_0^2/8} \). The conclusion follows by noting that \( \Pi (\|f - f_0\|_\infty < \epsilon_n) \leq \Pi (\|f - f_0\|_{2,n} < \epsilon_n) \). \( \square \)

**Lemma 2.** There exists a test function \( \Phi_n \) for \( H_0 : f = f_0 \) vs \( H_1 : f \in U_n \cap \mathcal{P}_n \) such that

\[
\mathbb{E}_{Y,X}^0 \Phi_n \leq e^{-Cn\epsilon_0^2}, \tag{12}
\]

\[
\sup_{f \in U_n \cap \mathcal{P}_n} \mathbb{E}_{Y,X}^f (1 - \Phi_n) \leq e^{-Cn\epsilon_0^2}. \tag{13}
\]

for some absolute constant \( C \).

**Proof.** Let \( \Phi_n = 1(\|\hat{f}_n - f_0\|_1 > M\epsilon_n/2) \). The error bounds follow from (BT), (DT) and (BS), (DS). \( \square \)

Using a standard line of argument for establishing convergence rates in Bayesian nonparametric models [Ghosal et al., 2000], we have \( \mathbb{E}_{Y,X}^0 \Pi(U_n \mid Y_{1:n}, X_{1:n}) \leq \sum_{i=1}^{4} b_{i,n} \), where \( b_{1,n} = \mathbb{E}_{Y,X}^f \Phi_n \), \( b_{2,n} = e^{n\epsilon_0^2} \sup_{f \in U_n \cap \mathcal{P}_n} \mathbb{E}_{Y,X}^f (1 - \Phi_n)/\Pi (\|f - f_0\|_\infty < \epsilon_n) \), \( b_{3,n} = e^{n\epsilon_0^2} \Pi(\mathcal{P}_n)/\Pi (\|f - f_0\|_\infty < \epsilon_n) \) and \( b_{4,n} = \mathbb{P}_{Y,X}^0 (A_n^c) \). The Theorem then follows from Lemma 1 and 2.
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