

# Nonparametric Bayesian Aggregation for Massive Data

**Zuofeng Shang**

*Department of Mathematical Sciences  
New Jersey Institute of Technology  
Newark, NJ 07102, USA*

ZUOFENGSHANG@GMAIL.COM

**Botao Hao**

*Department of Statistics  
Purdue University  
West Lafayette, IN 47906, USA*

HAO22@PURDUE.EDU

**Guang Cheng**

*Department of Statistics  
Purdue University  
West Lafayette, IN 47906, USA*

CHENGG@PURDUE.EDU

**Editor:** Francis Bach

## Abstract

We develop a set of scalable Bayesian inference procedures for a general class of nonparametric regression models. Specifically, nonparametric Bayesian inferences are separately performed on each subset randomly split from a massive dataset, and then the obtained local results are aggregated into global counterparts. This aggregation step is explicit without involving any additional computation cost. By a careful partition, we show that our aggregated inference results obtain an oracle rule in the sense that they are equivalent to those obtained directly from the entire data (which are computationally prohibitive). For example, an aggregated credible ball achieves desirable credibility level and also frequentist coverage while possessing the same radius as the oracle ball.

**Keywords:** Credible region, divide-and-conquer, Gaussian process prior, linear functional, nonparametric Bayesian inference

## 1. Introduction

With rapid development in modern technology, massive data sets are becoming more and more common. An important feature of massive data is their large volume which hinders applications of traditional statistical methods. For example, due to huge data amount and limited CPU memory, it is often impossible to process the entire data in a single machine. In the parallel computing environment, a common practice is to distribute massive data to multiple processors, and then aggregate local results in an efficient way. A series of frequentist methods such as Kleiner et al. (2011); McDonald et al. (2010); Zhang et al. (2015a); Zhao et al. (2016) have been proposed in this Divide-and-Conquer (D&C) framework.

In Bayesian community, there are quite a few computational or methodological works developed for massive data such as scalable algorithms for Bayesian variable selection Boom et al. (2015); Wang et al. (2014) and scalable posterior sampling in parametric models Wang and Dunson (2013); Wang et al. (2015). Theoretical guarantees of D&C methods have been

recently obtained in robust estimation Minsker et al. (2017), posterior interval estimation Srivastava et al. (2018), credible sets of signal in Gaussian white noise Szabó and van Zanten (2019); Szabo and van Zanten (2018). Rather, the present paper puts focus on uncertainty quantification of the model parameter in general nonparametric regression, primarily in theoretical aspects. For instance, how to aggregate individual posterior means into a global one that maintains frequentist optimality? How to aggregate individual credible balls into a global one with a minimal possible radius? And how many divisions and what kind of priors should be chosen to guarantee Bayesian and frequentist validity of the aggregated ball? We attempt to address these questions in a univariate nonparametric regression setup.

Specifically, we develop a set of aggregation procedures in Bayesian nonparametric regression. As a first step, nonparametric Bayesian regression is separately fitted based on each subsample randomly split from a massive dataset. A variety of finite sample valid credible balls (credible intervals) for regression functions (their linear functionals Rivoirard et al. (2012), e.g., local values) are then constructed from each individual posterior distribution based on MCMC. In the second step, we aggregate these credible balls (credible intervals) into global counterparts analytically without involving any additional computation. For example, the center of an aggregated ball is obtained by weighted averaging Fourier coefficients of all individual (approximate) posterior modes, while the radius is given through an explicit formula on individual radii. A notable advantage of this distributed strategy is its dramatically faster computational speed, and this computational advantage becomes more obvious as data size grows.

Our aggregation procedures are proven to obtain an oracle rule in the sense that they are equivalent to those obtained directly from the entire data, i.e., called as oracle results which are computationally prohibitive in practice. For example, our aggregated posterior means are proven to achieve optimal estimation rate, and our aggregated credible ball achieves desirable credibility level and also frequentist coverage while possessing asymptotically the same radius as the oracle ball. These oracle results hold when the assigned Gaussian process priors in each subset are properly chosen and the number of subsets does not grow too fast. A fundamental theory underlying Bayesian aggregation is a *uniform* version of nonparametric Gaussian approximation theorem, also called as Bernstein-von Mises theorem. Developed based on our recent work Shang and Cheng (2017), this theory states that a sequence of individual posterior distributions converge to Gaussian processes uniformly over the number of subsets.

The rest of this paper is organized as follows. Section 3 describes our Bayesian nonparametric model with a Gaussian process prior, based on which our main results are developed in Section 4. Specifically, a uniform nonparametric Gaussian approximation theorem is established in Section 4.1, and all the Bayesian aggregation procedures together with their theoretical guarantee are provided in Sections 4.2–4.6. Section 5 provides a simulation study to justify our methods. Section 6 applies the proposed procedures to a real dataset of large size. Main proofs are provided in Appendix. Other results and additional plots are given in a supplementary document Shang and Cheng.

## 2. Nonparametric Bayesian Aggregation: An Illustration

In this section, we provide a concrete example to demonstrate the intuition of our nonparametric Bayesian aggregation procedure. Our example is based on the special uniform design and periodic Sobolev space which makes our aggregation procedure explicit and easy to understand. Section 2.1 describes our nonparametric Bayesian model, and Section 2.2 demonstrates our algorithm and its numeric performance. General aggregation procedures will be proposed in Sections 3 and 4 with asymptotic properties investigated as well.

### 2.1. Nonparametric Bayesian model

Suppose that we observe the data  $Z_i = (Y_i, X_i)$ ,  $i = 1, \dots, N$ , generated from the following Gaussian regression model with uniform design

$$Y_i|f, X_i \sim N(f(X_i), 1), \quad X_1, \dots, X_N \stackrel{iid}{\sim} Unif[0, 1]. \quad (1)$$

Randomly split  $\{1, 2, \dots, N\}$  into  $s$  subsets  $I_1, I_2, \dots, I_s$  with  $|I_1| = \dots = |I_s| = n$  (so  $N = ns$ ). Denote  $\mathbf{D}_j = \{Z_i|i \in I_j\}$  the  $j$ -th subsample for  $j = 1, \dots, s$  and  $\mathbf{D} = \cup_{j=1}^s \mathbf{D}_j$  the entire sample.

Suppose that  $f$  belongs to an  $m$ -order periodic Sobolev space  $S_0^m[0, 1]$  where  $S_0^m[0, 1]$  is the collection of all functions on  $[0, 1]$  of the form

$$f(x) = \sqrt{2} \sum_{k=1}^{\infty} f_k \cos(2\pi kx) + \sqrt{2} \sum_{k=1}^{\infty} g_k \sin(2\pi kx) \quad (2)$$

with real coefficients  $f_k, g_k$  satisfying

$$\sum_{k=1}^{\infty} (f_k^2 + g_k^2)(2\pi k)^{2m} < \infty. \quad (3)$$

Here,  $m > 1/2$  is a constant describing the smoothness of the functions. Wahba (1990) introduced a Gaussian process (GP) prior on  $f$  which has an interesting smoothing spline interpretation. Specifically, she assumed that the coefficients  $f_k, g_k$  in (2) are independent and normally distributed as follows:

$$f_k, g_k \sim N\left(0, [4\pi k]^{2m+\beta} + n\lambda(2\pi k)^{2m}\right)^{-1}, \quad k = 1, 2, \dots, \quad (4)$$

where  $\beta > 1$  and  $\lambda \geq 0$  are predecided constants. In particular,  $\beta$  represents the “relative smoothness” of the prior to the parameter space and  $\lambda$  represents the amount of rescaling. Rescaling priors are also considered by Szabó and van Zanten (2019); Szabó and van Zanten (2018) for constructing credible sets of signals in Gaussian white noise. It can be examined that if  $f$  satisfies (2) and (4), then  $f$  is a Gaussian process with mean zero and isotropic covariance function

$$K_0(x, x') = 2 \sum_{k=1}^{\infty} \frac{\cos(2\pi k(x - x'))}{(2\pi k)^{2m+\beta} + n\lambda(2\pi k)^{2m}}, \quad x, x' \in [0, 1]. \quad (5)$$

Wahba (1990) showed that the above GP prior (4) generates a posterior distribution corresponding to a penalized likelihood function (with  $\lambda$  the penalty parameter). This

provides a Bayesian interpretation for smoothing splines. Below we provide some details to justify this argument.

Let  $\Pi_\lambda$  denote the probability distribution of  $f$  under (4). To derive the posterior distribution, we need to find the “prior density” of  $f$ . Unlike the parametric settings where the prior densities are Radon-Nikodym (RN) derivatives w.r.t. Lebesgue measure, in the current infinite-dimensional setting it is impossible to do so since there is no Lebesgue measure on  $S_0^m[0, 1]$  (see Hunt et al. (1992)). Instead, we need to characterize the prior density of  $f$  as an RN derivative w.r.t. other kinds of measures such as Gaussian measure. Following Wahba (1990),  $\Pi_\lambda$  and  $\Pi \equiv \Pi_0$  (corresponding to  $\lambda = 0$ ) are equivalent probability measures, and the RN derivative of  $\Pi_\lambda$  w.r.t.  $\Pi$  is

$$\begin{aligned} \frac{d\Pi_\lambda}{d\Pi}(f) &= \prod_{k=1}^{\infty} (1 + n\lambda(2\pi k)^{-\beta})^{-1} \times \exp\left(-\frac{n\lambda}{2} \sum_{k=1}^{\infty} (f_k^2 + g_k^2)(2\pi k)^{2m}\right) \\ &= \prod_{k=1}^{\infty} (1 + n\lambda(2\pi k)^{-\beta})^{-1} \times \exp\left(-\frac{n\lambda}{2} \int_0^1 f^{(m)}(x)^2 dx\right) \\ &= \prod_{k=1}^{\infty} (1 + n\lambda(2\pi k)^{-\beta})^{-1} \times \exp\left(-\frac{n\lambda}{2} J(f)\right), \end{aligned} \quad (6)$$

where  $J(f) = \int_0^1 f^{(m)}(x)^2 dx$ . Note that  $\prod_{k=1}^{\infty} (1 + n\lambda(2\pi k)^{-\beta})^{-1}$  converges thanks to  $\beta > 1$  so that (6) is a valid expression. (6) provides an expression for the prior density of  $f$ , which induces the following posterior distribution for  $f$  given subsample  $j$ :

$$\begin{aligned} dP(f|\mathbf{D}_j) &\propto P(\mathbf{D}_j|f) d\Pi_\lambda(f) \\ &\propto \exp\left(-\frac{1}{2} \sum_{i \in I_j} (Y_i - f(X_i))^2 - \frac{n\lambda}{2} J(f)\right) d\Pi(f), \quad j = 1, \dots, s. \end{aligned} \quad (7)$$

Recall that  $I_j$  indexes the  $j$ -th subsample. The right hand-side of (7) corresponds to penalized likelihood function  $\ell_j(f) = -\frac{1}{2n} \sum_{i \in I_j} (Y_i - f(X_i))^2 - \frac{\lambda}{2} J(f)$  which has been well studied in smoothing spline literature (Wahba (1990)). Theoretically, we recommend to choose  $\lambda \asymp N^{-\frac{2m}{2m+\beta}}$  which will be proven to yield optimal Bayesian inference; see Sections 3 and 4. The duality between the posterior and smoothing spline, i.e., (7), enables us to easily choose  $\lambda$  for practical use, e.g., GCV considered by Wahba (1990).

## 2.2. Nonparametric Bayesian Aggregation

First of all, we calculate  $\check{f}_{j,n} = E\{f|\mathbf{D}_j\}$ ,  $j = 1, \dots, s$ , the posterior means based on individual posterior distributions (7). Then we construct a  $(1-\alpha)$ -th credible ball centering at  $\check{f}_{j,n}$  with radius  $r_{j,n}(\alpha)$ . That is,  $r_{j,n}(\alpha) > 0$  such that  $P(f \in S_0^m[0, 1] : \|f - \check{f}_{j,n}\|_{L^2} \leq r_{j,n}(\alpha) | \mathbf{D}_j) = 1 - \alpha$ , where  $\|\cdot\|_{L^2}$  is the usual  $L^2$ -norm, i.e.,  $\|f\|_{L^2} = \sqrt{\int_0^1 f(x)^2 dx}$ . In practice,  $\check{f}_{j,n}$  and  $r_{j,n}(\alpha)$  can be both estimated by the posterior samples. For instance, generate  $M$  independent samples  $f_{j1}, \dots, f_{jM}$  from (7); estimate  $\check{f}_{j,n}$  by their average and estimate  $r_{j,n}(\alpha)$  by the  $(1-\alpha)$ -th percentile of  $\|f_{jl} - \check{f}_{j,n}\|_{L^2}$  for  $1 \leq l \leq M$ . We postpone the computational details of the sampling procedure to Section 8.5.

We next present a concrete aggregation scheme (procedures (1)–(3) below) to construct a credible ball based on these individual results  $\{\check{f}_{j,n}, r_{j,n}(\alpha)\}_{j=1}^s$ . Specifically, an aggregated

credible ball for  $f$ , denoted  $R_N(\alpha)$ , is constructed with its center/radius obtained through *weighted* averaging the individual centers/radii. Unlike simple averaging commonly used in frequentist setting (see Zhang et al. (2015a)), our procedures for posterior mean aggregation and radius aggregation are weighted averaging with weights  $w_{s,N,\lambda,k}$  defined in (10). These weights are used to calibrate the prior effect such that the aggregation procedure can have satisfactory asymptotic property. The details of our procedure are demonstrated as follows:

1. *Posterior mean aggregation.* For  $j$ -th subsample and  $k \geq 1$ , find

$$\check{f}_{j,n,k} = \sqrt{2} \int_0^1 \check{f}_{j,n}(x) \cos(2\pi kx) dx, \quad \check{g}_{j,n,k} = \sqrt{2} \int_0^1 \check{f}_{j,n}(x) \sin(2\pi kx) dx, \quad (8)$$

where  $\check{f}_{j,n}$  is the posterior mean based on subsample  $j$ . Then we aggregate these quantities through the following formulas:

$$\check{f}_{N,\lambda,k} = \sum_{j=1}^s \check{f}_{j,n,k} / s, \quad \check{g}_{N,\lambda,k} = \sum_{j=1}^s \check{g}_{j,n,k} / s. \quad (9)$$

In the end, we let

$$\check{f}_{N,\lambda}(x) = \sum_{k=1}^{\infty} w_{s,N,\lambda,k} \left\{ \check{f}_{N,\lambda,k} \sqrt{2} \cos(2\pi kx) + \check{g}_{N,\lambda,k} \sqrt{2} \sin(2\pi kx) \right\}, \quad (10)$$

where  $w_{s,N,\lambda,k} = \frac{s(2\pi k)^{2m+\beta} + N(1+\lambda(2\pi k)^{2m})}{(2\pi k)^{2m+\beta} + N(1+\lambda(2\pi k)^{2m})}$  for  $k \geq 1$ .

2. *Posterior radius aggregation.* Aggregate the radii  $r_{j,n}(\alpha)$  through the following formula:

$$r_N(\alpha) = \sqrt{A_{N,s} \left( \frac{1}{s} \sum_{j=1}^s r_{j,n}(\alpha)^2 \right) + B_{N,s}}, \quad (11)$$

where

$$\begin{aligned} A_{N,s} &= \sqrt{C_2/D_2} s^{-\frac{4m+2\beta-1}{2(2m+\beta)}}, \\ B_{N,s} &= \left( 2C_1 - 2D_1 \sqrt{C_2/D_2} s^{-\frac{1}{2(2m+\beta)}} \right) N^{-\frac{2m+\beta-1}{2m+\beta}}, \\ C_k &= \int_0^\infty (1 + (2\pi x)^{2m} + (2\pi x)^{2m+\beta})^{-k} dx, \quad k = 1, 2, \\ D_k &= \int_0^\infty (1 + (2\pi x)^{2m})^{-k} dx, \quad k = 1, 2. \end{aligned} \quad (12)$$

3. *Aggregated credible ball:*

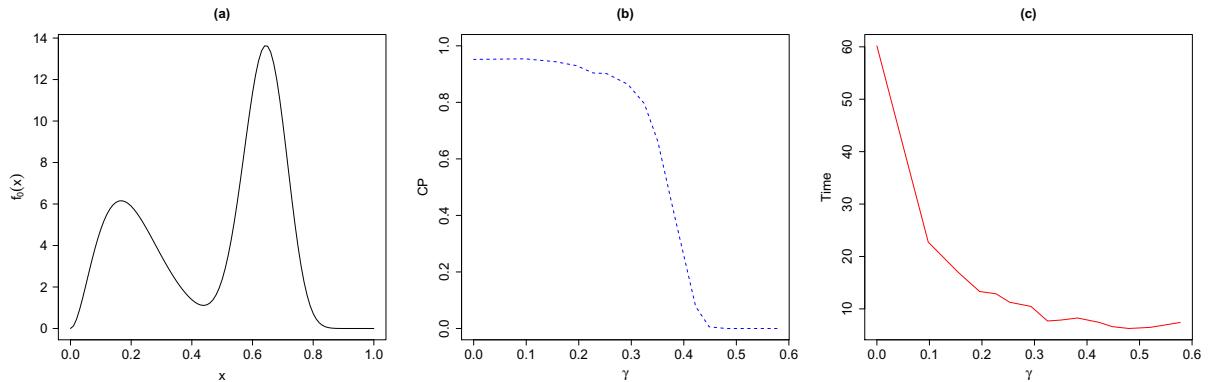
$$R_N(\alpha) = \{f \in S_0^m[0, 1] : \|f - \check{f}_{N,\lambda}\|_{L^2} \leq r_N(\alpha)\}. \quad (13)$$

Algorithms based on weighted averaging have been proposed in numerous computational aspects. For instance, Huang and Gelman (2005); Neiswanger et al. (2013); Scott et al. (2016) proposed computational procedures for efficiently aggregating local MCMC samples in which

the aggregation steps involve proper weight averaging. Such algorithms are particularly useful to produce MCMC samples from the oracle posterior which can be used for various inferential purposes, e.g., estimation and testing. The present paper focuses on inferences, e.g., construction of credible balls, in a special class of nonparametric regression models, and has more extensive theoretical guarantees.

In practice, one can approximate the integral (8) through discretization; see Section 8.5. Theorem 3 will show that  $R_N(\alpha)$  given in (13) asymptotically covers  $1 - \alpha$  mass of the posterior based on the full data set and includes the true function with probability approaching one. More theoretical study on  $R_N(\alpha)$  such as its center and radius can be found in Sections 4.2 and 4.3. Note that these sections present an aggregation procedure in a more general context, which covers (13) as a special case.

A toy simulation study was carried out to examine the proposed procedures (1)–(3). Specifically, we examine the computing time and coverage probability (CP) of  $R_N(\alpha)$  for various choices of  $s$ . The CP is defined as the relative frequency of the sets that cover the truth. We choose  $m = \beta = 2$  in our GP prior (4). Results are summarized in Figure 1. Plot (a) displays the true function  $f_0$  under which data were generated. Plot (b) displays how the CP varies as  $\gamma := \log(s)/\log(N)$ . Plot (c) displays that the computing time decreases when  $\gamma$  increases. There seems to be a transition for CP vs.  $\gamma$ , i.e., CP is uniformly close to one when  $0 \leq \gamma < 0.3$  and approaches zero when  $\gamma > 0.4$ . In conclusion,  $R_N(\alpha)$  possesses both satisfactory frequentist coverage and computational efficiency when  $\gamma \approx 0.2$ . Other choices of  $\gamma$  either lower CP or slow down the computing. Thus, under a proper choice of  $s$ , our aggregation procedure can maintain good statistical properties and reduce computing burden at the same time. Careful readers may have noticed that the CP approaches one rather than the credibility level  $(1 - \alpha)$ . This issue can be addressed by a modified aggregated set proposed in Section 4.4. More comprehensive simulation results are provided in Section 5 to examine various aggregation procedures such as the pointwise credible intervals.



**Figure 1.** Examination of our aggregation procedures (1)–(3). Results are based on  $N = 1200$  observations generated from (1) and a GP prior (4) with  $m = \beta = 2$  and  $\lambda = N^{-2/3}$ . (a) True regression function  $f_0(x) = 2.4\beta_{30,17}(x) + 1.6\beta_{3,11}(x)$ , where  $\beta_{a,b}$  is the probability density function for Beta( $a, b$ ). (b) Coverage probability (CP) of  $R_N(0.95)$  vs.  $\gamma$ . (c) Computing time (in seconds) of  $R_N(0.95)$  vs.  $\gamma$ .

### 3. A Nonparametric Bayesian Framework Based on General Design and Space

In this section, we introduce a more general Bayesian nonparametric framework based on general design and function space under which the aggregation results will be obtained. Suppose that the data  $\{Y_i, X_i\}_{i=1}^N$  follow a nonparametric regression model:

$$Y_i|f, X_i \stackrel{\text{ind.}}{\sim} N(f(X_i), \sigma^2), \quad X_1, \dots, X_N \stackrel{\text{iid}}{\sim} \pi(x), \quad (14)$$

where  $\pi(\cdot)$  is a probability density on  $\mathbb{I} = (0, 1)$ , and  $f$  belongs to an  $m$ -order Sobolev space  $S^m(\mathbb{I})$ :

$$S^m(\mathbb{I}) = \{f \in L^2(\mathbb{I}) | f^{(0)}, f^{(1)}, \dots, f^{(m-1)} \text{ are abs. cont. and } f^{(m)} \in L^2(\mathbb{I})\}. \quad (15)$$

In particular,  $S_0^m[0, 1]$  is a proper subset of  $S^m(\mathbb{I})$ . Throughout, we let  $m > 1/2$  such that  $S^m(\mathbb{I})$  is a reproducing kernel Hilbert space (RKHS). For technical convenience, assume  $\sigma^2 = 1$  and  $0 < \inf_{x \in \mathbb{I}} \pi(x) \leq \sup_{x \in \mathbb{I}} \pi(x) < \infty$ . When  $\sigma^2$  is unknown, our approach can still be applied with  $\sigma^2$  replaced by its consistent estimate.

For any  $f, g \in S^m(\mathbb{I})$ , define  $V(f, g) = E\{f(X)g(X)\}$  and  $J(f, g) = \int_0^1 f^{(m)}(x)g^{(m)}(x)dx$ . Following Shang et al. (2013), there exists a sequence of eigenfunctions  $\varphi_1, \varphi_2, \dots \in S^m(\mathbb{I})$  and a sequence of eigenvalues  $0 = \rho_1 = \rho_2 = \dots = \rho_m < \rho_{m+1} \leq \rho_{m+2} \leq \dots$  such that  $\rho_\nu \asymp \nu^{2m}$  and

$$V(\varphi_\nu, \varphi_\mu) = \delta_{\nu\mu}, \quad J(\varphi_\nu, \varphi_\mu) = \rho_\nu \delta_{\nu\mu}, \quad \nu, \mu \geq 1, \quad (16)$$

where  $\delta_{\nu\mu}$  is the Kronecker's delta.

We next place a prior distribution  $\Pi_\lambda$  on  $f$ , where  $\Pi_\lambda$  is a probability measure on  $S^m(\mathbb{I})$  and  $\lambda \geq 0$  is a hyperparameter. Similar to Section 2, we will characterize  $\Pi_\lambda$  through its Radon-Nikodym (RN) derivative w.r.t.  $\Pi$ , with  $\Pi$  a pre-given probability measure  $\Pi$  on  $S^m(\mathbb{I})$ . Specifically, assume that the RN derivative of  $\Pi_\lambda$  w.r.t.  $\Pi$  satisfies

$$\frac{d\Pi_\lambda}{d\Pi}(f) \propto \exp\left(-\frac{n\lambda}{2} J(f)\right), \quad (17)$$

where  $J(f)$  is defined in (3). Interestingly, it is possible to explicitly construct  $\Pi_\lambda$  and  $\Pi$  such that (17) holds. To see this, let

$$G_\lambda(\cdot) = \sum_{\nu=m+1}^{\infty} w_\nu \varphi_\nu(\cdot), \quad (18)$$

where  $w_\nu$ 's are independent of the observations satisfying  $w_\nu \sim N(0, 1/(\rho_\nu^{1+\beta/(2m)} + n\lambda\rho_\nu))$ ,  $\nu > m$ . Let  $G(\cdot) = G_{\lambda=0}(\cdot)$ . Suppose  $\Pi_\lambda$  and  $\Pi$  are probability measures induced by  $G_\lambda$  and  $G$ , i.e.,  $\Pi_\lambda(S) = P(G_\lambda \in S)$  and  $\Pi(S) = P(G \in S)$  for any measurable  $S \subseteq S^m(\mathbb{I})$ . It follows by Hájek's lemma (see Shang and Cheng (2017)) that (17) holds. In (18),  $\lambda \geq 0$  and  $\beta > 1$  are both hyper-parameters characterizing the smoothness of the prior. It is easy to check that the sample path of  $G_\lambda$  belongs to  $S^m(\mathbb{I})$  for any  $\beta > 1$  almost surely. As demonstrated in a simulation study, the GCV-selected  $\lambda$  is sufficient to provide satisfactory results.

## 4. Main Results

In this section, we present a series of main results that are built upon a uniform Gaussian approximation theorem (Section 4.1). Three classes of aggregation procedures are then proposed: aggregated credible balls in both strong and weak topology, and aggregated credible intervals for linear functionals. These results can be classified into two types: *finite sample* construction (Sections 4.3, 4.4 and 4.5) and *asymptotic* construction (Section 4.6). The former construction is often time-consuming since its radius (interval length) is obtained through  $s$  posterior sampling, while the latter employs a large-sample limit of the radius given by an explicit formula. The computational gain will be illustrated by the simulations in Section 5. Similar to Section 2, let  $I_1, I_2, \dots, I_s$  be a random partition of  $\{1, 2, \dots, N\}$  such that  $\cup_{j=1}^s I_j = \{1, 2, \dots, N\}$  with  $|I_j| = n$  for  $j = 1, \dots, s$  and  $N = ns$ .

### 4.1. A Uniform Gaussian Approximation Theorem

A fundamental theory underlying Bayesian aggregation is developed in this section. It is a *uniform* version of Gaussian approximation theorem that characterizes the limit shapes of a sequence of individual posterior distributions. This uniform validity holds if the number of posterior distributions does not grow too fast. Also, Bayesian aggregation procedures possess frequentist validity if  $\lambda$  is chosen properly.

Similar to (7), we note that each sub-posterior distribution can be written as

$$dP(f|\mathbf{D}_j) \propto \exp(n\ell_{jn}(f))d\Pi(f),$$

where  $\ell_{jn}(f) = n^{-1} \sum_{i \in I_j} (Y_i - f(X_i))^2 - (\lambda/2)J(f)$ . Define

$$\widehat{f}_{j,n} = \arg \max_{f \in S^m(\mathbb{I})} \ell_{jn}(f), \quad j = 1, \dots, s. \quad (19)$$

Suppose that  $\widehat{f}_{j,n}$  admits the following Fourier expansion:

$$\widehat{f}_{j,n}(\cdot) = \sum_{\nu=1}^{\infty} \widehat{f}_{\nu}^{(j)} \varphi_{\nu}(\cdot), \quad 1 \leq j \leq s. \quad (20)$$

Define  $h = \lambda^{1/(2m)}$  with  $h^* := N^{-\frac{1}{2m+\beta}}$ . We remark that  $h^*$  is an optimal choice for our aggregation procedure as will be shown later.

**Theorem 1** (*Uniform Gaussian Approximation*) Suppose that  $f_0$  admits a Fourier expansion  $f_0(\cdot) = \sum_{\nu=1}^{\infty} f_{\nu}^0 \varphi_{\nu}(\cdot)$  which further satisfies

$$\text{Condition (S):} \quad \sum_{\nu=1}^{\infty} |f_{\nu}^0|^2 \rho_{\nu}^{1+\frac{\beta-1}{2m}} < \infty$$

If the following holds

$$m > 1 + \frac{\sqrt{3}}{2} \approx 1.866, \quad 1 < \beta < 2m + \frac{1}{2m} - 1, \quad s = o(N^{\frac{\beta-1}{2m+\beta}}) \quad \text{and} \quad h \asymp h^*, \quad (21)$$

then we have as  $N \rightarrow \infty$ ,

$$\sup_{S \in \mathcal{S}} \max_{1 \leq j \leq s} |P(S|\mathbf{D}_j) - P_{0j}(S)| = O_{P_{f_0}} \left( \sqrt{s} N^{-\frac{4m^2+2m\beta-10m+1}{4m(2m+\beta)}} (\log N)^{\frac{5}{2}} \right), \quad (22)$$

where  $\mathcal{S}$  is the Borel  $\sigma$ -algebra on  $S^m(\mathbb{I})$  with respect to  $\Pi$ , and  $P_{0j}$ 's are GPs defined by

$$P_{0j}(S) = \frac{\int_S \exp\left(-\frac{n}{2}\|f - \widehat{f}_{j,n}\|^2\right) d\Pi(f)}{\int_{S^m(\mathbb{I})} \exp\left(-\frac{n}{2}\|f - \widehat{f}_{j,n}\|^2\right) d\Pi(f)}, \quad S \in \mathcal{S}. \quad (23)$$

Proof of Theorem 1 is rooted in Shang and Cheng (2017) who essentially considered  $s = 1$ . Substantial efforts have been made here to quantify a range of partition size  $s$  such that local posteriors can be uniformly approximated by GPs. The explicit structure of the GPs provides a guideline for our aggregation procedures which will be introduced in subsequent sections. It should be emphasized that our aggregation of GPs is weighted-averaging which is different from product-based ones such as Cao and Fleet (2014).

Condition (S) amounts to requiring known regularity of the truth  $f_0 \in S^{m+\frac{\beta-1}{2}}(\mathbb{I})$ . This can be seen from the inequality  $\sum_{\nu=1}^{\infty} |f_{\nu}^0|^2 \nu^{2m+\beta-1} < \infty$  since  $\rho_{\nu} \asymp \nu^{2m}$ . This condition essentially means that  $f_0$  has derivatives up to order  $m + \frac{\beta-1}{2}$  (when this order is integer-valued). Combined with (21) this means that the regularity of  $f_0$  belongs to  $(m, 2m + \frac{1}{4m} - 1)$ , i.e., the truth function is jointly confined by both functional space and the prior. The  $\|\cdot\|$ -norm used in (23) is defined as follows. For any  $g, \tilde{g} \in S^m(\mathbb{I})$ , define

$$\langle g, \tilde{g} \rangle = V(g, \tilde{g}) + \lambda J(g, \tilde{g}) \quad (24)$$

and its squared norm  $\|g\|^2 = \langle g, g \rangle$ . Clearly,  $\langle \cdot, \cdot \rangle$  is a valid inner product on  $S^m(\mathbb{I})$ .

**Remark 1** We remark that (21) can be replaced by a more general rate condition:

$$nh^{2m+1} \geq 1, \quad a_n = O(\tilde{r}_n), \quad b_n \leq 1, \quad r_n^2 b_n \leq \tilde{r}_n^2, \quad n\tilde{r}_n^2 b_n = o(1),$$

where  $r_n = (nh)^{-1/2} + h^m$ ,  $\tilde{r}_n = (nh/\log 2s)^{-1/2} + h^{m+\frac{\beta-1}{2}}$ ,  $a_n = n^{-1/2}h^{-\frac{6m-1}{4m}}r_n \log N$ ,  $b_n = n^{-1/2}h^{-\frac{6m-1}{4m}}(\log N)^{3/2}$ . Here, we provide a technical explanation for the terms  $r_n, \tilde{r}_n, a_n, b_n$ . Specifically,  $r_n$  can be viewed as the rate of convergence of local ordinary penalized MLE (19),  $\tilde{r}_n$  can be viewed as the posterior contraction rate of the local Bayesian mode,  $a_n, b_n$  are error bounds of the higher-order remainders in the Taylor expansions of the individual penalized likelihood functions. Uniform Gaussian approximation for general  $h$  (not necessarily  $h \asymp h^*$ ) can be established under such condition.

