Posterior contraction in Gaussian process regression using Wasserstein approximations

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We study posterior rates of contraction in Gaussian process regression with potentially unbounded covariate domain. Our argument relies on developing a Gaussian approximation to the posterior of the leading coefficients of a Karhunen–Loève expansion of the Gaussian process. The salient feature of our result is deriving such an approximation in the $L^2$ Wasserstein distance and relating the speed of the approximation to the posterior contraction rate using a coupling argument. Specific illustrations are provided for the Gaussian (or squared exponential) and Matérn covariance kernels.

Keywords: kernel regression; Gaussian process; Hermite polynomials; posterior contraction; random design; Wasserstein distance.

1. Introduction

Gaussian process (GP) priors [24] are popularly used in a variety of machine learning applications including regression, classification, density estimation, latent variable modeling, unsupervised learning, to name a few. GP priors also share a deep connection with frequentist-reproducible kernel Hilbert space (RKHS)-based regularization methods; see, for example, Chapter 6 of [24]. Paralleling the development of scalable algorithms for GP regression, there has been substantial progress in recent years in understanding frequentist properties of the posterior arising from a Gaussian process prior. A standard way of evaluating frequentist properties of Bayesian procedures is to consider whether the amount of posterior mass assigned to a neighbourhood of the true data-generating parameter (a function in the present setting) converges to one with increasing sample size. If the neighbourhood size is fixed, the above phenomenon is termed posterior consistency, while if the neighbourhood size is allowed to shrink to zero, then the (best possible) shrinking rate is termed the posterior contraction rate. [10,17] established posterior consistency of GP priors, while posterior contraction rates in a variety of contexts were derived in [5,23,29,30,32,33] among others; see also [25] for an information-theoretic approach. In particular, it has been established in various contexts that the posterior distribution contracts at an optimal rate (up to a logarithmic term) in a frequentist minimax sense.

The above references exclusively deal with compactly supported functions as parameters, even though the priors in principle are random functions on full Euclidean spaces. In fact, the influential article [32] remarks that
Consistency of a posterior on the full space can be expected only if the tails of the functions are restricted. If they are not, then one would still expect that the posterior restricted to compact subsets contracts at some rate. At the moment there seem to exist no results that would yield such a rate (or even consistency).

In this article, we take a step towards addressing this question borrowing inspiration from the kernel regression literature [14, 26], where a $L^2$ norm weighted by a possibly unbounded covariate density is commonly used as a measure of discrepancy. We focus on the non-parametric regression model with Gaussian errors

$$Y_i = f(X_i) + \epsilon_i, \quad \epsilon_i \sim N(0, \sigma^2), \quad i = 1, \ldots, n,$$

where $X_i \in \mathcal{X}$ are covariates and $f : \mathcal{X} \to \mathbb{R}$ is an unknown regression function with possibly unbounded domain $\mathcal{X} \subset \mathbb{R}^d$, which is assigned a zero-mean GP prior. We operate in a random design setting, where the covariates are drawn according to a distribution $\rho$ on $\mathcal{X}$ and study contraction of the posterior in an $L^2(\rho)$ norm, i.e., the $L^2$ norm on $\mathbb{R}^d$ weighted with respect to the covariate density $\rho$. This choice ensures that the large covariate values are weighted down, which can be considered as a way of restricting the tails of the function as in the comment by [32] above.

In deriving the posterior rate of contraction, we expand the GP prior via a Karhunen–Loève expansion [2] and then derive a Gaussian approximation to the posterior distribution of the leading coefficients of the expansion. The Gaussian approximation is derived in an $L^2$ Wasserstein metric, which is particularly suited for the present situation for reasons described in the sequel. Using a careful coupling argument, the speed of such Gaussian approximations are related to the posterior contraction rate, a result that is new to the best of our knowledge. Another key ingredient of our method is to control the effect of truncating the Karhunen–Loève expansion in the posterior. This typically requires bounds on the concentration of the prior around the true function in the sup-norm, which is difficult to control for unbounded covariates. A second contribution of this article is to develop a general result (Theorem 3.4) to bound (with high probability) the integrated log-likelihood ratio from below by a quantity involving prior concentration around the true function in the $L^2(\rho)$ norm instead of the sup-norm. We believe this result may be of independent interest in random-design Gaussian regression. We may comment here that in addition to dealing with unbounded covariates, the proposed technique has an added advantage of making the bias–variance trade-off in the posterior explicit as in kernel ridge regression theory.

While we make general assumptions on the covariance kernel to prove our results, verifying them in a specific context requires suitable control over the eigenfunctions of the kernel. This can potentially be a non-trivial exercise, in particular if the covariance kernel involves a parameter which is sample size dependent. We illustrate this in case of a squared-exponential kernel, for which explicit expressions of the eigenfunctions are available [24]. We develop precise bounds on the eigenfunctions making the role of a scale parameter explicit, which should be more broadly useful. We also prove a concentration result for the Matérn class of covariance kernels under a compact design assumption using our general technique.

2. Preliminaries

For a square matrix $B$, $\text{tr}(B)$ and $|B|$, respectively, denote the trace and the determinant of $B$. If $B$ is positive semi-definite (psd), then let $B^{1/2}$ denote its unique psd square root, so that $(B^{1/2})^2 = B$. $B$ is positive definite (pd) if and only if $B^{1/2}$ is pd [4], and in such cases, we can unambiguously define
\(B^{-1/2} = (B^{-1})^{1/2}\). Given two psd matrices \(B_1\) and \(B_2\), we write \(B_1 \succeq B_2\) if \(B_1 - B_2\) is psd. For a \(p \times d\) matrix \(A = (a_{ij})\) with \(p \geq d\), the singular values of \(A\) are the eigenvalues of \((A^T A)^{1/2}\). We shall use \(s_{\text{max}}(A)\) and \(s_{\text{min}}(A)\) to denote the largest and smallest non-zero singular values respectively; the condition number \(\kappa(A) = s_{\text{max}}(A) / s_{\text{min}}(A)\). The Frobenius norm \(\|A\|_F\) and the operator norm \(\|A\|_2\) are defined in the usual way, with \(\|A\|_F := \sqrt{\text{tr}(A^T A)}\) and \(\|A\|_2 := s_{\text{max}}(A)\). Note that \(\|A\|_2^2 = \|A^T A\|_2\).

For a vector \(x \in \mathbb{R}^d\), \(\|x\|\) will denote its Euclidean norm. Let \(\ell_2 = \{\theta = (\theta_1, \theta_2, \ldots) : \sum_{j=1}^{\infty} \theta_j^2 < \infty\}\) denote the space of square-summable sequences, with \(\|\theta\|_{\ell_2} = (\sum_{j=1}^{\infty} \theta_j^2)^{1/2}\). Let \(\Theta_\alpha = \{\theta \in \ell_2 : \sum_{j=1}^{\infty} j^{2\alpha} \theta_j^2 < \infty\}\) denote the Sobolev space of sequences with ‘smoothness’ \(\alpha > 0\) and denote the Sobolev norm \(\|\theta\|_\alpha = (\sum_{j=1}^{\infty} j^{2\alpha} \theta_j^2)^{1/2}\). For a density \(\rho\) on \(X \subset \mathbb{R}^d\), let \(L^2(\mathcal{X}) = \{g : \int g(x)^2 \rho(x) \, dx < \infty\}\) denote the space of square-integrable functions with respect to \(\rho\). \(L^2(\mathcal{X})\) is a Hilbert space under the inner product \(\langle g_1, g_2 \rangle = \int g_1(x) g_2(x) \rho(x) \, dx\); the resulting norm will be denoted by \(\|\cdot\|_{2,\rho}\), so that \(\|g\|_{2,\rho}^2 = \int g(x)^2 \rho(x) \, dx\).

The Sobolev space \(H^\alpha[0, 1]^d\) is the set of functions \(f_0 : [0, 1]^d \to \mathbb{R}\) that are restrictions of a function \(f_0 : \mathbb{R}^d \to \mathbb{R}\) with Fourier transform \(\hat{f}_0(\lambda)\), satisfying

\[
\|f_0\|_\alpha^2 = \int \left(1 + \|\lambda\|^2\right)^\alpha |\hat{f}_0(\lambda)|^2 \, d\lambda < \infty,
\]

where \(\|f_0\|_\alpha\) is the Sobolev norm of \(f_0\). Roughly speaking, for integer \(\alpha\), a function belongs to \(H^\alpha\) if it has partial derivatives up to order \(\alpha\) that are all square integrable. This follows because the \(\alpha\)th derivative of a function \(f_0\) has Fourier transform \(\lambda \mapsto (i\lambda)^\alpha \hat{f}_0(\lambda)\).

Throughout \(C, C', C_1, C_2, \ldots\) are generically used to denote positive constants whose values might change from one line to another, but are independent from everything else. \(\lesssim / \gtrsim\) denote inequalities up to a constant multiple. \(a \asymp b\) when we have both \(a \lesssim b\) and \(a \gtrsim b\).

### 2.1 The \(L^p\) Wasserstein distances

Given two probability measures \(P\) and \(Q\) on \(\mathbb{R}^d\), the total variation distance \(d_{TV}(P, Q) := \sup_{A} |P(A) - Q(A)|\), where the supremum is over all Borel subsets of \(\mathbb{R}^d\) and the Kullback–Leibler divergence \(D(P||Q)\) are defined in the usual way. For \(p \geq 1\), the \(L^p\) Wasserstein distance with respect to the Euclidean metric (henceforth \(W_p\) in short), denoted \(d_{W,p}(P, Q)\), is defined as

\[
d_{W,p}(P, Q) = \inf_{\text{joint}(P, Q)} \left(\mathbb{E} \|X - Y\|^p\right)^{1/p},
\]

where \(\text{joint}(P, Q)\) denotes all random vectors \((X, Y) \in \mathbb{R}^d \times \mathbb{R}^d\), such that \(X \sim P, Y \sim Q\). The Wasserstein distances have their origins in the problem of optimal transport; refer to [15,18] for background and properties. Explicit expressions are available for the \(W_2\) distance between two \(d\)-dimensional Gaussian measures. In particular, if \(P \equiv N_d(\mu_1, \Sigma_1), Q \equiv N_d(\mu_2, \Sigma_2)\) and \(\Sigma_1, \Sigma_2 = \Sigma_2 = \Sigma_1\), then

\[
d_{W,2}(P, Q) = \|\mu_1 - \mu_2\|^2 + \|\Sigma_{1/2} - \Sigma_{2/2}\|_F^2.
\]

For \(d = 1\), the \(W_2\) distance is identical to the Fréchet distance [12].
3. Posterior contraction in random design GP regression

Write the non-parametric regression model (1.1) in vector form as

\[ Y = F + \varepsilon, \quad \varepsilon \sim N(0, \sigma^2 I_n), \]  

(3.1)

where \( Y = (Y_1, \ldots, Y_n)^T \) and \( F = (f(X_1), \ldots, f(X_n))^T \). We shall assume the error variance \( \sigma^2 \) to be known throughout this article. Let \( f_0 : \mathcal{X} \to \mathbb{R} \) denote the true data-generating function and define \( F_0 = (f_0(X_1), \ldots, f_0(X_n))^T \).

As mentioned in the Introduction, we operate in a random design setting where we assume that the covariates \( X_i \) are independent and identically distributed according to a known density \( \rho \) on \( \mathcal{X} \) and \( Y_i \mid X_i \sim N(f_0(X_i), \sigma^2) \) independently for \( i = 1, \ldots, n \). Letting \( h(y, x) = N(y \mid f_0(x), \sigma^2) \rho(x) \), the true joint density of \((Y, X)\) is an \( n \)-fold product of \( h \). We shall use \( \mathbb{E}_0 \) to denote an expectation with respect to the true joint distribution of \((Y, X)\); \( \mathbb{E}_X \) and \( \mathbb{E}_{0X} \) will respectively denote an expectation with respect to the marginal distribution of \( X \) and the conditional of \( Y \) given \( X \). Similarly, \( \mathbb{P}_0, \mathbb{P}_X \) and \( \mathbb{P}_{0|X} \) will denote probabilities under the respective distributions.