Theorem 3.5 in Shang and Cheng (2017) shows that  $P_{0j}$  (conditional on  $\mathbf{D}_j$ ) is induced by a Gaussian process, denoted as  $W^j$ , in the sense that  $P_{0j}(S) = P(W^j \in S | \mathbf{D}_j)$  for any  $S \in \mathcal{S}$ . Define

$$\tau_{\nu}^2 = \rho_{\nu}^{1+\frac{\beta}{2m}}, \quad \nu \geq 1. \quad (25)$$

Then we have

$$W^j(\cdot) = \sum_{\nu=1}^{\infty} (a_{n,\nu} \widehat{f}_{\nu}^{(j)} + b_{n,\nu} \tau_{\nu} v_{\nu}) \varphi_{\nu}(\cdot), \quad j = 1, 2, \dots, s,$$

where  $a_{n,\nu} = n(1 + \lambda\rho_{\nu})(\tau_{\nu}^2 + n(1 + \lambda\rho_{\nu}))^{-1}$ ,  $b_{n,\nu} = (\tau_{\nu}^2 + n(1 + \lambda\rho_{\nu}))^{-1/2}$  and  $v_{\nu} \sim N(0, \tau_{\nu}^{-2})$ . For convenience, define the mean functions of  $W^j$  as

$$\tilde{f}_{j,n}(\cdot) := \sum_{\nu=1}^{\infty} a_{n,\nu} \widehat{f}_{\nu}^{(j)} \varphi_{\nu}(\cdot), \quad j = 1, \dots, s, \quad (26)$$

such that we can re-express  $W^j$  as

$$W^j = \tilde{f}_{j,n} + W_n, \quad j = 1, \dots, s,$$

where  $W_n(\cdot) := \sum_{\nu=1}^{\infty} b_{n,\nu} \tau_{\nu} v_{\nu} \varphi_{\nu}(\cdot)$  is a zero-mean GP. Note that the posterior mode  $\tilde{f}_{j,n}$  is very close to  $\widehat{f}_{j,n}$  since  $\|\widehat{f}_{j,n} - \tilde{f}_{j,n}\| = o_{P_{f_0}}(1)$  uniformly for  $1 \leq j \leq s$ ; see the proof of Theorem 3. The above characterization of  $W^j$  is useful for the subsequent Bayesian aggregation procedures.

#### 4.2. Aggregated posterior means

In this section, we propose a method to aggregate the posterior means  $\check{f}_{j,n} := E\{f|\mathbf{D}_j\}$ , for  $j = 1, \dots, s$ . The aggregated mean function, denoted as  $\check{f}_{N,\lambda}(\cdot)$ , can be viewed as a nonparametric Bayesian estimate of  $f$ , and will be used to construct aggregated credible balls/intervals to be introduced later.

Our aggregation procedure is

$$\check{f}_{N,\lambda}(\cdot) = \sum_{\nu=1}^{\infty} \frac{a_{N,\nu}}{a_{n,\nu}} V \left( \frac{1}{s} \sum_{j=1}^s \check{f}_{j,n}, \varphi_{\nu} \right) \varphi_{\nu}(\cdot). \quad (27)$$

Note that when the model is Gaussian and  $f \in S_0^m(0, 1)$ , (27) becomes (10). Next we will show that the aggregation procedure (27) yields minimax optimality in the following theorem.

**Theorem 2** *Under conditions of Theorem 1, the following result holds:*

$$\max_{1 \leq j \leq s} \|\check{f}_{j,n} - \tilde{f}_{j,n}\| = O_{P_{f_0}} \left( \tilde{r}_n \sqrt{s} N^{-\frac{4m^2+2m\beta-10m+1}{4m(2m+\beta)}} (\log N)^{\frac{5}{2}} \right), \quad (28)$$

If, in addition,  $3/2 < \beta < 2m + 1/(2m) - 3/2$  and  $s$  satisfies

$$s = o \left( N^{\frac{4m^2+2m\beta-11m+1}{8m(2m+\beta)}} (\log N)^{-\frac{3}{2}} \right), \quad (29)$$

then it holds that

$$\|\check{f}_{N,\lambda} - f_0\|_2 = O_{P_{f_0}} \left( N^{-\frac{2m+\beta-1}{2(2m+\beta)}} \right), \quad (30)$$

where  $\|f\|_2 = \sqrt{V(f)}$  denotes the  $V$ -norm.

According to van der Vaart et al. (2008b), the rate in (30) is minimax optimal given Condition (S).

#### 4.3. Aggregated credible region in strong topology

In this section, we construct an aggregated credible region based on  $s$  individual credible regions (w.r.t. a weighted  $\ell^2$ -norm). Specifically,  $s$  radii are combined in an explicit manner. This aggregated region possesses nominal posterior mass asymptotically, and is further proven to cover the true function with probability tending to one. This nice frequentist

property is achieved as long as  $s$  is not diverging fast and the assigned GP prior in each subset is chosen by setting  $h \asymp h^*$ , i.e.,  $\lambda \asymp N^{-2m/(2m+\beta)}$ . The conservative frequentist coverage can be improved to the nominal level if we use a weaker norm in defining credible region; see Section 4.4.

Based on each subset  $\mathbf{D}_j$ , the individual credible ball is constructed as follows:

$$R_{j,n}(\alpha) = \{f \in S^m(\mathbb{I}) : \|f - \check{f}_{j,n}\|_2 \leq r_{j,n}(\alpha)\}.$$

The credible ball centers around the posterior mean  $\check{f}_{j,n}$ , while its radius  $r_{j,n}(\alpha)$  is directly sampled from MCMC such that  $P(R_{j,n}(\alpha) | \mathbf{D}_j) = 1 - \alpha$  for any  $\alpha \in (0, 1)$ . We will construct an “aggregated” region centering at  $\check{f}_{N,\lambda}$  with radius explicitly constructed as follows:

$$r_N(\alpha) = \sqrt{\frac{1}{N} \left[ \zeta_{1,N} + \sqrt{\frac{\zeta_{2,N}}{\zeta_{2,n}} \left( \frac{n}{s} \sum_{j=1}^s r_{j,n}^2(\alpha) - \zeta_{1,n} \right)} \right]}, \quad (31)$$

where

$$\zeta_{k,n} = \sum_{\nu=1}^{\infty} \left( \frac{n}{\tau_{\nu}^2 + n(1 + \lambda\rho_{\nu})} \right)^k \text{ for } k = 1, 2.$$

The final aggregated credible region is obtained as

$$R_N(\alpha) := \{f \in S^m(\mathbb{I}) : \|f - \check{f}_{N,\lambda}\|_2 \leq r_N(\alpha)\}. \quad (32)$$

Our theorem below confirms that  $R_N(\alpha)$  indeed possesses (asymptotic) posterior mass  $(1 - \alpha)$ , and more importantly, proves that it covers the true function  $f_0$  with probability tending to one.

**Theorem 3** *Suppose that  $f_0$  satisfies Condition  $(S)$ ,  $m > 1 + \frac{\sqrt{3}}{2}$ ,  $3/2 < \beta < 2m+1/(2m)-3/2$ ,  $s = o(N^{\frac{\beta-1}{2m+\beta}})$ , (29) and  $h \asymp h^*$ . Then for any  $\alpha \in (0, 1)$ ,  $P(R_N(\alpha) | \mathbf{D}) = 1 - \alpha + o_{P_{f_0}}(1)$  and  $\lim_{n \rightarrow \infty} P_{f_0}(f_0 \in R_N(\alpha)) = 1$ .*

From the proof of Theorem 3, we point out that when  $s = 1$ , the posterior mass of the aggregated credible region is exactly  $1 - \alpha$ , consistent with Shang and Cheng (2017). This remark also applies to other aggregated procedures to be presented later.

**Remark 2** *When  $h \asymp h^*$ , the radius of the aggregated ball  $r_N(\alpha) \asymp N^{-\frac{2m+\beta-1}{2(2m+\beta)}}$  according to the discussions in Section 4.6. This is the optimal rate at which a posterior ball contracts based on the entire sample; see van der Vaart et al. (2008b).*

#### 4.4. Aggregated credible region in weak topology

In this section, we invoke a weaker norm (than that used in Section 4.3) to construct an aggregated credible region. Under this new norm (inspired by Castillo et al. (2013, 2014)), it is proven that the frequentist coverage *exactly* matches with the asymptotic credibility level. The requirement on  $s$  and  $h$  in this section remains the same as Section 4.3.

We define a weaker norm than  $\|\cdot\|_2$ , denoted  $\|\cdot\|_{\omega}$ . For any  $f \in S^m(\mathbb{I})$  with  $f = \sum_{\nu} f_{\nu} \varphi_{\nu}$ , define  $\|f\|_{\omega}^2 = \sum_{\nu=1}^{\infty} \omega_{\nu} f_{\nu}^2$ , where  $\omega_{\nu} = (\nu(\log 2\nu))^{-\tau}$  for some constant  $\tau > 1$ . Since  $\omega_{\nu} < 1$  for

all  $\nu \geq 1$ , we have  $\|f\|_\omega \leq \|f\|_2$ . Under the new  $\|\cdot\|_\omega$ -norm, each individual  $(1 - \alpha)$  credible region is constructed as

$$R_{j,n}^\omega(\alpha) = \{f \in S^m(\mathbb{I}) : \|f - \check{f}_{j,n}\|_\omega \leq r_{\omega,j,n}(\alpha)\},$$

where  $r_{\omega,j,n}(\alpha)$  is directly obtained from posterior sampling such that  $P(R_{j,n}^\omega(\alpha) | \mathbf{D}_j) = 1 - \alpha$ .

Under  $\|\cdot\|_\omega$ -norm, the aggregated credible region is constructed as:

$$R_N^\omega(\alpha) := \{f \in S^m(\mathbb{I}) : \|f - \check{f}_{N,\lambda}\|_\omega \leq r_{\omega,N}(\alpha)\}, \quad (33)$$

where the radius is given as

$$r_{\omega,N}(\alpha) = \sqrt{\frac{1}{s^2} \sum_{j=1}^s r_{\omega,j,n}^2(\alpha)}. \quad (34)$$

Interestingly, Section 4.6 illustrates that the aggregated radius  $r_{\omega,N}(\alpha)$  contracts at root- $N$  rate.

Our theorem below shows that the frequentist coverage of  $R_N^\omega(\alpha)$  exactly matches with the asymptotic posterior mass, both of which achieve the nominal level  $(1 - \alpha)$ .

**Theorem 4** Suppose that  $f_0$  satisfies Condition (S),  $m > 1 + \sqrt{3}/2$ ,  $2 \leq \beta < \frac{(2m-1)^2}{2m}$ ,  $s = o(N^{\frac{\beta-1}{2m+\beta}})$ ,  $s = o(N^{\frac{4m^2+2m\beta-12m+1}{8m(2m+\beta)}}(\log N)^{-\frac{3}{2}})$ , and  $h \asymp h^*$ . Then for any  $\alpha \in (0, 1)$ ,  $P(R_N^\omega(\alpha) | \mathbf{D}) = 1 - \alpha + o_{P_{f_0}}(1)$  and  $\lim_{n \rightarrow \infty} P_{f_0}(f_0 \in R_N^\omega(\alpha)) = 1 - \alpha$ .

#### 4.5. Aggregated credible interval for linear functional

In this section, we construct aggregated credible intervals for a class of linear functionals of  $f$ , denoted as  $F(f)$ . Examples include the evaluation functional, i.e.,  $F(f) = f(x)$ , and integral functional, i.e.,  $F(f) = \int_0^1 f(x)dx$ . Specifically, the interval is centered at  $F(\check{f}_{N,\lambda})$  with an length aggregated through  $s$  lengths obtained from posterior sampling. Posterior and frequentist coverage properties of this aggregated interval depends on the functional form  $F(\cdot)$ . Again, our theory holds when  $s$  is mildly diverging and  $h \asymp h^*$ .

Let  $F : S^m(\mathbb{I}) \mapsto \mathbb{R}$  be a linear  $\Pi$ -measurable functional satisfying the following Condition (F):  $\sup_{\nu \geq 1} |F(\varphi_\nu)| < \infty$ , and there exist constants  $\kappa > 0$  and  $r \in [0, 1]$  such that for any  $f \in S^m(\mathbb{I})$ ,

$$|F(f)| \leq \kappa h^{-r/2} \|f\|. \quad (35)$$

It follows by Shang and Cheng (2017) that the evaluation functional satisfies Condition (F) with  $r = 1$  and the integral functional satisfies Condition (F) with  $r = 0$ .

Based on each  $\mathbf{D}_j$ , we obtain from posterior samples the following  $(1 - \alpha)$  credible interval:

$$CI_{j,n}^F(\alpha) := \{f \in S^m(\mathbb{I}) : |F(f) - F(\check{f}_{j,n})| \leq r_{F,j,n}(\alpha)\},$$

where  $r_{F,j,n}(\alpha)$  is a radius such that  $P(CI_{j,n}^F(\alpha) | \mathbf{D}_j) = 1 - \alpha$ . The aggregated credible interval is constructed as

$$CI_N^F(\alpha) := \{f \in S^m(\mathbb{I}) : |F(f) - F(\check{f}_{N,\lambda})| \leq \bar{r}_{F,N}(\alpha)\} \quad (36)$$

where

$$r_{F,N}(\alpha) = \frac{\theta_{1,N}}{\theta_{1,n}} \sqrt{\frac{1}{s} \sum_{j=1}^s r_{F,j,n}(\alpha)^2} \quad \text{and} \quad \theta_{k,n}^2 = \sum_{\nu=1}^{\infty} \frac{F(\varphi_{\nu})^2}{(\tau_{\nu}^2 + n(1 + \lambda\rho_{\nu}))^k} \quad \text{for } k = 1, 2. \quad (37)$$

The shrinking rate of  $\bar{r}_{F,N}(\alpha)$  depends on the functional form  $F$ ; see Section 4.6.

Our theorem below investigates the asymptotic properties of  $CI_F^N(\alpha)$  in terms of both posterior and frequentist coverage.

**Theorem 5** Suppose that  $f_0 = \sum_{\nu=1}^{\infty} f_{\nu}^0 \varphi_{\nu}$  satisfies Condition  $(S')$ :  $\sum_{\nu=1}^{\infty} |f_{\nu}^0|^2 \nu^{2m+\beta} < \infty$ ,  $E_{f_0}\{\epsilon^4 | X\} \leq M_4$  a.s. for some constant  $M_4 > 0$ ,  $N^k \theta_{k,N}^2 \gtrsim h^{-r}$  for  $k = 1, 2$ ,  $m > 1 + \frac{\sqrt{3}}{2}$ ,  $2 \leq \beta < \frac{(2m-1)^2}{2m}$ ,  $s = o(N^{\frac{\beta-1}{2m+\beta}})$ ,  $s = o(N^{\frac{4m^2+2m\beta-12m+1}{8m(2m+\beta)}} (\log N)^{-\frac{3}{2}})$ , (29) and  $h \asymp h^*$ . Then for any  $\alpha \in (0, 1)$ ,  $P(CI_N^F(\alpha) | \mathbf{D}) = 1 - \alpha + o_{P_{f_0}}(1)$ , and  $\liminf_{N \rightarrow \infty} P_{f_0}(f_0 \in CI_N^F(\alpha)) \geq 1 - \alpha$  given that Condition  $(F)$  holds. Moreover, if  $0 < \sum_{\nu=1}^{\infty} F(\varphi_{\nu})^2 < \infty$ , then  $\lim_{N \rightarrow \infty} P_{f_0}(f_0 \in CI_N^F(\alpha)) = 1 - \alpha$ .

Note that Condition  $(S')$  is slightly stronger than Condition  $(S)$  required in Theorem 1. Indeed, this condition essentially means that  $f_0$  has derivatives up to order  $m + \frac{\beta}{2}$  (when this order is integer-valued). Hence, Theorem 5 requires a more smooth true function  $f_0$ .

It was shown in Shang and Cheng (2017) that the integral functional  $F_x(f) := \int_0^x f(z) dz$  for any  $x \in [0, 1]$  satisfies (35) with  $r = 0$  and  $0 < \sum_{\nu=1}^{\infty} F_x(\varphi_{\nu})^2 < \infty$ . Therefore, the  $(1 - \alpha)$ -th credible interval of  $F_x(f)$  achieves exactly  $(1 - \alpha)$  frequentist coverage, while that for the evaluation functional is more conservative. These theoretical findings will be empirically verified in Section 5.

#### 4.6. Asymptotic aggregated inference

In practice, the centers  $\check{f}_{N,\lambda}$ ,  $F(\check{f}_{N,\lambda})$  and the radii  $r_{j,n}(\alpha)$ ,  $r_{\omega,j,n}(\alpha)$ ,  $r_{F,j,n}(\alpha)$  in Sections 4.3 – 4.5 are directly obtained from posterior samples. Sometimes posterior sampling is time consuming and inefficient, particularly as  $s \rightarrow \infty$ . This computational consideration motivates us to propose an *asymptotic* approach in which one replaces the above centers/radii by their large sample limits. Our new asymptotic inference procedures dramatically improve the computing speed, as displayed in simulations; see Section 5.

Define

$$\tilde{f}_{N,\lambda}(\cdot) = \sum_{\nu=1}^{\infty} \frac{a_{N,\nu}}{a_{n,\nu}} V \left( \frac{1}{s} \sum_{j=1}^s \tilde{f}_{j,n}(\varphi_{\nu}) \right) \varphi_{\nu}(\cdot). \quad (38)$$

Clearly,  $\tilde{f}_{N,\lambda}$  is a counterpart of  $\check{f}_{N,\lambda}$  (27) with  $\check{f}_{j,n}$  therein replaced by  $\tilde{f}_{j,n}$ . By a careful examination of the proofs of Theorems 3 – 5, it can be shown that the following limits hold:

$$\begin{aligned} \|\check{f}_{N,\lambda} - \tilde{f}_{N,\lambda}\| &= o_{P_{f_0}}(N^{-1/2} h^{-1/4}), \\ \max_{1 \leq j \leq s} \left| \frac{nr_{j,n}^2(\alpha) - \zeta_{1,n}}{\sqrt{2\zeta_{2,n}}} - z_{\alpha} \right| &= o_{P_{f_0}}(1), \\ \max_{1 \leq j \leq s} |\sqrt{n}r_{\omega,j,n}(\alpha) - \sqrt{c_{\alpha}}| &= o_{P_{f_0}}(1), \\ \max_{1 \leq j \leq s} |r_{F,j,n}(\alpha)/\theta_{1,n} - z_{\alpha/2}| &= o_{P_{f_0}}(1), \end{aligned} \quad (39)$$

where  $z_\alpha = \Phi^{-1}(1 - \alpha)$  with  $\Phi(\cdot)$  being the c.d.f. of standard normal random variable, and  $c_\alpha > 0$  satisfies  $P(\sum_{\nu=1}^{\infty} d_\nu \eta_\nu^2 \leq c_\alpha) = 1 - \alpha$  with  $\eta_\nu$  being independent standard normal random variables.

It yields from (39) that the following approximation relationships hold uniformly for  $1 \leq j \leq s$ :

$$r_{j,n}(\alpha) \approx \sqrt{\frac{\zeta_{1,n} + \sqrt{2\zeta_{2,n}}z_\alpha}{n}}, \quad r_{\omega,j,n}(\alpha) \approx \sqrt{\frac{c_\alpha}{n}} \quad \text{and} \quad r_{F,j,n}(\alpha) \approx \theta_{1,n} z_{\alpha/2},$$

which further implies (by the aggregation formulae (31), (34) and (37))

$$\begin{aligned} r_N(\alpha) &\approx r_N^\dagger(\alpha) := \sqrt{\frac{\zeta_{1,N} + \sqrt{2\zeta_{2,N}}z_\alpha}{N}}, \\ r_{\omega,N}(\alpha) &\approx r_{\omega,N}^\dagger(\alpha) := \sqrt{\frac{c_\alpha}{N}}, \\ r_{F,N}(\alpha) &\approx r_{F,N}^\dagger(\alpha) := \theta_{1,N} z_{\alpha/2}. \end{aligned} \tag{40}$$

Thus, we have the following *asymptotic* counterparts of  $R_N(\alpha)$ ,  $R_N^\omega(\alpha)$  and  $CI_N^F(\alpha)$ :

$$R_N^\dagger(\alpha) := \{f \in S^m(\mathbb{I}) : \|f - \tilde{f}_{N,\lambda}\|_2 \leq r_N^\dagger(\alpha)\}, \tag{41}$$

$$R_N^{\dagger\omega}(\alpha) := \{f \in S^m(\mathbb{I}) : \|f - \tilde{f}_{N,\lambda}\|_\omega \leq r_{\omega,N}^\dagger(\alpha)\}, \tag{42}$$

$$CI_N^{\dagger F}(\alpha) := \{f \in S^m(\mathbb{I}) : |F(f) - F(\tilde{f}_{N,\lambda})| \leq r_{F,N}^\dagger(\alpha)\}. \tag{43}$$

Our theorem below shows that the posterior coverage and frequentist coverage of the above computationally efficient alternatives remain the same as those for  $R_N(\alpha)$ ,  $R_N^\omega(\alpha)$  and  $CI_N^F(\alpha)$  under the same set of conditions.

**Theorem 6** *Suppose that all assumptions in Theorems 3 – 5 hold. Then for any  $\alpha \in (0, 1)$ ,  $R_N^\dagger(\alpha)$ ,  $R_N^{\dagger\omega}(\alpha)$  and  $CI_N^{\dagger F}(\alpha)$  possess exactly the same posterior and frequentist properties as  $R_N(\alpha)$ ,  $R_N^\omega(\alpha)$  and  $CI_N^F(\alpha)$ , respectively.*

As a byproduct, (40) implies the contraction rate of each aggregated credible ball/interval in Sections 4.3 – 4.6. It is easy to see that  $r_{\omega,N}(\alpha) \asymp N^{-1/2}$ . As for  $r_{F,N}(\alpha)$ , it depends on the functional form  $F$ . For example, when  $F$  is an evaluation functional, it holds that  $\theta_{1,N}^2 \asymp (Nh)^{-1}$ , leading to  $N^{-\frac{2m+\beta-1}{2(2m+\beta)}}$  when  $h \asymp h^*$ ; when  $F$  is an integral functional, we have  $r_{F,N}(\alpha) \asymp N^{-1/2}$  since  $\theta_{1,N}^2 \asymp N^{-1}$ . As for  $r_N(\alpha)$ , it can be shown by a simple fact  $\zeta_{1,N}, \zeta_{2,N} \asymp h^{-1}$  that  $r_N(\alpha) \asymp (Nh)^{-1/2} \asymp N^{-\frac{2m+\beta-1}{2(2m+\beta)}}$  when  $h \asymp h^*$ . This contraction rate turns out to be optimal based on the entire sample; see van der Vaart et al. (2008b). However, if we choose  $h$  in the scale of subsample size  $n$ , e.g.,  $h \asymp n^{-\frac{1}{2m+\beta}}$ , similar arguments show that  $r_N(\alpha) \asymp N^{-\frac{2m+\beta-1}{2(2m+\beta)}} s^{-\frac{1}{2(2m+\beta)}}$ . Hence, such a region contracts faster than the optimal rate, which results in unsatisfactory frequentist coverage.

Table 1 summarizes six aggregated credible regions/intervals from Sections 4.3 – 4.5 in terms of their centers and radii.

**Table 1.** Summary of Aggregated  $(1 - \alpha)$  Credible Regions/Intervals

Type	Name	Notation	Center	Radius
Finite-sample	strong CR for $f$	$R_N(\alpha)$	$\check{f}_{N,\lambda}$	$r_N(\alpha)$
	weak CR for $f$	$R_N^\omega(\alpha)$	$\check{f}_{N,\lambda}$	$r_{\omega,N}(\alpha)$
	CI for $F(f)$	$CI_N^F(\alpha)$	$F(\check{f}_{N,\lambda})$	$r_{F,N}(\alpha)$
Asymptotic	strong CR for $f$	$R_N^\dagger(\alpha)$	$\tilde{f}_{N,\lambda}$	$r_N^\dagger(\alpha)$
	weak CR for $f$	$R_N^{\dagger\omega}(\alpha)$	$\tilde{f}_{N,\lambda}$	$r_{\omega,N}^\dagger(\alpha)$
	CI for $F(f)$	$CI_N^{\dagger F}(\alpha)$	$F(\tilde{f}_{N,\lambda})$	$r_{F,N}^\dagger(\alpha)$

## 5. Simulation Study

In this section, statistical properties of the proposed aggregated procedures are examined using a simulation study. We generated samples from the following model

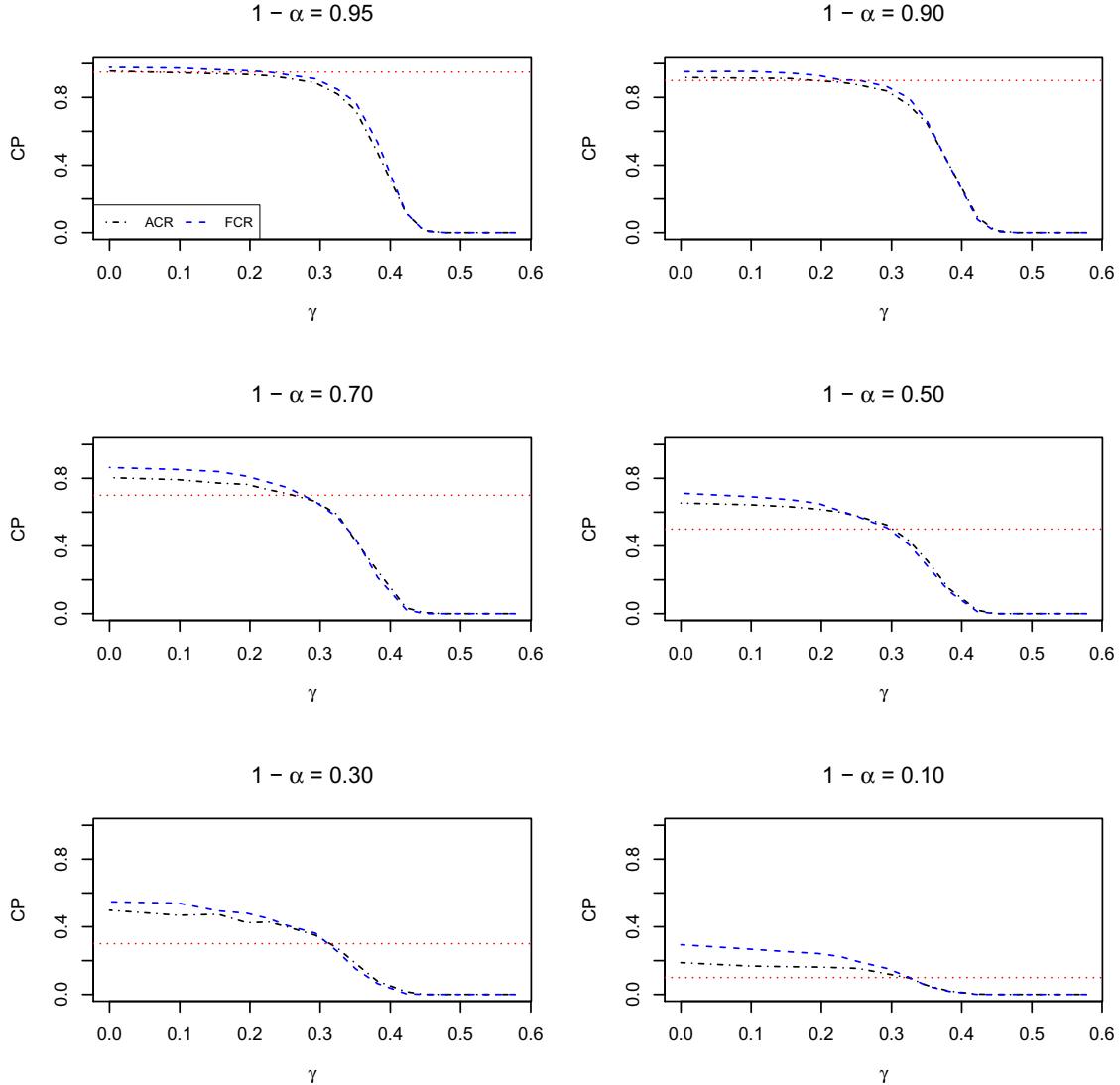
$$Y_{ij} = f_0(X_{ij}) + \epsilon_{ij}, \quad i = 1, 2, \dots, n, j = 1, 2, \dots, s, \quad (44)$$

where  $X_{ij} \stackrel{iid}{\sim} Unif[0, 1]$ ,  $\epsilon_{ij} \stackrel{iid}{\sim} N(0, 1)$ , and  $\epsilon_{ij}$  are independent of  $X_{ij}$ . The true regression function was chosen to be  $f_0(x) = 2.4\beta_{30,17}(x) + 1.6\beta_{3,11}(x)$ , where  $\beta_{a,b}$  is the probability density function for  $Beta(a, b)$ .

Consider GP prior  $f \sim \sum_{\nu=1}^n w_\nu \varphi_\nu$ , where  $w_\nu$  are defined in (18). The proposed Bayesian procedures were examined. Specifically, we computed the frequentist coverage proportions (CP) of the credible regions (32), (33), (41), (42), and credible intervals (36), (43). In particular, (32), (33) and (36) were constructed based on posterior samples, as described in Sections 4.2–4.5; whereas (41), (42) and (43) were constructed based on asymptotic theory developed in Section 4.6. To ease presentation, we call (32) and (33) as finite-sample credible regions (FCR), and call (41) and (42) as asymptotic credible regions (ACR).

The calculation of CP was based on 500 independent experiments. Specifically, the CP is the proportion of the credible regions/intervals containing  $f_0/F(f_0)$  (for a linear functional  $F$ ). Two types of  $F$  were considered: (1) the evaluation functional  $F_x(f) = f(x)$  for any  $x \in [0, 1]$ , and (2) the integral functional  $F_x(f) = \int_0^x f(z)dz$  for any  $x \in [0, 1]$ . In both cases, we consider  $F_x$  with  $x$  being 15 evenly spaced points in  $[0.05, 0.95]$ . To make the study more complete, a set of credibility levels were examined, i.e.,  $1 - \alpha = 0.1, 0.3, 0.5, 0.7, 0.9, 0.95$ . In each experiment,  $N = 1200$  independent samples were generated from the model (44). For ACR and FCR, we chose the number of divisions  $s = 1, 2, 3, 4, 5, 6, 8, 10, 12, 15, 20, 24, 30, 40, 60$ . Define  $\gamma = \log s / \log N$ . Note that  $s = 1$  (equivalently,  $\gamma = 0$ ) means “no division.”

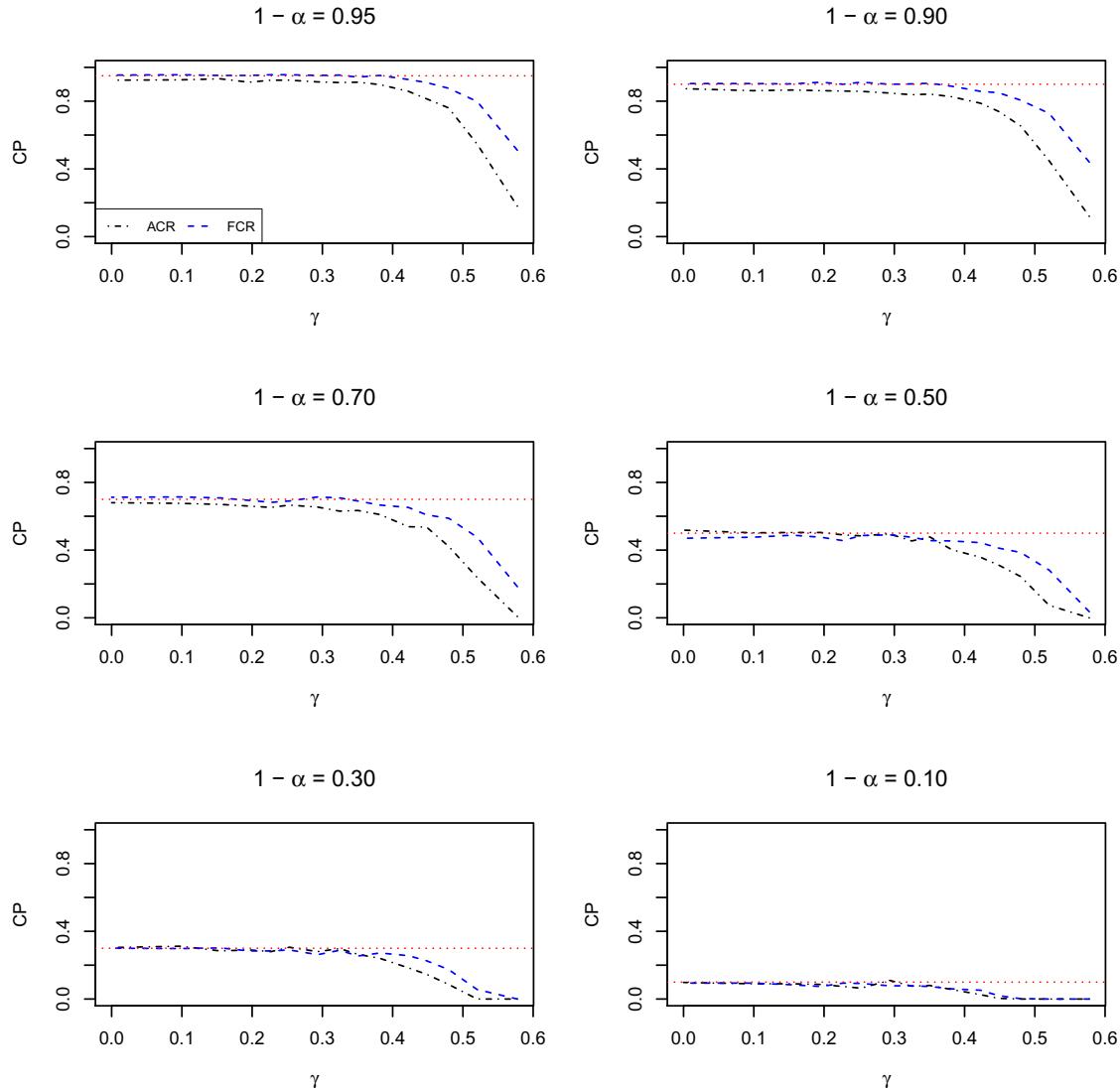
Figure 2 demonstrates the results for FCR and ACR based on strong topology, i.e., (32) and (41). The red dotted line indicates the  $(1 - \alpha)$  credibility level. It can be seen that the CP of both FCR and ACR is above the credibility levels when  $\gamma$  is small, while it suddenly drops to zero as  $\gamma$  is beyond some threshold, say 0.3. This observation supports our theory that  $s$  should not grow too fast, and that the credible regions based on strong



**Figure 2.** *CP of ACR and FCR based on strong topology. Dotted red lines indicate credibility levels.*

topology tends to be more “conservative.” Figure 3 demonstrates the results for FCR and ACR based on weak topology, i.e., (33) and (42). We observe that the CP of both ACR and FCR approaches the desired credibility levels when  $\gamma \leq 0.3$ , but quickly drops to zero when  $\gamma$  becomes large. This observation also supports our theory that the use of weak topology leads to a more satisfactory frequentist coverage.

For credible intervals of linear functionals, we chose the number of divisions  $s = 1, 6, 15, 60$ . Figures 4 and 5 display the results for evaluation functional and integral functional, respectively, based on posterior samples. It can be seen that when  $s = 60$ , the CP of the credible intervals for the evaluation functional drops to zero at most of the  $x$  points, indicating the failure in covering the true values of the function. However, when  $s = 1, 6, 15$ , the CP is



**Figure 3.** *CP of ACR and FCR based on weak topology. Dotted red lines indicate credibility levels.*

above the credibility levels except for the points where the true function  $f_0$  has peaks; see (a) of Figure 1. The observation that the CP stays above  $(1 - \alpha)$  coincides with our theory that the credible interval of the evaluation functional is conservative. On the other hand, it can be seen that when  $s = 60$ , the CP of the credible intervals for the integral functional becomes far below the credibility levels at most  $x$ . However, when  $s = 1, 6, 15$ , the CP is close to the credibility levels at all  $x$ . This finding coincides with our theory that the the credible interval of the integral functional achieves exactly  $(1 - \alpha)$  frequentist coverage. The above results also support our claim that  $s$  cannot grow too fast for guaranteeing frequency validity. Credible intervals based on asymptotic theory, i.e., (43), were summarized in Figures 11 and 12 of the supplement document Shang and Cheng. Interpretations of these results are similar to those based on finite posterior samples.

The supplement document Shang and Cheng also includes Figures 13 – 16 which demonstrate how the radii/lengths of the aggregated credible regions/intervals change along with  $\gamma$ , the size of the subsample. It can be observed that when  $\gamma \leq 0.3$ , indicating that the full sample is divided into at most twelve subsamples, the radii of the aggregated regions/intervals are almost identical to the radii of the regions/intervals directly constructed from the full sample, i.e.,  $\gamma = 0$ . This means that our aggregated procedures, based on a suitable amount of divisions, indeed mimic the oracle procedures. However, when  $\gamma$  increases to 0.6, the distinctions between the the aggregated and oracle procedures quickly become obvious.

We also repeated the above study for  $N = 1800$  and  $2400$ . The plots corresponding to these studies are given in supplement document; see Section S.8.6 of Shang and Cheng. The interpretations of these additional results are similar as above.

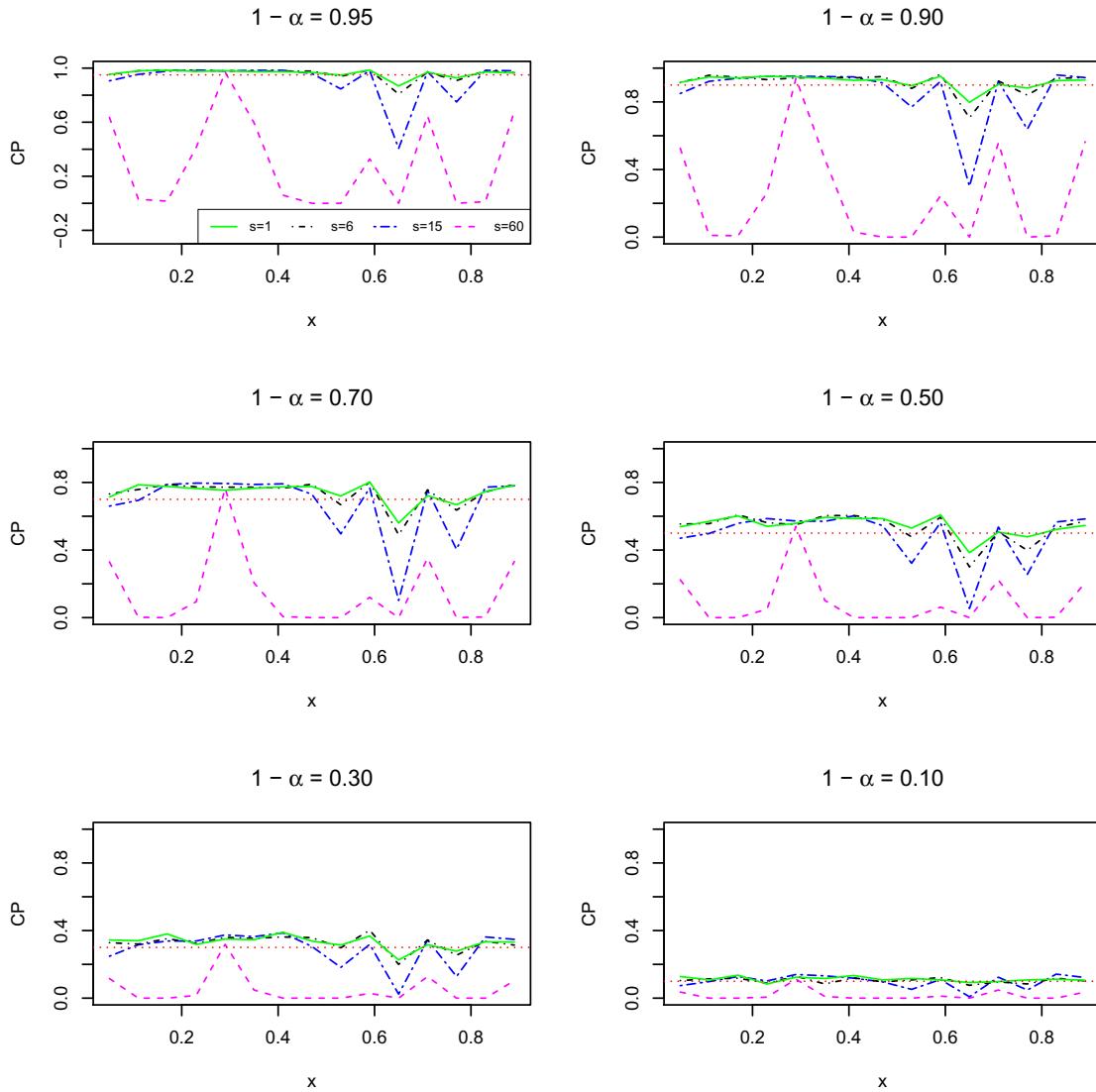
To the end of this section, computing efficiency is investigated. Figure 6 displays the results based on a single experiment for various choices of  $N$ . Specifically, we look at the value of the quantity  $\rho = 1 - (T/T_0)$  versus a collection of  $\gamma$ 's for FCR and ACR, where  $T_0$  ( $T$ ) is the computing time without using D&C (based on D&C). We observe that  $T$  is substantially smaller than  $T_0$ , and this computation efficiency (as reflected by the value of  $\rho$ ) becomes more obvious as  $\gamma$  grows for each fixed  $N$ . This can also be seen as  $N$  grows for each fixed  $\gamma$ . However, this reduction in computing time does not affect the performances of the aggregated credible regions when  $0 \leq \gamma \leq 0.3$ , as demonstrated in Figures 2, 3, 13–16.

## 6. Real Data Analysis

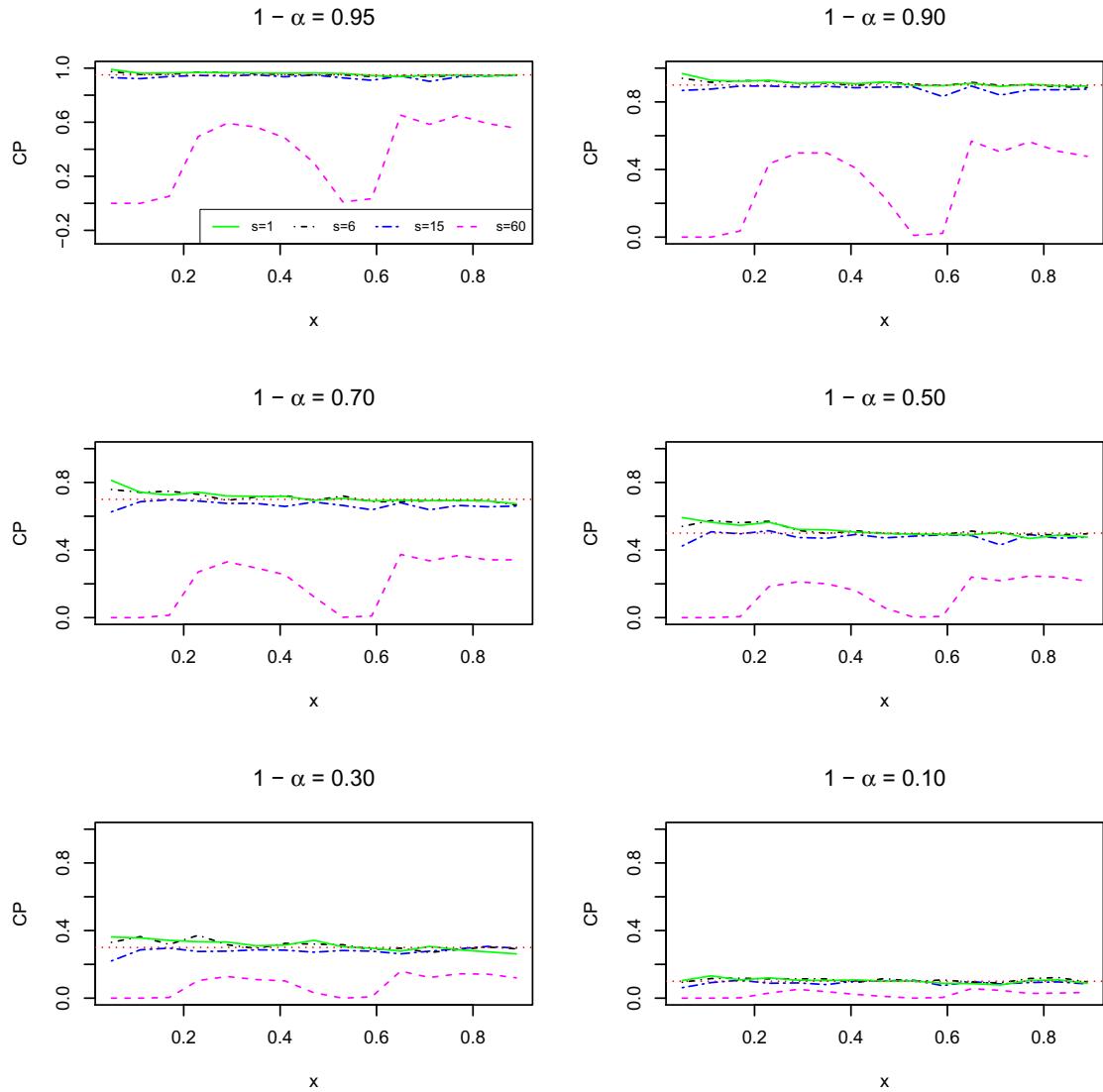
In this section, we apply our methods to Million Song Data (MSD) and Flight Delay Data (FDD).

### 6.1. Million Song Data

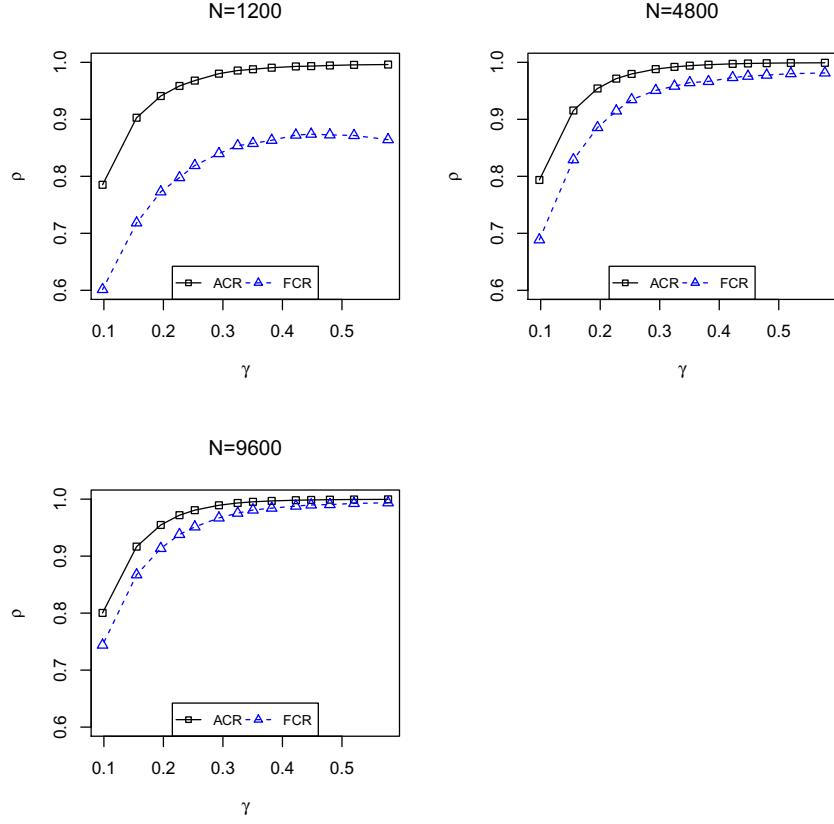
As a real application, we apply our aggregation procedure to analyze MSD. The MSD is a perfect example of large dataset, a freely-available collection of audio features and metadata for a million contemporary popular music tracks. Each observation is a song track released between the year 1922 and 2011. The response variable  $Y_i$  is the year when the song was released and the covariate  $X_i$  is the timbre average of the song. The main purpose is to explore a relationship, denoted as  $f$ , between song features and years in a nonparametric regression model, i.e., year =  $f(\text{timbre}) + \text{error}$ . The above model is useful to



**Figure 4.**  $CP$  of  $F_x(f) = f(x)$  against  $x$  based on posterior samples of  $f$ . Dotted red lines indicate credibility levels.



**Figure 5.**  $CP$  of  $F_x(f) = \int_0^x f(z)dz$  against  $x$  based on posterior samples of  $f$ . Dotted red lines indicate credibility levels.



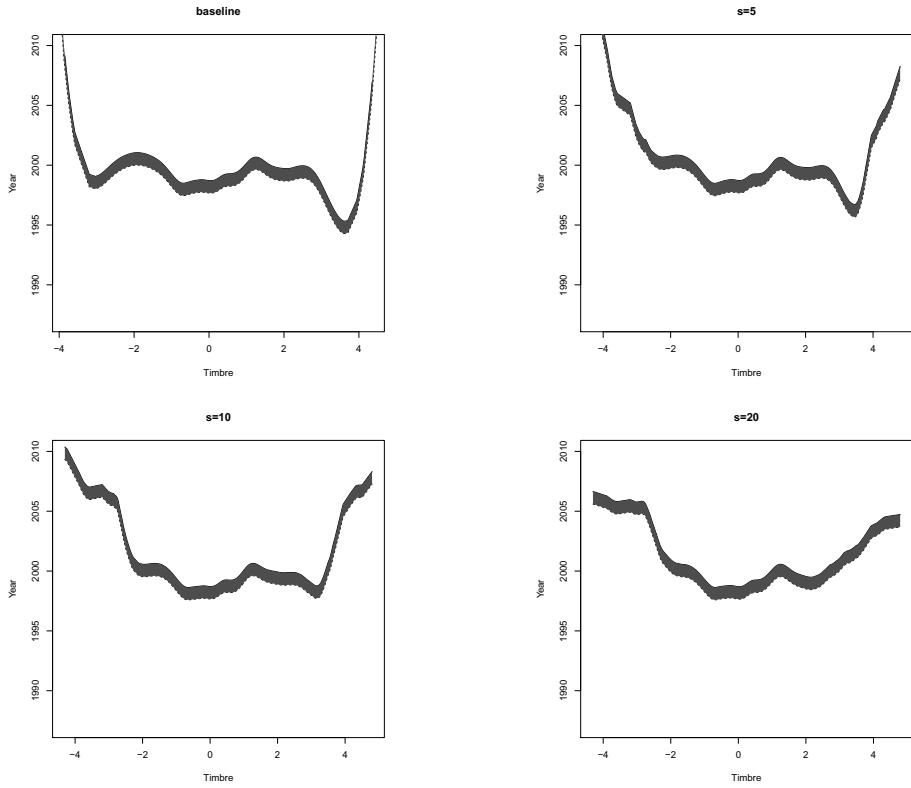
**Figure 6.**  $\rho$  versus  $\gamma$  based on FCR and ACR for single experiment.

predict production year based on song timbre. Due to enormous sample size, processing the entire data is infeasible. In frequentist setting, a distributed kernel ridge regression method was proposed by Zhang et al. (2015a,b) for estimation purposes (without quantifying uncertainty).

In the Bayesian setup, we applied our aggregation procedure to construct 95% credible sets for  $f$  based on a subset of  $N = 10,000$  songs released from the year 1996 to 2010. We randomly split the observations to  $s = 5, 10, 20$  subsets. We also compared our results with the baseline method in which all ten thousand observations were used. Credible sets are displayed as gray areas in Figure 7. We find that the shapes of all credible sets are overall the same when the timbre ranges from -4 to 4, e.g., all display a W-shape, although the results are a bit sensitive near the endpoints. Therefore, the overall pattern of the sets appears to be insensitive to the above selections of  $s$ .

## 6.2. Flight Delay Data

We applied our aggregation procedure to one more real data set, the FDD. The data consists of flight arrival and departure information for all commercial flights within the United States, from October 1987 to April 2008. The main purpose is to find the key factors that have an

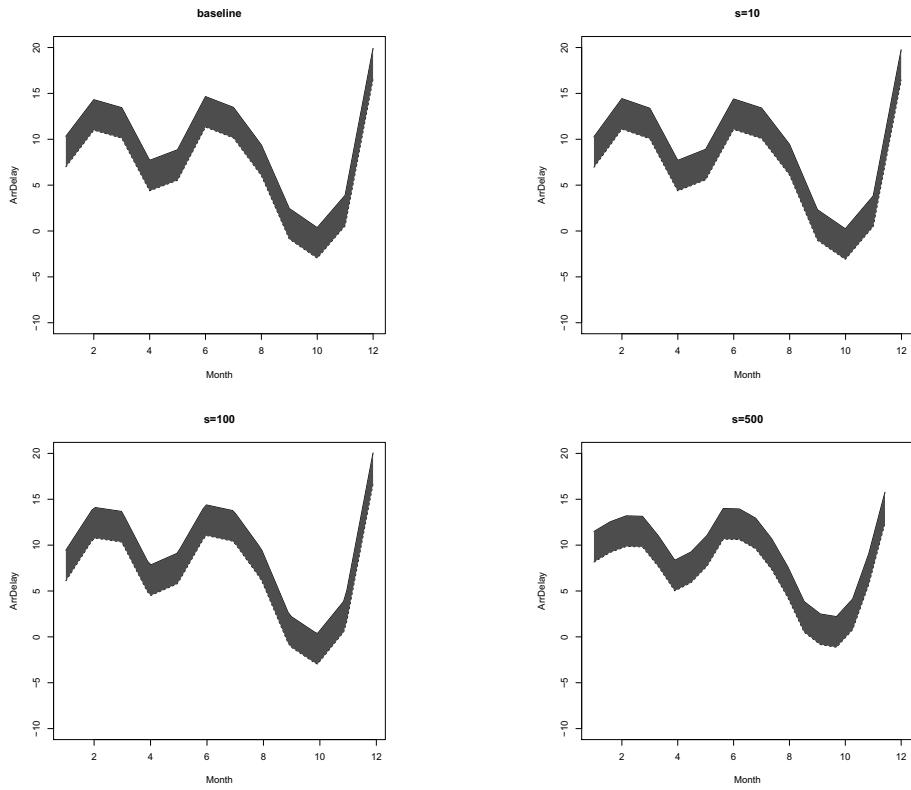


**Figure 7.** 95% Credible sets (grey areas) for  $f$  based on a subset of 10,000 samples in Million Song Data. The first plot refers to the baseline method where the whole samples were used. The rest three plots refer to the aggregation procedure which was applied to 5, 10, 20 random splits.

impact on the flight delay. We considered the relationship (denoted  $f$ ) between month and the length of the flight delay, i.e., length of flight delay =  $f(\text{month}) + \text{error}$ . Negative length of delay implies that the flight arrived earlier. We applied the same Bayesian aggregation procedure as described in MSD to a randomly selected subset of  $N = 10,000$  flight information in the year 2007. We randomly split the observations to  $s = 10, 100, 500$  subsamples, based on which the aggregated credible sets for  $f$  were constructed. We also compared the results with the baseline where all the ten thousand samples were used. Credible sets are displayed as gray areas in Figure 8. Again, the shapes of the four credible sets appear to be almost the same for all  $s$ .

### 6.3. Computation Efficiency

We compare the overall execute computation time of both MSD and FDD on different numbers of splits, e.g. computational time per machine  $\times$  number of machines in Figure 9-10. It can be seen that the computing time dramatically decreases as the number of splits increases, which reflects the scalability of our proposed algorithm.



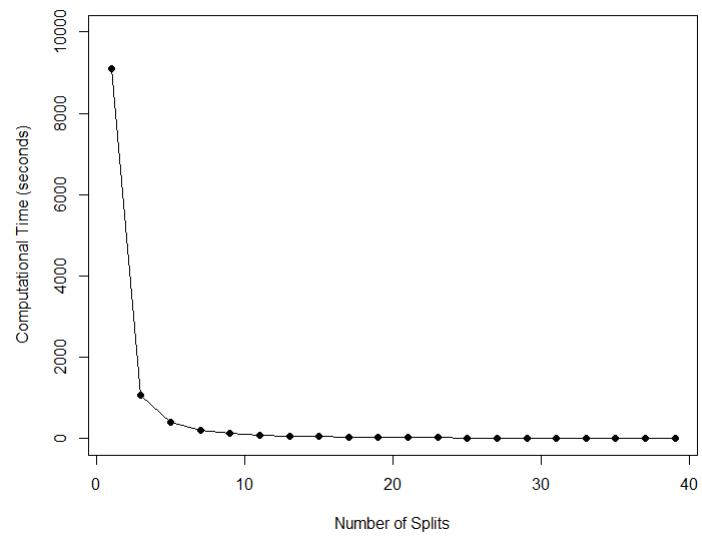
**Figure 8.** 95% Credible sets (grey areas) for  $f$  based on a subset of 10,000 samples in Flight Delay Data. The first plot refers to the baseline method where the whole samples were used. The rest three plots refer to the aggregation procedure which was applied to 10, 100, 500 random splits.

## 7. Conclusions

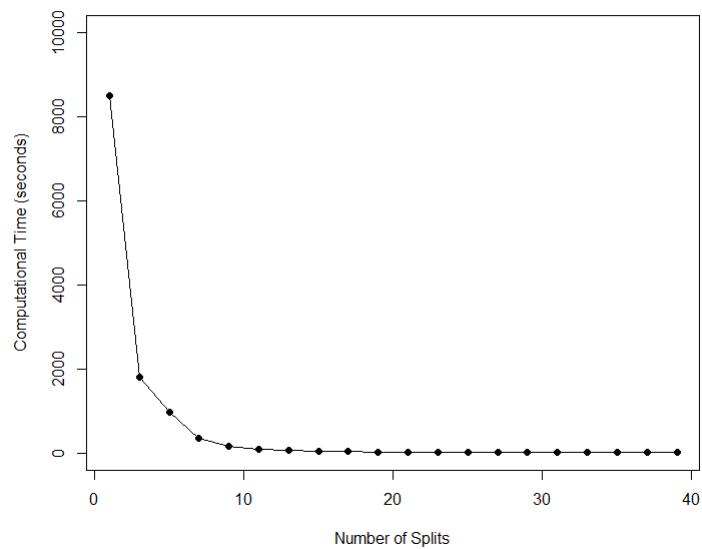
This paper proposes algorithms for aggregating individual posterior results such as modes, balls, intervals, into their global counterparts. The algorithms are easy-to-implement which are particularly useful in big data scenarios. We also experimented the proposed algorithms through simulated and real data sets. A notable contribution of this article is to provide rigorously justified theoretical guarantees. The major tool for proving our theoretical results is a uniform Gaussian approximation theorem which shows that the individual posterior distributions converge uniformly to Gaussian processes provided that the number of subsets is not too large.

## Acknowledgments

Shang's research is sponsored by NSF grants DMS 1821157 and DMS 1764280. Guang Cheng would like to acknowledge support by NSF DMS-1712907, DMS-1811812, DMS-1821183, and Office of Naval Research (ONR N00014-18-2759). In addition, Guang Cheng is a member of Institute for Advanced Study, Princeton and visiting Fellow of SAMSI for the Deep Learning Program in the Fall of 2019; he would like to thank both Institutes for their hospitality.



**Figure 9.** Computational time of aggregation procedures for MSD.



**Figure 10.** Computational time of aggregation procedures for FDD.

## 8. APPENDIX

This appendix section contains the proofs of the main results. Section 8.1 contains proof of Theorem 1 and relevant preliminary results. Section 8.2 includes the proof of Theorem 2. Sections 8.3 and 4.4 includes the proofs of Theorems 3 and 4, i.e., coverage properties of the credible sets based on strong and weak topology respectively.

All proofs crucially depend on an eigensystem designed for simultaneous diagonalization of the two bilinear functionals  $U, V$  induced from likelihood and prior, respectively. In fact,  $(\varphi_\nu, \rho_\nu)$  is a solution of the following ordinary differential system (whose existence and uniqueness is guaranteed by Birkhoff (1908)):

$$\begin{aligned} (-1)^m \varphi_\nu^{(2m)}(\cdot) &= \rho_\nu \pi(\cdot) \varphi_\nu(\cdot), \\ \varphi_\nu^{(j)}(0) &= \varphi_\nu^{(j)}(1) = 0, \quad j = m, m+1, \dots, 2m-1, \end{aligned} \quad (1)$$

Properties of this eigen-system are summarized in Proposition 1, whose proof can be found in (Shang et al., 2013, Proposition 2.2).

**Proposition 1** *It holds that  $\sup_{\nu \in \mathbb{N}} \|\varphi_\nu\|_\infty < \infty$ , and that the sequence  $\rho_\nu$  is nondecreasing with  $\rho_1 = \dots = \rho_m = 0$ , and  $\rho_\nu > 0$  for  $\mu > m$ . Moreover,  $\rho_\nu \asymp \nu^{2m}$  and*

$$V(\varphi_\mu, \varphi_\nu) = \delta_{\mu\nu}, \quad J(\varphi_\mu, \varphi_\nu) = \rho_\mu \delta_{\mu\nu}, \quad \mu, \nu \in \mathbb{N}, \quad (2)$$

where  $\delta_{\mu\nu}$  is the Kronecker's delta. In particular, any  $f \in S^m(\mathbb{I})$  admits a Fourier expansion  $f = \sum_\nu V(f, \varphi_\nu) \varphi_\nu$  with convergence held in the  $\|\cdot\|$ -norm.

### 8.1. Proofs in Section 4.1

The proof of Theorem 1 requires the following technical result which derives a local contraction rate  $\tilde{r}_n$  uniformly over  $s$ :  $\tilde{r}_n = (nh/\log 2s)^{-1/2} + h^{m+\frac{\beta-1}{2}}$ . The proof can be found in (Shang and Cheng).