Consider a GP(0, \( \sigma^2 K \)) prior on \( f \), where \( K(\cdot, \cdot) \) is a positive definite correlation function, i.e., \( K(x, x) = 1 \) for all \( x \in \mathcal{X} \). We shall generically use \( \Pi \) and \( \Pi(\cdot \mid Y, X) \) to denote the prior and posterior distribution of \( f \). Under suitable regularity conditions, Mercer’s theorem \cite{Mercer} guarantees that the kernel \( K \) admits an eigen expansion of the form \( K(x, x') = \sum_{j=1}^{\infty} \lambda_j \phi_j(x) \phi_j(x') \) in \( L^2(\mathcal{X}) \), where \( \{\phi_j\} \) is an orthonormal system in \( L^2(\mathcal{X}) \) (\( \int \phi_j(x) \phi_i(x) \rho(x) \, dx = \delta_{ij} \)) and \( \{\lambda_j\} \) the corresponding non-negative eigenvalues, which satisfy

\[ \int K(x, x') \phi_j(x') \rho(x') \, dx' = \lambda_j \phi_j(x), \quad j = 1, 2, \ldots \]  

(3.2)

By the Karhunen–Loève Theorem \cite{Mercer}, the GP itself can be expanded as

\[ f(x) = \sigma \sum_{j=1}^{\infty} \sqrt{\lambda_j} Z_j \phi_j(x), \]  

(3.3)

where \( Z_j \)s are i.i.d. \( N(0, 1) \). If the series representation above is truncated to the first \( k \) terms and the resulting random function is denoted by \( f' \), then it follows from (3.2) and the orthogonality of the eigenfunctions \( \phi_j \) that

\[ E \| f - f' \|_{L^2(\rho)}^2 = \sigma^2 \sum_{j=k+1}^{\infty} \lambda_j. \]  

The accuracy of the truncation relies on the rate of decay of the eigenvalues, which is related to the smoothness of the GP. For example, if the sample paths of a GP are infinite smooth, then the eigenvalues decay exponentially fast, so that relatively few leading terms in the expansion (3.3) offer a close reconstruction of the original process.

Given a GP(0, \( \sigma^2 K \)) prior, we shall consider such truncations of (3.3) to define priors which we refer to as truncated Gaussian process (tGP) priors:

\[ f'(x) = \sum_{j=1}^{k_0} \theta_j \phi_j(x), \quad \theta_j \sim N(0, \sigma^2 \lambda_j). \]  

(3.4)

Let \( \theta' = (\theta_1, \ldots, \theta_{k_0})^T \) denote the \( k_0 \)-dimensional vector of coefficients in (3.4) and \( \Lambda = \text{diag}(\lambda_1, \ldots, \lambda_{k_0}) \), so that \( \theta' \sim N(0, \sigma^2 \Lambda) \). One may consider the tGP priors (3.4) as sieve approximations to the original GP prior, where the basis functions \( \phi_j \)s and the prior variances \( \lambda_j \)s are determined by the choice of the
kernel $K$. We denote such priors by $\text{tGP}_{kn}(0,K)$; the truncation level $k_n$ will be suppressed when clear from the context.

We note here that the tGP prior is solely introduced to obtain theoretical understanding of the original GP prior and the resulting posterior. When working with a GP prior, one can conveniently direct attention to the coefficient vector $\theta'$, which is finite dimensional, albeit with the dimension possibly increasing with sample size $n$. In fact, defining the $n \times k_n$ (random) matrix $\Phi = (\phi_j(x_i))_{1 \leq i \leq n, 1 \leq j \leq k_n}$, one can write model (3.1) equipped with a tGP prior (3.4) as

$$Y \sim \mathcal{N}(F, \sigma^2 I_n), \quad F = \Phi \theta', \quad \theta' \sim \mathcal{N}_{k_n}(0, \sigma^2 \Lambda). \quad (3.5)$$

Using standard Gaussian conjugacy, the posterior distribution of $\theta'$ under (3.5) is

$$\tilde{\mathcal{W}}'(\cdot | X, Y) \equiv \mathcal{N}(\tilde{\theta}, \tilde{\Sigma}), \quad \tilde{\theta} = (\Phi^T \Phi + \Lambda^{-1})^{-1} \Phi^T Y, \quad \tilde{\Sigma} = \sigma^2 (\Phi^T \Phi + \Lambda^{-1})^{-1}. \quad (3.6)$$

From (3.6), the posterior distribution of $F = \Phi \theta'$ is also Gaussian. With a slight abuse of terminology, we shall refer to the posterior distribution (3.6) of $\theta'$ as the tGP posterior induced by the tGP prior. The role of the tGP in deriving posterior rates of contraction for the original GP prior is made precise through the following general rate theorem for GP priors. We first state our assumption regarding the true data-generating function $f$, and introduce some notations.

**T1** The true data-generating function $f_0 \in L_p^2(\mathcal{X})$, so that $f_0 = \sum_{j=1}^\infty \theta_0 \phi_j$ with $\theta_0 = \{f_0, \phi_j\} = \int f_0(x) \phi_j(x) \rho(x) \, dx$. The convergence of the infinite sum is in an $L_p^2$ sense, i.e., $\|f_0 - \sum_{j=1}^J \theta_0 \phi_j\|_{2,p} \to 0$ as $J \to \infty$.

Define $f'_0 = \sum_{j=1}^{k_n} \theta_0 \phi_j$, $\theta'_0 = (\theta_0)_{1 \leq j \leq k_n} \in \mathbb{R}^{k_n}$. Also define $\|\theta'_0\|_H = \sum_{j=1}^{k_n} \frac{\theta_j^2}{\lambda_j} = \|\Lambda^{-1/2} \theta'_0\|^2$.

**Theorem 3.1** Consider model (1.1) with a GP prior $f \sim \mathcal{GP}(0, \sigma^2 K)$, where the kernel $K$ has eigenfunctions $\{\phi_j\}$ and eigenvalues $\{\lambda_j\}$ with respect to the covariate density $\rho$ as in (3.2). Assume the true function $f_0$ satisfies (T1). For $k_n < n$, let $\tilde{\mathcal{W}}'(\cdot | X, Y)$ denote the tGP posterior as in (3.6). Let $\epsilon_n \to 0$ be a sequence with $n \epsilon_n^2 \to \infty$ and $\|f_0 - f'_0\|_{2,p} \lesssim \epsilon_n$. Then, for any $M > 0$,

$$\mathbb{E}_0 T(\|f - f_0\|_{2,p} > M \epsilon_n | Y, X) \leq T_{1n} + T_{2n}, \quad (3.7)$$

where

$$T_{1n} = \frac{\mathbb{E}_0 \left\{ \int_{\mathcal{A}_n(X)} dW_2 \left[ \tilde{\mathcal{W}}'(\cdot | Y, X, N_{kn}(\theta'_0, \sigma_n^2 I_{kn})) \right] \right\} - M^2 \epsilon_n^2/4}{\mathbb{P}_X(\mathcal{X}_n^2 > M^2 n \epsilon_n^2/4) + \mathbb{P}_X(A_n^c)}, \quad (3.8)$$

$$T_{2n} = \mathbb{E}_0 T(\|f - f'_0\|_{2,p} > M \epsilon_n | Y, X). \quad (3.9)$$

In (3.8), $\mathcal{X}_n^2$ denotes a $\chi^2$ random variable with $r$ degrees of freedom and $A_n \subset \mathcal{X}_n$ is any set in the $\sigma$-field generated by $X_1, \ldots, X_n$.

It immediately follows from (3.7) that, for a given $\epsilon_n$, if the sequences $T_{1n}, T_{2n} \to 0$, then $\epsilon_n$ is an upper bound to the posterior contraction rate [16] in the $L_p^2$ norm; note that no assumptions regarding the support of the covariate density $\rho$ is made. Theorem 3.1 thus relates the posterior contraction rate of a GP prior to (i) the speed of a posterior Wasserstein approximation of the induced tGP prior $(T_{1n})$, 

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and (ii) the associated truncation error ($T_{2n}$). To obtain the best possible rate out of Theorem 3.1, one needs to choose the truncation level $k_n$ (and to a lesser extent the set $A_n$) in an optimal fashion. The role of these quantities will become more explicit once we provide manageable bounds to $T_{1n}$ and $T_{2n}$ in the subsequent sections. To that end, we need to make additional assumptions on the eigenfunctions $\{\phi_i\}$ and eigenvalues $\{\lambda_j\}$ of the kernel $K$ stated below. Recall $A = \text{diag}(\lambda_1, \ldots, \lambda_{k_n})$ and $\Phi = (\phi_j(X_i))_{1 \leq i \leq n, 1 \leq j \leq k_n}$.

Assume

(A1) $\|A^{-1}\|_2 < n/4$.

(A2) $\sup_{x \in X} |\phi_j(x)| \leq L_n$ for all $j = 1, \ldots, k_n$, with $L_n^2 k_n \log k_n < n$.

Assumption (A1) typically implies a bound on the growth rate of $k_n$; for example, if the eigenvalues decay polynomially, $\lambda_j \asymp j^{-2\beta}$ for some $\beta > 0$, then $\|A^{-1}\|_2 = \lambda^{-1}_{k_n} \asymp k_n^{-2\beta}$, and hence (A1) is satisfied for all $k_n \gtrsim n^{1/(2\beta+1)}$. Assumption (A2) is readily satisfied if all the eigenfunctions $\phi_j$ are uniformly bounded in magnitude by a constant. However, (A2) is more general and allows the sup-norm of the top $k_n$ eigenfunctions to increase with $n$ subject to a growth condition; note that no assumption is made regarding the trailing eigenfunctions. Allowing the sup-norm bound to grow with $n$ is important when the kernel is indexed by one or more hyper parameters which may depend on $n$. A specific illustration is provided in the context of the squared-exponential covariance kernel (4.1) in Section 4. It turns out a non-trivial exercise to bound the eigenfunctions (4.1), making the dependence on the bandwidth parameter $a$ explicit.

3.1 Wasserstein approximations to tGP posteriors

To bound $T_{1n}$, one primarily needs a handle on the squared $W_2$ distance between the tGP posterior $\tilde{Y}^\rho(\cdot \mid Y, X)$ in (3.6) and a Gaussian $N_{k_n}(\theta_0^t, \sigma^2 I_{k_n}/n)$ distribution. Inspecting the proof of Theorem 3.1, it may seem a more obvious choice for $T_{1n}$ is

$$T^*_{1n} = \mathbb{E}_{\rho \sim d_{TV}} \left[ \tilde{Y}^\rho(\cdot \mid Y, X), N_{k_n}(\theta_0^t, \frac{\sigma^2}{n} I_{k_n}) \right] + P(\chi_{k_n}^2 > M^2 n e_2^2 / 4),$$

where $d_{TV}$ denotes the total variation distance. However, such approximations in the total variation distance require a prior flatness condition [7] which is not satisfied by the tGP priors. We find that bounding the $W_2$ distance between the tGP posterior and the asymptotic Gaussian distribution is less demanding in the present setting compared with the total variation distance. However, the connection between such an approximation result in the $W_2$ distance and posterior contraction rates in the $L_2^n$ norm is not immediately clear. We devise a coupling argument to relate the two quantities in the proof of Theorem 3.1.

The $\mathcal{H}_{A_n}(X)$ term in $T_{1n}$ is introduced as a technical device to control the expectation of the squared Wasserstein distance on $A_n$; we appropriately choose $A_n$ in a way so that $A_n^{-1}$ receives vanishingly small probability under $\mathbb{P}_X$. Before proceeding further, we settle with a choice of $A_n$ in the following Lemma 3.2.