**Proposition 1** *If  $f_0$  satisfies Condition **(S)** and the following Rate Condition **(R)** holds:*

$$nh^{2m+1} \geq 1, \quad a_n = O(\tilde{r}_n), \quad b_n \leq 1, \quad r_n^2 b_n \leq \tilde{r}_n^2.$$

Let  $a \geq 0$  be a fixed constant. Then for any  $\varepsilon \in (0, 1)$ , there exist positive constants  $M', N'$  s.t. for any  $n \geq N'$ ,

$$P_{f_0} \left( \max_{1 \leq j \leq s} \{E\{\|f - f_0\|^a I(\|f - f_0\| \geq M' \tilde{r}_n) | \mathbf{D}_j\} \geq M' s^2 \exp(-n \tilde{r}_n^2 / \log(2s))\} \right) \leq \varepsilon \quad (3)$$

We remark that Proposition 1 significantly generalizes the classical results in Ghosal et al. (2000); van der Vaart et al. (2008a).

**Proof** [Proof of Theorem 1] Let  $M_1, M_2$  be large positive constants. For any fixed constant  $a \geq 0$ , consider three events:

$$\begin{aligned} \mathcal{E}'_n &= \left\{ \max_{1 \leq j \leq s} \|\widehat{f}_{j,n} - f_0\| \leq M_1 \tilde{r}_n \right\} \\ \mathcal{E}''_n &= \left\{ \max_{1 \leq j \leq s} E\{\|f - f_0\|^a I(\|f - f_0\| \geq M_2 \tilde{r}_n) | \mathbf{D}_j\} \leq M_2 s^2 \exp(-n \tilde{r}_n^2 / \log(2s)) \right\} \\ \mathcal{E}'''_n &= \left\{ \max_{1 \leq j \leq s} E_{0j}\{\|f - f_0\|^a I(\|f - f_0\| \geq M_2 \tilde{r}_n)\} \leq M_2 \exp(-n \tilde{r}_n^2) \right\} \end{aligned}$$

where  $E_{0j}$  means expectation taken under  $P_{0j}$ . It follows from Shang and Cheng and Proposition 1 that we can choose  $M_1 > M_2$  (both large enough) s.t.  $P_{f_0}(\mathcal{E}'_n \cap \mathcal{E}''_n) \geq 1 - \varepsilon_1/2$  where  $\varepsilon_1 > 0$  is an arbitrary constant. Meanwhile, by (Shang and Cheng) we have, on  $\mathcal{E}'_n$ , for any  $1 \leq j \leq s$ ,

$$\begin{aligned}
 & E_{0j}\{\|f - f_0\|^a I(\|f - f_0\| \geq M_2 \tilde{r}_n)\} \\
 &= \frac{\int_{\|f-f_0\| \geq M_2 \tilde{r}_n} \|f - f_0\|^a \exp\left(-\frac{n}{2}\|f - \hat{f}_{j,n}\|^2\right) d\Pi(f)}{\int_{S^m(\mathbb{I})} \exp\left(-\frac{n}{2}\|f - \hat{f}_{j,n}\|^2\right) d\Pi(f)} \\
 &\leq \frac{\int_{\|f-f_0\| \geq M_2 \tilde{r}_n} \|f - f_0\|^a \exp\left(-\frac{n}{2}\|f - \hat{f}_{j,n}\|^2\right) d\Pi(f)}{\int_{\|f-f_0\| \leq \tilde{r}_n} \exp\left(-\frac{n}{2}\|f - \hat{f}_{j,n}\|^2\right) d\Pi(f)} \\
 &\leq \exp\left(-\left((M_2 - M_1)^2/2 - (M_1 + 1)^2/2 - c_3/4\right)n\tilde{r}_n^2\right) C(a, \Pi), \tag{4}
 \end{aligned}$$

where  $c_3 > 0$  is a universal constant and  $C(a, \Pi) = \int_{S^m(\mathbb{I})} \|f - f_0\|^a d\Pi(f)$ . We can choose  $M_2 > C(a, \Pi)$  so that the quantity (4) is less than  $M_2 \exp(-n\tilde{r}_n^2)$ . So  $\mathcal{E}'_n$  implies  $\mathcal{E}'''_n$ , so that  $P_{f_0}(\mathcal{E}'''_n) \geq P_{f_0}(\mathcal{E}'_n \cap \mathcal{E}''_n) \geq 1 - \varepsilon_1/2$ . Define  $\mathcal{E}_n = \mathcal{E}'_n \cap \mathcal{E}''_n \cap \mathcal{E}'''_n$ , then it can be seen that  $P_{f_0}(\mathcal{E}_n) \geq 1 - \varepsilon_1$ .

Let  $T_j$  be defined as

$$T_{j2}(f) = -\frac{1}{2n} \sum_{i \in I_j} [\Delta f](X_i)^2 - E_X\{(\Delta f)(X)^2\}. \tag{5}$$

Following Lemma 9, for any  $1 \leq j \leq s$ ,

$$\ell_{jn}(f) - \ell_{jn}(\hat{f}_{j,n}) + \frac{1}{2}\|f - \hat{f}_{j,n}\|^2 = T_j(f). \tag{6}$$

It follows from the proof of Proposition 1 that on  $\mathcal{E}_n$ , for any  $f \in S^m(\mathbb{I})$  satisfying  $\|f - f_0\| \leq M_2 \tilde{r}_n$  and  $1 \leq j \leq s$ ,

$$|T_j(f)| \leq D \times \tilde{r}_n^2 b_n, \tag{7}$$

where  $D = D(M_1, M_2)$  is a positive constant depending only on  $M_1, M_2$ . Recall that our assumption says that  $\varepsilon_2 \equiv nD\tilde{r}_n^2 b_n = o(1)$ .

For  $1 \leq j \leq s$ , define

$$\begin{aligned}
 J_{nj1} &= \int_{S^m(\mathbb{I})} \exp\left(n(\ell_{jn}(f) - \ell_{jn}(\hat{f}_{j,n}))\right) d\Pi(f), \\
 J_{nj2} &= \int_{S^m(\mathbb{I})} \exp\left(-\frac{n}{2}\|f - \hat{f}_{j,n}\|^2\right) d\Pi(f), \\
 \bar{J}_{nj1} &= \int_{\|f-f_0\| \leq M_2 \tilde{r}_n} \exp\left(n(\ell_{jn}(f) - \ell_{jn}(\hat{f}_{j,n}))\right) d\Pi(f), \\
 \bar{J}_{nj2} &= \int_{\|f-f_0\| \leq M_2 \tilde{r}_n} \exp\left(-\frac{n}{2}\|f - \hat{f}_{j,n}\|^2\right) d\Pi(f).
 \end{aligned}$$

For simplicity, let  $\varepsilon_3 = M_2 s^2 \exp(-n\tilde{r}_n^2 / \log(2s))$ . On  $\mathcal{E}_n$  (with  $a = 0$ ) and for any  $1 \leq j \leq s$ ,

$$0 \leq \frac{J_{nj1} - \bar{J}_{nj1}}{J_{nj1}} \leq M_2 s^2 \exp(-n\tilde{r}_n^2 / \log(2s)) = \varepsilon_3, \quad 0 \leq \frac{J_{nj2} - \bar{J}_{nj2}}{J_{nj2}} \leq \exp(-n\tilde{r}_n^2) \leq \varepsilon_3.$$

By some algebra, it can be shown that the above inequalities lead to

$$(1 - \varepsilon_3) \cdot \frac{\bar{J}_{nj2}}{\bar{J}_{nj1}} \leq \frac{J_{nj2}}{J_{nj1}} \leq \frac{1}{1 - \varepsilon_3} \cdot \frac{\bar{J}_{nj2}}{\bar{J}_{nj1}}. \quad (8)$$

Meanwhile, on  $\mathcal{E}_n$  and for any  $1 \leq j \leq s$ , using (7) and the elementary inequality  $|\exp(x) - 1| \leq 2|x|$  for  $|x| \leq \log 2$ , we get that

$$\begin{aligned} |\bar{J}_{nj2} - \bar{J}_{nj1}| &\leq \int_{\|f-f_0\| \leq M_2 \tilde{r}_n} \exp\left(-\frac{n}{2} \|f - \hat{f}_{j,n}\|^2\right) \times |\exp(nT_j(f)) - 1| d\Pi(f) \\ &\leq 2\varepsilon_2 \bar{J}_{nj2}, \end{aligned}$$

leading to that

$$\frac{1}{1 + 2\varepsilon_2} \leq \frac{\bar{J}_{nj2}}{\bar{J}_{nj1}} \leq \frac{1}{1 - 2\varepsilon_2}. \quad (9)$$

Combining (8) and (9), on  $\mathcal{E}_n$  and for any  $1 \leq j \leq s$ ,  $\frac{1-\varepsilon_3}{1+2\varepsilon_2} \leq \frac{J_{nj2}}{J_{nj1}} \leq \frac{1}{(1-2\varepsilon_2)(1-\varepsilon_3)}$ . When  $n$  is large,  $\varepsilon_3 \leq \varepsilon_2$  and both quantities are small, the above inequalities lead to

$$-4\varepsilon_2 \leq \frac{1-\varepsilon_3}{1+2\varepsilon_2} - 1 \leq \frac{J_{nj2}}{J_{nj1}} - 1 \leq \frac{1}{(1-2\varepsilon_2)(1-\varepsilon_3)} - 1 \leq 4\varepsilon_2 \quad (10)$$

For simplicity, denote  $R_{nj}(f) = nT_j(f)$ . For any  $S \in \mathcal{S}$ , let  $S' = S \cap \{f \in S^m(\mathbb{I}) : \|f - f_0\| \leq M_2 \tilde{r}_n\}$ . Then on  $\mathcal{E}_n$ , we get that  $\max_{1 \leq j \leq s} |P(S|\mathbf{D}_j) - P_{0j}(S)| \leq \max_{1 \leq j \leq s} |P(S'|\mathbf{D}_j) - P_{0j}(S')| + 2\varepsilon_3$ . Moreover, it follows from (10) that on  $\mathcal{E}_n$  and for any  $1 \leq j \leq s$ ,

$$\begin{aligned} &|P(S'|\mathbf{D}_j) - P_{0j}(S')| \\ &= \left| \int_{S'} \left( \frac{\exp(n(\ell_{jn}(f) - \ell_{jn}(\hat{f}_{j,n})))}{J_{nj1}} - \frac{\exp(-\frac{n}{2} \|f - \hat{f}_{j,n}\|^2)}{J_{nj2}} \right) d\Pi(f) \right| \\ &\leq \int_{S'} \exp\left(-\frac{n}{2} \|f - \hat{f}_{j,n}\|^2\right) \times \left| \frac{\exp(R_{nj}(f))}{J_{nj1}} - \frac{1}{J_{nj2}} \right| d\Pi(f) \\ &\leq \int_{S'} \exp\left(-\frac{n}{2} \|f - \hat{f}_{j,n}\|^2\right) \times \frac{|\exp(R_{nj}(f)) - 1|}{J_{nj2}} d\Pi(f) \\ &\quad + \int_{S'} \exp\left(-\frac{n}{2} \|f - \hat{f}_{j,n}\|^2\right) \times \exp(R_{nj}(f)) \times \left| \frac{1}{J_{nj1}} - \frac{1}{J_{nj2}} \right| d\Pi(f) \\ &\leq 2\varepsilon_2 \frac{\int_{S'} \exp\left(-\frac{n}{2} \|f - \hat{f}_{j,n}\|^2\right) d\Pi(f)}{J_{nj2}} \\ &\quad + \exp(\varepsilon_2) \times \left| \frac{1}{J_{nj1}} - \frac{1}{J_{nj2}} \right| \times \int_{S'} \exp\left(-\frac{n}{2} \|f - \hat{f}_{j,n}\|^2\right) d\Pi(f) \\ &\leq 2\varepsilon_2 + \exp(\varepsilon_2) \times \left| \frac{J_{nj2}}{J_{nj1}} - 1 \right| \leq 2\varepsilon_2 + 4\varepsilon_2 \exp(\varepsilon_2) \leq 14\varepsilon_2. \end{aligned}$$

Note that the right hand side is free of  $S$ . Then we get that on  $\mathcal{E}_n$ ,  $\sup_{S \in \mathcal{S}} \max_{1 \leq j \leq s} |P(S|\mathbf{D}_j) - P_{0j}(S)| \leq 14\varepsilon_2 + 2\varepsilon_3 \leq 16\varepsilon_2$ . This implies that for sufficiently large  $n$ ,

$$\begin{aligned} & P_{f_0} \left( \sup_{S \in \mathcal{S}} \max_{1 \leq j \leq s} |P(S|\mathbf{D}_j) - P_{0j}(S)| > 16\varepsilon_2 \right) \\ & \leq P_{f_0}(\mathcal{E}_n^c) + P_{f_0} \left( \mathcal{E}_n, \sup_{S \in \mathcal{S}} \max_{1 \leq j \leq s} |P(S|\mathbf{D}_j) - P_{0j}(S)| > 16\varepsilon_2 \right) = P_{f_0}(\mathcal{E}_n^c) \leq \varepsilon_1. \end{aligned}$$

The desirable result follows by the simple fact  $\varepsilon_2 \lesssim \sqrt{s}N^{-\frac{4m^2+2m\beta-10m+1}{4m(2m+\beta)}} (\log N)^{\frac{5}{2}}$  when  $h \asymp h^*$ .  $\blacksquare$

## 8.2. Proofs in Section 4.2

**Proof** [Proof of Theorem 2] We first show (28). Let  $A_n = \{f \in S^m(\mathbb{I}) : \|f - f_0\| \geq M\tilde{r}_n\}$  and  $B_j = \{f \in S^m(\mathbb{I}) : dP(f|\mathbf{D}_j) \geq dP_{0j}(f)\}$  for  $1 \leq j \leq s$ . By Proposition 1, Theorem 1 and (4) with  $a = 1$  therein, we can choose  $M > 0$  sufficiently large such that

$$\begin{aligned} & \max_{1 \leq j \leq s} \|E(f|\mathbf{D}_j) - E_{0j}(f)\| \\ &= \max_{1 \leq j \leq s} \left\| \int (f - f_0) dP(f|\mathbf{D}_j) - \int (f - f_0) dP_{0j}(f) \right\| \\ &\leq \max_{1 \leq j \leq s} \left\| \int_{A_n} (f - f_0) dP(f|\mathbf{D}_j) \right\| + \max_{1 \leq j \leq s} \left\| \int_{A_n} (f - f_0) dP_{0j}(f) \right\| \\ &\quad + \max_{1 \leq j \leq s} \left\| \int_{A_n^c} (f - f_0) (dP(f|\mathbf{D}_j) - dP_{0j}(f)) \right\| \\ &\leq \max_{1 \leq j \leq s} E\{\|f - f_0\| I(f \in A_n) | \mathbf{D}_j\} + \max_{1 \leq j \leq s} E_{0j}\{\|f - f_0\| I(f \in A_n)\} \\ &\quad + M\tilde{r}_n \max_{1 \leq j \leq s} \int_{A_n^c} |dP(f|\mathbf{D}_j) - dP_{0j}(f)| \\ &= O_{P_{f_0}} \left( s^2 \exp(-n\tilde{r}_n^2 / \log(2s)) + \exp(-n\tilde{r}_n^2) + \tilde{r}_n \sqrt{s} N^{-\frac{4m^2+2m\beta-10m+1}{4m(2m+\beta)}} (\log N)^{\frac{5}{2}} \right) \\ &= O_{P_{f_0}} \left( \tilde{r}_n \sqrt{s} N^{-\frac{4m^2+2m\beta-10m+1}{4m(2m+\beta)}} (\log N)^{\frac{5}{2}} \right) \equiv O_{P_{f_0}}(L_N), \end{aligned}$$

where the second last equality uses Theorem 1 and the fact that, uniformly for  $j$ ,

$$\begin{aligned} & \int_{A_n^c} |dP(f|\mathbf{D}_j) - dP_{0j}(f)| \\ &= |P(A_n^c \cap B_j | \mathbf{D}_j) - P_{0j}(A_n^c \cap B_j)| + |P(A_n^c \cap B_j^c | \mathbf{D}_j) - P_{0j}(A_n^c \cap B_j^c)|. \end{aligned}$$

Then (28) follows from the trivial fact that  $E_{0j}\{f\} = E(W^j | \mathbf{D}_j) = \tilde{f}_{j,n}$ .

Next we show (30). By direct examinations we can verify the following Rate Conditions (R):

$$n\tilde{r}_n^2 b_n = o(1), N\tilde{r}_N^2 b_N = o(1), Nh^{1/2}a_N^2 = o(1), Nh^{1/2}a_n^2 = o(1).$$

Define  $Rem_{j,n} = \tilde{f}_{j,n} - f_0 - S_{j,n}(f_0)$  for  $j = 1, 2, \dots, s$ . It follows by Lemma 6 of Shang and Cheng that  $\max_{1 \leq j \leq s} \|Rem_{j,n}\| = O_{P_{f_0}}(a_n)$ .

It is easy to see that  $a_{N,\nu}/a_{n,\nu} \leq s$  for all  $\nu \geq 1$ . Then it holds from (38) that

$$\begin{aligned} \|\check{f}_{N,\lambda} - \tilde{f}_{N,\lambda}\|^2 &= \sum_{\nu \geq 1} \left( \frac{a_{N,\nu}}{a_{n,\nu}} \right)^2 V \left( \frac{1}{s} \sum_{j=1}^s (\check{f}_{j,n} - \tilde{f}_{j,n}), \varphi_\nu \right)^2 (1 + \lambda \rho_\nu) \\ &\leq s^2 \left\| \frac{1}{s} \sum_{j=1}^s (\check{f}_{j,n} - \tilde{f}_{j,n}) \right\|^2 = O_{P_{f_0}}(s^2 L_N^2) = o_{P_{f_0}}(N^{-1} h^{-1/2}). \end{aligned} \quad (11)$$

The last equality owes to the condition  $s^4 \log(2s) = o\left(N^{\frac{4m^2+2m\beta-11m+1}{2m(2m+\beta)}} (\log N)^{-5}\right)$  and  $\beta > 3/2$ .

By direct examinations, we have

$$\begin{aligned} \tilde{f}_{N,\lambda} - f_0 &= \sum_{\nu=1}^{\infty} \left( a_{N,\nu} \left( \frac{1}{s} \sum_{j=1}^s V(\tilde{f}_{j,n}, \varphi_\nu) \right) - f_\nu^0 \right) \varphi_\nu \\ &= \sum_{\nu=1}^{\infty} \left( a_{N,\nu} \left( \frac{1}{s} \sum_{j=1}^s V(Re m_{j,n} + f_0 + S_{j,n}(f_0), \varphi_\nu) \right) - f_\nu^0 \right) \varphi_\nu \\ &= \sum_{\nu=1}^{\infty} a_{N,\nu} V\left(\frac{1}{s} \sum_{j=1}^s Re m_{j,n}, \varphi_\nu\right) \varphi_\nu + \sum_{\nu=1}^{\infty} (a_{N,\nu} - 1) f_\nu^0 \varphi_\nu \\ &\quad + \sum_{\nu=1}^{\infty} a_{N,\nu} V\left(\frac{1}{N} \sum_{i=1}^N \epsilon_i K_{X_i}, \varphi_\nu\right) \varphi_\nu - \sum_{\nu=1}^{\infty} a_{N,\nu} V(\mathcal{P}_\lambda f_0, \varphi_\nu) \varphi_\nu. \end{aligned} \quad (12)$$

Denote the four terms in the above equation by  $T_1, T_2, T_3, T_4$ .

Since  $a_{N,\nu} \leq 1$ , it is easy to see that

$$\begin{aligned} \|T_1\|_2^2 &= \sum_{\nu=1}^{\infty} a_{N,\nu}^2 |V\left(\frac{1}{s} \sum_{j=1}^s Re m_{j,n}, \varphi_\nu\right)|^2 \\ &\leq \sum_{\nu=1}^{\infty} |V\left(\frac{1}{s} \sum_{j=1}^s Re m_{j,n}, \varphi_\nu\right)|^2 = \left\| \frac{1}{s} \sum_{j=1}^s Re m_{j,n} \right\|_2^2 \leq (\max_{1 \leq j \leq s} \|Re m_{j,n}\|)^2 = O_{P_{f_0}}(a_n^2). \end{aligned} \quad (13)$$

Using  $h \asymp N^{-1/(2m+\beta)}$  and a direct algebra we get that

$$\|T_2\|_2^2 = \sum_{\nu=1}^{\infty} (a_{N,\nu} - 1)^2 |f_\nu^0|^2 \asymp \sum_{\nu=1}^{\infty} \left( \frac{\nu^{2m+\beta}}{\nu^{2m+\beta} + N(1 + \lambda \nu^{2m})} \right)^2 |f_\nu^0|^2 = o(N^{-\frac{2m+\beta-1}{2m+\beta}}) = o(N^{-1} h^{-1}).$$

Meanwhile, it follows by Proposition Shang and Cheng that

$$\begin{aligned} \|T_4\|_2^2 &= \sum_{\nu=1}^{\infty} a_{N,\nu}^2 |f_\nu^0|^2 \left( \frac{\lambda \rho_\nu}{1 + \lambda \rho_\nu} \right)^2 \leq \sum_{\nu=1}^{\infty} |f_\nu^0|^2 \left( \frac{\lambda \rho_\nu}{1 + \lambda \rho_\nu} \right)^2 \\ &\lesssim \sum_{\nu=1}^{\infty} |f_\nu^0|^2 (h \nu)^{2m+\beta-1} \frac{(h \nu)^{2m-\beta+1}}{(1 + (h \nu)^{2m})^2} = o(N^{-\frac{2m+\beta-1}{2m+\beta}}) = o(N^{-1} h^{-1}). \end{aligned}$$

Define  $R(x, x') = \sum_{\nu=1}^{\infty} a_{N,\nu} \frac{\varphi_\nu(x) \varphi_\nu(x')}{1 + \lambda \rho_\nu}$  for any  $x, x' \in \mathbb{I}$ . Also define  $R_x(\cdot) = R(x, \cdot)$ . It is easy to see that  $R_x \in S^m(\mathbb{I})$  for any  $x \in \mathbb{I}$ . Then it can be shown that  $T_3 = \frac{1}{N} \sum_{i=1}^N \epsilon_i R_{X_i}$ ,

leading to

$$\|T_3\|_2^2 = V(T_3, T_3) = \frac{1}{N^2} \sum_{i=1}^N \epsilon_i^2 V(R_{X_i}, R_{X_i}) + \frac{2}{N^2} \sum_{i < k} \epsilon_i \epsilon_k V(R_{X_i}, R_{X_k}).$$

Since  $E_{f_0}\{\epsilon^2 V(R_X, R_X)\} = O(h^{-1})$ , we have  $E_{f_0}\{\|T_3\|_2^2\} = O(N^{-1}h^{-1})$ . Therefore,  $\|\tilde{f}_{N,\lambda} - f_0\|_2^2 = O_{P_{f_0}}(N^{-1}h^{-1}) = O_{P_{f_0}}\left(N^{-\frac{2m+\beta-1}{2m+\beta}}\right)$ . This together with (11) leads to (30).  $\blacksquare$

### 8.3. Proofs in Section 4.3

Before proving Theorem 3, we give some preliminary notation and results. Define an ‘‘oracle’’ penalized likelihood  $\ell_{N,\lambda}(f) = -\frac{1}{2N} \sum_{i=1}^N (Y_i - f(X_i))^2 - \frac{\lambda}{2} J(f)$ . Applying Theorem 1 to  $s = 1$ , we have

$$\sup_{S \in \mathcal{S}} |P(S|\mathbf{D}) - P_0(S)| = o_{P_{f_0}}(1), \quad (14)$$

where  $P_0(S) = \frac{\int_S \exp\left(-\frac{N}{2}\|f - \tilde{f}_{N,\lambda}^{or}\|^2\right) d\Pi(f)}{\int_{S^m(\mathbb{I})} \exp\left(-\frac{N}{2}\|f - \tilde{f}_{N,\lambda}^{or}\|^2\right) d\Pi(f)}$  and  $\tilde{f}_{N,\lambda}^{or} = \arg \max_{f \in S^m(\mathbb{I})} \ell_{N,\lambda}(f)$  is the ‘‘oracle’’ smoothing spline estimator based on full data. Consider a generalized Fourier expansion of  $\tilde{f}_{N,\lambda}^{or}$ :  $\tilde{f}_{N,\lambda}^{or}(\cdot) = \sum_{\nu=1}^{\infty} V(\tilde{f}_{N,\lambda}^{or}, \varphi_{\nu}) \varphi_{\nu}(\cdot)$ . By Theorem 5.2 in Shang and Cheng (2017), we have  $P_0(S) = P(W^{or} \in S|\mathbf{D})$  for any  $S \in \mathcal{S}$ , where  $W^{or}(\cdot) = \sum_{\nu=1}^{\infty} (a_{N,\nu} V(\tilde{f}_{N,\lambda}^{or}, \varphi_{\nu}) + b_{N,\nu} \tau_{\nu} v_{\nu}) \varphi_{\nu}(\cdot)$ . Here,  $a_{n,\nu}$ ,  $b_{n,\nu}$  are analogous to ones in the definition of  $W^j(\cdot)$  in Section 4.1, and  $v_{\nu} \sim N(0, \tau_{\nu}^{-2})$  and  $\tau_{\nu}^2$  are given in (25). Define the mean functions of  $W^{or}$  as  $\tilde{f}_{N,\lambda}^{or}(\cdot) := \sum_{\nu=1}^{\infty} a_{N,\nu} V(\tilde{f}_{N,\lambda}^{or}, \varphi_{\nu}) \varphi_{\nu}(\cdot)$ . So we can re-express  $W^{or}$  as  $W^{or} = \tilde{f}_{N,\lambda}^{or} + W_N$ , where  $W_N(\cdot) := \sum_{\nu=1}^{\infty} b_{N,\nu} \tau_{\nu} v_{\nu} \varphi_{\nu}(\cdot)$  is a zero-mean GP.

The following result describes the distribution of  $W_n$  and  $W_N$ .

**Lemma 2** As  $N \rightarrow \infty$ ,  $\frac{n\|W_n\|_2^2 - \zeta_{1,n}}{\sqrt{2\zeta_{2,n}}} \xrightarrow{d} N(0, 1)$ , and  $\frac{N\|W_N\|_2^2 - \zeta_{1,N}}{\sqrt{2\zeta_{2,N}}} \xrightarrow{d} N(0, 1)$ .

**Proof** [Proof of Theorem 3] We can show that Rate Conditions **(R)** hold by direct calculations.

It is sufficient to investigate the  $P_{f_0}$ -probability of the event  $\{\|f_0 - \check{f}_{N,\lambda}\|_2 \leq r_N(\alpha)\}$ . To achieve this goal, we first prove the following fact:

$$\max_{1 \leq j \leq s} |z_{j,n}(\alpha) - z_{\alpha}| = o_{P_{f_0}}(1), \quad (15)$$

where  $z_{\alpha} = \Phi^{-1}(1 - \alpha)$  and  $\Phi$  is the c.d.f. of  $N(0, 1)$ , and  $z_{j,n}(\alpha) = (nr_{j,n}(\alpha)^2 - \zeta_{1,n})/\sqrt{2\zeta_{2,n}}$ . The proof of the theorem follows by (15) and a careful analysis of  $f_0 - \check{f}_{N,\lambda}$ .

We first show (15). It follows by Theorem 1 that for any  $j = 1, 2, \dots, s$ ,

$$\begin{aligned} |P(R_{j,n}(\alpha)|\mathbf{D}_j) - P_{0j}(R_{j,n}(\alpha))| &\leq \max_{1 \leq k \leq s} |P(R_{j,n}(\alpha)|\mathbf{D}_k) - P_{0k}(R_{j,n}(\alpha))| \\ &\leq \sup_{S \in \mathcal{S}} \max_{1 \leq k \leq s} |P(S|\mathbf{D}_k) - P_{0k}(S)| = o_{P_{f_0}}(1). \end{aligned}$$

Together with  $P(R_{j,n}(\alpha)|\mathbf{D}_j) = 1 - \alpha$ , we have  $\max_{1 \leq j \leq s} |P_{0j}(R_{j,n}(\alpha)) - (1 - \alpha)| = o_{P_{f_0}}(1)$ . Let  $\Delta_j = \check{f}_{j,n} - \tilde{f}_{j,n}$  for  $1 \leq j \leq s$ . It is clear that

$$\begin{aligned} P_{0j}(R_{j,n}(\alpha)) &= P(W^j \in R_{j,n}(\alpha)|\mathbf{D}_j) = P(\|W_n + \Delta_j\|_2 \leq r_{j,n}(\alpha)|\mathbf{D}_j) \\ &= P(\|W_n\|_2^2 + 2\langle W_n, \Delta_j \rangle_2 + \|\Delta_j\|_2^2 \leq r_{j,n}(\alpha)^2|\mathbf{D}_j), \end{aligned} \quad (16)$$

and, for any  $\varepsilon \in (0, 1)$ ,

$$\begin{aligned} P(|\langle W_n, \Delta_j \rangle_2|^2 \geq \|\Delta_j\|_2^2/(n\varepsilon)|\mathbf{D}_j) &\leq n\varepsilon E\{|\langle W_n, \Delta_j \rangle_2|^2|\mathbf{D}_j\}/\|\Delta_j\|_2^2 \\ &= \frac{n\varepsilon}{\|\Delta_j\|_2^2} \sum_{\nu \geq 1} b_{n,\nu}^2 |V(\Delta_j, \varphi_\nu)|^2 \leq \frac{n\varepsilon}{\|\Delta_j\|_2^2} \times \frac{\|\Delta_j\|_2^2}{n} = \varepsilon, \end{aligned} \quad (17)$$

and by Theorem 2,  $\max_{1 \leq j \leq s} \|\Delta_j\|_2^2 = O_{P_{f_0}}(L_N^2)$ , where  $L_N = \tilde{r}_n \sqrt{s} N^{-\frac{4m^2+2m\beta-10m+1}{4m(2m+\beta)}} (\log N)^{\frac{5}{2}}$ . By (29),  $\zeta_{k,n} \asymp n^{1/(2m+\beta)}$  (Lemma 2), and direct examinations it holds that

$$\max_{1 \leq j \leq s} \frac{n\|\Delta_j\|_2^2}{\sqrt{\zeta_{2,n}}} = o_{P_{f_0}}(1). \quad (18)$$

Combining (16) and (17) we get that

$$\begin{aligned} P_{0j}(R_{j,n}(\alpha)) &\geq \Phi_n \left( z_{j,n}(\alpha) - \frac{n\|\Delta_j\|_2^2}{\sqrt{\zeta_{2,n}}} - \frac{2n\|\Delta_j\|_2}{\sqrt{n\varepsilon\zeta_{2,n}}} \right) - \varepsilon, \\ P_{0j}(R_{j,n}(\alpha)) &\leq \Phi_n \left( z_{j,n}(\alpha) - \frac{n\|\Delta_j\|_2^2}{\sqrt{\zeta_{2,n}}} + \frac{2n\|\Delta_j\|_2}{\sqrt{n\varepsilon\zeta_{2,n}}} \right) + \varepsilon, \end{aligned}$$

where  $\Phi_n$  is the c.d.f. of  $U_n$ . It follows by Lemma 2 and Polya's theorem (Chow and Teicher (2012)) that  $\Phi_n$  uniformly converges to  $\Phi(\cdot)$ , the c.d.f. of standard normal variable. Therefore, when  $n$  becomes large enough,

$$\begin{aligned} \left| \Phi_n \left( z_{j,n}(\alpha) - \frac{n\|\Delta_j\|_2^2}{\sqrt{\zeta_{2,n}}} - \frac{2n\|\Delta_j\|_2}{\sqrt{n\varepsilon\zeta_{2,n}}} \right) - \Phi \left( z_{j,n}(\alpha) - \frac{n\|\Delta_j\|_2^2}{\sqrt{\zeta_{2,n}}} - \frac{2n\|\Delta_j\|_2}{\sqrt{n\varepsilon\zeta_{2,n}}} \right) \right| &\leq \varepsilon, \\ \left| \Phi_n \left( z_{j,n}(\alpha) - \frac{n\|\Delta_j\|_2^2}{\sqrt{\zeta_{2,n}}} + \frac{2n\|\Delta_j\|_2}{\sqrt{n\varepsilon\zeta_{2,n}}} \right) - \Phi \left( z_{j,n}(\alpha) - \frac{n\|\Delta_j\|_2^2}{\sqrt{\zeta_{2,n}}} + \frac{2n\|\Delta_j\|_2}{\sqrt{n\varepsilon\zeta_{2,n}}} \right) \right| &\leq \varepsilon, \end{aligned}$$

where implies that

$$\begin{aligned} \Phi \left( z_{j,n}(\alpha) - \frac{n\|\Delta_j\|_2^2}{\sqrt{\zeta_{2,n}}} - \frac{2n\|\Delta_j\|_2}{\sqrt{n\varepsilon\zeta_{2,n}}} \right) &\leq P_{0j}(R_{j,n}(\alpha)) + 2\varepsilon = \Phi(z_\alpha) + 2\varepsilon + o_{P_{f_0}}(1), \\ \Phi \left( z_{j,n}(\alpha) - \frac{n\|\Delta_j\|_2^2}{\sqrt{\zeta_{2,n}}} + \frac{2n\|\Delta_j\|_2}{\sqrt{n\varepsilon\zeta_{2,n}}} \right) &\geq P_{0j}(R_{j,n}(\alpha)) - 2\varepsilon = \Phi(z_\alpha) - 2\varepsilon + o_{P_{f_0}}(1). \end{aligned}$$

Since (18) implies that  $\frac{n\|\Delta_j\|_2^2}{\sqrt{\zeta_{2,n}}}$  and  $\frac{2\sqrt{n}\|\Delta_j\|_2}{\sqrt{\zeta_{2,n}}}$  are both  $o_{P_{f_0}}(1)$  uniformly for  $j$ , so (15) holds.