**Lemma 3.2** Assume the eigenfunctions $\{\phi_j\}$ of the kernel $K$ with respect to the covariate density $\rho$ satisfy (A2). Define $A_n = (\|\Phi^T \Phi - n I_{k_n}\|_2 < n/2)$. Then, $\mathbb{P}_X(A_n^c) < k_n e^{-Cn/(k_n L_n^2)}$. 
Remark 3.1 On the set $A_n$, $\Phi$ satisfies

$$\|\Phi^T\Phi\|_2 \leq 3n/2, \quad s_{\text{min}}(\Phi^T\Phi) \geq n/2, \quad \kappa(\Phi^T\Phi) \leq 3, \quad \text{tr}[(\Phi^T\Phi)^{-1}] \leq \frac{2k_n}{n}. \quad (3.10)$$

Lemma 3.2 follows from a measure concentration phenomenon, which under appropriate conditions on the summands ensures that a sum of independent symmetric random matrices is concentrated around its expectation with high probability. We can write $\Phi^T\Phi = \sum_{i=1}^n \phi(i)(\phi(i))^T + \phi(0)(\phi(0))^T \in \mathbb{R}^{kn}_+$ independent for $i = 1, \ldots, n$. Using the orthonormality of the eigenfunctions $\{\phi_j\}$, $(E_X\phi(i)(\phi(i))^T)_{jl} = \int \phi_j(x)\phi_l(x)\rho(x)\,dx = \delta_{jl}$, and hence $E_X\Phi^T\Phi = nI_{kn}$. We specifically apply a version of matrix Bernstein inequality [28] to prove the concentration of $\Phi^T\Phi$ around $nI_{kn}$; the proof is deferred to Section 6. The sup-norm bound on the eigenfunctions $\phi_j$s in Lemma 3.2 is used to bound the operator norms of the matrices $\phi(i)(\phi(i))^T$.

We are now in a position to state our approximation result in the $W_2$ distance that provides a simple bound to the first term of $T_{1n}$ in (3.8). Recall $\theta_0^f, f_0^l$ from (T1).

Theorem 3.3 Assume the true function $f_0$ satisfies (T1) and the eigenfunctions $\{\phi_j\}$ and eigenvalues $\{\lambda_j\}$ of the kernel $K$ with respect to the covariate density $\rho$ satisfy (A1) and (A2). Let $A_n \in \mathcal{X}^n$ be the set defined in Lemma 3.2. The tGP posterior $\tilde{W}^\prime(\cdot \mid Y, X)$ from (3.6) satisfies

$$E_0 \left\{ \|W_{A_n}(X) d_{W,2}^2 \left[ \tilde{W}^\prime(\cdot \mid Y, X), N_{kn} \left( \theta_0^f, \frac{\sigma^2}{n}I_{kn} \right) \right] \right\} \leq \sigma^2 \frac{k_n}{n} + \left\| \theta_0^f \right\|_2^2 \frac{2}{n} + \left\| f_0 - f_0^l \right\|_{2,\rho}^2. \quad (3.11)$$

While $f_0$ is only assumed to be an element of $L_\rho^2(\mathcal{X})$ in Theorem 3.3, additional smoothness assumption can be utilized to obtain more precise bounds on the truncation error $\left\| f_0 - f_0^l \right\|_{2,\rho}$ in (3.11). The bound (3.11) indicates a typical bias–variance-type trade-off: increasing the truncation level $k_n$ will improve the truncation error $\left\| f_0 - f_0^l \right\|_{2,\rho}$, however, at the expense of the first two terms increasing. Typically, if $f_0$ is $\alpha$-smooth, then the first two sums contribute a $k_n/n$ factor and the truncation error is of the order $k_n^{\alpha-2}$; with $k_n/n + k_n^{\alpha-2}$ attaining its minimum when $k_n = n^{1/(\alpha+1)}$. The $\left\| \theta_0^f \right\|_W^2$ term can be considered an RKHS-type penalty; indeed, it is the RKHS norm of $\theta_0^f$ relative to a $N(0, A)$ distribution [31].

### 3.2 Handling the truncation error

We now focus attention on the term $T_{2n}$ in (3.7). To this end, we rely on a standard argument in Bayesian non-parametrics: if the prior probability of a set is exponentially small, then its posterior probability converges to zero. Such an argument is commonly used to derive upper [16] and lower [9] bounds to the posterior convergence rate. However, a crucial ingredient for the above argument to work is to obtain suitable lower bounds to the log-likelihood ratio integrated with respect to the prior. The only such result that we are aware of in the random design setting is from [33], who derive a bound for the empirical $L_2$ norm, and then use a functional Bernstein inequality to extrapolate to the $L_\rho^2$ norm. Their result requires the prior draws from the GP to be bounded with probability one, which may not be the case for non-compact covariates. In Theorem 3.4 below, we develop a general result to bound (with high probability) the integrated log-likelihood ratio from below by a quantity involving the prior concentration around the true function in the $L_\rho^2$ norm. A proof of Theorem 3.4 can be found in Section 6.
THEOREM 3.4 Recall $F = (f(X_1), \ldots, f(X_n))^T$, $F_0 = (f_0(X_1), \ldots, f_0(X_n))^T$ and $X_1, \ldots, X_n$ are independently and identically distributed according to the density $\rho$. For $\mu \in \mathbb{R}^n$, let $p_{n, \mu} (\cdot)$ denote the $N_n (\mu, I_n)$ density. Let $\Pi$ be a prior on $L_p^2$ and $\tilde{\epsilon}_n \to 0$ be a sequence such that $n\tilde{\epsilon}_n^2 \to \infty$. Then,

$$
\mathbb{P}_0 \left( \int \frac{p_n f(Y)}{p_{n, f_0}(Y)} \Pi (df) \geq e^{-n\tilde{\epsilon}_n^2} \Pi (f : \|f - f_0\|_{2, \rho} < \tilde{\epsilon}_n) \right) \geq 1 - C \frac{\log (n\tilde{\epsilon}_n^2)}{\sqrt{n\tilde{\epsilon}_n^2}}.
$$

(3.12)

Using Theorem 3.4 along with a standard argument (see, for example, Theorem 2.1 of [16]), we can bound

$$
T_{2n} \leq \frac{\Pi \left( \|f - f_1\|_{2, \rho}^2 > M^2 \epsilon_n^2 \right)}{e^{-n\tilde{\epsilon}_n^2} \Pi \left( \|f - f_0\|_{2, \rho} \leq \tilde{\epsilon}_n \right)} + C \frac{\log (n\tilde{\epsilon}_n^2)}{\sqrt{n\tilde{\epsilon}_n^2}}.
$$

(3.13)

Using Theorem 3.3 and Theorem 3.4, we arrive at the following corollary to Theorem 3.1.

COROLLARY 3.5 Consider model (1.1) with a GP prior $f \sim \text{GP}(0, \sigma^2 K)$. Assume the true function $f_0$ satisfies (T1). Let $\epsilon_n \to 0$ satisfy $n\epsilon_n^2 \to \infty$. Let $k_n < n$ be such that

(C0) The eigenfunctions $\{\phi_j\}_{j=1}^{k_n}$ and eigenvalues $\{\lambda_j\}_{j=1}^{k_n}$ of the kernel $K$ with respect to the covariate density $\rho$ satisfy (A1) and (A2).

(C1) $\max \{k_n, \|\theta_0\|_{2, \Pi}^2 \} = o(n\epsilon_n^2)$.

(C2) $\|f_0 - f_0\|_{2, \rho}^2 = o(\epsilon_n^2)$.

(C3) There exists a sequence $\tilde{\epsilon}_n \to 0$ with $n\tilde{\epsilon}_n^2 \to \infty$ such that

$$
\frac{\Pi \left( \|f - f_1\|_{2, \rho}^2 > M^2 \epsilon_n^2 \right)}{e^{-n\tilde{\epsilon}_n^2} \Pi \left( \|f - f_0\|_{2, \rho} \leq \tilde{\epsilon}_n \right)} \to 0.
$$

(3.14)

Then, for a large constant $M > 0$,

$$
\lim_{n \to \infty} \mathbb{E}_0 \Pi \left( \|f - f_0\|_{2, \rho} > M\epsilon_n | Y, X \right) = 0.
$$

(3.15)

Proof. The quantity in (3.15) is bounded by $T_{1n} + T_{2n}$ from Theorem 3.1. Invoking Theorem 3.3,

$$
T_{1n} \lesssim \frac{\max \{k_n, \|\theta_0\|_{2, \Pi}^2 \}}{n\epsilon_n^2} + \frac{\|f_0 - f_0\|_{2, \rho}^2}{\epsilon_n^2} + \frac{\mathbb{P} \left( \chi_{kn}^2 > M^2 n\epsilon_n^2 / 4 \right)}{\mathbb{P}_X (A_n^0)}.
$$

The first two quantities in the above display converge to zero by (C1) and (C2). By (C1) and a standard deviation inequality for chi-square distributions, $\mathbb{P} (\chi_{kn}^2 > M^2 n\epsilon_n^2 / 4) \to 0$ for $M > 2$. By Lemma 3.2, $\mathbb{P}_X (A_n^0) \leq k_n e^{-Cn/(knL^2)} \to 0$ by (C0). The proof is completed using the bound (3.13) for $T_{2n}$. \qed

In (3.14), the prior tail probability in the numerator $\Pi \left( \|f - f_1\|_{2, \rho}^2 > M^2 \epsilon_n^2 \right) = \Pi \left( \sum_{j=k_n+1}^{\infty} \lambda_j Z_j^2 > M^2 \epsilon_n^2 \right)$, with $Z_j$s i.i.d. $\text{N}(0, 1)$. Using a version of Bernstein’s inequality for sub-exponential random
variables (Proposition 5.16 of [34]), one can suitably bound this probability. Secondly, the prior concentration in $L^2$ norm in the denominator $\Pi \left( \|f - f_0\|_{2, p} \leq \tilde{\varepsilon}_n \right) = \Pi \left( \|\theta - \theta_0\|_{2, \ell^2} \leq \tilde{\varepsilon}_n \right)$ with $\theta_j \sim N(0, \lambda_j)$; this can be bounded from below using Anderson’s inequality (Lemma B.2 in Appendix B). We provide specific illustrations of these arguments for the squared-exponential kernel below.

4. Applications to popular Gaussian process kernels

4.1 Squared-exponential kernel

As a non-trivial application of the general results in the previous section, we consider Gaussian process regression with a squared-exponential kernel $K_n(x, x') = \exp(-a^2 \|x - x'\|^2)$, a popular choice in machine learning applications. It is well-known that the realizations of a GP with squared-exponential kernel are infinitely smooth, and hence are not suitable to model rougher functions. It has only been recently understood [29] that the parameter $a$ plays the role of an ‘inverse bandwidth’, and scaling the parameter $a$ with the sample size enables better approximation of rougher functions. The work by [29] motivates this from a rescaling perspective; i.e., choosing a large value of $a$ is equivalent to tracing the trajectory of a smooth process (with $a = 1$) over a larger domain, incurring more roughness. In the regression context (1.1), [29] derived optimal posterior convergence rates in the empirical $L^2$ norm using a rescaling $a \equiv a_n = n^{1/(2a + 1)}$, where the true function is $\alpha$-smooth on a compact domain in $\mathbb{R}$. Using a gamma prior on $a$, [32] extended their result showing that the rate of contraction is adaptive over any $\alpha$-smooth compactly supported function. In a more recent article, [23] extended the results in [29] for integrated $L^1$ norm. All these articles make exclusive use of the reproducing kernel Hilbert space theory from [31] and bounds on sup-norm small ball probabilities of Gaussian processes over compact domain [20–22].

As a concrete example, consider the squared-exponential kernel $K_n(x, x') = \exp(-a^2 \|x - x'\|^2)$ indexed by a length-scale parameter $a$. For Gaussian covariate distributions $\rho$, explicit expressions for the eigenfunctions and eigenvalues are known [24]. Specifically, when the dimension $d = 1$, with a Gaussian covariate density $\rho(x) = \sqrt{2b/\pi} e^{-2bx^2}$ and $c = \sqrt{b^2 + 2ab^2}$,

$$\phi_j(x) = \frac{(c/b)^{1/4}}{\sqrt{2}^{j-1} (j-1)!} e^{-(c-b)x^2/2} H_{j-1}(\sqrt{2c} x), \quad \lambda_j = \left( \frac{2b}{b + a^2 + c} \right)^{1/2} \left( \frac{a^2}{b + a^2 + c} \right)^{j-1},$$

(4.1)

where $H_k(x) = (-1)^n e^{x^2} \frac{d^k}{dx^k} e^{-x^2}, k = 0, 1, \ldots$ denote the Hermite polynomials. The eigen-expansion of the squared-exponential kernel offers a complementary perspective into the rescaling phenomenon. Consider the expression for the eigenvalues of the squared-exponential kernel in (4.1). It is well-known that the rate of decay of the eigenvalues is closely connected to the smoothness of the process (3.3). When $a = 1$, the eigenvalues $\lambda_j$ decay exponentially fast in $j$, indicating the infinite smoothness of the sample paths. Although the rate of decay remains exponential in $j$ for any fixed value of $a$, it is effectively slowed down for large values of $a$; see Fig. 1 for an illustration.

In this section, we apply the results developed in Section 4 (specifically Corollary 3.5) to derive posterior rates of contraction for the above rescaled GP priors with the covariates drawn i.i.d. from a Gaussian density on the real line. To the best of our knowledge, no existing posterior contraction rate result for the squared-exponential (or other) kernel allows unbounded covariate support. Using a tensor-product basis approach, it is possible to extend our results to covariates in $\mathbb{R}^d$.

---

1 Many references term $H_k$ the ‘physicist’s Hermite polynomial’ to distinguish from the ‘probabilist’s Hermite polynomial’ $h_k(x) = 2^{-k/2} H_k(x/\sqrt{2})$. 
4.2 Matérn kernel

The Matérn family form another popular class of covariance kernels routinely used in machine learning and spatial statistics. However, unlike the Gaussian kernel in the previous subsection, we are not aware of a Mercer decomposition of the Matérn kernel, which necessitates further work to bound the eigenvalues. For simplicity of exposition, we assume the covariates are compactly supported and consider Matérn kernels on $[0, 1] \times [0, 1]$ given by

$$K_a(x, y) = k_a(|x - y|),$$

for $x, y \in [0, 1]$, where

$$k_a(t) = \frac{2^{1-v}}{\Gamma(v)} \left\{ \sqrt{2v} |t| \right\}^v B_v\left\{\sqrt{2v} a|t|\right\}, \quad t \in [-1, 1],$$

(4.2)

where $a > 0$, and $B_v$ is the modified Bessel function of the second kind for $0 < v < \infty$. We now characterize the eigen system of $K_a(x, y)$ defined on $[0, 1] \times [0, 1]$. Since an exact Mercer expansion is unavailable, we propose to estimate the eigenvalues with respect to the Fourier basis, which form an orthonormal basis of $L^2, \rho([0, 1])$, with $\rho$ the uniform distribution on $[0, 1]$. Specifically, let

$$\phi_{2j-1}(x) = \sin(j\pi x), \quad \phi_{2j}(x) = \cos(j\pi x), \quad j = 1, 2, \ldots,$$

denote the Fourier basis and consider a Mercer expansion

$$K_a(x, y) = \sum_{j=0}^{\infty} \lambda_j \phi_j(x)\phi_j(y),$$

where $\lambda_j$ is the $j$th largest eigenvalue. We now derive estimates on the sizes of the leading eigenvalues in Proposition 4.1 below.

**Proposition 4.1** If $K_a(x, y)$ is given by (4.2), then

$$\lambda_0 \asymp a^{-1}, \quad \lambda_{2j-1} = \lambda_{2j} \asymp a^{-1}(1 + j^2 / a^2)^{-(\nu+1)/2}, j = 1, \ldots, n^\kappa$$

(4.3)

for any $\kappa > 0$, provided $a \geq C(\nu, \kappa) \log n$ for a constant $C(\nu, \kappa) > 0$ depending on $\nu$ and $\kappa$. 

---

![Figure 1](https://academic.oup.com/imaiai/article-abstract/doi/10.1093/imaiai/iax003/3782822/Posterior-contraction-in-Gaussian-process/16000000)

*Fig. 1.* The top 50 eigenvalues $\lambda_j$ of the squared-exponential kernel in (4.1) plotted against the index $j$ for four different values of $a$. Left panel: the index $j$ runs from 1 to 20. Right panel: $j$ runs from 21 to 50. With increasing $a$, the rate of decay is slowed down.
Proof. Clearly, $k_a(\cdot)$ is an even function over $[-1, 1]$. Consider its Fourier series expansion

$$k_a(t) = \sum_{\nu=0}^{\infty} \alpha_{\nu} \cos(\nu \pi t), \quad t \in [-1, 1],$$

where we used the fact that the Fourier coefficients for the sine basis are zero because $K$ is an even function. In the above display,

$$\alpha_{\nu} = \int_{-1}^{1} k_a(t) \cos(\nu \pi t) \, dt = \int_{-1}^{1} k_a(t) e^{i \nu \pi t} \, dt, \quad u \geq 1,$$

where, in the last step, we again used the fact that $k_a(t)$ is an even function. Use the identity that for any $x, y$,

$$\cos(x - y) = \cos(x) \cos(y) + \sin(x) \sin(y),$$

we obtain

$$K_a(x, y) = k_a(|x - y|) = \sum_{\nu=0}^{\infty} \alpha_{\nu} \left[ \cos(\nu \pi x) \cos(\nu \pi y) + \sin(\nu \pi x) \sin(\nu \pi y) \right], \quad x, y \in [0, 1].$$

Thus,

$$\lambda_0 = \int_{-1}^{1} k_a(t) \, dt, \quad \lambda_{2j-1} = \lambda_{2j} = \int_{-1}^{1} k_a(t) e^{i \nu \pi t} \, dt, \quad j \geq 1.$$

The spectral density of the Matern kernel is given by

$$h^a(\psi) := \frac{1}{2\pi} \int e^{i \nu \psi} k_a(t) \, dt = C \left( 1 + \frac{\psi^2}{a^2} \right)^{-(\nu+1)/2}.$$  

We now argue that by choosing $a \geq C \log n$ for a suitably large constant $C$, one can ensure that $\int_{|u| \leq 1} k_a(u) \, e^{i \nu u} \, du$ is of the same order as $\int_{-\infty}^{\infty} k_a(u) \, e^{i \nu u} \, du$. This is true, since

$$\int_{|u| \geq 1} k_a(u) \, e^{i \nu u} \, du \leq \int_{|u| \geq 1} k_a(u) \, du = C_1 \int_{|u| \geq C_2 a} t^\nu B_v(t) \approx e^{-C_3 a}$$

for $j = 0, 1, 2, \ldots$, where the last inequality follows from Theorem 2.5 and (A.5) of [13]. Since $e^{-C_3 a}$ can be made smaller than $\lambda_{2j}$ by choosing $a \geq C(\nu, \kappa) \log n$, we can estimate $\lambda_{2j-1} = \lambda_{2j} \approx h^a(j \pi)$, delivering the proof of the Proposition. \qed

5. Posterior contraction rate

5.1 Squared-exponential kernel

For the first part of this section, let $\{\phi_j\}$ and $\{\lambda_j\}$ denote the eigenfunctions and eigenvalues (4.1) of the squared-exponential kernel with inverse-bandwidth parameter $a$; the dependence on $a$ is suppressed.
for notational convenience. In order to apply Theorem 3.5 to the squared-exponential kernel, we need sup-norm bounds on the $k_n$ leading eigenfunctions $\phi_j$s. Since we are concerned with rescaled processes where the parameter $a$ is sample size dependent, it is important to precisely characterize the role of $a$ in the bound.

A well-known inequality for the Hermite polynomial is Cramer’s bound [27], which states that for any $l \geq 1$, $|H_l(z)| \leq C\sqrt{2\pi}! e^{z^2/2}$ for all $z \in \mathbb{R}$, where $C \leq 2$ is a global constant that does not depend on $z$ or $l$. A direct use of this bound leads to $|\phi_{j+1}(x)| \lesssim (c/b)^{1/4} e^{bx^2}$, which is clearly not sufficient as we are dealing with unbounded covariates. Since the Hermite functions are polynomials, the exponential bound provided by Cramer’s inequality is wasteful in the tails. We derive a bound for the leading eigenfunctions $\phi_j$s in Lemma 5.1 below; refer to Appendix A for a proof. We did not find an existing reference proving this result. The main idea is to use Cramer’s bound in a neighbourhood of the origin, while for suitably large values of $x$, use a combination of Cramer’s bound with a different bound obtained by exploiting an integral representation of the Hermite polynomials.

**Lemma 5.1** Let $\phi_j$s be the eigenfunctions of the squared-exponential kernel as in (4.1). Then, $\max_{0 \leq j \leq k} \sup_{x \in \mathbb{R}} |\phi_j(x)| \lesssim a^{1/4} e^{bx^2}$ for large $a$.

We are now in a position to state the rate theorem. Set $a_n = n^{1/(2\alpha+1)}$ in (4.1). We define the true class of functions $\mathcal{F}$ with ‘smoothness $\alpha$’ as linear combinations of the eigenfunctions $\phi_j$ with the coefficient vector in the Sobolev class $\Theta_\alpha$. Formally,

$$\mathcal{F} = \left\{ f_0 : f_0 = \sum_{j=1}^\infty \theta_j \phi_j, \theta_j = (\theta_{01}, \theta_{02}, \ldots) \in \Theta_\alpha \right\}. \quad (5.1)$$

**Theorem 5.2** Consider the non-parametric regression model (1.1). Assume the covariates $X_i$ are drawn i.i.d. from a Gaussian density $\rho(x) = \sqrt{2b/\pi} e^{-2bx^2}$ and the true function $f_0 \in \mathcal{F}$ as in (5.1) with $\alpha > 1/[4(1 - 2b)]$. Let $f \sim \text{GP}(0, \sigma^2 K)$ with squared-exponential covariance kernel $K_u(x, x') = \exp(-a^2 |x - x'|^2)$. Choose $a \equiv a_n = n^{1/(2\alpha+1)}$. Then, an upper bound to the posterior contraction rate (3.15) in $L_2^\nu$ norm is $\epsilon_n = n^{-\alpha/(2\alpha+1)} \log n$.

**Remark 5.1** From [29], the rescaling $a_n = n^{1/(2\alpha+1)}$ is the optimal choice for $\alpha$ smooth functions on a compact domain and leads to the optimal rate $n^{-\alpha/(2\alpha+1)}$ up to a logarithmic term. Theorem 5.2 obtains a similar result for non-compact domains in a random design setting. The lower bound on the smoothness $\alpha$ is typically necessitated in random design settings; see for example, [6,8]. In particular, when $b = 1/4$, so that $\rho$ corresponds to the standard normal density, we require $\alpha > 1/[4(1 - 2b)] = 1/2$.

### 5.2 Matérn kernel

In this section, we illustrate the use Corollary 3.5 to deliver optimal convergence rate using Matérn kernel. We focus on the case where the true function $f_0 : [0, 1] \to \mathbb{R}$, so that we can leverage on the eigenvalue estimates from Proposition 4.1.

**Theorem 5.3** Consider the non-parametric regression model (1.1). Assume the covariates $X_i$ are drawn i.i.d. from an uniform density $\rho(x) = 1_{[0,1]}(x)$ and the true function $f_0 \in \mathcal{F}$, but with $\phi_j$ as defined in (4.3). Let $f \sim \text{GP}(0, \sigma^2 K_a)$, where $K_a$ is the Matérn covariance kernel defined in (4.2) with $\nu = \alpha$. 