Next we prove the theorem. Consider expansion (12). Only focus on  $T_3$ . Define  $W(N) = 2 \sum_{1 \leq i < k \leq N} \epsilon_i \epsilon_k V(R_{X_i}, R_{X_k})$ . Let  $W_{ik} = 2\epsilon_i \epsilon_k V(R_{X_i}, R_{X_k})$ , then  $W(N) = \sum_{1 \leq i < k \leq N} W_{ik}$ . Note that  $W(N)$  is clean in the sense of de Jong (1987). Let  $\sigma^2(N) = E_{f_0}\{W(N)^2\}$  and  $G_I, G_{II}, G_{IV}$  be defined as  $G_I = \sum_{i < j} E_{f_0}\{W_{ij}^4\}$ ,  $G_{II} = \sum_{i < j < k} (E_{f_0}\{W_{ij}^2 W_{ik}^2\} + E_{f_0}\{W_{ji}^2 W_{jk}^2\} + E_{f_0}\{W_{ki}^2 W_{kj}^2\})$ , and

$$G_{IV} = \sum_{i < j < k < l} (E_{f_0}\{W_{ij} W_{ik} W_{lj} W_{lk}\} + E_{f_0}\{W_{ij} W_{il} W_{kj} W_{kl}\} + E_{f_0}\{W_{ik} W_{il} W_{jk} W_{jl}\}).$$

Since  $\varphi_\nu$  are uniformly bounded, we get that  $\|R_x\|_2^2 = \sum_{\nu=1}^{\infty} \frac{|\varphi_\nu(x)|^2}{(1+N^{-1}\tau_\nu^2+\lambda\rho_\nu)^2} \lesssim h^{-1}$ , where “ $\lesssim$ ” is free of  $x$ . This implies that  $G_I = O(N^2 h^{-4})$  and  $G_{II} = O(N^3 h^{-4})$ .

It can also be shown that for pairwise distinct  $i, k, t, l$ ,

$$\begin{aligned} E_{f_0}\{W_{ik} W_{il} W_{tk} W_{tl}\} &= 2^4 E_{f_0}\{\epsilon_i^2 \epsilon_k^2 \epsilon_t^2 \epsilon_l^2 V(R_{X_i}, R_{X_k}) V(R_{X_i}, R_{X_l}) V(R_{X_t}, R_{X_k}) V(R_{X_t}, R_{X_l})\} \\ &= 2^4 \sum_{\nu=1}^{\infty} \frac{a_{N,\nu}^8}{(1+\lambda\rho_\nu)^8} = O(h^{-1}), \end{aligned}$$

which implies that  $G_{IV} = O(N^4 h^{-1})$ . In the mean time, a straight algebra leads to that

$$\sigma^2(N) = 4 \binom{N}{2} \sum_{\nu=1}^{\infty} \frac{a_{N,\nu}^4}{(1+\lambda\rho_\nu)^4} = 4 \binom{N}{2} \sum_{\nu=1}^{\infty} \left( \frac{N}{\tau_\nu^2 + N(1+\lambda\rho_\nu)} \right)^4 = 2N(N-1)\zeta_{4,N} \asymp N^2 h^{-1}.$$

Since  $Nh^2 \asymp N^{1-2/(2m+\beta)} \rightarrow \infty$ , we get that  $G_I, G_{II}$  and  $G_{IV}$  are all of order  $o(\sigma^4(N))$ . Then it follows by de Jong (1987) that as  $N \rightarrow \infty$ ,  $\frac{W(N)}{N\sqrt{2\zeta_{4,N}}} \xrightarrow{d} N(0, 1)$ . Since  $\zeta_{4,N} \asymp h^{-1}$ , the above equation leads to that  $W(N)/N = O_{P_{f_0}}(h^{-1/2})$ .

It follows by direct examination that  $Var_{f_0}\{\sum_{i=1}^N \epsilon_i^2 V(R_{X_i}, R_{X_i})\} \leq N E_{f_0}\{\epsilon_i^4 \|R_{X_i}\|_2^4\} = O(Nh^{-2})$ , leading to that  $\sum_{i=1}^N \epsilon_i^2 V(R_{X_i}, R_{X_i}) = E_{f_0}\{\sum_{i=1}^N \epsilon_i^2 V(R_{X_i}, R_{X_i})\} + O_{P_{f_0}}(N^{1/2}h^{-1}) = N\zeta_{2,N} + O_{P_{f_0}}(N^{1/2}h^{-1})$ . Therefore, it follows by Rate Condition (R), i.e.,  $Nha_n^2 = o(1)$ , and the analysis on  $T_1, T_2, T_3, T_4$  in (12) that

$$Nh\|\tilde{f}_{N,\lambda} - f_0\|_2^2 = Nh\|T_3\|_2^2 + O_{P_{f_0}}(Nha_n^2) + o_{P_{f_0}}(1) = h\zeta_{2,N} + o_{P_{f_0}}(1). \quad (19)$$

In the end, note from (15) and  $\zeta_{k,n} \asymp n^{\alpha_1}$  for  $\alpha_1 = 1/(2m+\beta)$  (see proof of Lemma 2) that  $\frac{n}{s} \sum_{j=1}^s r_{j,n}(\alpha)^2 = \zeta_{1,n} + \sqrt{2\zeta_{2,n}}z_\alpha + o_{P_{f_0}}(\sqrt{\zeta_{2,n}})$ , which leads to that

$$Nr_N(\alpha)^2 = \zeta_{1,N} + \sqrt{2\zeta_{2,N}}z_\alpha + o_{P_{f_0}}(h^{-1/2}). \quad (20)$$

Therefore,  $Nhr_N(\alpha)^2 = h\zeta_{1,N}(1 + o_{P_{f_0}}(1))$ . Since  $\liminf_{N \rightarrow \infty} (h\zeta_{1,N} - h\zeta_{2,N}) > 0$ , we get by (11) that, with  $P_{f_0}$ -probability approaching one,  $\|\tilde{f}_{N,\lambda} - f_0\|_2 \leq r_N(\alpha)$ . Meanwhile, it follows by Shang and Cheng that  $\|\tilde{f}_{N,\lambda}^{or} - f_0 - S_{N,\lambda}(f_0)\|_2 = O_{P_{f_0}}(a_N)$  and  $\|\frac{1}{s} \sum_{j=1}^s \widehat{f}_{j,n} - f_0 - \frac{1}{s} \sum_{j=1}^s S_{j,n}(f_0)\|_2 = O_{P_{f_0}}(a_n)$ , where  $S_{N,\lambda}(f_0) = \frac{1}{N} \sum_{i=1}^N \epsilon_i K_{X_i} - \mathcal{P}_\lambda f_0$ . Note that  $S_{N,\lambda}(f_0) = \frac{1}{s} \sum_{j=1}^s S_{j,n}(f_0)$ , which leads to  $\|\tilde{f}_{N,\lambda}^{or} - \frac{1}{s} \sum_{j=1}^s \widehat{f}_{j,n}\|_2 = O_{P_{f_0}}(a_n + a_N)$ . Since  $a_{N,\nu} \leq 1$ , we get

that

$$\begin{aligned}
 N\|\tilde{f}_{N,\lambda}^{or} - \tilde{f}_{N,\lambda}\|^2 &= N \sum_{\nu=1}^{\infty} a_{N,\nu}^2 V \left( \tilde{f}_{N,\lambda}^{or} - \frac{1}{s} \sum_{j=1}^s \tilde{f}_{j,n}, \varphi_{\nu} \right)^2 (1 + \lambda \rho_{\nu}) \\
 &\leq N \sum_{\nu=1}^{\infty} V \left( \tilde{f}_{N,\lambda}^{or} - \frac{1}{s} \sum_{j=1}^s \tilde{f}_{j,n}, \varphi_{\nu} \right)^2 (1 + \lambda \rho_{\nu}) \\
 &= N\|\tilde{f}_{N,\lambda}^{or} - \frac{1}{s} \sum_{j=1}^s \tilde{f}_{j,n}\|^2 = O_{P_{f_0}}(Na_n^2 + Na_N^2) \\
 &= o_{P_{f_0}}(h^{-1/2}), \quad (\text{by condition } Nh^{1/2}a_n^2 + Nh^{1/2}a_N^2 = o(1))
 \end{aligned} \tag{21}$$

Using (11) we get that  $N\|\tilde{f}_{N,\lambda}^{or} - \check{f}_{N,\lambda}\|_2^2 = o_{P_{f_0}}(h^{-1/2})$ . Since  $E\{|\langle W_N, \tilde{f}_{N,\lambda}^{or} - \check{f}_{N,\lambda} \rangle_2|^2 | \mathbf{D}\} = \sum_{\nu \geq 1} b_{N,\nu}^2 V(\tilde{f}_{N,\lambda}^{or} - \check{f}_{N,\lambda}, \varphi_{\nu})^2 \leq \|\tilde{f}_{N,\lambda}^{or} - \check{f}_{N,\lambda}\|_2^2/N = o_{P_{f_0}}(N^{-2}h^{-1/2})$ , we have that  $N\|W^{or} - \check{f}_{N,\lambda}\|_2^2 = N\|W_N\|_2^2 + o_{P_{f_0}}(h^{-1/2})$ . It follows by  $P\left(\frac{N\|W_N\|_2^2 - \zeta_{1,N}}{\sqrt{2\zeta_{2,N}}} \leq z_{\alpha}\right) \rightarrow 1 - \alpha$ , (14) and (20) that  $P(R_N(\alpha) | \mathbf{D}) = 1 - \alpha + o_{P_{f_0}}(1)$ . This completes the proof.  $\blacksquare$

#### 8.4. Proofs in Section 4.4

Before proving Theorem 4, let us present a preliminary lemma.

**Lemma 3** *As  $N \rightarrow \infty$ ,  $N\|W_N\|_{\omega}^2 \xrightarrow{d} \sum_{\nu=1}^{\infty} d_{\nu} \eta_{\nu}^2$ , and  $n\|W_n\|_{\omega}^2 \xrightarrow{d} \sum_{\nu=1}^{\infty} d_{\nu} \eta_{\nu}^2$ , where  $\eta_{\nu}$  are independent standard normal random variables.*

**Proof** [Proof of Theorem 4] By direct examinations, one can show that Rate Conditions  $(\mathbf{R}')$ :  $n\tilde{r}_n^2 b_n = o(1)$ ,  $N\tilde{r}_N^2 b_N = o(1)$ ,  $Na_N^2 = o(1)$  and  $Na_n^2 = o(1)$  are all satisfied.

We first have the following fact:

$$\max_{1 \leq j \leq s} |\sqrt{nr}_{\omega,j,n}(\alpha) - \sqrt{c_{\alpha}}| = o_{P_{f_0}}(1), \tag{22}$$

where  $c_{\alpha} > 0$  satisfies  $P(\sum_{\nu=1}^{\infty} d_{\nu} \eta_{\nu}^2 \leq c_{\alpha}) = 1 - \alpha$  with  $\eta_{\nu}$  being independent standard normal random variables. It follows from (22) that

$$Nr_{\omega,N}(\alpha)^2 = c_{\alpha} + o_{P_{f_0}}(1). \tag{23}$$

By Theorem 2 and the condition  $s = o(N^{\frac{4m^2+2m\beta-12m+1}{8m(2m+\beta)}} (\log N)^{-\frac{3}{2}})$  we have the following  $\max_{1 \leq j \leq s} n\|\Delta_j\|_{\omega}^2 = \max_{1 \leq j \leq s} n\|\Delta_j\|_2^2 = O_{P_{f_0}}(nL_N^2) = o_{P_{f_0}}(1)$ . Also, for arbitrarily small  $\varepsilon \in (0, 1)$ ,  $P(|\langle W_n, \Delta_j \rangle_{\omega}|^2 \geq \|\Delta_j\|_{\omega}^2/(n\varepsilon) | \mathbf{D}_j) \leq \varepsilon$ . The proof of (22) is then similar to the proof of (15) and details are omitted.

Let  $T_1, T_2, T_3, T_4$  be defined in (12). It follows from the proof of Theorem 3 that  $\|T_1\|_{\omega}^2 \leq \|T_1\|_2^2 = O_{P_{f_0}}(a_n^2)$ , so  $N\|T_1\|_{\omega}^2 = O_{P_{f_0}}(Na_n^2) = o_{P_{f_0}}(1)$  due to the condition  $Na_n^2 = o(1)$ . It follows by condition  $h \asymp N^{-1/(2m+\beta)}$ , dominated convergence theorem and direct

examinations,

$$\begin{aligned}\|T_2\|_\omega^2 &= \sum_{\nu=1}^{\infty} d_\nu (a_{N,\nu} - 1)^2 |f_\nu^0|^2 \asymp N^{-2} \sum_{\nu=1}^{\infty} d_\nu \frac{\nu^{2m+\beta+1}}{(1 + (h\nu)^{2m} + (h\nu)^{2m+\beta})^2} \times \nu^{2m+\beta-1} |f_\nu^0|^2 \\ &\lesssim N^{-1} \sum_{\nu=1}^{\infty} \frac{(h\nu)^{2m+\beta+1}}{(1 + (h\nu)^{2m} + (h\nu)^{2m+\beta})^2} \times \nu^{2m+\beta-1} |f_\nu^0|^2 = o(N^{-1}),\end{aligned}$$

and

$$\begin{aligned}\|T_4\|_\omega^2 &= \sum_{\nu=1}^{\infty} d_\nu a_{N,\nu}^2 \left( \frac{\lambda \rho_\nu}{1 + \lambda \rho_\nu} \right)^2 |f_\nu^0|^2 \lesssim \sum_{\nu=1}^{\infty} d_\nu \frac{(h\nu)^{2m-\beta+1}}{(1 + (h\nu)^{2m} + (h\nu)^{2m+\beta})^2} \times |f_\nu^0|^2 (h\nu)^{2m+\beta-1} \\ &\lesssim h^{2m+\beta} \sum_{\nu=1}^{\infty} \frac{(h\nu)^{2m-\beta}}{(1 + (h\nu)^{2m} + (h\nu)^{2m+\beta})^2} \times |f_\nu^0|^2 \nu^{2m+\beta-1} = o(N^{-1}).\end{aligned}$$

By direct examination it can be shown that  $T_3 = \frac{1}{N} \sum_{i=1}^N \epsilon_i \sum_{\nu=1}^{\infty} \frac{\varphi_\nu(X_i) \varphi_\nu}{1 + \lambda \rho_\nu + N^{-1} \tau_\nu^2}$ . It follows by Shang and Cheng (2017) that, as  $N \rightarrow \infty$ ,  $N \|T_3\|_\omega^2 \xrightarrow{d} \sum_{\nu=1}^{\infty} d_\nu \eta_\nu^2$ . By the above analysis on  $T_1$  through  $T_4$ , and  $N \|\check{f}_{N,\lambda} - \tilde{f}_{N,\lambda}\|_\omega^2 = O_{P_{f_0}}(Ns^2 L_N^2) = o_{P_{f_0}}(1)$ , we get that  $N \|\check{f}_{N,\lambda} - f_0\|_\omega^2 \xrightarrow{d} \sum_{\nu=1}^{\infty} d_\nu \eta_\nu^2$ . It follows by (23) that  $\lim_{N \rightarrow \infty} P_{f_0}(f_0 \in R_N^\omega(\alpha)) = 1 - \alpha$ .

It follows by  $N \|\check{f}_{N,\lambda}^{or} - \check{f}_{N,\lambda}\|_2^2 = O_{P_{f_0}}(Na_N^2 + Na_n^2) = o_{P_{f_0}}(1)$  (see (21)),  $P(N \|W_N\|_2^2 \leq c_\alpha) \rightarrow 1 - \alpha$ , (23) and (14) that  $P(R_N^\omega(\alpha) | \mathbf{D}) = 1 - \alpha + o_{P_{f_0}}(1)$ . Proof is completed.  $\blacksquare$

## 8.5. Computational Details

In this subsection, we provide some computational details relating to Section 2.2. For convenience, we rewrite model (2.1) as following:

$$Y_{ji} = f(X_{ji}) + \epsilon_{ji}, \quad j = 1, \dots, s, \quad i = 1, \dots, n.$$

*Calculation of posterior means.* In order to calculate the posterior mean  $\check{f}_{j,n}$ , we have to generate samples of  $f$  from its posterior distribution  $P(f | \{Y_{ji}, X_{ji}\}_{i=1}^n)$ . In practice, directly sampling the function  $f$  from  $P(f | \{Y_{ji}, X_{ji}\}_{i=1}^n)$  is impossible. Instead, we generate some samples from  $(f(X_{j1}), \dots, f(X_{jn}))^\top$ . As  $n$  is large,  $(f(X_{j1}), \dots, f(X_{jn}))^\top$  can represent the whole curve of  $f$ . Firstly, let us derive the posterior distribution for  $(f(X_{j1}), \dots, f(X_{jn}))^\top$ . For the  $j$ -th subsample, the likelihood function is written by

$$Y_{j1}, \dots, Y_{jn} | X_{j1}, \dots, X_{jn} \sim N((f(X_{j1}), \dots, f(X_{jn}))^\top, I_n).$$

Since  $f$  follows a GP prior with mean zero and covariance function  $K_0$ , where  $K_0$  is given in (5), the prior of  $(f(X_{j1}), \dots, f(X_{jn}))^\top$  is multivariate Gaussian:

$$(f(X_{j1}), \dots, f(X_{jn}))^\top \sim N(0, K_j),$$

where  $K_j$  is the covariance matrix satisfying

$$K_j = \begin{bmatrix} K_0(X_{j1}, X_{j1}), & \cdots & K_0(X_{j1}, X_{jn}) \\ \vdots & \ddots & \vdots \\ K_0(X_{jn}, X_{j1}) & \cdots & K_0(X_{jn}, X_{jn}) \end{bmatrix}.$$

$K_0(x, x')$  involves an infinite summation which is practically infeasible. Instead, the infinite sum is approximated by a finite one, i.e.,

$$K_0(x, x') \approx 2 \sum_{k=1}^M \frac{\cos(2\pi k(x - x'))}{(2\pi k)^{2m+\beta} + n\lambda(2\pi k)^{2m}}.$$

In our numerical study, we found that  $M = 100$  can already provide a good approximation. Due to the conjugacy, the posterior distribution of  $(f(X_{j1}), \dots, f(X_{jn}))^\top$  also follows a multivariate Gaussian distribution

$$(f(X_{j1}), \dots, f(X_{jn}))^\top \mid \{Y_{ji}, X_{ji}\}_{i=1}^n \sim N\left(K_j(K_j + \frac{1}{n}I_n)^{-1}(Y_{j1}, \dots, Y_{jn})^\top, K_j(K_j + \frac{1}{n}I_n)^{-1}\frac{1}{n}\right).$$

Next we generate  $M$  independent samples, denoted  $(f^{(l)}(X_{j1}), \dots, f^{(l)}(X_{jn}))^\top, l = 1, \dots, M$ , from above multivariate Gaussian distribution. Therefore, the posterior mean can be approximated by

$$\left(\check{f}_{jn}(X_{j1}), \dots, \check{f}_{jn}(X_{jn})\right)^\top = \left(\frac{1}{M} \sum_{l=1}^M f^{(l)}(X_{j1}), \dots, \frac{1}{M} \sum_{l=1}^M f^{(l)}(X_{jn})\right)^\top.$$

*Calculation of posterior radius.* Once we have  $M$  independent samples  $\{(f^{(l)}(X_{j1}), \dots, f^{(l)}(X_{jn}))\}_{l=1}^M$ , we are able to approximate  $\|f^{(l)} - \check{f}_{jn}\|_{L^2}$  by

$$L_l = \left(\frac{1}{n} \sum_{i=1}^n (f^{(l)}(X_{ji}) - \check{f}_{jn}(X_{ji}))^2\right)^{\frac{1}{2}}, \text{ for } l = 1, \dots, M.$$

Finally, the radius  $r_{j,n}(\alpha)$  is approximated by the upper  $\alpha$ -th percentile of  $\{L_1, \dots, L_M\}$ .

*Calculation of the integral.* We approximate (8) by

$$\check{f}_{j,n,k} \approx \frac{\sqrt{2}}{n} \sum_{i=1}^n \check{f}_{jn}(X_{ji}) \cos(2\pi k X_{ji}) dx, \quad \check{g}_{j,n,k} \approx \frac{\sqrt{2}}{n} \sum_{i=1}^n \check{f}_{jn}(X_{ji}) \sin(2\pi k X_{ji}) dx.$$

In (12),  $C_k$  and  $D_k$  also involve two integrals. Since they are independent of samples, any numerical method for integral calculation is applicable. We also approximate  $\check{f}_{N,\lambda}(x)$  in (10) by

$$\check{f}_{N,\lambda}(x) \approx \sum_{k=1}^M w_{s,N,\lambda,k} \left\{ \check{f}_{N,\lambda,k} \sqrt{2} \cos(2\pi k x) + \check{g}_{N,\lambda,k} \sqrt{2} \sin(2\pi k x) \right\}.$$

## References

George D Birkhoff. Boundary value and expansion problems of ordinary linear differential equations. *Transactions of the American Mathematical Society*, 9(4):373–395, 1908.

Willem van den Boom, Galen Reeves, and David B Dunson. Scalable approximations of marginal posteriors in variable selection. *arXiv preprint arXiv:1506.06629*, 2015.

Robert H Cameron and William T Martin. Transformations of weiner integrals under translations. *Annals of Mathematics*, pages 386–396, 1944.

Yanshuai Cao and David J Fleet. Generalized product of experts for automatic and principled fusion of gaussian process predictions. *arXiv preprint arXiv:1410.7827*, 2014.

Ismaël Castillo, Richard Nickl, et al. Nonparametric bernstein–von mises theorems in gaussian white noise. *The Annals of Statistics*, 41(4):1999–2028, 2013.

Ismaël Castillo, Richard Nickl, et al. On the bernstein–von mises phenomenon for nonparametric bayes procedures. *The Annals of Statistics*, 42(5):1941–1969, 2014.

Yuan Shih Chow and Henry Teicher. *Probability theory: independence, interchangeability, martingales*. Springer Science & Business Media, 2012.

Peter de Jong. A central limit theorem for generalized quadratic forms. *Probability Theory and Related Fields*, 75(2):261–277, 1987.

Subhashis Ghosal, Jayanta K Ghosh, Aad W Van Der Vaart, et al. Convergence rates of posterior distributions. *Annals of Statistics*, 28(2):500–531, 2000.

Jorgen Hoffmann-Jorgensen, Lawrence A Shepp, and Richard M Dudley. On the lower tail of gaussian seminorms. *The Annals of Probability*, pages 319–342, 1979.

Zaijing Huang and Andrew Gelman. Sampling for bayesian computation with large datasets. *Available at SSRN 1010107*, 2005.

Brian R Hunt, Tim Sauer, and James A Yorke. Prevalence: a translation-invariant almost every on infinite-dimensional spaces. *Bulletin of the American mathematical society*, 27(2):217–238, 1992.

Ariel Kleiner, Ameet Talwalkar, Purnamrita Sarkar, and Michael I Jordan. Bootstrapping big data. In *Advances in neural information processing systems, workshop: Big learning: Algorithms, systems, and tools for learning at scale*, 2011.

Michael R Kosorok. *Introduction to empirical processes and semiparametric inference*. Springer, 2008.

James Kuelbs, Wenbo V Li, and Werner Linde. The gaussian measure of shifted balls. *Probability Theory and Related Fields*, 98(2):143–162, 1994.

Cheng Li, Sanvesh Srivastava, and David B Dunson. Simple, scalable and accurate posterior interval estimation. *Biometrika*, 104(3):665–680, 2017.

Wenbo Li et al. A gaussian correlation inequality and its applications to small ball probabilities. *Electronic Communications in Probability*, 4:111–118, 1999.

Ryan McDonald, Keith Hall, and Gideon Mann. Distributed training strategies for the structured perceptron. In *Human Language Technologies: The 2010 Annual Conference of the North American Chapter of the Association for Computational Linguistics*, pages 456–464. Association for Computational Linguistics, 2010.

Stanislav Minsker, Sanvesh Srivastava, Lizhen Lin, and David B Dunson. Robust and scalable bayes via a median of subset posterior measures. *The Journal of Machine Learning Research*, 18(1):4488–4527, 2017.

Carl N Morris et al. Natural exponential families with quadratic variance functions: statistical theory. *The Annals of Statistics*, 11(2):515–529, 1983.

Willie Neiswanger, Chong Wang, and Eric Xing. Asymptotically exact, embarrassingly parallel mcmc. *arXiv preprint arXiv:1311.4780*, 2013.

Iosif Pinelis et al. Optimum bounds for the distributions of martingales in banach spaces. *The Annals of Probability*, 22(4):1679–1706, 1994.

Vincent Rivoirard, Judith Rousseau, et al. Bernstein–von mises theorem for linear functionals of the density. *The Annals of Statistics*, 40(3):1489–1523, 2012.

Walter Rudin et al. *Principles of mathematical analysis*, volume 3. McGraw-hill New York, 1964.

Steven L Scott, Alexander W Blocker, Fernando V Bonassi, Hugh A Chipman, Edward I George, and Robert E McCulloch. Bayes and big data: The consensus monte carlo algorithm. *International Journal of Management Science and Engineering Management*, 11(2):78–88, 2016.

Hao Botao Shang, Zuofeng and Guang Cheng. Supplementary document to “nonparametric bayesian aggregation for massive data.”.

Zuofeng Shang and Guang Cheng. Gaussian approximation of general non-parametric posterior distributions. *Information and Inference: A Journal of the IMA*, 7(3):509–529, 2017.

Zuofeng Shang, Guang Cheng, et al. Local and global asymptotic inference in smoothing spline models. *The Annals of Statistics*, 41(5):2608–2638, 2013.

Sanvesh Srivastava, Cheng Li, and David B Dunson. Scalable bayes via barycenter in wasserstein space. *The Journal of Machine Learning Research*, 19(1):312–346, 2018.

Botond Szabo and Harry van Zanten. Adaptive distributed methods under communication constraints. *arXiv preprint arXiv:1804.00864*, 2018.

Botond Szabó and Harry van Zanten. An asymptotic analysis of distributed nonparametric methods. *Journal of Machine Learning Research*, 20(87):1–30, 2019.

Sara Van De Geer and SA Van De Geer. *Empirical Processes in M-estimation*. Cambridge UP, 2006.

Aad W van der Vaart, J Harry van Zanten, et al. Reproducing kernel hilbert spaces of gaussian priors. In *Pushing the limits of contemporary statistics: contributions in honor of Jayanta K. Ghosh*, pages 200–222. Institute of Mathematical Statistics, 2008a.

Aad W van der Vaart, J Harry van Zanten, et al. Rates of contraction of posterior distributions based on gaussian process priors. *The Annals of Statistics*, 36(3):1435–1463, 2008b.

Grace Wahba. *Spline models for observational data*, volume 59. Siam, 1990.

Xiangyu Wang and David B Dunson. Parallelizing mcmc via weierstrass sampler. *arXiv preprint arXiv:1312.4605*, 2013.

Xiangyu Wang, Peichao Peng, and David B Dunson. Median selection subset aggregation for parallel inference. In *Advances in neural information processing systems*, pages 2195–2203, 2014.

Xiangyu Wang, Fangjian Guo, Katherine A Heller, and David B Dunson. Parallelizing mcmc with random partition trees. In *Advances in neural information processing systems*, pages 451–459, 2015.

Yuchen Zhang, John Duchi, and Martin Wainwright. Divide and conquer kernel ridge regression: A distributed algorithm with minimax optimal rates. *The Journal of Machine Learning Research*, 16(1):3299–3340, 2015a.

Yuchen Zhang, Martin Wainwright, and Michael Jordan. Distributed estimation of generalized matrix rank: Efficient algorithms and lower bounds. In *International Conference on Machine Learning*, pages 457–465, 2015b.

Tianqi Zhao, Guang Cheng, and Han Liu. A partially linear framework for massive heterogeneous data. *Annals of statistics*, 44(4):1400, 2016.

*Supplementary document to Nonparametric Bayesian Aggregation for Massive Data*

This supplementary document is structured as follows.

- Section S.8.1 contains the proofs of Lemmas 2 and 3.
- Section S.8.2 contains the proofs of the main results in Section 4.5 and 4.6 that were not included in the main paper.
- Section S.8.3 proves Proposition 1, i.e., a uniform contraction rate result. Preliminary results relevant to the proof of Proposition 1 are provided in Section S.8.4.
- Section S.8.5 includes a result that characterizes the posterior tail moments of  $\|f - f_0\|^a$  for any  $a \geq 0$ .
- Section S.8.6 includes additional simulation results supplementary to Section 5.