Choose \( a \equiv a_n = \log n \). Then, an upper bound to the posterior contraction rate (3.15) in \( L^2_{\rho} \) norm is \( \epsilon_n = n^{-\alpha/(2\alpha+1)} \log n \), where \( t = (2\alpha + 2)/(2\alpha + 1) \).

### 5.3 Comparison with existing results

Posterior concentration rates using GP priors with squared-exponential covariance kernel were obtained in [23,29,32,33]. However, they consider functions defined on a compact interval with covariates generated either according to fixed design [29,32] or according to random design [23,33]. Theorem 5.2 is the first posterior contraction result with GP priors with squared-exponential kernel that can handle functions defined on an unbounded domain with covariates drawn according to a random design.

For the Matérn covariance kernel, analogous results are known both in fixed and in random design; see Theorem 5 of [33]. Observe that if \( \phi_j \) are as defined in (4.3), (5.1) essentially defines the Sobolev space \( H^\alpha[0,1] \). Hence, our Theorem 5.3 recovers the result in Theorem 5 of [33].

### 6. Proof of main results

**Proof of Theorem 3.1**

Using triangle inequality \( \| f - f_0 \|_{2,\rho} \leq \| f' - f_0' \|_{2,\rho} + \| f - f' \|_{2,\rho} + \| f_0 - f_0' \|_{2,\rho} \), and since \( \| f_0 - f_0' \|_{2,\rho} \leq \epsilon_n \), by assumption, we can bound

\[
\Pi\left(\| f - f_0 \|_{2,\rho} > M\epsilon_n \mid Y, X \right) \leq \Pi\left(\| f' - f_0' \|_{2,\rho} > M\epsilon_n \mid Y, X \right) + \Pi\left(\| f - f' \|_{2,\rho} > M\epsilon_n \mid Y, X \right).
\]

Further, using the orthonormality of the eigenfunctions,

\[
\Pi\left(\| f' - f_0' \|_{2,\rho} > M\epsilon_n \mid Y, X \right) = \tilde{\mathbb{V}}(\| \theta' - \theta_0' \| > M\epsilon_n \mid Y, X).
\]

Therefore, taking expectation,

\[
\mathbb{E}_0\Pi \left(\| f - f_0 \|_{2,\rho} > M\epsilon_n \mid Y, X \right) \leq \mathbb{E}_0\tilde{\mathbb{V}}(\| \theta' - \theta_0' \| > M\epsilon_n \mid Y, X) + T_{2n}. \tag{6.1}
\]

Let \( U_n = \{\| \theta' - \theta_0' \| \leq M\epsilon_n\}. \) We shall show below that \( \mathbb{E}_0\tilde{\mathbb{V}}(U_n^c \mid Y, X) \leq T_{1n} \), which will complete the proof of the theorem. For any \( A_n \subset \mathcal{X}^n \) in the \( \sigma \)-field generated by \( X_1, \ldots, X_n \), bound

\[
\mathbb{E}_0\tilde{\mathbb{V}}(U_n^c \mid Y, X) \leq \mathbb{E}_0\tilde{\mathbb{V}}(U_n^c \mid Y, X)\mathbb{P}_X(A_n^c) + \mathbb{P}_X(A_n^c). \tag{6.2}
\]

We now elucidate a coupling argument to bound the \( \tilde{\mathbb{V}}(U_n^c \mid Y, X) \) term in (6.2). Given \( (Y, X) \), let \( (\theta_T, \theta_A) \in \mathbb{R}^k \times \mathbb{R}^k \) be a pair of random variables such that \( \theta_T \sim Q_T \equiv \tilde{\mathbb{V}}(\cdot \mid Y, X) \), and \( \theta_A \sim Q_A \equiv N(\theta_0', \sigma^2 I_n/n) \) and \( \mathbb{E}\| \theta_T - \theta_A \|^2 = \mathbb{E} d_{0,2}(Q_T, Q_A) \), where \( \mathbb{E} \) denotes an expectation with respect to the joint distribution of \( (\theta_T, \theta_A) \) given \( Y, X \). In other words, \( (\theta_T, \theta_A) \in \text{joint}(Q_T, Q_A) \) are *optimally coupled*, i.e., the infimum in (2.1) is attained by \( (\theta_T, \theta_A) \). Such an optimal coupling can be always constructed in general; see [18] for a a constructive proof for normal distributions. We then have

\[
\tilde{\mathbb{V}}(U_n^c \mid Y, X) = P(\theta_T \in U_n^c) \leq P(\theta_T \in U_n^c, \| \theta_T - \theta_A \| \leq M\epsilon_n/2) + P(\| \theta_T - \theta_A \| > M\epsilon_n/2) \tag{6.3}
\]
\[
\begin{align*}
&\leq P \left( \|\theta_\Lambda - \theta_0\| > M\epsilon_n / 2 \right) + \frac{4E \|\theta_T - \theta_\Lambda\|^2}{M^2\epsilon_n^2} \\
&= P \left( \chi_{kn}^2 > M^2n\epsilon_n^2 / 4 \right) + \frac{4d_{W,2}^2(Q_T, Q_\Lambda)}{M^2\epsilon_n^2}.
\end{align*}
\] (6.4)

In the above display, the first line simply uses that the marginal distribution of \(\theta_T\) is \(\tilde{W}^n(\cdot \mid Y, X)\) by construction. From the first to the second line (6.3), we use a union bound. For the first term in (6.3), we first use triangle inequality to conclude that if \(\theta_T \in U^n\), i.e., \(\|\theta_T - \theta_0\| > M\epsilon_n\) and \(\|\theta_T - \theta_\Lambda\| \leq M\epsilon_n/2\), then \(\|\theta_\Lambda - \theta_0\| \geq \|\theta_T - \theta_0\| - \|\theta_T - \theta_\Lambda\| > M\epsilon_n/2\). Next, by construction, \((\theta_\Lambda - \theta_0) \mid Y, X \sim N(0, \sigma^2/nI_{kn})\), which implies \(P(\|\theta_\Lambda - \theta_0\| > M\epsilon_n/2) = P(\chi_{kn}^2 > M^2n\epsilon_n^2 / 4)\). For the \(P(\|\theta_T - \theta_0\| > M\epsilon_n/2)\) term in (6.3), we first use Markov’s inequality and then exploit the fact that \((\theta_T, \theta_0)\) are ‘optimally coupled’, i.e., \(E \|\theta_T - \theta_\Lambda\|^2 = d_{W,2}^2(Q_T, Q_\Lambda)\). This leaves us at (6.4). Finally, substituting the bound (6.4) in (6.2), we have

\[
\mathbb{E}_0 \tilde{W}^n(U^n \mid Y, X) \leq \mathbb{E}_0 \left\{ \|\nabla \tilde{W}^n(\cdot \mid Y, X, N_{kn}(\theta_0, \chi_{kn}^2/nI_{kn})) \|_2 \right\} / M^2\epsilon_n^2 / 4 + P(\chi_{kn}^2 > M^2n\epsilon_n^2 / 4) + \mathbb{P}(A_n^c).
\]

The quantity in the right-hand side in the above display is \(T_{1n}\), and the theorem is proved.

**Proof of Lemma 3.2 and Remark 3.1**

We make use of the following version of a matrix Bernstein inequality from [28]: let \(Z_i, i = 1, \ldots, n\) be a sequence of independent self-adjoint \(d \times d\) matrices with \(\mathbb{E}Z_i = 0\) and \(\|Z_i\|_2 \leq B\) almost surely for some \(B > 0\). Let \(\eta^2 = \sum_{i=1}^n \mathbb{E}Z_i^2\). Then, for any \(t > 0\),

\[
\mathbb{P} \left( \left\| \sum_{i=1}^n Z_i \right\| > t \right) \leq d \exp \left( - \frac{t^2/2}{\eta^2 + Bt/3} \right).
\] (6.5)

Set \(\phi^{(i)} = (\phi(X_i))_{1 \leq i \leq kn} \in \mathbb{R}^{kn}\) and \(Z_i = \phi^{(i)}(\phi^{(i)})^T - I_{kn}\), so that \(\sum_{i=1}^n Z_i = \Phi^T \Phi - nI_{kn}\). The \(Z_i\)s are independent symmetric matrices with \(\mathbb{E}Z_i = 0\), since from the orthonormality of the eignefunctions \(\{\phi_j\}\),

\[
(\mathbb{E} \phi^{(i)}(\phi^{(i)})^T)_{jl} = \int \phi_j(x)\phi_l(x)\rho(x) \, dx = \delta_{jl}.
\]

We also have \(\|\phi^{(i)}\|_2 = \|\phi^{(i)}\|_2 = 1 + \sum_{j=1}^{kn} |\phi_j^2(X_i)| \leq 1 + k_nL_n^2 \leq k_nL_n^2\). Therefore, the conditions for applying (6.5) are satisfied.

We have \(Z_i^2 = \|\phi^{(i)}\|^2 \phi^{(i)}(\phi^{(i)})^T - 2\phi^{(i)}(\phi^{(i)})^T + I_{kn} < \|\phi^{(i)}\|^2 \phi^{(i)}(\phi^{(i)})^T + I_{kn} < k_nL_n^2\phi^{(i)}(\phi^{(i)})^T + I_{kn}\), so that \(\mathbb{E}Z_i^2 \leq k_nL_n^2\), and hence by triangle inequality, \(\eta^2 \leq nk_nL_n^2\). Substituting \(t = n/2\) and \(B = k_nL_n^2\) in (6.5), we have

\[
\mathbb{P}(\|\Phi^T \Phi - nI_{kn}\| > n/2) \leq k_n \exp \left( - \frac{Cn^2}{\eta^2 + Bn/2} \right) \leq k_n e^{-Cn/(knL_n^2)},
\]

since \(\eta^2 + Bn/6 \leq nk_nL_n^2 + nk_nL_n^2/6 \leq Cnk_nL_n^2\) and \(e^{-1/x}\) is increasing in \(x\).

Remark 3.1 follows, since on \(A_n\),

(i) using triangle inequality, \(\|\Phi^T \Phi\|_2 \leq 3n/2\).

(ii) using Lemma A.1 (ii), \(s_{\min}(\Phi^T \Phi) \geq n - \|\Phi^T \Phi - nI_{kn}\| \geq n/2\).
(iii) using (i) and (ii), $\kappa(\Phi^T\Phi) \leq 3$.
(iv) $\text{tr} [(\Phi^T\Phi)^{-1}] \leq k_n \|(\Phi^T\Phi)^{-1}\|_2 = k_n/s_{\text{min}}(\Phi^T\Phi) \leq 2k_n/n$.

**Proof of Theorem 3.3**

Given $Y, X$, recall that $Q_T$ and $Q_n$, respectively, denote the probability measures $\mathcal{W}(\cdot \mid Y, X) \equiv N_{k_n}(\tilde{\theta}, \tilde{\Sigma})$ and $N_{k_n}(\theta_0, \sigma_0^2 I_{k_n}/n)$. By the tower property of conditional expectation,

$$
\mathbb{E}_0[\mathcal{W}_n(X) d_{W,2}(Q_T, Q_A)] = \mathbb{E}_X[\mathcal{W}_n(X) \mathbb{E}_{0|X} d_{W,2}(Q_T, Q_A)].
$$

(6.6)

Since $\tilde{\Sigma}$ and $\sigma^2 I_{k_n}/n$ (trivially) commute, apply (2.2) to write

$$
d_{W,2}(Q_T, Q_A) = \|\tilde{\theta} - \theta_0\|^2 + \|\tilde{\Sigma}^{1/2} - \frac{\sigma}{\sqrt{n}} I_{k_n}\|^2_F.
$$

(6.7)

Thus,

$$
\mathbb{E}_{0|X} d_{W,2}^2(Q_T, Q_A) = \mathbb{E}_{0|X} \|\tilde{\theta} - \theta_0\|^2 + \|\tilde{\Sigma}^{1/2} - \frac{\sigma}{\sqrt{n}} I_{k_n}\|^2_F,
$$

(6.8)

since the second term does not involve $Y$. We now proceed to bound each of these two terms in (6.8) on the set $A_n$. To that end, we shall apply Lemma 3.2 and, in particular, the consequences of Lemma 3.2 summarized in Remark 3.1 multiple times below. We also make use of Lemma B.1 on multiple occasions.

Recall $\tilde{\theta} = (\Phi^T\Phi + A^{-1})^{-1}$ and define $\theta_T = (\Phi^T\Phi)^{-1}\Phi^TY$. Using $\|a + b\|^2 \leq 2(\|a\|^2 + \|b\|^2)$, bound

$$
\mathbb{E}_{0|X} (\tilde{\theta} - \theta_0^T)^2 \leq \mathbb{E}_{0|X} \|\tilde{\theta} - \theta_T\|^2 + \mathbb{E}_{0|X} \|\theta_T - \theta_0^T\|^2.
$$

(6.9)

Let us first deal with $\mathbb{E}_{0|X} \|\theta_T - \theta_0^T\|^2$. Let $F_0 = (f_0(X_1), \ldots, f_0(X_n))^T$, so that $F_0 = \mathbb{E}_{0|X} Y$. By (T1), we can write $F_0 = \Phi\theta_0^T + R$, where $R = (R_1, \ldots, R_n)^T$ with $R_i = f_i(X_i) - f_0(X_i)$. Write $\mathbb{E}_{0|X} \|\theta_T - \theta_0^T\|^2 = \mathbb{E}_{0|X} \|\tilde{\theta} - \theta_T\|^2 + \mathbb{E}_{0|X} \|\theta_T - \theta_0^T\|^2$. The first term $\mathbb{E}_{0|X} \|\tilde{\theta} - \theta_T\|^2 = \sigma^2 \text{tr} [(\Phi^T\Phi)^{-1}] \leq \sigma^2 k_n/n$ on $A_n$. For the second term, write $\mathbb{E}_{0|X} \|\theta_T - \theta_0^T\|^2 = \|\Phi^T\Phi - \Phi^T\Phi F_0\|^2 = \|\Phi^T\Phi - \Phi^T\Phi\|^2 \mathbb{E}_{0|X} \|\theta_T - \theta_0^T\|^2$.

Finally,

$$
\|\Phi^T\Phi - \Phi^T\Phi F_0\|^2 \leq \|\Phi^T\Phi - \Phi^T\Phi\|^2 \mathbb{E}_{0|X} \|\theta_T - \theta_0^T\|^2 \leq \|\Phi^T\Phi - \Phi^T\Phi\|^2 \mathbb{E}_{0|X} \|\theta_T - \theta_0^T\|^2.
$$

(6.10)

and the last quantity is bounded above by a constant multiple of $1/\sqrt{n}$ on $A_n$. Therefore,

$$
\mathbb{E}_{0|X} \|\tilde{\theta} - \theta_0^T\|^2 \leq \sigma^2 k_n/n + \|R\|^2/n.
$$

(6.11)
So the goal now is to bound each one of $\|BF_0\|^2$ and $\|B\|_F^2$ on $A_n$. We have

$$BF_0 = (\Phi^T\Phi)^{-1} \Delta(\Phi^T\Phi)\theta_0^* + (\Phi^T\Phi)^{-1} \Delta \Phi^TR = (\Phi^T\Phi)^{-1} \Lambda^{-1}\theta_0^* + (\Phi^T\Phi)^{-1} \Delta \Phi^TR,$$

where

$$\theta_0^* = (\Phi^T\Phi + \Lambda^{-1})^{-1}(\Phi^T\Phi)\theta_0'.$$

Bound

$$\|BF_0\|^2 \leq 2\left(\|(\Phi^T\Phi)^{-1}\Lambda^{-1}\theta_0^*\|^2 + \|(\Phi^T\Phi)^{-1}\Delta \Phi^TR\|^2\right).$$

Bound

$$\|\Delta\|_2^2 \leq \|\Lambda^{-1}\|_2^2/\{s_{\min}(\Phi^T\Phi) - \|\Lambda^{-1}\|_2\} \lesssim 1$$ on $A_n$,

since $\|\Lambda^{-1}\|_2^2 < n/4$ by (A1). Therefore,

$$\|(\Phi^T\Phi)^{-1}\Delta \Phi^TR\| \lesssim \|\Phi^T\|/s_{\min}(\Phi^T\Phi)\|R\| \lesssim \|R\|/\sqrt{n}$$ on $A_n$,

using an argument as in the paragraph after the display (6.9). Next, $\|(\Phi^T\Phi)^{-1}\Lambda^{-1}\theta_0^*\| \leq \|\Lambda^{-1/2}/s_{\min}(\Phi^T\Phi)\|\Lambda^{-1/2}\theta_0^*\| \leq \|\Lambda^{-1/2}\theta_0^*\|/\sqrt{n}$ on $A_n$. After some manipulation, we can write

$$\theta_0^* = \theta_0' - \Delta^T\theta_0',$$

so that

$$\|\Lambda^{-1/2}\theta_0^*\| \leq \|\Lambda^{-1/2}\theta_0'\| + \|\Lambda^{-1/2}\Delta^T\theta_0'\| \leq \|\Lambda^{-1/2}\theta_0'\| + \|\Lambda^{-1/2}(\Phi^T\Phi + \Lambda^{-1})^{-1}\Lambda^{-1/2}\theta_0^*\| \lesssim \|\Lambda^{-1/2}\theta_0^*\| = \|\theta_0^*\|_F,$$

since $\|\Lambda^{-1/2}(\Phi^T\Phi + \Lambda^{-1})^{-1}\Lambda^{-1/2}\|_2 = \|\Delta\|_2$, which we already know is $\lesssim 1$ on $A_n$. Thus, we conclude that $\|BF_0\|^2 \lesssim \|R\|^2/n + \|\theta_0^*\|_F^2/n$ on $A_n$. Finally,

$$\|B\|_F^2 \leq k_n/\sqrt{\Sigma} \|\Delta\|_2^2 \|\Phi^T\|_F^2 \lesssim \frac{k_n}{\sqrt{n}}$$

on $A_n$, since we have already shown that $\|\Delta\|_2 \lesssim 1$ and $\|\Phi^T\|_F/s_{\min}(\Phi^T\Phi) \lesssim 1/\sqrt{n}$ on $A_n$. Substituting all the inequalities in (6.11),

$$\|\kappa_{A_n}(X)E_{0|X}\|_{F} \lesssim \|\Delta\|_2^2 \lesssim \frac{\|R\|^2}{n} + \|\theta_0'\|_F^2/n + \sigma^2 k_n/n.$$  \hspace{1cm} (6.12)

Substituting the inequalities obtained in (6.10) and (6.12) in (6.9),

$$\|\kappa_{A_n}(X)E_{0|X}\|_{F} \lesssim \sigma \frac{k_n}{n} + \|\theta_0'\|_F^2/n + \|R\|^2/n.$$  \hspace{1cm} (6.13)

Now we consider the term $\|\tilde{\Sigma}^{1/2} - \frac{\sigma^4}{\sigma^2} I_{k_n}\|^2_F$ in (6.8). Recalling the expression of $\tilde{\Sigma}$, $\tilde{\Sigma}^{1/2} = \sigma (\Phi^T\Phi + \Lambda^{-1})^{-1/2}$, and since $n/4 \leq s_{\min}(\Phi^T\Phi + \Lambda^{-1}) \leq \|\Phi^T\Phi + \Lambda^{-1}\| \leq 2n$ on $A_n$, all eigenvalues of $\tilde{\Sigma}$ are
of the form $C \sigma / \sqrt{n}$ on $A_n$. Since the squared Frobenius norm of a matrix is the sum of the squared eigenvalues, we conclude that $\| \tilde{\Sigma}^{1/2} - \frac{\sigma}{\sqrt{n}} I_n \|^2 \lesssim \sigma^2 k_n / n$ on $A_n$. This, in conjunction with (6.13), when substituted in (6.8) yield

$$W_{A_n}(X) \mathbb{E}_{0|X} d_{W,2}(Q_T, Q_{\lambda}) \leq \sigma^2 k_n / n + \frac{\|\theta_0\|^2}{n} + \frac{\| R \|^2}{n}. \quad (6.14)$$

Recall from (6.6) that our objective is to bound the $\mathbb{E}_X$ expectation of the left-hand side of (6.14). The only term depending on $X$ in the right-hand side of (6.14) is $\| R \|^2$ and $\mathbb{E}_X \| R \|^2 = n \| f_0 - f_0 \|^2_{2,\rho}$. Therefore, taking an expectation with respect to $\mathbb{E}_X$ on both sides of (6.14), the conclusion follows.

**Proof of Theorem 3.4**

Let

$$D_n = \int \frac{p_{n,f}(Y)}{p_{n,f_0}(Y)} \Pi(df), \quad G_n = \int \log \left\{ \frac{p_{n,f}(Y)}{p_{n,f_0}(Y)} \right\} \Pi(df).$$

Following a standard argument, it is enough to show the desired lower bound on $\mathbb{P}_0(D_n \geq e^{-n\epsilon_n^2})$ for any probability measure $\Pi$ supported on $\mathcal{F}_n = \{ f : \| f - f_0 \|_{2,\rho} < \epsilon_n \}$. By Jensen’s inequality, log $D_n \geq G_n$, so that $\mathbb{P}_0(D_n \geq e^{-n\epsilon_n^2}) \geq \mathbb{P}_0(G_n \geq -n\epsilon_n^2)$. Our goal below is to bound $\mathbb{P}_0(G_n \geq -n\epsilon_n^2)$ from below, or equivalently, bound $\mathbb{P}_0(G_n \leq -n\epsilon_n^2)$ from above.

A simple calculation yields

$$G_n = \mu_{0X}(Y - F_0) - \sigma_{0X}^2 / 2,$$

where $\mu_{0X} = \int (F - F_0) \Pi(df) \in \mathbb{R}^n$ and $\sigma_{0X}^2 = \int \| F - F_0 \|^2 \Pi(df)$. Since $Y \sim N(F_0, I_n)$, we have $G_n \mid X \sim N(-\sigma_{0X}^2 / 2, \| \mu_{0X} \|^2)$.

The marginal expectation of $G_n$, $\mathbb{E}_0 G_n = -\mathbb{E}_{0X} \sigma_{0X}^2 / 2 = -n\sigma_0^2 / 2$, where $\sigma_0^2 = \int \| f - f_0 \|^2_{2,\rho} \Pi(df)$. Since $\Pi$ is supported on $\mathcal{F}_n$, clearly $\sigma_0^2 \leq \epsilon_n^2$.

The Paley–Zygmund inequality (see, for example, [11]) states that for any non-negative random variable $Z$ with finite second moment and $\delta \in (0, 1)$, $P(Z \geq \delta EZ) \geq (1 - \delta^2)(EZ)^2 / (EZ)^2$. In particular, if $(EZ)^2 / (EZ)^2 \geq 1 - \gamma$ for $\gamma > 0$ small, then

$$P(Z < \delta EZ) \leq 1 - (1 - \delta^2)(1 - \gamma) \lesssim \delta + \gamma. \quad (6.15)$$

We shall invoke (6.15) with the non-negative random variable $Z_n = e^{\lambda G_n}$ for some $t_n \in (0, 1/2)$ and $\delta_n \in (0, 1)$ to be chosen below. A key ingredient of such an exercise is to obtain a lower bound on $(\mathbb{E}_0 Z_n)^2 / (\mathbb{E}_0 Z_n^2)$.