### S.8.1. Proofs of Lemmas 2 and 3

**Proof** [Proof of Lemma 2] We only show the first limit distribution since the proof of the second one is similar.

Let  $\eta_\nu = \tau_\nu v_\nu$ . Then  $\eta_\nu$  is a sequence of *iid* standard normals. Note that

$$\|W_n\|_2^2 = \sum_{\nu=1}^{\infty} \frac{\eta_\nu^2}{\tau_\nu^2 + n(1 + \lambda\rho_\nu)}.$$

Let  $U_n = (n\|W_n\|_2^2 - \zeta_{1,n})/\sqrt{2\zeta_{2,n}}$ , then we have

$$U_n = \frac{1}{\sqrt{2\zeta_{2,n}}} \sum_{\nu=1}^{\infty} \frac{n(\eta_\nu^2 - 1)}{\tau_\nu^2 + n(1 + \lambda\rho_\nu)}.$$

By straightforward calculations and Taylor's expansion of  $\log(1 - x)$ , it can be shown that the logarithm of the moment generating function of  $U_n$  equals

$$\log E\{\exp(tU_n)\} = t^2/2 + O\left(t^3\zeta_{2,n}^{-3/2}\zeta_{3,n}\right). \quad (\text{S.1})$$

Without loss of generality, assume that  $N = n^a$  for some  $a \geq 1$ . Then  $\alpha_1 := \min\{1/(2m + \beta), a/(2m + \beta)\} = 1/(2m + \beta)$ . It follows by (Shang and Cheng, 2017, Lemma S.1) that  $\zeta_{2,n} \asymp n^{\alpha_1}$  and  $\zeta_{3,n} \asymp n^{\alpha_1}$ , so the remainder term in (S.1) is  $O(n^{-\alpha_1/2}) = o(1)$ . So  $\lim_{n \rightarrow \infty} E\{\exp(tU_n)\} = \exp(t^2/2)$ . Proof is completed.  $\blacksquare$

**Proof** [Proof of Lemma 3] The proof follows by moment generating function approach and direct calculations.  $\blacksquare$

### S.8.2. Proofs in Sections 4.5 and 4.6

This section contains the proofs in Sections 4.5 and 4.6.

## PROOFS IN SECTION 4.5

**Proof** [Proof of Theorem 5] Recall in the proof of Theorem 4 we showed that Rate Conditions  $(\mathbf{R}')$  are satisfied.

It is easy to see that

$$F(W_n) \stackrel{d}{=} N(0, \theta_{1,n}^2), \quad \text{and} \quad F(W_N) \stackrel{d}{=} N(0, \theta_{1,N}^2). \quad (\text{S.2})$$

For  $1 \leq j \leq s$ , define  $R_{j,n}^F(\alpha) = \{f \in S^m(\mathbb{I}) : |F(f) - F(\check{f}_{j,n})(\alpha)| \leq r_{F,j,n}(\alpha)\}$ . It follows by Theorem 1 that  $\max_{1 \leq j \leq s} |1 - \alpha - P_{0j}(R_{j,n}^F(\alpha))| = o_{P_{f_0}}(1)$ . Since  $s = o(N^{\frac{4m^2+2m\beta-12m+1}{8m(2m+\beta)}} (\log N)^{-\frac{3}{2}})$ , it can be examined that  $N L_N^2 = o(1)$ . Together with the condition  $h^{-r} \lesssim N \theta_{1,N}^2$  and the fact  $\theta_{k,n} \leq \theta_{k,n}$ , one can verify that  $h^{-r} \lesssim N \theta_{1,N}^2 \leq N \theta_{1,n}^2 = o(L_N^{-2} \theta_{1,n}^2)$ . So we have by (35) and Theorem 2 that

$$\max_{1 \leq j \leq s} |F(\Delta_j)| = O_{P_{f_0}}(h^{-r/2} L_N) = o_{P_{f_0}}(\theta_{1,n}).$$

Combined with (S.2) we get that

$$\begin{aligned} P_{0j}(R_{j,n}^F(\alpha)) &= P(|F(W_n) - F(\Delta_j)| \leq r_{F,j,n}(\alpha) | \mathbf{D}_j) \\ &= \Phi\left(\frac{r_{F,j,n}(\alpha) + F(\Delta_j)}{\theta_{1,n}}\right) + \Phi\left(\frac{r_{F,j,n}(\alpha) - F(\Delta_j)}{\theta_{1,n}}\right) - 1 \\ &= 2\Phi\left(\frac{r_{F,j,n}(\alpha)}{\theta_{1,n}}\right) - 1 + o_{P_{f_0}}(1), \quad \text{uniformly for } 1 \leq j \leq s. \end{aligned}$$

The above argument leads to  $\Phi(r_{F,j,n}(\alpha)/\theta_{1,n}) = 1 - \alpha/2 + o_{P_{f_0}}(1)$  uniformly for  $1 \leq j \leq s$ , which further leads to the following

$$\max_{1 \leq j \leq s} |r_{F,j,n}(\alpha)/\theta_{1,n} - z_{\alpha/2}| = o_{P_{f_0}}(1). \quad (\text{S.3})$$

Consider the decomposition (12) with  $T_1, T_2, T_3, T_4$  being defined therein. It follows by (13) and rate condition  $N a_n^2 = o(1)$  that  $N \|T_1\|^2 = O_{P_{f_0}}(N a_n^2) = o_{P_{f_0}}(1)$ . Meanwhile, it follows by Condition  $(\mathbf{S}')$ ,  $N^{-1} \asymp h^{2m+\beta}$  and  $\lambda = h^{2m}$  and direct examinations that

$$\begin{aligned} N \|T_2\|^2 &= N \sum_{\nu=1}^{\infty} (a_{N,\nu} - 1)^2 |f_{\nu}^0|^2 (1 + \lambda \rho_{\nu}) \\ &\asymp N \sum_{\nu=1}^{\infty} \left( \frac{\nu^{2m+\beta}}{\nu^{2m+\beta} + N(1 + \lambda \nu^{2m})} \right)^2 |f_{\nu}^0|^2 (1 + \lambda \nu^{2m}) \\ &\asymp \sum_{\nu=1}^{\infty} \frac{(h\nu)^{2m+\beta} + (h\nu)^{4m+\beta}}{(1 + (h\nu)^{2m} + (h\nu)^{2m+\beta})^2} \times |f_{\nu}^0|^2 \nu^{2m+\beta} = o(1), \end{aligned}$$

and

$$\begin{aligned} N \|T_4\|^2 &= N \sum_{\nu=1}^{\infty} a_{N,\nu}^2 \left( \frac{\lambda \rho_{\nu}}{1 + \lambda \rho_{\nu}} \right)^2 |f_{\nu}^0|^2 (1 + \lambda \rho_{\nu}) \\ &\asymp \sum_{\nu=1}^{\infty} \frac{(h\nu)^{2m-\beta}}{1 + (h\nu)^{2m}} \times |f_{\nu}^0|^2 \nu^{2m+\beta} = o(1). \end{aligned}$$

By (11) and  $Ns^2L_N^2 = o(1)$  we get  $\|\check{f}_{N,\lambda} - \tilde{f}_{N,\lambda}\| = o_{P_{f_0}}(N^{-1/2})$ . Therefore,  $\|\check{f}_{N,\lambda} - f_0 - T_3\| \leq \|\check{f}_{N,\lambda} - \tilde{f}_{N,\lambda}\| + \|T_1 + T_2 + T_4\| = o_{P_{f_0}}(N^{-1/2})$ . It follows from (35) that  $|F(\check{f}_{N,\lambda} - f_0) - F(T_3)| = o_{P_{f_0}}(h^{-r/2}N^{-1/2})$ .

Note that  $F(T_3) = \frac{1}{N} \sum_{i=1}^N \epsilon_i F(R_{X_i})$ , where the kernel  $R$  is defined in the proof of Theorem 3. We will derive asymptotic distribution for  $F(T_3)$ . Let  $s_N^2 = \text{Var}_{f_0}(\sum_{i=1}^N \epsilon_i F(R_{X_i}))$ . It is easy to show that

$$s_N^2 = N^3 \sum_{\nu=1}^{\infty} \frac{F(\varphi_{\nu})^2}{(\tau_{\nu}^2 + N(1 + \lambda\rho_{\nu}))^2} = N^3 \theta_{2,N}^2.$$

Clearly, by uniform boundedness of  $\varphi_{\nu}$  and  $F(\varphi_{\nu})$ , we get

$$|F(R_x)| = \left| \sum_{\nu=1}^{\infty} a_{N,\nu} \frac{\varphi_{\nu}(x) F(\varphi_{\nu})}{1 + \lambda\rho_{\nu}} \right| \lesssim h^{-1},$$

where the “ $\lesssim$ ” is free of  $x \in \mathbb{I}$ , and

$$E_{f_0}\{\epsilon^2 F(R_X)^2\} = N^2 \sum_{\nu=1}^{\infty} \frac{F(\varphi_{\nu})^2}{(\tau_{\nu}^2 + N(1 + \lambda\rho_{\nu}))^2} = N^2 \theta_{2,N}^2. \quad (\text{S.4})$$

Then for any  $\delta > 0$ , by condition  $E_{f_0}\{\epsilon^4|X\} \leq M_4$  a.s.,

$$\begin{aligned} & \frac{1}{s_N^2} \sum_{i=1}^N E_{f_0}\{\epsilon_i^2 F(R_{X_i})^2 I(|\epsilon_i F(R_{X_i})| \geq \delta s_N)\} \\ & \leq \frac{N}{s_N^2} (\delta s_N)^{-2} E_{f_0}\{\epsilon^4 F(R_X)^4\} \\ & \lesssim \frac{N}{s_N^2} (\delta s_N)^{-2} h^{-2} E_{f_0}\{\epsilon^2 F(R_X)^2\} \lesssim \delta^{-2} N^{-1} h^{-2+r} = o(1), \end{aligned}$$

where the last  $o(1)$ -term follows by  $h \asymp h^*$  and  $2 - r < 2m + \beta$ . By Lindeberg's central limit theorem, as  $N \rightarrow \infty$ ,

$$\frac{F(T_3)}{\sqrt{N}\theta_{2,N}} = \frac{1}{s_N} \sum_{i=1}^N \epsilon_i F(R_{X_i}) \xrightarrow{d} N(0, 1). \quad (\text{S.5})$$

By condition  $N^2\theta_{2,N}^2 \gtrsim h^{-r}$ , we have

$$\left| \frac{F(\check{f}_{N,\lambda} - f_0 - T_3)}{\sqrt{N}\theta_{2,N}} \right| = o_{P_{f_0}}\left(\frac{h^{-r/2}N^{-1/2}}{\sqrt{N}\theta_{2,N}}\right) = o_{P_{f_0}}(1).$$

It follows by (S.3) that

$$r_{F,N}(\alpha) = \theta_{1,N} \sqrt{\frac{1}{s} \sum_{j=1}^s r_{F,j,n}(\alpha)^2 / \theta_{1,n}^2} = \theta_{1,N} z_{\alpha/2}(1 + o_{P_{f_0}}(1)), \quad (\text{S.6})$$

leading to that

$$\frac{r_{F,N}(\alpha)}{\sqrt{N}\theta_{2,N}} = \frac{\theta_{1,N}}{\sqrt{N}\theta_{2,N}} \times z_{\alpha/2}(1 + o_{P_{f_0}}(1)).$$

It can be shown that

$$\frac{\theta_{1,N}^2}{N\theta_{2,N}^2} = \frac{\sum_{\nu=1}^{\infty} \frac{F(\varphi_{\nu})^2}{1+\lambda\rho_{\nu}+N^{-1}\tau_{\nu}^2}}{\sum_{\nu=1}^{\infty} \frac{F(\varphi_{\nu})^2}{(1+\lambda\rho_{\nu}+N^{-1}\tau_{\nu}^2)^2}} \geq 1,$$

together with (S.5) we get that

$$\begin{aligned} & P_{f_0}(|F(f_0) - F(\check{f}_{N,\lambda})| \leq r_{F,N}(\alpha)) \\ &= P_{f_0}\left(\left|\frac{F(\check{f}_{N,\lambda} - f_0 - T_3)}{\sqrt{N}\theta_{2,N}} + \frac{F(T_3)}{\sqrt{N}\theta_{2,N}}\right| \leq \frac{r_{F,N}(\alpha)}{\sqrt{N}\theta_{2,N}}\right) \\ &\geq P_{f_0}\left(\left|\frac{F(\check{f}_{N,\lambda} - f_0 - T_3)}{\sqrt{N}\theta_{2,N}} + \frac{F(T_3)}{\sqrt{N}\theta_{2,N}}\right| \leq z_{\alpha/2}(1 + o_{P_{f_0}}(1))\right) \\ &\rightarrow 1 - \alpha. \end{aligned} \tag{S.7}$$

Notice that when  $0 < \sum_{\nu=1}^{\infty} F(\varphi_{\nu})^2 < \infty$ ,  $\frac{\theta_{1,N}^2}{N\theta_{2,N}^2} \rightarrow 1$ , leading to that the probability in (S.7) approaches exactly  $1 - \alpha$ .

In the end, we show that  $P(R_N^F(\alpha)|\mathbf{D}) = 1 - \alpha + o_{P_{f_0}}(1)$ , where  $R_N^F(\alpha) = \{f \in S^m(\mathbb{I}) : |F(f) - F(\check{f}_{N,\lambda})| \leq r_{F,N}(\alpha)\}$ . By rate condition  $N(a_N^2 + a_n^2) = o(1)$ , proof of (21) leading to  $\|\tilde{f}_{N,\lambda}^{or} - \tilde{f}_{N,\lambda}\| = O_{P_{f_0}}(a_N + a_n)$ , and (35) we have

$$\frac{F(\tilde{f}_{N,\lambda}^{or} - \tilde{f}_{N,\lambda})}{\theta_{1,N}} = O_{P_{f_0}}\left(\frac{h^{-r/2}(a_N + a_n)}{\theta_{1,N}}\right) = o_{P_{f_0}}(1),$$

where the last  $o(1)$ -term follows by condition  $N\theta_{1,N}^2 \gtrsim h^{-r}$  and Rate Condition (R'). From (S.6) we get that

$$\begin{aligned} P_0(R_N^F(\alpha)) &= P(W^{or} \in R_N^F(\alpha)|\mathbf{D}) \\ &= P(|F(W^{or}) - F(\check{f}_{N,\lambda})| \leq r_{F,N}(\alpha)|\mathbf{D}) \\ &= P\left(\left|\frac{F(\tilde{f}_{N,\lambda}^{or} - \tilde{f}_{N,\lambda})}{\theta_{1,N}} + \frac{F(W_N)}{\theta_{1,N}}\right| \leq \frac{r_{F,N}(\alpha)}{\theta_{1,N}}\right| \mathbf{D}\right) \\ &= 1 - \alpha + o_{P_{f_0}}(1). \end{aligned} \tag{S.8}$$

So it follows from (14) that  $P(R_N^F(\alpha)|\mathbf{D}) = 1 - \alpha + o_{P_{f_0}}(1)$ . Proof is completed.  $\blacksquare$

#### PROOFS IN SECTION 4.6

**Proof** [Proof of Theorem 6] It follows from (20) that  $r_N(\alpha) - r_N^{\dagger}(\alpha) = o_{P_{f_0}}(N^{-1}h^{-1/2})$ , which together with (19) leads to that  $\lim_{n \rightarrow \infty} P_{f_0}(f_0 \in R_N^{\dagger}(\alpha)) = 1$ . It follows from Lemma 2, (14) and the proof of Theorem 3 that  $P(R_N^{\dagger}(\alpha)|\mathbf{D}) = 1 - \alpha + o_{P_{f_0}}(1)$ .

It follows from (23) that  $r_{\omega,N}(\alpha)^2 - r_{\omega,N}^{\dagger}(\alpha)^2 = o_{P_{f_0}}(N^{-1})$ . Then the desired results on  $R_N^{\dagger\omega}(\alpha)$  directly follow from the proof of Theorem 4.

It follows by (S.6) that  $r_{F,N}^\dagger(\alpha) = r_{F,N}(\alpha)(1 + o_{P_{f_0}}(1))$ . Then the desired results on  $CI_N^{\dagger F}(\alpha)$  follow from (S.7) and (S.8).  $\blacksquare$

### S.8.3. Proofs of Proposition 1 and relevant results

The goal of this section is to prove Proposition 1 and relevant results. Before proofs, we exactly describe the Fréchet derivatives of the likelihood function that will be technically useful. Suppose that  $(Y, X)$  follows model (14) based on  $f$ . Let  $g, g_k \in S^m(\mathbb{I})$  for  $k = 1, 2$ . For  $j = 1, 2, \dots, s$ , the Fréchet derivative of  $\ell_{jn}$  can be identified as

$$D\ell_{jn}(g)g_1 = \frac{1}{n} \sum_{i \in I_j} (Y_i - g(X_i)) \langle K_{X_i}, g_1 \rangle - \langle \mathcal{P}_\lambda g, g_1 \rangle := \langle S_{j,n}(g), g_1 \rangle.$$

Define  $S_\lambda(g) = E\{S_{j,n}(g)\}$ . We also use  $DS_\lambda$  and  $D^2S_\lambda$  to represent the second- and third-order Fréchet derivatives of  $S_\lambda$ . Note that  $S_{j,n}(\widehat{f}_{j,n}) = 0$ , and  $S_{j,n}(f)$  can be expressed as

$$S_{j,n}(f) = \frac{1}{n} \sum_{i \in I_j} (Y_i - f(X_i)) K_{X_i} - \mathcal{P}_\lambda f. \quad (\text{S.9})$$

The Fréchet derivative of  $S_{j,n}$  is denoted  $DS_{j,n}(g)g_1g_2$ . These derivatives can be explicitly written as

$$D^2\ell_{jn}(g)g_1g_2 := DS_{j,n}(g)g_1g_2 = -\frac{1}{n} \sum_{i \in I_j} g_1(X_i)g_2(X_i) - \langle \mathcal{P}_\lambda g_1, g_2 \rangle,$$

The proof of Proposition 1 requires a series of preliminary lemmas. Define  $H^m(b) = \{f \in S^m(\mathbb{I}) : J(f) \leq b^2\}$ . We first state a basic lemma about a concentration phenomenon of smoothing spline estimates in the distributed setup.

**Lemma 4** *If  $b, r, h, M$  are positives satisfying the following Rate Condition (H):*

1.  $h^{1/2}r \leq 1$ ,
2.  $c_K^2 M^{1/2}rh^{-1/2}B(h) \leq 1/2$ , where  $B(h) = A(h, 2)$  with  $A(h, \varepsilon)$  given in (S.19),

*then, for any  $1 \leq j \leq s$ , the following two results hold:*

1.  $\sup_{f \in H^m(b)} P_f(\|\widehat{f}_{j,n} - f\| \geq \delta_n) \leq 2 \exp(-Mnhr^2)$ , where  $\delta_n = bh^m + 2c_K(C_\epsilon + M)r$  with  $C_\epsilon = E\{(|\epsilon| + 1)^2 \exp(|\epsilon| + 1)\}$  an absolute constant;
2.  $\sup_{f \in H^m(b)} P_f(\|\widehat{f}_{j,n} - f - S_{j,n}(f)\| > a_n) \leq 2 \exp(-Mnhr^2)$ , where  $a_n = c_K^2 M^{1/2}h^{-1/2}rB(h)\delta_n$ . Here,  $S_{j,n}(f)$  is the Fréchet derivative of the likelihood function  $\ell_{jn}(f)$ ; see (S.9) for its exact expression.

**Lemma 5** *For any fixed constants  $M > 1$  and  $b > 0$ , let*

$$r = (nh/\log 2s)^{-1/2}, \delta_n = bh^m + 2c_K(C_\epsilon + M)r, \quad (\text{S.10})$$

$$a_n = c_K^2 M^{1/2} h^{-1/2} r B(h) \delta_n. \quad (\text{S.11})$$

Then as  $n \rightarrow \infty$ ,

$$P_{f_0} \left( \max_{1 \leq j \leq s} \|\widehat{f}_{j,n} - f_0\| \geq \delta_n \right) \leq 6sN^{-M} \rightarrow 0,$$

and

$$P_{f_0} \left( \max_{1 \leq j \leq s} \|\widehat{f}_{j,n} - f_0 - S_{j,n}(f_0)\| > a_n \right) \leq 8sN^{-M} \rightarrow 0.$$

**Proof** [Proof of Lemma 5] The result is a straightforward consequence of Lemma 4.  $\blacksquare$

**Lemma 6** *It holds that*

$$\max_{1 \leq j \leq s} \|\widehat{f}_{j,n} - f_0 - S_{j,n}(f_0)\| = O_{P_{f_0}}(a_n). \quad (\text{S.12})$$

**Proof** [Proof of Lemma 6] The proof follows by Lemma 5, and simple fact that  $B(h) \lesssim h^{-\frac{2m-1}{4m}}$ .  $\blacksquare$

**Lemma 7** *Under Condition (S), we get  $\max_{1 \leq j \leq s} \|\widehat{f}_{j,n} - f_0\| = O_{P_{f_0}}(\tilde{r}_n)$ .*

**Proof** [Proof of Lemma 7] Recall that

$$S_{j,n}(f_0) = -\frac{1}{n} \sum_{i \in I_j} (Y_i - f_0(X_i)) K_{X_i} - \mathcal{P}_\lambda f_0.$$

It was shown by Shang et al. (2013) that  $\mathcal{P}_\lambda \varphi_\nu = \frac{\lambda \varphi_\nu}{1 + \lambda \varphi_\nu} \varphi_\nu$ . Since  $f_0$  satisfies Condition (S),

$$\begin{aligned} \|\mathcal{P}_\lambda f_0\|^2 &= \left\langle \sum_{\nu=1}^{\infty} f_\nu^0 \frac{\lambda \rho_\nu}{1 + \lambda \rho_\nu} \varphi_\nu, \sum_{\nu=1}^{\infty} f_\nu^0 \frac{\lambda \rho_\nu}{1 + \lambda \rho_\nu} \varphi_\nu \right\rangle \\ &= \sum_{\nu=1}^{\infty} |f_\nu^0|^2 \frac{\lambda^2 \rho_\nu^2}{1 + \lambda \rho_\nu} \\ &= \lambda^{1+\frac{\beta-1}{2m}} \sum_{\nu=1}^{\infty} |f_\nu^0|^2 \rho_\nu^{1+\frac{\beta-1}{2m}} \frac{(\lambda \rho_\nu)^{1-\frac{\beta-1}{2m}}}{1 + \lambda \rho_\nu} = O(h^{2m+\beta-1}), \end{aligned}$$

where the last equation follows by  $\lambda = h^{2m}$ ,  $\sup_{x \geq 0} \frac{x^{1-\frac{\beta-1}{2m}}}{1+x} < \infty$ , and Condition (S). On the other side, it follows by the proof of (S.22) that

$$\begin{aligned} P_{f_0} \left( \max_{1 \leq j \leq s} \left\| \sum_{i \in I_j} (Y_i - f_0(X_i)) K_{X_i} \right\| \geq L(M) n (nh/\log 2s)^{-1/2} \right) \\ \leq 2s \exp(-Mnh(nh/\log 2s)^{-1}) = (2s)^{1-M} \rightarrow 0, \text{ as } M \rightarrow \infty, \end{aligned}$$

where  $L(M) := c_K(C_\epsilon + M)$ . This implies that

$$\max_{1 \leq j \leq s} \left\| \sum_{i \in I_j} (Y_i - f_0(X_i)) K_{X_i} \right\| = O_{P_{f_0}}(n(nh/\log 2s)^{-1/2}),$$

and hence,

$$\max_{1 \leq j \leq s} \|S_{j,n}(f_0)\| = O_{P_{f_0}}((nh/\log 2s)^{-1/2} + h^{m+\frac{\beta-1}{2}}) = O_{P_{f_0}}(\tilde{r}_n).$$

Together with (S.12) of Lemma 6 and the rate condition  $a_n \lesssim \tilde{r}_n$ , we get that  $\max_{1 \leq j \leq s} \|\widehat{f}_{j,n} - f_0\| = O_{P_{f_0}}(\tilde{r}_n)$ .  $\blacksquare$

Consider a function class

$$\mathcal{G} = \{g \in S^m(\mathbb{I}) : \|g\|_\infty \leq 1, J(g, g) \leq c_K^{-2}h^{-2m+1}\}. \quad (\text{S.13})$$

**Lemma 8** *For any fixed constant  $M > 1$ , as  $n \rightarrow \infty$ ,*

$$P_{f_0} \left( \max_{1 \leq j \leq s} \sup_{g \in \mathcal{G}} \|Z_{j,n}(g)\| \leq B(h)\sqrt{M \log N} \right) \rightarrow 1,$$

where  $Z_{j,n}(g) = \frac{1}{\sqrt{n}} \sum_{i \in I_j} [\psi_{j,n}(Z_i; g) K_{X_i} - E\{\psi_{j,n}(Z_i; g) K_{X_i}\}]$ ,  $\psi_{j,n}(Z_i; g) = c_K^{-1}h^{1/2}g(X_i)$ .

**Proof** [Proof of Lemma 8] It is easy to see that  $\psi_{j,n}(Z_i; g)$  satisfies the Lipschitz continuity condition (S.20). Then the result directly follows by Lemma 12 (see appendix).  $\blacksquare$

**Lemma 9** *For  $j = 1, \dots, s$ ,*

1.  $\ell_{jn}(f) - \ell_{jn}(\widehat{f}_{j,n}) = I_{j,n}(f)$ , where  $I_{j,n}(f) = \int_0^1 \int_0^1 s D S_{j,n}(\widehat{f}_{j,n} + ss'(f - \widehat{f}_{j,n}))(f - \widehat{f}_{j,n})(f - \widehat{f}_{j,n}) ds ds'$  for any  $f \in S^m(\mathbb{I})$ ;
2.  $I_{j,n}(f) = T_j(f) - \frac{1}{2}\|f - \widehat{f}_{j,n}\|^2$ , where recall that (see 5)

$$T_j(f) = -\frac{1}{2n} \sum_{i \in I_j} [f - \widehat{f}_{j,n}](X_i)^2 - E_X\{(f - \widehat{f}_{j,n})(X)^2\}. \quad (\text{S.14})$$

**Proof** [Proof of Lemma 9] Let  $\Delta f = f - \widehat{f}_{j,n}$ . Therefore,

$$\begin{aligned} I_{j,n}(f) &= -\frac{1}{n} \int_0^1 \int_0^1 s \sum_{i \in I_j} (\Delta f)(X_i)^2 ds ds' - \lambda J(\Delta f, \Delta f)/2 \\ &= -\frac{1}{2n} \sum_{i \in I_j} [\Delta f](X_i)^2 - E_X\{(\Delta f)(X)^2\} - \frac{1}{2}\|\Delta f\|^2 \\ &= T_j(f) - \frac{1}{2}\|\Delta f\|^2. \end{aligned}$$

By Taylor's expansion in terms of Fréchet derivatives,  $\ell_{jn}(f) - \ell_{jn}(\widehat{f}_{j,n}) = S_{j,n}(\widehat{f}_{j,n})(f - \widehat{f}_{j,n}) + I_{j,n}(f) = I_{j,n}(f)$ .  $\blacksquare$

**Lemma 10** *There exists a universal constant  $c_3 > 0$  s.t.*

$$\Pi(\|f - f_0\| \leq \tilde{r}_n) \geq \exp(-c_3 \tilde{r}_n^{-\frac{2}{2m+\beta-1}}),$$

where recall that  $\Pi$  is the probability measure induced by  $G$ .

**Proof** [Proof of Lemma 10] Note that  $\lambda \leq \tilde{r}_n^{\frac{4m}{2m+\beta-1}}$ . Then it follows by Lemma 13 (with  $d_n$  therein replaced by  $\tilde{r}_n$ ) and the proof of Theorem 7 that

$$\begin{aligned} \Pi(\|f - f_0\| \leq \tilde{r}_n) &= P(\|G - f_0\| \leq \tilde{r}_n) \\ &\geq P(V(G - f_0) \leq \tilde{r}_n^2/2, \lambda J(G - f_0) \leq \tilde{r}_n^2/2) \\ &\geq P(V(G - f_0) \leq \tilde{r}_n^2/2, J(G - f_0) \leq \tilde{r}_n^{\frac{2(\beta-1)}{2m+\beta-1}}/2) \\ &= P(\tilde{V}(\tilde{G} - \tilde{f}_0) \leq \tilde{r}_n^2/2, \tilde{J}(\tilde{G} - \tilde{f}_0) \leq \tilde{r}_n^{\frac{2(\beta-1)}{2m+\beta-1}}/2) \\ &\geq P(\tilde{V}(\tilde{G} - \omega) \leq (1/\sqrt{2} - 1/2)^2 \tilde{r}_n^2, \tilde{J}(\tilde{G} - \omega) \leq (1/\sqrt{2} - 1/2)^2 \tilde{r}_n^{\frac{2(\beta-1)}{2m+\beta-1}}) \\ &\geq \exp(-\|\omega\|_\beta^2/2) \\ &\quad \times P(\tilde{V}(\tilde{G}) \leq (1/\sqrt{2} - 1/2)^2 \tilde{r}_n^2, \tilde{J}(\tilde{G}) \leq (1/\sqrt{2} - 1/2)^2 \tilde{r}_n^{\frac{2(\beta-1)}{2m+\beta-1}}) \\ &\geq \exp(-\|\omega\|_\beta^2/2) P(\tilde{V}(\tilde{G}) \leq (1/\sqrt{2} - 1/2)^2 \tilde{r}_n^2/2) \\ &\quad \times P(\tilde{J}(\tilde{G}) \leq (1/\sqrt{2} - 1/2)^2 \tilde{r}_n^{\frac{2(\beta-1)}{2m+\beta-1}}/2) \\ &\geq \exp(-c_3 \tilde{r}_n^{-\frac{2}{2m+\beta-1}}), \end{aligned}$$

where  $c_3 > 0$  is a universal constant. ■

**Proof** [Proof of Proposition 1] Fix any  $\varepsilon \in (0, 1)$ . Let  $M_1$  be a large constant so that (thanks to Lemma 7) the event

$$\mathcal{E}'_n = \left\{ \max_{1 \leq j \leq s} \|\hat{f}_{j,n} - f_0\| \leq M_1 \tilde{r}_n \right\} \quad (\text{S.15})$$

has probability approaching one. Meanwhile, for a fixed constant  $M > 1$ , define

$$\mathcal{E}''_n = \left\{ \max_{1 \leq j \leq s} \sup_{g \in \mathcal{G}} \|Z_{j,n}(g)\| \leq B(h) \sqrt{M \log N} \right\}. \quad (\text{S.16})$$

By Lemma 8 we have that  $\mathcal{E}''_n$  has  $P_{f_0}$ -probability approaching one. Thus, it holds that, when  $n$  becomes large,  $P_{f_0}(\mathcal{E}_n) \geq 1 - \varepsilon/2$ , where  $\mathcal{E}_n := \mathcal{E}'_n \cap \mathcal{E}''_n$ . In the rest of the proof we simply assume that  $\mathcal{E}_n$  holds.