By Jensen’s inequality, $\mathbb{E}_0 Z_n \geq e^{\lambda \mathbb{E}_0 G_n} = e^{-n\sigma_0^2 / 2}$, which implies $(\mathbb{E}_0 Z_n)^2 \geq e^{-n\lambda \sigma_0^2 / 2}$. We next need to bound $\mathbb{E}_0 Z_n^2 = \mathbb{E}_0 e^{2\lambda G_n}$ from above. Since $G_n \mid X$ is conditionally Gaussian, we have sufficient control over the moment generating function $\mathcal{M}_{G_n}(\lambda) = \mathbb{E}_0 e^{\lambda G_n}$ for $\lambda \in (0, 1)$. Using the iterative property of conditional expectations, we can write $\mathbb{E}_0 e^{\lambda G_n} = \mathbb{E}_0[\mathbb{E}_0 e^{\lambda G_n}]$. Recalling $G_n \mid X \sim N(-\sigma_{0X}^2 / 2, \| \mu_{0X} \|^2)$, we have

$$\mathbb{E}_{0X}(e^{\lambda G_n}) = e^{-\lambda \sigma_{0X}^2 / 2} e^{\mu_{0X}^2 / 2} \leq e^{-(\lambda - \lambda^2)\sigma_{0X}^2 / 2},$$

where the second step follows since by an application of Cauchy–Schwartz inequality, $\| \mu_{0X} \|^2 \leq \sigma_{0X}^2$. Since $\lambda \in (0, 1)$, the quantity $\lambda - \lambda^2$ in the exponent is positive. Therefore, by Jensen’s inequality,
Consider the function $E$. By choice of $\lambda$ after some algebra, it can be shown that $\lambda_j \asymp a_n^{-1} e^{-j/\alpha_n}$ subsequently, since after some algebra, it can be shown that $\lambda_j \asymp a_n^{-1} e^{-j/\alpha_n}$. Recall $a_n = n^{1/(2\alpha + 1)}$ and choose $k_n = n^{1/(2\alpha + 1)} \log \{ n^{2\alpha/(2\alpha + 1)} \}$ in Corollary 3.5. We first verify that (C0)–(C3) are satisfied.

We start with (C0), which requires verifying (A1) and (A2). For (A1), we have

$$\| A^{-1} \|_2 = \lambda_{k_n}^{-1} \asymp \alpha_n e^{k_n/\alpha_n} \lesssim n$$

by choice of $k_n$. From Lemma 5.1, we have that for any $j = 1, \ldots, k_n, \sup_{x \in \mathbb{R}} |\phi_j(x)| \leq a_n^{1/4} e^{k_n/\alpha_n}$.

Setting $L_n = a_n^{1/4} e^{k_n/\alpha_n}$, we have

$$L_n^2 k_n \log k_n \lesssim n^{(4\alpha + 3)/2(2\alpha + 1)} \log n \lesssim n$$

as long as $\alpha > 1/\{4(1 - 2b)\}$, verifying (A2).
We next verify (C1). Clearly, \( k_n = o(n \epsilon_n^2) \). So it remains to establish that \( \| \theta'_n \|^2_H = o(n \epsilon_n^2) \). Bound

\[
\| \theta'_n \|^2_H \asymp a_n \sum_{j=1}^{k_n} e^{j/\alpha_n} \theta_{ij}^2 \leq a_n \| \theta_0 \|^2_a \max_{1 \leq j \leq k_n} e^{j/\alpha_n} j^{-2\alpha}.
\]

The function \( x \rightarrow e^{x/\alpha_n} x^{-2\alpha} \) is monotonically decreasing on the interval \((0, 2a_\alpha a_n)\) and monotonically increasing on \((2a_\alpha a_n, \infty)\). Therefore, \( \max_{1 \leq j \leq k_n} e^{j/\alpha_n} j^{-2\alpha} \leq \max_{j=1}^{k_n} e^{j/\alpha_n} j^{-2\alpha} \). We have \( 1/a_n < 1 \), and hence \( e^{j/\alpha_n} j^{-2\alpha} \) evaluated at \( j = 1 \) can be bounded above by \( e^{j/\alpha_n} j^{-2\alpha} \) evaluated at \( j = k_n \) is bounded above by \( n^{2a/(2a_\alpha + 1)} k_n^{-2\alpha} = o(1) \). Hence \( \| \theta'_0 \|^2_H / n \epsilon_n^2 \leq a_n / n \epsilon_n^2 \to 0 \) as \( n \to \infty \).

To verify (C2), we need to show that \( \| f_0 - f'_0 \|_{2, \rho} \leq \epsilon_n \). Indeed,

\[
\| f_0 - f'_0 \|^2_{2, \rho} = \sum_{j=1}^{k_n+1} \lambda_j \| f_j \|^2_{L^2} = \sum_{j=1}^{k_n+1} \lambda_j \| f_j \|^2_{L^2} < k_n^{-2\alpha} \sum_{j=k_n+1}^{\infty} 2^{2\alpha} \lambda_j \| f_0 \|^2 = o(\epsilon_n^2).
\]

It now remains to verify (C3). As noted in the paragraph after (3.13), the numerator in (3.14) can be expressed as \( \Pi (\| f - f' \|^2_{2, \rho} > M^2 \epsilon_n^2) = \Pi (\sum_{j=1}^{\infty} \lambda_j Z_j^2 > M^2 \epsilon_n^2) \) with \( Z_j \)'s i.i.d. \( N(0, 1) \). Noting that \( \sum_{j=1}^{\infty} \lambda_j \leq e^{-\epsilon_0 / \alpha_n} = n^{-2a/(2a_\alpha + 1)} \leq \epsilon_0^2 \),

\[
\Pi \left( \sum_{j=1}^{\infty} \lambda_j Z_j^2 > M^2 \epsilon_n^2 \right) \leq \Pi \left\{ \sum_{j=1}^{\infty} \lambda_j (Z_j^2 - 1) > M^2 \epsilon_n^2 / 2 \right\}.
\]

\((Z_j^2 - 1)\)'s are mean-zero sub-exponential random variables. By an application of Bernstein’s inequality for linear combinations of mean-zero sub-exponential random variables (Proposition 5.16 of [34]),

\[
\Pi \left\{ \sum_{j=1}^{\infty} \lambda_j (Z_j^2 - 1) > M^2 \epsilon_n^2 / 2 \right\} \leq 2 \exp \left\{ - C \min \left\{ \frac{1}{K^2} \sum_{j=1}^{\infty} \lambda_j^2, \frac{M^2 \epsilon_n^2}{K (\max_{j=1}^{\infty} \lambda_j)} \right\} \right\}
\]

\[
\leq 2 \exp \left\{ - C \min \left\{ a_n M^4 \epsilon_n^4 e^{-2a_\alpha / \alpha_n}, a_n M^2 \epsilon_n^2 e^{(k_n + 1)/\alpha_n} \right\} \right\}
\]

\[
= 2 \exp \left\{ - C \min \left\{ a_n M^4 \log^4 n, a_n M^2 \log^2 n \right\} \right\} = 2 \exp(-CM^2 n^{1/(2a_\alpha + 1)} \log^2 n),
\]

where \( K, C, C' \) are global constants. The second inequality in the previous display is due to \( \sum_{j=1}^{\infty} \lambda_j^2 \asymp (1/2a_n) e^{-2a_\alpha / \alpha_n} \) and \( \max_{j=1}^{\infty} \lambda_j = (1/a_n) e^{-k_n / \alpha_n} \).

Next, the term in the denominator of (3.14), \( \Pi (\| f - f_0 \|_{2, \rho} \leq \tilde{\epsilon}_n) = \tilde{\nu}(\| \theta - \theta_0 \|_{L^2} \leq \tilde{\epsilon}_n) \), where \( \theta = (\theta_1, \theta_2, \ldots) \) with \( \theta_j \sim N(0, \lambda_j) \) and \( \theta_0 = (\theta_0_1, \theta_0_2, \ldots) \). Set \( \tilde{\epsilon}_n = C n^{-a/(2a_\alpha + 1)} \) for some constant \( C \). We show below that

\[
\tilde{\nu}(\| \theta - \theta_0 \|_{L^2} \leq \tilde{\epsilon}_n) \geq \exp(-C' n^{1/(2a_\alpha + 1)} \log^2 n).
\]
\[ \sum_{j=k_n+1}^{\infty} \theta_{0j}^2 \leq \| \bar{\theta}_0 \|^2 k_n^{-2\alpha} \] is bounded by \( \tilde{\mathcal{W}}(\sum_{j=k_n+1}^{\infty} \theta_j^2 \leq \tilde{\epsilon}_n^2/4) \).

By Markov’s inequality,
\[ \tilde{\mathcal{W}} \left( \sum_{j=k_n+1}^{\infty} \theta_j^2 \leq \tilde{\epsilon}_n^2/4 \right) \geq 1 - 4/\tilde{\epsilon}_n^2 \sum_{j=k_n+1}^{\infty} E\theta_j^2 \geq 1 - \frac{4 \varepsilon_n^{-2}}{\tilde{\epsilon}_n^2} \sum_{j=k_n+1}^{\infty} E\theta_j^2 \geq 1/2 \] (6.21)

for large \( C \). We used above that \( \sum_{j=k_n+1}^{\infty} \theta_j^2 \leq \tilde{\mathcal{W}}(\| \theta' - \theta_0 \|^2 \leq \tilde{\epsilon}_n^2/2) \). By Anderson’s inequality (Lemma B.2 in Appendix B),
\[ \tilde{\mathcal{W}}(\| \theta' - \theta_0 \|^2 \leq \tilde{\epsilon}_n^2/2) \geq e^{-\frac{1}{2}\| \theta_0 \|^2_{\mathcal{H}}} \tilde{\mathcal{W}}(\| \theta \|^2 \leq \tilde{\epsilon}_n^2/2). \] (6.22)

We have already shown that \( \| \theta_0 \|^2_{\mathcal{H}} \leq a_n \), so that \( e^{-\frac{1}{2}\| \theta_0 \|^2_{\mathcal{H}}} \geq e^{-C_n n^{0.5} \| \bar{\theta}_0 \|^2} \). Therefore, suffices to bound \( \tilde{\mathcal{W}}(\| \theta \|^2 \leq \tilde{\epsilon}_n^2/2) \). Recall \( \theta_j^2/\lambda_j \sim \chi^2_1 \), therefore \( \theta_j^2 \) has a density \( (\sqrt{2\pi}x)^{-1} a_n \) \( e^{1/(2a_n)} \exp(-a_n e^{i/\alpha} x/2) \) \( \mathcal{K}_{1,0}(x) \). Let \( dx \) denote \( dx_1 \ldots dx_n \) in short and set \( D_n = a_n / \sqrt{2\pi} \). Then,
\[ \tilde{\mathcal{W}} \left( \sum_{i=1}^{k_n} \theta_i^2 \leq \tilde{\epsilon}_n^2/2 \right) = D_n^{k_n} e^{k_n(k_n+1)/4n \alpha} \prod_{j=1}^{k_n} \exp \left( -a_n e^{i/\alpha} x_j/2 \right) dx \]
\[ \geq \left( D_n \tilde{\epsilon}_n \right)^{k_n} e^{k_n(k_n+1)/4n \alpha} \prod_{j=1}^{k_n} \exp \left( -a_n e^{i/\alpha} x_j/2 \right) \int \exp \left( -a_n e^{i/\alpha} x_j/2 \right) dx \]
\[ \frac{D_n \tilde{\epsilon}_n}{\sqrt{2}} \left( D_n \tilde{\epsilon}_n \right)^{k_n} e^{k_n(k_n+1)/4n \alpha} \frac{\Gamma(1/2)k_n}{\Gamma(k_n/2)} \int_0^1 \exp \left( -a_n e^{i/\alpha} x_j/2 \right) dx j^{k_n-1} dt. \] (6.23)

From the first to the second line, we replace \( j \) by \( k_n \), perform a change of variable and drop the \( \tilde{\epsilon}_n \) term appearing inside the exponent as \( \tilde{\epsilon}_n \ll 1 \). The last equality follows from the Dirichlet integral formula (Lemma B.3 in Appendix B). Using \( \Gamma(1/2) = \sqrt{\pi} \) and the standard inequality (see, for example, [1]) \( \Gamma(\alpha) \leq \sqrt{2\pi e^2} e^{-\alpha^2/2} \) for \( \alpha > 1 \), we can simplify (6.23) to write
\[ \tilde{\mathcal{W}} \left( \sum_{i=1}^{k_n} \theta_i^2 \leq \tilde{\epsilon}_n^2/2 \right) \geq \sqrt{k_n} e^{k_n(k_n+1)/4n \alpha} \left( a_n \tilde{\epsilon}_n^2 e^{k_n/2} \right) \int_0^1 \exp \left( -a_n e^{i/\alpha} x_j/2 \right) dx j^{k_n-1} dt. \] (6.24)

The integral in the above display can be bounded from below by \( 2 e^{-1/k_n} \alpha_n e^{k_n/4} \) \( k_n/2 \). Substituting this bound and simplifying, the lower bound is
\[ \frac{1}{k_n} e^{k_n(k_n+1)/4n \alpha} e^{-k_n^2/2k_n} \left( 2e\tilde{\epsilon}_n^2 \right)^{k_n/2} \geq e^{-C_n n^{1/(2\alpha+1)} \log^2 n}. \]

Combining with (6.22), (6.20) is proved.