For some positive constant  $M_0$ , it follows by Theorem 7 that

$$\max_{1 \leq j \leq s} E\{\|f - f_0\|^a I(\|f - f_0\| \geq M_0 r_n) | \mathbf{D}_j\} = O_{P_{f_0}}(s^2 \exp(-nr_n^2)).$$

Let  $C' > M_1$  be a constant to be further determined later, then we have that

$$\begin{aligned} &\max_{1 \leq j \leq s} E\{\|f - f_0\|^a I(\|f - f_0\| \geq 2C' \tilde{r}_n) | \mathbf{D}_j\} \\ &\leq \max_{1 \leq j \leq s} E\{\|f - f_0\|^a I(\|f - f_0\| \geq M_0 r_n) | \mathbf{D}_j\} \\ &\quad + \max_{1 \leq j \leq s} E\{\|f - f_0\|^a I(2C' \tilde{r}_n \leq \|f - f_0\| \leq M_0 r_n) | \mathbf{D}_j\}. \end{aligned}$$

The first term is  $O_{P_{f_0}}(s^2 \exp(-nr_n^2))$ . Thus, when  $n$  is sufficiently large,

$$P_{f_0} \left( \max_{1 \leq j \leq s} E\{\|f - f_0\|^a I(\|f - f_0\| \geq M_0 r_n) | \mathbf{D}_j\} \geq M' s^2 \exp(-nr_n^2)/2 \right) \leq \varepsilon/2$$

for a large constant  $M' > 0$ .

Next we only need to handle the second term. Let  $\Delta f = f - \widehat{f}_{j,n}$ . It follows by Lemma 9 that  $I_{j,n}(f) = T_j(f) - \frac{1}{2}\|\Delta f\|^2$ , and  $\ell_{jn}(f) - \ell_{jn}(\widehat{f}_{j,n}) = I_{j,n}(f)$ . Therefore,

$$\begin{aligned} & E\{\|f - f_0\|^a I(f \in A_n) | \mathbf{D}_j\} \\ &= \frac{\int_{A_n} \|f - f_0\|^a \exp(n(\ell_{jn}(f) - \ell_{jn}(\widehat{f}_{j,n}))) d\Pi(f)}{\int_{S^m(\mathbb{I})} \exp(n(\ell_{jn}(f) - \ell_{jn}(\widehat{f}_{j,n}))) d\Pi(f)} = \frac{\int_{A_n} \|f - f_0\|^a \exp(nI_{j,n}(f)) d\Pi(f)}{\int_{S^m(\mathbb{I})} \exp(nI_{j,n}(f)) d\Pi(f)}, \end{aligned}$$

where  $A_n = \{f \in S^m(\mathbb{I}) : 2C'\widetilde{r}_n \leq \|f - f_0\| \leq M_0 r_n\}$ .

Let

$$J_{j1} = \int_{S^m(\mathbb{I})} \exp(nI_{j,n}(f)) d\Pi(f), \quad J_{j2} = \int_{A_n} \|f - f_0\|^a \exp(nI_{j,n}(f)) d\Pi(f).$$

Then on  $\mathcal{E}_n$  and for  $\|f - f_0\| \leq \widetilde{r}_n$ , we have  $\|f - \widehat{f}_{j,n}\| \leq \|f - f_0\| + \|\widehat{f}_{j,n} - f_0\| \leq (M_1 + 1)\widetilde{r}_n$ .

Let  $d_n = c_K(M_1 + 1)h^{-1/2}\widetilde{r}_n$ . It follows by similar arguments as above (S.23) that  $d_n^{-1}\Delta f \in \mathcal{G}$ . Note that on  $\mathcal{E}_n$  and for  $\|f - f_0\| \leq \widetilde{r}_n$ , for all  $1 \leq j \leq s$ ,

$$\begin{aligned} |T_j(f)| &= \frac{1}{2n} \left| \sum_{i \in I_j} [\Delta f](X_i)^2 - E_X\{(\Delta f)(X)^2\} \right| \\ &= \frac{1}{2n} \left| \left\langle \sum_{i \in I_j} [\Delta f](X_i) K_{X_i} - E_X\{(\Delta f)(X) K_X\}, \Delta f \right\rangle \right| \\ &\leq \frac{1}{2n} \|\Delta f\| \times \left\| \sum_{i \in I_j} [\Delta f](X_i) K_{X_i} - E_X\{(\Delta f)(X) K_X\} \right\| \\ &= \frac{c_K h^{-1/2} d_n \|\Delta f\|}{2\sqrt{n}} \times \|Z_{j,n}(d_n^{-1}\Delta f)\| \\ &\leq \frac{c_K h^{-1/2} d_n \|\Delta f\|}{2\sqrt{n}} B(h) \sqrt{M \log N} \\ &\leq D(c_K, M, M_1) \times n^{-1/2} h^{-\frac{6m-1}{4m}} \widetilde{r}_n^2 \sqrt{\log N} \leq D(c_K, M, M_1) \times \widetilde{r}_n^2 b_n, \quad (\text{S.17}) \end{aligned}$$

where  $D(c_K, M, M_1)$  is constant depending only on  $c_K, M_1, M$ .

It follows that on  $\mathcal{E}_n$  and for all  $1 \leq j \leq s$ ,

$$\begin{aligned} J_{j1} &\geq \int_{\|f - f_0\| \leq \widetilde{r}_n} \exp(nI_{j,n}(f)) d\Pi(f) \\ &= \int_{\|f - f_0\| \leq \widetilde{r}_n} \exp\left(nT_j(f) - \frac{n}{2}\|f - \widehat{f}_{j,n}\|^2\right) d\Pi(f) \\ &\geq \exp\left(-[D(c_K, M, M_1)b_n + (M_1 + 1)^2/2]n\widetilde{r}_n^2\right) \Pi(\|f - f_0\| \leq \widetilde{r}_n). \end{aligned}$$

Since  $\Pi(\|f - f_0\| \leq \tilde{r}_n) \geq \exp(-c_3 \tilde{r}_n^{-\frac{2}{2m+\beta-1}})$  (Lemma 10), together with  $\tilde{r}_n \geq (nh)^{-1/2} + h^{m+\frac{\beta-1}{2}} \geq 2n^{-\frac{2m+\beta-1}{2(2m+\beta)}}$ , we get that  $n\tilde{r}_n^{2+\frac{2}{2m+\beta-1}} \geq n(4n^{-\frac{2m+\beta-1}{2m+\beta}})^{1+\frac{1}{2m+\beta-1}} = 4$ . Therefore,  $\tilde{r}_n^{-\frac{2}{2m+\beta-1}} \leq n\tilde{r}_n^2/4$ , leading to

$$\Pi(\|f - f_0\| \leq \tilde{r}_n) \geq \exp\left(-\frac{c_3}{4}n\tilde{r}_n^2\right). \quad (\text{S.18})$$

This implies by rate conditions  $b_n \leq 1$  that, on  $\mathcal{E}_n$  and for any  $1 \leq j \leq s$ ,

$$\begin{aligned} J_{j1} &\geq \exp\left(-[D(c_K, M, M_1)b_n + (M_1 + 1)^2/2 + c_3/4]n\tilde{r}_n^2\right) \\ &\geq \exp\left(-[D(c_K, M, M_1) + (M_1 + 1)^2/2 + c_3/4]n\tilde{r}_n^2\right). \end{aligned}$$

Next we handle  $J_{j2}$ . The idea is similar to how we handle  $J_{j1}$  but with technical difference. Let  $\Delta f = f - \hat{f}_{j,n}$ . Note that  $\tilde{r}_n^2 \leq r_n^2 \log(2s)$ , and hence, on  $\mathcal{E}_n$ , for any  $f \in A_n$ , i.e.,  $\|f - f_0\| \leq M_0 r_n$ , we get that  $\|\Delta f\| = \|\hat{f}_{j,n} - f\| \leq \|\hat{f}_{j,n} - f_0\| + \|f - f_0\| \leq M_1 \tilde{r}_n + M_0 r_n \leq (M_0 + M_1)r_n \sqrt{\log(2s)}$ . Let  $d_{*n} = c_K(M_0 + M_1)h^{-1/2}r_n \sqrt{\log(2s)}$ . Then  $d_{*n}^{-1}\Delta f \in \mathcal{G}$ . Using previous similar arguments handling  $T_j(f)$ , we have that on  $\mathcal{E}_n$ , for any  $f \in A_n$  and  $1 \leq j \leq s$ ,

$$\begin{aligned} |T_j(f)| &\leq \frac{\|\Delta f\|}{2\sqrt{n}} c_K h^{-1/2} d_{*n} \cdot B(h) \sqrt{M \log N} \\ &\leq \frac{1}{2} c_K^2 (M_0 + M_1)^2 M^{1/2} n^{-1/2} h^{-1} r_n^2 B(h) (\log N)^{3/2} \\ &\leq D(c_K, M, M_0, M_1) \times n^{-1/2} r_n^2 h^{-\frac{6m-1}{4m}} (\log N)^{3/2} \\ &= D(c_K, M, M_0, M_1) \times r_n^2 b_n \leq D(c_K, M, M_0, M_1) \times \tilde{r}_n^2, \end{aligned}$$

where  $D(c_K, M, M_0, M_1)$  is constant only depending on  $c_K, M, M_0, M_1$  and the last inequality follows by rate condition  $r_n^2 b_n \leq \tilde{r}_n^2$ . It is easy to see that on  $\mathcal{E}_n$  and for any  $f \in A_n$  and  $1 \leq j \leq s$ ,  $\|\hat{f}_{j,n} - f\| \geq \|f - f_0\| - \|\hat{f}_{j,n} - f_0\| \geq (2C' - M_1)\tilde{r}_n$ , leading to that

$$J_{j2} \leq \exp\left(-\left(\frac{(2C' - M_1)^2}{2} - D(c_K, M, M_0, M_1)\right)n\tilde{r}_n^2\right) C(a, \Pi),$$

where  $C(a, \Pi) = \int_{S^m(\mathbb{I})} \|f - f_0\|^a d\Pi(f)$  is the  $a$ th prior moment of  $\|f - f_0\|$  which is finite. Choose  $C' > M_1$  to be large such that

$$\frac{(2C' - M_1)^2}{2} \geq 1 + D(c_K, M, M_1) + D(c_K, M, M_0, M_1) + (M_1 + 1)^2/2 + c_3/4.$$

Therefore, on  $\mathcal{E}_n$ ,

$$\max_{1 \leq j \leq s} E\{\|f - f_0\|^a I(f \in A_n) | \mathbf{D}_j\} \leq \frac{\max_{1 \leq j \leq s} J_{j2}}{\min_{1 \leq j \leq s} J_{j1}} \leq \exp(-n\tilde{r}_n^2) C(a, \Pi).$$

So we get that

$$P_{f_0} \left( \max_{1 \leq j \leq s} E\{\|f - f_0\|^a I(f \in A_n) | \mathbf{D}_j\} \geq \exp(-n\tilde{r}_n^2) C(a, \Pi) \right) \leq P_{f_0}(\mathcal{E}_n^c) \leq \varepsilon/2.$$

By  $\tilde{r}_n^2 \leq r_n^2 \log(2s)$ , the above leads to that

$$\begin{aligned} P_{f_0} \left( \max_{1 \leq j \leq s} E\{\|f - f_0\|^a I(\|f - f_0\| \geq 2C' \tilde{r}_n) | \mathbf{D}_j\} \right. \\ \left. \geq (M' + C(a, \Pi)) s^2 \exp(-n \tilde{r}_n^2 / \log(2s)) \right) \leq \varepsilon. \end{aligned}$$

Proof is completed. ■

#### S.8.4. Proofs of other results in Section S.8.3

Let  $N(\varepsilon, \mathcal{G}, \|\cdot\|_\infty)$  be the  $\varepsilon$ -packing number in terms of supremum norm, where recall that the space  $\mathcal{G}$  is defined in (S.13). The following result can be found in Van De Geer and Van De Geer (2006).

**Lemma 11** *There exists a universal constant  $c_0 > 0$  s.t. for any  $\varepsilon > 0$ ,*

$$\log N(\varepsilon, \mathcal{G}, \|\cdot\|_\infty) \leq c_0 (\sqrt{2} c_K^{-1})^{1/m} h^{-\frac{2m-1}{2m}} \varepsilon^{-1/m}.$$

For  $r \geq 0$ , define  $\Psi(r) = \int_0^r \sqrt{\log(1 + \exp(x^{-1/m}))} dx$ . For arbitrary  $\varepsilon > 0$ , define

$$\begin{aligned} A(h, \varepsilon) &= \frac{32\sqrt{6}}{\tau} \sqrt{2} c_K^{-1} c_0^m h^{-(2m-1)/2} \Psi \left( \frac{1}{2\sqrt{2}} c_K c_0^{-m} h^{(2m-1)/2} \varepsilon \right) \\ &\quad + \frac{10\sqrt{24}\varepsilon}{\tau} \sqrt{\log \left( 1 + \exp \left( 2c_0 ((\sqrt{2})^{-1} c_K h^{(2m-1)/2} \varepsilon)^{-1/m} \right) \right)}, \end{aligned} \quad (\text{S.19})$$

where  $\tau = \sqrt{\log 1.5} \approx 0.6368$ .

We have the following useful lemma.

**Lemma 12** *For any  $1 \leq j \leq s$  and  $f \in S^m(\mathbb{I})$ , suppose that  $\psi_{j,n,f}(z; g)$  is a measurable function defined upon  $z = (y, x) \in \mathcal{Y} \times \mathbb{I}$  and  $g \in \mathcal{G}$  satisfying  $\psi_{j,n,f}(z; 0) = 0$  and the following Lipschitz continuity condition: for any  $i \in I_j$  and  $g_1, g_2 \in \mathcal{G}$ ,*

$$|\psi_{j,n,f}(Z_i; g_1) - \psi_{j,n,f}(Z_i; g_2)| \leq c_K^{-1} h^{1/2} \|g_1 - g_2\|_\infty. \quad (\text{S.20})$$

*Then for any constant  $t \geq 0$  and  $n \geq 1$ ,*

$$\sup_{f \in S^m(\mathbb{I})} P_f \left( \sup_{g \in \mathcal{G}} \|Z_{j,n,f}(g)\|_f > t \right) \leq 2 \exp \left( -\frac{t^2}{B(h)^2} \right),$$

*where  $B(h) = A(h, 2)$  and*

$$Z_{j,n,f}(g) = \frac{1}{\sqrt{n}} \sum_{i \in I_j} [\psi_{j,n,f}(Z_i; g) K_{X_i} - E_f \{\psi_{j,n,f}(Z_i; g) K_{X_i}\}].$$

**Proof** [Proof of Lemma 12] For any  $f \in S^m(\mathbb{I})$  and  $n \geq 1$ , and any  $g_1, g_2 \in \mathcal{G}$ , we get that

$$\|(\psi_{j,n,f}(Z_i; g_1) - \psi_{j,n,f}(Z_i; g_2)) K_{X_i}\| \leq c_K^{-1} h^{1/2} \|g_1 - g_2\|_\infty c_K h^{-1/2} = \|g_1 - g_2\|_\infty.$$

By Theorem 3.5 of Pinelis et al. (1994), for any  $t > 0$ ,  $P_f(\|Z_{j,n,f}(g_1) - Z_{j,n,f}(g_2)\| \geq t) \leq 2 \exp\left(-\frac{t^2}{8\|g_1 - g_2\|_\infty^2}\right)$ . Then by Lemma 8.1 in Kosorok (2008), we have

$$\|\|Z_{j,n,f}(g_1) - Z_{j,n,f}(g_2)\|\|_{\psi_2} \leq \sqrt{24}\|g_1 - g_2\|_\infty,$$

where  $\|\cdot\|_{\psi_2}$  denotes the Orlicz norm associated with  $\psi_2(s) := \exp(s^2) - 1$ . Recall  $\tau = \sqrt{\log 1.5} \approx 0.6368$ . Define  $\phi(x) = \psi_2(\tau x)$ . Then it can be shown by elementary calculus that  $\phi(1) \leq 1/2$ , and for any  $x, y \geq 1$ ,  $\phi(x)\phi(y) \leq \phi(xy)$ . By a careful examination of the proof of Lemma 8.2, it can be shown that for any random variables  $\xi_1, \dots, \xi_l$ ,

$$\|\max_{1 \leq i \leq l} \xi_i\|_{\psi_2} \leq \frac{2}{\tau} \psi_2^{-1}(l) \max_{1 \leq i \leq l} \|\xi_i\|_{\psi_2}. \quad (\text{S.21})$$

Next we use a “chaining” argument. Let  $T_0 \subset T_1 \subset T_2 \subset \dots \subset T_\infty := \mathcal{G}$  be a sequence of finite nested sets satisfying the following properties:

- for any  $T_q$  and any  $s, t \in T_q$ ,  $\|s - t\|_\infty \geq \varepsilon 2^{-q}$ ; each  $T_q$  is “maximal” in the sense that if one adds any point in  $T_q$ , then the inequality will fail;
- the cardinality of  $T_q$  is upper bounded by

$$\log |T_q| \leq \log N(\varepsilon 2^{-q}, \mathcal{G}, \|\cdot\|_\infty) \leq c_0(\sqrt{2}c_K^{-1})^{1/m} h^{-(2m-1)/(2m)}(\varepsilon 2^{-q})^{-1/m},$$

where  $c_0 > 0$  is absolute constant;

- each element  $t_{q+1} \in T_{q+1}$  is uniquely linked to an element  $t_q \in T_q$  which satisfies  $\|t_q - t_{q+1}\|_\infty \leq \varepsilon 2^{-q}$ .

For arbitrary  $s_{k+1}, t_{k+1} \in T_{k+1}$  with  $\|s_{k+1} - t_{k+1}\|_\infty \leq \varepsilon$ , choose two chains (both being of length  $k+2$ )  $t_q$  and  $s_q$  with  $t_q, s_q \in T_q$  for  $0 \leq q \leq k+1$ . The ending points  $s_0$  and  $t_0$  satisfy

$$\begin{aligned} \|s_0 - t_0\|_\infty &\leq \sum_{q=0}^k [\|s_q - s_{q+1}\|_\infty + \|t_q - t_{q+1}\|_\infty] + \|s_{k+1} - t_{k+1}\|_\infty \\ &\leq 2 \sum_{q=0}^k \varepsilon 2^{-q} + \varepsilon \leq 5\varepsilon, \end{aligned}$$

and hence,  $\|\|Z_{j,n,f}(s_0) - Z_{j,n,f}(t_0)\|_f\|_{\psi_2} \leq 5\sqrt{24}\varepsilon$ . It follows by the proof of Theorem 8.4 of Kosorok (2008) and (S.21) that

$$\begin{aligned}
 & \left\| \max_{s_{k+1}, t_{k+1} \in T_{k+1}} \|Z_{j,n,f}(s_{k+1}) - Z_{j,n,f}(t_{k+1}) - (Z_{j,n,f}(s_0) - Z_{j,n,f}(t_0))\| \right\|_{\psi_2} \\
 & \leq 2 \sum_{q=0}^k \left\| \max_{\substack{u \in T_{q+1}, v \in T_q \\ u, v \text{ link each other}}} \|Z_{j,n,f}(u) - Z_{j,n,f}(v)\| \right\|_{\psi_2} \\
 & \leq \frac{4}{\tau} \sum_{q=0}^k \psi_2^{-1}(N(2^{-q-1}\varepsilon, \mathcal{G}, \|\cdot\|_\infty)) \\
 & \quad \times \max_{\substack{u \in T_{q+1}, v \in T_q \\ u, v \text{ link each other}}} \left\| \|Z_{j,n,f}(u) - Z_{j,n,f}(v)\| \right\|_{\psi_2} \\
 & \leq \frac{4\sqrt{24}}{\tau} \sum_{q=0}^k \sqrt{\log(1 + N(\varepsilon 2^{-q-1}, \mathcal{G}, \|\cdot\|_\infty))} \varepsilon 2^{-q} \\
 & \leq \frac{8\sqrt{24}}{\tau} \sum_{q=1}^{k+1} \sqrt{\log\left(1 + \exp\left(c_0 c_K^{-1/m} h^{-(2m-1)/(2m)} (\varepsilon 2^{-q})^{-1/m}\right)\right)} \varepsilon 2^{-q} \\
 & \leq \frac{32\sqrt{6}}{\tau} \int_0^{\varepsilon/2} \sqrt{\log\left(1 + \exp\left(c_0 c_K^{-1/m} h^{-(2m-1)/(2m)} x^{-1/m}\right)\right)} dx \\
 & = \frac{32\sqrt{6}}{\tau} c_K^{-1} c_0^m h^{-(2m-1)/2} \Psi\left(\frac{1}{2} c_K c_0^{-m} h^{(2m-1)/2} \varepsilon\right).
 \end{aligned}$$

On the other hand,

$$\begin{aligned}
 \left\| \max_{\substack{u, v \in T_0 \\ \|u-v\|_\infty \leq 5\varepsilon}} \|Z_{j,n,f}(u) - Z_{j,n,f}(v)\|_f \right\|_{\psi_2} & \leq \frac{2}{\tau} \psi_2(|T_0|^2) \max_{\substack{u, v \in T_0 \\ \|u-v\|_\infty \leq 5\varepsilon}} \left\| \|Z_{j,n,f}(u) - Z_{j,n,f}(v)\|_f \right\|_{\psi_2} \\
 & \leq \frac{2}{\tau} \psi_2^{-1}(N(\varepsilon, \mathcal{G}, \|\cdot\|_\infty)^2) (5\sqrt{24}\varepsilon).
 \end{aligned}$$

Therefore,

$$\begin{aligned}
 \left\| \max_{\substack{s, t \in T_{k+1} \\ \|s-t\|_\infty \leq \varepsilon}} \|Z_{j,n,f}(s) - Z_{j,n,f}(t)\| \right\|_{\psi_2} & \leq \frac{32\sqrt{6}}{\tau} c_K^{-1} c_0^m h^{-(2m-1)/2} \Psi\left(\frac{1}{2} c_K c_0^{-m} h^{(2m-1)/2} \varepsilon\right) \\
 & \quad + \frac{2}{\tau} \psi_2^{-1}(N(\varepsilon, \mathcal{G}, \|\cdot\|_\infty)^2) (5\sqrt{24}\varepsilon) \\
 & \leq \frac{32\sqrt{6}}{\tau} c_K^{-1} c_0^m h^{-(2m-1)/2} \Psi\left(\frac{1}{2} c_K c_0^{-m} h^{(2m-1)/2} \varepsilon\right) \\
 & \quad + \frac{10\sqrt{24}\varepsilon}{\tau} \sqrt{\log\left(1 + \exp\left(2c_0(c_K h^{(2m-1)/2} \varepsilon)^{-1/m}\right)\right)} \\
 & = A(h, \varepsilon).
 \end{aligned}$$

Now for any  $g_1, g_2 \in \mathcal{G}$  with  $\|g_1 - g_2\|_\infty \leq \varepsilon/2$ . Let  $k \geq 2$ , hence,  $2^{1-k} \leq 1 - \|g_1 - g_2\|_\infty/\varepsilon$ . Since  $T_k$  is “maximal”, there exist  $s_k, t_k \in T_k$  s.t.  $\max\{\|g_1 - s_k\|_\infty, \|g_2 - t_k\|_\infty\} \leq \varepsilon 2^{-k}$ . It is

easy to see that  $\|s_k - t_k\|_\infty \leq \varepsilon$ . So

$$\begin{aligned} \|Z_{j,n,f}(g_1) - Z_{j,n,f}(g_2)\| &\leq \|Z_{j,n,f}(g_1) - Z_{j,n,f}(s_k)\| + \|Z_{j,n,f}(g_2) - Z_{j,n,f}(t_k)\| \\ &\quad + \|Z_{j,n,f}(s_k) - Z_{j,n,f}(t_k)\| \\ &\leq 4\sqrt{n}\varepsilon 2^{-k} + \max_{\substack{u,v \in T_k \\ \|u-v\|_\infty \leq \varepsilon}} \|Z_{j,n,f}(u) - Z_{j,n,f}(v)\|. \end{aligned}$$

Therefore, letting  $k \rightarrow \infty$  we get that

$$\begin{aligned} &\left\| \sup_{\substack{g_1, g_2 \in \mathcal{G} \\ \|g_1 - g_2\|_\infty \leq \varepsilon/2}} \|Z_{j,n,f}(g_1) - Z_{j,n,f}(g_2)\| \right\|_{\psi_2} \\ &\leq 4\sqrt{n}\varepsilon 2^{-k}/\sqrt{\log 2} + \left\| \max_{\substack{u,v \in T_k \\ \|u-v\|_\infty \leq \varepsilon}} \|Z_{j,n,f}(u) - Z_{j,n,f}(v)\| \right\|_{\psi_2} \\ &\leq 4\sqrt{n}\varepsilon 2^{-k}/\sqrt{\log 2} + A(h, \varepsilon) \rightarrow A(h, \varepsilon). \end{aligned}$$

Taking  $\varepsilon = 2$  in the above inequality, we get that

$$\left\| \sup_{\substack{g_1, g_2 \in \mathcal{G} \\ \|g_1 - g_2\|_\infty \leq 1}} \|Z_{j,n,f}(g_1) - Z_{j,n,f}(g_2)\| \right\|_{\psi_2} \leq A(h, 2) = B(h).$$

By Lemma 8.1 in Kosorok (2008), we have

$$P_f \left( \sup_{g \in \mathcal{G}} \|Z_{j,n,f}(g)\| \geq t \right) \leq 2 \exp \left( -\frac{t^2}{B(h)^2} \right).$$

Note that the right hand side in the above does not depend on  $f$ . This completes the proof.  $\blacksquare$

**Proof** [Proof of Lemma 4] Let  $f \in H^m(b)$  be the parameter based on which the data are drawn. It is easy to see that  $DS_\lambda(f)g = -E\{g(X)K_X\} - \mathcal{P}_\lambda g$ ,  $\forall g \in S^m(\mathbb{I})$ . Therefore, for any  $g, \tilde{g} \in S^m(\mathbb{I})$ ,  $\langle DS_\lambda(f)g, \tilde{g} \rangle = -\langle g, \tilde{g} \rangle$ , implying  $DS_\lambda(f) = -id$ .

The proof of (1) is finished in two parts.

**Part I:** For any  $f \in S^m(\mathbb{I})$ , define an operator mapping  $S^m(\mathbb{I})$  to  $S^m(\mathbb{I})$ :

$$T_{1f}(g) = g + S_\lambda(f + g), \quad g \in S^m(\mathbb{I}).$$

First observe that, under  $P_f$  with  $f \in H^m(b)$ ,

$$\|S_\lambda(f)\| = \|\mathcal{P}_\lambda f\| = \sup_{\|g\|=1} |\langle \mathcal{P}_\lambda f, g \rangle| \leq \sqrt{\lambda J(f)} \leq h^m b.$$

Let  $r_{1n} = bh^m$ . Let  $\mathbb{B}(r_{1n}) = \{g \in S^m(\mathbb{I}) : \|g\| \leq r_{1n}\}$  be the  $r_{1n}$ -ball. For any  $g \in \mathbb{B}(r_{1n})$ , using  $DS_\lambda(f) = -id$ , it is easy to see that  $\|T_{1f}(g)\| = \|S_\lambda(f)\| \leq bh^m = r_{1n}$ . Therefore,  $T_{1f}$

maps  $\mathbb{B}(r_{1n})$  to itself. For any  $g_1, g_2 \in \mathbb{B}(r_{1n})$ , by Taylor's expansion we have

$$\begin{aligned}\|T_{1f}(g_1) - T_{1f}(g_2)\| &= \|g_1 - g_2 + S_\lambda(f + g_1) - S_\lambda(f + g_2)\| \\ &= \|g_1 - g_2 + \int_0^1 DS_\lambda(f + g_2 + sg)gds\| = 0.\end{aligned}$$

This shows that  $T_{1f}$  is a contraction mapping which maps  $\mathbb{B}(r_{1n})$  into  $\mathbb{B}(r_{1n})$ . By contraction mapping theorem (see Rudin et al. (1964)),  $T_{1f}$  has a unique fixed point  $g' \in \mathbb{B}(r_{1n})$  satisfying  $T_{1f}(g') = g'$ . Let  $f_\lambda = f + g'$ . Then  $S_\lambda(f_\lambda) = 0$  and  $\|f_\lambda - f\| \leq r_{1n}$ .

**Part II:** For any  $f \in H^m(b)$ , under (14) with  $f$  being the truth, let  $f_\lambda$  be the function obtained in **Part I** s.t.  $\|f_\lambda - f\| \leq r_{1n}$ . Define an operator

$$T_{2f}(g) = g + S_{j,n}(f_\lambda + g), \quad g \in S^m(\mathbb{I}).$$

Rewrite  $T_{2f}$  as

$$T_{2f}(g) = [DS_{j,n}(f_\lambda)g - DS_\lambda(f_\lambda)g] + S_{j,n}(f_\lambda).$$

Denote the above two terms by  $I_{1f}, I_{2f}$ , respectively.

For any  $i \in I_j$ , let  $R_i = (Y_i - f_\lambda(X_i))K_{X_i} - E_f\{(Y - f_\lambda(X))K_X\}$ . Obviously,

$$\begin{aligned}\|E_f\{(Y - f_\lambda(X))K_X\}\| &= \sup_{\|g\|=1} |\langle E_f\{(Y - f_\lambda(X))K_X\}, g \rangle| \\ &= \sup_{\|g\|=1} |E_f\{(Y - f_\lambda(X))g(X)\}| \leq \|f - f_\lambda\| \leq r_{1n}.\end{aligned}$$

Therefore,  $\|R_i\| \leq c_K h^{-1/2} |Y_i - f_\lambda(X_i)| + r_{1n}$  which leads to that

$$E \left\{ \exp \left( \frac{\|R_i\|}{c_K h^{-1/2}} \right) \right\} \leq E(\exp(|\epsilon_i| + 1)) \leq C_\epsilon,$$

where  $C_\epsilon = E\{(|\epsilon| + 1)^2 \exp(|\epsilon| + 1)\}$ . Let  $\delta = hr/c_K$ . By condition  $rh^{1/2} \leq 1$ , we have

$$E\{\exp(\delta\|R_i\|) - 1 - \delta\|R_i\|\} \leq E\{(\delta\|R_i\|)^2 \exp(\delta\|R_i\|)\} \leq c_K^2 C_\epsilon \delta^2 h^{-1}.$$

It follows by Theorem 3.2 of Pinelis et al. (1994) that, for  $L(M) := c_K(C_\epsilon + M)$ ,

$$\begin{aligned}P_f \left( \left\| \sum_{i \in I_j} R_i \right\|_f \geq L(M)nr \right) &\leq 2 \exp(-L(M)\delta nr + c_K^2 C_\epsilon nh^{-1} \delta^2) \\ &= 2 \exp(-Mnhr^2).\end{aligned} \tag{S.22}$$

We note that the right hand side in (S.22) does not depend on  $f$ . Moreover, it is easy to see that  $S_{j,n}(f_\lambda) = S_{j,n}(f_\lambda) - S_\lambda(f_\lambda) = \frac{1}{n} \sum_{i \in I_j} R_i$ . Let

$$\mathcal{E}_{n,1} = \{\|S_{j,n}(f_\lambda)\| \leq L(M)r\},$$

then  $\sup_{f \in H^m(C)} P_f(\mathcal{E}_{n,1}^c) \leq 2 \exp(-Mnhr^2)$ . Define  $\psi_{j,n}(X_i; g) = c_K^{-1} h^{1/2} g(X_i)$ ,  $i \in I_j$ , and  $Z_{j,n}(g) = \frac{1}{\sqrt{n}} \sum_{i \in I_j} [\psi_{j,n}(X_i; g) K_{X_i} - E_f\{\psi_{j,n}(X_i; g) K_{X_i}\}]$ . By Lemma 12,  $\sup_{f \in H^m(b)} P_f(\mathcal{E}_{n,2}^c) \leq 2 \exp(-Mnhr^2)$ , where  $\mathcal{E}_{n,2} = \{\sup_{g \in \mathcal{G}} \|Z_{j,n}(g)\| \leq \sqrt{Mnhr^2} B(h)\}$ .