Finally, the ratio of the bounds in (6.19) and (6.20) converge to zero by choosing \( M \) large enough, completing the proof.
Proof of Theorem 5.3

As before, we will verify the conditions of Corollary 3.5 with \( \sigma^2 = 1 \). We replace \( \lambda_j \) by \((1/a_n)(j/a_n)^{(2\alpha+1)}\) with \( a_n = \log n \). Choose \( k_n = n^{1/(2\alpha+1)} \log^t n \), where \( t = (2\alpha + 2)/(2\alpha + 1) \) in Corollary 3.5. We first verify that (C0) – (C3) are satisfied.

We start with (C0), which requires verifying (A1) and (A2). For (A1), we have \( \|A^{-1}\| = \lambda_{k_n}^{-1} \gtrless n \) by choice of \( k_n \). From Lemma 5.1, we have that for any \( j = 1, \ldots, k_n \), \( \sup_{t \in [0,1]} |\phi_j(t)| \leq 1 \) verifying (A2).

We next verify (C1). Clearly, \( k_n = o(ne_n^2) \). So it remains to establish that \( \|\theta_0^\epsilon\|^2_{\Pi} = o(ne_n^2) \). Bound

\[
\|\theta_0^\epsilon\|^2_{\Pi} = \sum_{j=1}^{k_n} \lambda_j^{-1} \theta_{0j}^2 \leq k_n \|\theta_0^\epsilon\|^2_{a^n},
\]

Hence \( \|\theta_0^\epsilon\|^2_{\Pi}/(ne_n^2) \to 0 \). C2 can be verified exactly as in the proof of Theorem (5.2). It now remains to verify (C3). Note that \( \epsilon_n^2/(\sum_{j=k_n+1}^{\infty} \lambda_j^2) > ne_n^2 \) and \( \epsilon_n^2/(\sum_{j=k_n+1}^{\infty} \lambda_j) \geq n \epsilon_n^2 \), we have \( \Pi(\|f - f_0\|_{2,\rho} > M^2 \epsilon_n^2) \leq e^{-M^2n\epsilon_n^2} \). Since \( \theta_0 \in \Theta_0, f_0 \in H^a[0,1] \). It then follows from Lemma 3 and 4 of [33] that \( \Pi(\|f - f_0\|_{2,\rho} \leq \epsilon_n) \geq \exp\{-Cn\epsilon_n^2\} \) for some constant \( C > 0 \) verifying (C3). The proof is completed by choosing \( M_n \) to be large enough.

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Appendix A. Proof of Lemma 5.1

It suffices to show that for any $t > 0$, $\max_{0 \leq s \leq a} \sup_{x \in R} |\phi_{j+1}(x)| \lesssim a^{1/4} e^{bt}$ for large $a$. For fixed $b$, clearly $c = \sqrt{b^2 + 2ba^2} \approx a$. Therefore, $\phi_0(x) = (c/b)^{1/4} \lesssim a^{1/4}$, so enough to take the max over $1 \leq j \leq at$. 
Finally, since both $\phi_{j+1}$ and $H_j$ are symmetric functions, it suffices to consider the supremum over $x$ on $(0, \infty)$.

The Hermite polynomials have an integral representation

$$H_j(z) = \frac{2^j}{\sqrt{\pi}} \int_{-\infty}^{\infty} (z + it)^j e^{-t^2} \, dt. \quad (A.1)$$

For $z > 0$, using $|\int f \, d\mu| \leq \int |f| \, d\mu$, we have

$$|H_j(z)| \leq \frac{2^j}{\sqrt{\pi}} \int (z^2 + t^2)^{j/2} e^{-t^2} \, dt$$

$$= \frac{2^{j+1} z^{j+1}}{\sqrt{\pi}} \int_0^{\infty} (1 + t^2)^{j/2} e^{-z^2 t^2} \, dt. \quad (A.2)$$

Let $g(t) = (1 + t^2)^{j/2} e^{-z^2 t^2}$; clearly, $\log g(t) = (j/2) \log(1 + t^2) - z^2 t^2/2$. Differentiating, $\frac{d}{dt} \log g(t) = j t/(1 + t^2) - z^2 t$. Setting $\frac{d}{dt} \log g(t) = 0$, we have $t(1 + t^2) - j/z^2 = 0$. Therefore, if $z^2 > j$, $g(t)$ attains maxima at $t = 0$ with $g(0) = 1$. On the other hand, if $z^2 \leq j$, $g(t)$ attains maxima at $t = (j/z^2 - 1)^{1/2}$. When $z^2 > j$, bounding $g(t) \leq 1$ in (A.2), we get the inequality

$$|H_j(z)| \leq \frac{2^{j+1} z^{j+1}}{\sqrt{\pi}} \int_0^{\infty} g(t) e^{-z^2 t^2} \, dt$$

$$\leq \frac{2^{j+1} z^{j+1}}{\sqrt{\pi}} \int_0^{\infty} e^{-z^2 t^2} \, dt$$

$$= \frac{2^{j+1} z^{j+1}}{\sqrt{\pi}} \frac{1}{\sqrt{2\pi}} \frac{1}{z}$$

$$= \sqrt{2} 2^j z^j. \quad (A.3)$$

We record this bound below:

**Lemma A.1** The Hermite polynomials satisfy $|H_j(z)| \leq \sqrt{2} 2^j z^j$ whenever $z^2 > j$.

Note that the exponential $e^{z^2/2}$ term in Cramer’s bound has been replaced by a polynomial $z^j$ term. When $z^2 = j$, ignoring constants, Cramer’ bound for $|H_j(z)|$ is $2^{j/2} \sqrt{j!} e^{j^2/2}$, while the same from Lemma A.1 is $2^j j^{j/2}$. Using $j! \approx j^{j+1/2} e^{-j}$, we see that both bounds give similar results when $z^2 \approx j$.

As discussed at the beginning, we now proceed to establish the bound for $|\phi_{j+1}(x)|$ for $1 \leq j \leq at$ and $x > 0$. For $x \in (0, \sqrt{t})$, use Cramer’s bound to obtain $|\phi_{j+1}(x)| \leq (c/b)^{1/4} e^{b x^2} \leq a^{1/4} e^{b x^2}$ when $x \in (0, \sqrt{t})$.

When $x > \sqrt{t}$, setting $z = \sqrt{2c} x$, we have $z^2 > 2ct > j$ for any $j \leq at$. Therefore, we have two bounds for $|H_j(z)|$: (i) $|H_j(z)| \lesssim \sqrt{2} j! e^{z^2}$ from Cramer’s bound and (ii) $|H_j(z)| \lesssim 2^j z^j$ from Lemma A.1. Using a combination of both delivers a tighter bound for $|\phi_{j+1}(x)|$. Let $\delta > 0$ be such that $c \delta > b$. 


Then, for any such $\delta$, we may write

$$|H_j(z)| = |H_j(z)|^{1-\delta}|H_j(z)|^{\delta} \lesssim \left\{ 2^{j(1-\delta)/2} (j!)^{(1-\delta)/2} e^{c(1-\delta)z^2} \right\} \left\{ 2^{j\delta} (2c)^{j\delta/2} z^{j\delta} \right\} = 2^{j/2+j\delta} (j!)^{(1-\delta)/2} z^{j\delta} e^{c(1-\delta)z^2}. \quad (A.4)$$

Substituting this bound in the expression for $\phi_{j+1}$, we have

$$|\phi_{j+1}(x)| \lesssim (c/b)^{1/4} \frac{2^{j\delta} c^{j\delta/2}}{(j!)^{1/2}} x^j e^{-(c\delta-b)x^2}.$$

The function $x \rightarrow x^j e^{-(c\delta-b)x^2}$ for $x > 0$ achieves its maximum at $x = [j\delta/(2(c\delta-b))]^{1/2}$. Substituting $x^2 = j\delta/(2(c\delta-b))$ in the above display and bounding $j! \geq (j/e)^j$,

$$|\phi_{j+1}(x)| \lesssim c^{1/4} \frac{2^{j\delta} c^{j\delta/2}}{(j!)^{1/2}} \left( \frac{j\delta}{2(c\delta-b)} \right)^{j\delta/2} e^{-j\delta/2} = c^{1/4} \frac{2^{j\delta/2}}{(j!)^{1/2}} \left( \frac{c\delta}{c\delta-b} \right)^{j\delta/2}.$$

Now choose $\delta = be/(c(e-2))$, so that $c\delta/(c\delta-b) = e/2$. Then, we have $|\phi_{j+1}(x)| \lesssim c^{1/4} e^{j\delta/2} \lesssim A^{1/4} e^{bt}$, since $j\delta/2 < at\delta/2 \lesssim ct\delta/2 \lesssim bt$.

**Appendix B. Some useful results**

Some matrix inequalities. Proofs can be found in standard texts; see for example, [3].

**Lemma B.1** For any two matrices $A, B$,

$$s_{\min}(A) \| B \|_F \leq \| AB \|_F \leq \| A \|_2 \| B \|_F \quad \text{(i)}$$

$$s_{\min}(A) \| B \|_2 \leq \| AB \|_2 \leq \| A \|_2 \| B \|_2. \quad \text{(ii)}$$

If $s_{\min}(A) \geq \| B \|_2$, then

$$s_{\min}(A - B) \geq s_{\min}(A) - \| B \|_2. \quad \text{(iii)}$$

A version of Anderson’s lemma from [31] provides a sharp bound on the probability of shifted balls under multivariate Gaussian distributions in terms of the centered probability and the size of the shift.

**Lemma B.2** Suppose $\xi \sim N_n(0, \Sigma)$ with $\Sigma$ p.d. and $\xi_0 \in \mathbb{R}^n$. Let $\|\xi_0\|_\Sigma^2 = \xi_0^T \Sigma^{-1} \xi_0$. Then, for any $t > 0$,

$$P \left( \| \xi - \xi_0 \|_2 < t \right) \geq e^{-\frac{1}{2} \|\xi_0\|_\Sigma^2} P \left( \|\xi\|_2 \leq t/2 \right).$$
The Dirichlet integral formula (formula 4.635 in [19]) to simplify integrals over the unit probability simplex.

**Lemma B.3** Let \( \psi(\cdot) \) be a Lebesgue integrable function and \( \alpha_j > 0, j = 1, \ldots, n \). Then,

\[
\int \frac{\prod_{j=1}^{n} \Gamma(\alpha_j)}{\Gamma(\sum_{j=1}^{n} \alpha_j)} \psi(t) t^{(\sum \alpha_j) - 1} dt.
\]