For any  $g \in S^m(\mathbb{I}) \setminus \{0\}$ , let  $\bar{g} = g/d'_n$ , where  $d'_n = c_K h^{-1/2} \|g\|$ . It follows that

$$\|\bar{g}\|_\infty \leq c_K h^{-1/2} \|\bar{g}\| = c_K h^{-1/2} \|g\|/d'_n = 1, \text{ and}$$

$$J(\bar{g}, \bar{g}) = d'^{-2} J(g, g) = h^{-2m} \frac{\lambda J(g, g)}{c_K^2 h^{-1} \|g\|^2} \leq h^{-2m} \frac{\|g\|^2}{c_K^2 h^{-1} \|g\|^2} \leq c_K^{-2} h^{-2m+1}.$$

Therefore,  $\bar{g} \in \mathcal{G}$ . Consequently, on  $\mathcal{E}_{n,2}$ , for any  $g \in S^m(\mathbb{I}) \setminus \{0\}$ , we get  $\|Z_{j,n}(\bar{g})\| \leq \sqrt{Mnhr^2} B(h)$ , which leads to that

$$\begin{aligned} \|DS_{j,n}(f_\lambda)g - DS_\lambda(f_\lambda)g\| &= \frac{1}{n} \left\| \sum_{i \in I_j} [g(X_i)K_{X_i} - E\{g(X_i)K_{X_i}\}] \right\|_f \\ &\leq c_K^2 M^{1/2} r h^{-1/2} B(h) \|g\| \leq \|g\|/2, \end{aligned} \quad (\text{S.23})$$

where the last inequality follows by condition  $c_K^2 M^{1/2} r h^{-1/2} B(h) \leq 1/2$ . Note that the above inequality also holds for  $g = 0$ .

Let  $r_{2n} = 2L(M)r$ . Therefore, it follows by (S.23) that, for any  $f \in H^m(b)$ , on  $\mathcal{E}_n := \mathcal{E}_{n,1} \cap \mathcal{E}_{n,2}$  and for any  $g \in \mathbb{B}(r_{2n})$ ,  $\|T_{2f}(g)\| \leq \|g\|/2 + r_{2n}/2 \leq r_{2n}$ . Meanwhile, for any  $g_1, g_2 \in \mathbb{B}(r_{2n})$ , replacing  $g$  by  $g_1 - g_2$  in (S.23), we get that  $\|T_{2f}(g_1) - T_{2f}(g_2)\| \leq \|g_1 - g_2\|/2$ . Therefore, for any  $f \in H^m(b)$ , on  $\mathcal{E}_n$ ,  $T_{2f}$  is a contraction mapping from  $\mathbb{B}(r_{2n})$  to itself. By contraction mapping theorem, there exists uniquely an element  $g'' \in \mathbb{B}(r_{2n})$  s.t.  $T_{2f}(g'') = g''$ . Let  $\widehat{f}_{j,n} = f_\lambda + g''$ . Clearly,  $S_{j,n}(\widehat{f}_{j,n}) = 0$ , and hence,  $\widehat{f}_{j,n}$  is the maximizer of  $\ell_{jn}$ ; see (19). So we get that, on  $\mathcal{E}_n$ ,  $\|\widehat{f}_{j,n} - f\|_f \leq \|f_\lambda - f\| + \|\widehat{f}_{j,n} - f_\lambda\| \leq r_{1n} + r_{2n} = bh^m + 2L(M)r$ . The desired conclusion follows by the trivial fact:  $\sup_{f \in H^m(b)} P_f(\mathcal{E}_n^c) \leq 4 \exp(-Mnhr^2)$ . Proof of (1) is completed.

Next we show (2).

For any  $f \in H^m(b)$ , let  $\widehat{f}_{j,n}$  be the penalized MLE of  $f$  obtained by (19). Let  $g_n = \widehat{f}_{j,n} - f$ ,  $\delta_n = bh^m + 2L(M)r$ ,  $d'_n = c_K h^{-1/2} \delta_n$ .

On  $\mathcal{E}_n$ , we have  $\|g_n\|_f \leq \delta_n$ . Let  $\bar{g} = g_n/d'_n$ . Clearly,  $\bar{g} \in \mathcal{G}$ . Then we get that

$$\begin{aligned} &\|S_{j,n}(f + g_n) - S_{j,n}(f) - (S_\lambda(f + g_n) - S_\lambda(f))\| \\ &= \frac{1}{n} \left\| \sum_{i \in I_j} [g_n(X_i)K_{X_i} - E\{g_n(X)K_X\}] \right\| \\ &= \frac{c_K d'_n}{\sqrt{nh}} \|Z_{j,n}(\bar{g})\| \leq c_K^2 M^{1/2} h^{-1/2} r B(h) \delta_n = a_n. \end{aligned} \quad (\text{S.24})$$

Since  $S_{j,n}(f + g_n) = 0$  and  $DS_\lambda(f) = -id$ , from (S.24) we have on  $\mathcal{E}_n$ ,

$$a_n \geq \|S_{j,n}(f) + DS_\lambda(f)g_n + \int_0^1 \int_0^1 s D^2 S_\lambda(f + ss' g_n) g_n g_n ds ds' \| = \|S_{j,n}(f) - g_n\|$$

which implies that  $\|\widehat{f}_{j,n} - f - S_{n,\lambda}(f)\| \leq a_n$ . Since  $\sup_{f \in H^m(bC)} P_f(\mathcal{E}_n^c) \leq 4 \exp(-Mnhr^2)$ , proof of (2) is completed.  $\blacksquare$

### S.8.5. An initial contraction rate

Theorem 7 below states that the  $s$  posterior measures uniformly contract at rate  $r_n = (nh)^{-1/2} + h^m$ , where recall that  $h = \lambda^{1/(2m)}$ . This is an initial rate result that holds irrespective the diverging rate of  $s$ .

**Theorem 7 (An Initial Contraction Rate)** Suppose  $f_0 = \sum_{\nu=1}^{\infty} f_{\nu}^0 \varphi_{\nu}$  satisfies Condition  $(S)$ . Let  $a \geq 0$  be a fixed constant. If  $r_n = o(h^{3/2})$ ,  $h^{1/2} \log N = o(1)$ ,  $nh^{2m+1} \geq 1$ , then there exists a universal constant  $M > 0$  s.t.

$$\max_{1 \leq j \leq s} E\{\|f - f_0\|^a I(\|f - f_0\| \geq Mr_n) | \mathbf{D}_j\} = O_{P_{f_0}}(s^2 \exp(-nr_n^2))$$

as  $n \rightarrow \infty$ , no matter  $s$  is fixed or diverges at any rate.

Before proving Theorem 7, we present a preliminary lemma.

Let  $\{\tilde{\varphi}_{\nu} : \nu \geq 1\}$  be a bounded orthonormal basis of  $L^2(\mathbb{I})$  under usual  $L^2$  inner product. For any  $b \in [0, \beta]$ , define

$$\tilde{H}_b = \left\{ \sum_{\nu=1}^{\infty} f_{\nu} \tilde{\varphi}_{\nu} : \sum_{\nu=1}^{\infty} f_{\nu}^2 \rho_{\nu}^{1+b/(2m)} < \infty \right\}.$$

Then  $\tilde{H}_b$  can be viewed as a version of Sobolev space with regularity  $m + b/2$ . Define  $\tilde{G} = \sum_{\nu=1}^{\infty} v_{\nu} \tilde{\varphi}_{\nu}$ , a centered GP, and  $\tilde{f}_0 = \sum_{\nu=1}^{\infty} f_{\nu}^0 \tilde{\varphi}_{\nu}$ . Define  $\tilde{V}(f, g) = \langle f, g \rangle_{L^2} = \int_0^1 f(x)g(x)dx$ , the usual  $L^2$  inner product,  $\tilde{J}(f) = \sum_{\nu=1}^{\infty} |\tilde{V}(f, \tilde{\varphi}_{\nu})|^2 \rho_{\nu}$ , a functional on  $\tilde{H}_0$ . For simplicity, denote  $\tilde{V}(f) = \tilde{V}(f, f)$ . Clearly,  $\tilde{f}_0 \in \tilde{H}_{\beta}$ . Since  $\tilde{G}$  is a Gaussian process with covariance function

$$\tilde{r}(s, t) = E\{\tilde{G}(s)\tilde{G}(t)\} = \sum_{\nu=1}^m \sigma_{\nu}^2 \tilde{\varphi}_{\nu}(s) \tilde{\varphi}_{\nu}(t) + \sum_{\nu>m} \rho_{\nu}^{-(1+\frac{\beta}{2m})} \tilde{\varphi}_{\nu}(s) \tilde{\varphi}_{\nu}(t),$$

it follows by van der Vaart et al. (2008a) that  $\tilde{H}_{\beta}$  is the RKHS of  $\tilde{G}$ . For any  $\tilde{H}_b$  with  $0 \leq b \leq \beta$ , define inner product

$$\left\langle \sum_{\nu=1}^{\infty} f_{\nu} \tilde{\varphi}_{\nu}, \sum_{\nu=1}^{\infty} g_{\nu} \tilde{\varphi}_{\nu} \right\rangle_b = \sum_{\nu=1}^m \sigma_{\nu}^{-2} f_{\nu} g_{\nu} + \sum_{\nu>m} f_{\nu} g_{\nu} \rho_{\nu}^{1+\frac{b}{2m}}.$$

Let  $\|\cdot\|_b$  be the norm corresponding to the above inner product. The following lemma is used in the proof of Theorem 7. Its proof can be found in Shang and Cheng (2017).

**Lemma 13** Let  $d_n$  be any positive sequence. If Condition  $(S)$  holds, then there exists  $\omega \in \tilde{H}_{\beta}$  such that

1.  $\tilde{V}(\omega - \tilde{f}_0) \leq \frac{1}{4} d_n^2$ ,
2.  $\tilde{J}(\omega - \tilde{f}_0) \leq \frac{1}{4} d_n^{\frac{2(\beta-1)}{2m+\beta-1}}$ ,
3.  $\|\omega\|_{\beta}^2 = O(d_n^{-\frac{2}{2m+\beta-1}})$ .

To ease reading, we sketch the proof of Theorem 7. We first show the following result: for any  $\varepsilon > 0$ , as  $n \rightarrow \infty$ ,

$$\max_{1 \leq j \leq s} \int_{\|f - f_0\|_\infty \geq \varepsilon} \|f - f_0\|^a dP(f|\mathbf{D}_j) = O_{P_{f_0}}(s^2 \exp(-nr_n^2)) \quad (\text{S.25})$$

To show (S.25), we can rewrite the posterior density of  $f$  by

$$p(f|\mathbf{D}_j) = \frac{\prod_{i \in I_j} (p_f/p_{f_0})(Z_i) \exp(-n\lambda J(f)/2) d\Pi(f)}{\int_{S^m(\mathbb{I})} \prod_{i \in I_j} (p_f/p_{f_0})(Z_i) \exp(-n\lambda J(f)/2) d\Pi(f)}, \quad 1 \leq j \leq s,$$

where recall that  $p_f(z)$  is the probability density of  $Z = (Y, X)$  under  $f$ . For  $1 \leq j \leq s$ , define

$$I_{j1} = \int_{S^m(\mathbb{I})} \prod_{i \in I_j} (p_f/p_{f_0})(Z_i) \exp(-n\lambda J(f)/2) d\Pi(f), \quad (\text{S.26})$$

$$I_{j2} = \int_{A_n} \|f - f_0\|^a \prod_{i \in I_j} (p_f/p_{f_0})(Z_i) \exp(-\frac{n\lambda}{2} J(f)) d\Pi(f), \quad (\text{S.27})$$

$$I'_{j2} = \int_{A'_n} \|f - f_0\|^a \prod_{i \in I_j} (p_f/p_{f_0})(Z_i) \exp(-\frac{n\lambda}{2} J(f)) d\Pi(f), \quad (\text{S.28})$$

where  $A_n = \{f \in S^m(\mathbb{I}) : \|f - f_0\| \geq 2\delta_n\}$  and  $A'_n = \{f \in S^m(\mathbb{I}) : \|f - f_0\| \geq \sqrt{2}Mr_n\}$ , with the quantities  $\delta_n, M$  specified later. Using LeCam's uniformly consistent test Ghosal et al. (2000), we will show that  $\max_{1 \leq j \leq s} I_{j2}/I_{j1}$  is of an exponential order (in the sense of  $P_{f_0}$ ). Then (S.25) holds by taking  $a = 0$  in  $I_{j2}$ . The proof of Theorem 7 will be completed by decomposing  $I'_{j2}/I_{j1}$  into three terms based on an auxiliary event  $\{f \in S^m(\mathbb{I}) : \|f - f_0\|_\infty \leq \varepsilon\}$  with each term of an exponential order.

**Proof** [Proof of Theorem 7] Note that there exists a universal constant  $c' > 0$  such that  $\Psi(x) \leq c'x^{1-1/(2m)}$  for any  $0 < x < 1$ . Therefore, there exists a universal constant  $c'' > 0$  s.t.  $B(h) \leq c''h^{-(2m-1)/(4m)}$ .

Define  $B_n = \{f \in S^m(\mathbb{I}) : V(f - f_0) \leq r_n^2, J(f - f_0) \leq r_n^{\frac{2(\beta-1)}{2m+\beta-1}}\}$ . Then

$$\begin{aligned} I_{j1} &\geq \int_{B_n} \prod_{i \in I_j} (p_f/p_{f_0})(Z_i) \exp(-n\lambda J(f)/2) d\Pi(f) \\ &= \int_{B_n} \exp\left(\sum_{i \in I_j} R_i(f, f_0)\right) \exp(-n\lambda J(f)/2) d\Pi(f), \end{aligned}$$

where  $R_i(f, f_0) = \log(p_f(Z_i)/p_{f_0}(Z_i)) = Y_i(f(X_i) - f_0(X_i)) - f(X_i)^2/2 + f_0(X_i)^2/2$  for any  $i \in I_j$ . Define  $d\Pi^*(f) = d\Pi(f)/\Pi(B_n)$ , a reduced probability measure on  $B_n$ . By Jensen's

inequality,

$$\begin{aligned}
 & \log \int_{B_n} \exp\left(\sum_{i \in I_j} R_i(f, f_0)\right) \exp(-n\lambda J(f)/2) d\Pi^*(f) \\
 & \geq \int_{B_n} \left( \sum_{i \in I_j} R_i(f, f_0) - n\lambda J(f)/2 \right) d\Pi^*(f) \\
 & = \int_{B_n} \sum_{i \in I_j} [R_i(f, f_0) - E_{f_0}\{R_i(f, f_0)\}] d\Pi^*(f) \\
 & \quad + n \int_{B_n} E_{f_0}\{R_i(f, f_0)\} d\Pi^*(f) - \int_{B_n} \frac{n\lambda J(f)}{2} d\Pi^*(f) \\
 & := J_{j1} + J_{j2} + J_{j3}.
 \end{aligned}$$

For any  $f \in B_n$ ,  $\|f - f_0\|^2 = V(f - f_0) + \lambda J(f - f_0) \leq r_n^2 + \lambda r_n^{\frac{2(\beta-1)}{2m+\beta-1}}$ . By (Shang and Cheng, 2017, Lemma A.9) and the condition  $h^{-3/2}r_n = o(1)$ , we can choose  $n$  to be sufficiently large so that  $\|f - f_0\|_\infty \leq ch^{-1/2}\|f - f_0\| \leq c\sqrt{h^{-1}r_n^2 + h^{2m-1}} \leq 1$ .

It follows by Taylor's expansion and  $E_{f_0}\{Y_i - f_0(X_i)|X_i\} = 0$ , that for any  $f \in B_n$ ,

$$|E_{f_0}\{R_i(f, f_0)\}| = E_{f_0}\{(f(X) - f_0(X))^2\}/2 \leq r_n^2/2.$$

Therefore,  $J_{j2} \geq -nr_n^2/2$  for any  $1 \leq j \leq s$ .

Since  $r_n^2 = o(1)$ , we can choose  $n$  to be large so that  $|E_{f_0}\{R_i(f, f_0)\}| \leq 1$ . Meanwhile, for any  $f \in B_n$ , for some  $s \in [0, 1]$ , we have

$$\begin{aligned}
 |R_i(f, f_0)| &= |Y_i(f(X_i) - f_0(X_i)) - f(X_i)^2/2 + f_0(X_i)^2/2| \\
 &= |Y_i - f_0(X_i) - \frac{1}{2}(f - f_0)(X_i)| \times |(f - f_0)(X_i)| \\
 &\leq |Y_i - f_0(X_i)| + 1/2 = |\epsilon_i| + 1/2.
 \end{aligned}$$

We have used  $\|f - f_0\|_\infty \leq 1$  in the above inequalities.

For any  $1 \leq i \leq N$ , define  $A_i = \{|\epsilon_i| \leq 2 \log N\}$ . It is easy to check that  $P_{f_0}(\cup_{i=1}^N A_i^c) \rightarrow 0$ , as  $N \rightarrow \infty$ . Define  $\xi_i = \int_{B_n} R_i(f, f_0) d\Pi^*(f) \times I_{A_i}$ , we get that  $|\xi_i| \leq 2 \log N + 1/2$ , a.s. It can also be shown by  $r_n^2 \gg 1/n \geq 1/N$  that, as  $n, N \rightarrow \infty$ ,

$$\begin{aligned}
 |E_{f_0}\{\int_{B_n} R_i(f, f_0) d\Pi^*(f) \times I_{A_i^c}\}| &\leq E_{f_0}\{(|\epsilon_i| + 1/2) \times I_{A_i^c}\} \\
 &\leq C_\epsilon(1/N + 1/N^2) \leq r_n^2,
 \end{aligned}$$

where  $C_\epsilon$  is an absolute constant.

Let  $\delta = 1/(\sqrt{n}r_n)$ . Note that by the condition  $h^{1/2} \log N = o(1)$  we have  $\delta \log N = (\log N)/(\sqrt{n}r_n) \leq h^{1/2} \log N = o(1)$ , we can let  $n$  be large so that  $\delta(2 \log N + 1) \leq 1$ . Let  $d_i = \xi_i - E_{f_0}\{\xi_i\}$  for  $i \in I_j$ , then it is easy to see that

$$|d_i| \leq |\xi_i| + |E_{f_0}\{\xi_i\}| \leq 2 \log N + 1, \text{ a.s.}$$

Let  $e_i = E_{f_0}\{\exp(\delta|d_i|) - 1 - \delta|d_i|\}$ . It can be shown using inequality  $\exp(x) - 1 - x \leq x^2 \exp(x)$  for  $x \geq 0$  and Cauchy-Schwartz inequality that

$$\begin{aligned}
|e_i| &\leq E_{f_0}\{\delta^2 d_i^2 \exp(\delta|d_i|)\} \\
&\leq e\delta^2 E_{f_0}\{d_i^2\} \\
&\leq e\delta^2 E_{f_0}\{\xi_i^2\} \\
&\leq e\delta^2 \int_{B_n} E_{f_0}\{R_i(f, f_0)^2\} d\Pi^*(f) \\
&\leq e\delta^2 \int_{B_n} E_{f_0}\{(|\epsilon_i| + 1/2)^2 (f - f_0)(X_i)^2\} d\Pi^*(f) \\
&\leq eC_\epsilon \delta^2 r_n^2,
\end{aligned}$$

where the last step follows from  $V(f - f_0) \leq r_n^2$  for any  $f \in B_n$ . Therefore, it follows by (Pinelis et al., 1994, Theorem 3.2) that

$$\begin{aligned}
&P_{f_0} \left( \max_{1 \leq j \leq s} \left| \sum_{i \in I_j} [\xi_i - E_{f_0}\{\xi_i\}] \right| \geq 4\sqrt{nr_n \log N} \right) \\
&\leq s P_{f_0} \left( \left| \sum_{i \in I_j} [\xi_i - E_{f_0}\{\xi_i\}] \right| \geq 4\sqrt{nr_n \log N} \right) \\
&\leq 2s \exp(-4\sqrt{nr_n}(\log N)\delta + eC_\epsilon \delta^2 nr_n^2) \\
&\leq 2s/N^2 \rightarrow 0, \text{ as } N \rightarrow \infty. \tag{S.29}
\end{aligned}$$

Since  $\sqrt{nr_n} \gg \log N$ , we can let  $n$  be large so that  $4\sqrt{nr_n} \log N \leq nr_n^2$ . Since on  $\cap_{i=1}^N A_i$ ,

$$J_{j1} = \sum_{i \in I_j} [\xi_i - E_{f_0}\{\xi_i\}] - n E_{f_0} \left\{ \int_{B_n} R_i(f, f_0) d\Pi^*(f) \times I_{A_i^c} \right\},$$

we get from (S.29) that with  $P_{f_0}$ -probability approaching one, for any  $1 \leq j \leq s$ ,

$$J_{j1} \geq -4\sqrt{nr_n} \log N - nr_n^2 \geq -2nr_n^2.$$

Meanwhile, for any  $f \in B_n$ ,  $J(f) \leq (1 + J(f_0)^{1/2})^2$ . Therefore,  $J_{j3} \geq -\frac{(1 + J(f_0)^{1/2})^2}{2} n \lambda$ . So, with probability approaching one, for any  $1 \leq j \leq s$ ,

$$I_{j1} \geq \exp \left( -5nr_n^2/2 - \frac{(1 + J(f_0)^{1/2})^2}{2} n \lambda \right) \Pi(B_n).$$

To proceed, we need a lower bound for  $\Pi(B_n)$ . It follows by Lemma 13 by replacing  $d_n$  therein by  $r_n$ , by Gaussian correlation inequality (see Theorem 1.1 of Li et al. (1999)), by Cameron-Martin theorem (see Cameron and Martin (1944) or (Kuelbs et al., 1994, eqn

(4.18))) and (Hoffmann-Jorgensen et al., 1979, Example 4.5) that

$$\begin{aligned}
 \Pi(B_n) &= P(V(G - f_0) \leq r_n^2, J(G - f_0) \leq r_n^{\frac{2(\beta-1)}{2m+\beta-1}}) \\
 &= P(\tilde{V}(\tilde{G} - \tilde{f}_0) \leq r_n^2, \tilde{J}(\tilde{G} - \tilde{f}_0) \leq r_n^{\frac{2(\beta-1)}{2m+\beta-1}}) \\
 &\geq P(\tilde{V}(\tilde{G} - \omega) \leq r_n^2/4, \tilde{J}(\tilde{G} - \omega) \leq r_n^{\frac{2(\beta-1)}{2m+\beta-1}}/4) \\
 &\geq \exp\left(-\frac{1}{2}\|\omega\|_\beta^2\right) P(\tilde{V}(\tilde{G}) \leq r_n^2/4, \tilde{J}(\tilde{G}) \leq r_n^{\frac{2(\beta-1)}{2m+\beta-1}}/4) \\
 &\geq \exp\left(-\frac{1}{2}\|\omega\|_\beta^2\right) P(\tilde{V}(\tilde{G}) \leq r_n^2/8) P(\tilde{J}(\tilde{G}) \leq r_n^{\frac{2(\beta-1)}{2m+\beta-1}}/8) \\
 &\geq \exp(-c_1 r_n^{-2/(2m+\beta-1)}), \tag{S.30}
 \end{aligned}$$

where  $c_1 > 0$  is a universal constant.

Since  $\beta > 1$  and  $r_n^2 = (nh)^{-1} + \lambda \geq n^{-2m/(2m+1)}$ , we get  $r_n^2 \geq \lambda$  and  $nr_n^{\frac{2(2m+\beta)}{2m+\beta-1}} \geq n^{1-\frac{2m(2m+\beta)}{(2m+1)(2m+\beta-1)}} > 1$ , so  $nr_n^2 > r_n^{-\frac{2}{2m+\beta-1}}$ . Consequently, with  $P_{f_0}$ -probability approaching one

$$\min_{1 \leq j \leq s} I_{j1} \geq \exp(-c_2 nr_n^2), \tag{S.31}$$

where  $c_2 = 5/2 + (1 + J(f_0)^{1/2})^2/2 + c_1$ .

Let  $b = 2\sqrt{c_2 + 1}$  and  $C \geq b^2/4$ . Next we examine  $I_{j2}$  defined in (S.27) with  $A_n = \{f \in S^m(\mathbb{I}) : \|f - f_0\| \geq 2\delta_n\}$ , for  $\delta_n = bh^m + 2c_K(C_\epsilon + C)r$ ,  $r = r_n h^{-1/2}$ . By the condition  $h^{-3/2}r_n = o(1)$  and  $B(h) \lesssim h^{-(2m-1)/(4m)}$  it can be easily checked that the Rate Condition **(H)**: is satisfied (when  $n$  becomes large) with  $M$  therein replaced by  $C$ . For  $1 \leq j \leq s$ , define test  $\phi_{j,n} = I(\|\widehat{f}_{j,n} - f_0\| \geq \delta_n)$ . It follows by part (1) of Theorem 4 that for any  $1 \leq j \leq s$ ,

$$E_{f_0}\{\phi_{j,n}\} = P_{f_0}(\|\widehat{f}_{j,n} - f_0\| \geq \delta_n) \leq 2 \exp(-Cnr_n^2),$$

and

$$\begin{aligned}
 \sup_{\substack{f \in H^m(b) \\ \|f - f_0\| \geq 2\delta_n}} E_f\{1 - \phi_{j,n}\} &= \sup_{\substack{f \in H^m(b) \\ \|f - f_0\| \geq 2\delta_n}} P_f(\|\widehat{f}_{j,n} - f_0\| < \delta_n) \\
 &\leq \sup_{\substack{f \in H^m(b) \\ \|f - f_0\| \geq 2\delta_n}} P_f(\|\widehat{f}_{j,n} - f\| \geq \delta_n) \leq 2 \exp(-Cnr_n^2).
 \end{aligned}$$

An immediate consequence is  $E_{f_0}\{\max_{1 \leq j \leq s} \phi_{j,n}\} \leq 2s \exp(-Cnr_n^2)$ , which implies  $\max_{1 \leq j \leq s} \phi_{j,n} = O_{P_{f_0}}(s \exp(-Cnr_n^2))$ .

Note that for any  $f \in A_n \setminus H^m(b)$ ,  $J(f) > b^2$ . Since  $nh^{2m+1} \geq 1$  leads to  $r_n^2 = (nh)^{-1} + \lambda \leq 2\lambda$ , it then holds that, for any  $1 \leq j \leq s$ ,

$$\begin{aligned}
& E_{f_0}\{I_{j2}(1 - \phi_{j,n})\} \\
&= \int_{A_n} \|f - f_0\|^a E_f\{1 - \phi_{j,n}\} \exp(-n\lambda J(f)/2) d\Pi(f) \\
&= \int_{A_n \setminus H^m(b)} \|f - f_0\|^a E_f\{1 - \phi_{j,n}\} \exp(-n\lambda J(f)/2) d\Pi(f) \\
&\quad + \int_{A_n \cap H^m(b)} \|f - f_0\|^a E_f\{1 - \phi_{j,n}\} \exp(-n\lambda J(f)/2) d\Pi(f) \\
&\leq (\exp(-b^2 n \lambda / 2) + 2 \exp(-Cnr_n^2)) C(a, \Pi) \\
&\leq 3 \exp(-b^2 nr_n^2 / 4) C(a, \Pi),
\end{aligned}$$

where the last inequality follows by  $C \geq b^2/4$  and  $\lambda \geq r_n^2/2$ . So

$$E_{f_0}\{\max_{1 \leq j \leq s} I_{j2}(1 - \phi_{j,n})\} \leq \sum_{j=1}^s E_{f_0}\{I_{j2}(1 - \phi_{j,n})\} \leq 3s \exp(-b^2 nr_n^2 / 4) C(a, \Pi),$$

which implies  $\max_{1 \leq j \leq s} I_{j2}(1 - \phi_{j,n}) = O_{P_{f_0}}(s \exp(-b^2 nr_n^2 / 4))$ . On the other hand, as  $n \rightarrow \infty$ ,

$$E_{f_0}\{\max_{1 \leq j \leq s} I_{j2}\} \leq s \int_{S^m(\mathbb{I})} \|f - f_0\|^2 d\Pi(f)$$

which implies that  $\max_{1 \leq j \leq s} I_{j2} = o_{P_{f_0}}(s)$ . Therefore,

$$\max_{1 \leq j \leq s} \frac{I_{j2}}{I_{j1}} \phi_{j,n} \leq \frac{\max_{1 \leq j \leq s} I_{j2} \times \max_{1 \leq j \leq s} \phi_{j,n}}{\min_{1 \leq j \leq s} I_{j1}} = O_{P_{f_0}}(s^2 \exp(-nr_n^2)). \quad (\text{S.32})$$

By the above arguments and (S.31), we have

$$\begin{aligned}
\max_{1 \leq j \leq s} \int_{A_n} \|f - f_0\|^a dP(f|\mathbf{D}_j) &= \max_{1 \leq j \leq s} \frac{I_{j2}}{I_{j1}} \\
&\leq \max_{1 \leq j \leq s} \frac{I_{j2}}{I_{j1}} \phi_{j,n} + \max_{1 \leq j \leq s} \frac{I_{j2}(1 - \phi_{j,n})}{I_{j1}} \\
&= O_{P_{f_0}}(s^2 \exp(-nr_n^2)) + O_{P_{f_0}}(s \exp(-b^2 nr_n^2 / 4) \exp(c_2 nr_n^2)) \\
&= O_{P_{f_0}}(s^2 \exp(-nr_n^2)).
\end{aligned}$$

By condition  $r_n h^{-3/2} = o(1)$  and the trivial fact  $\delta_n \asymp r_n h^{-1/2}$ , we have that  $h^{-1/2} \delta_n = o(1)$ . Therefore, eventually  $\int_{\|f - f_0\|_\infty \geq \varepsilon} \|f - f_0\|^a dP(f|\mathbf{D}_j) \leq \int_{A_n} \|f - f_0\|^a dP(f|\mathbf{D}_j)$  for all  $1 \leq j \leq s$ , which implies that (S.25) holds.

Now we will prove the theorem. Let  $I'_{j2}$  be defined as in (S.28) with  $A'_n = \{f \in S^m(\mathbb{I}) : \|f - f_0\| \geq \sqrt{2}Mr_n\}$  for a fixed number satisfying  $M > \max\{2, J(f_0)^{1/2} + \sqrt{2(c_2 + 1)}, 1 + \|f_0\|_\infty\}$  ( $M$  will be further described). Let  $A'_{n1} = \{f \in S^m(\mathbb{I}) : V(f - f_0) \geq M^2 r_n^2, \lambda J(f - f_0) \leq M^2 r_n^2\}$  and  $A'_{n2} = \{f \in S^m(\mathbb{I}) : \lambda J(f - f_0) \geq M^2 r_n^2\}$ . For any  $f \in A'_{n2}$ , it can be shown that

$$Mr_n \leq \sqrt{\lambda J(f - f_0)} \leq \sqrt{\lambda}(J(f)^{1/2} + J(f_0)^{1/2}) \leq (\lambda J(f))^{1/2} + J(f_0)^{1/2} r_n,$$

which leads to  $\lambda J(f) \geq (M - J(f_0)^{1/2})^2 r_n^2$ . So we have

$$\begin{aligned}
 & E_{f_0} \left\{ \max_{1 \leq j \leq s} \int_{A'_{n2}} \|f - f_0\|^a \prod_{i \in I_j} (p_f/p_{f_0})(Z_i) \exp\left(-\frac{n\lambda}{2} J(f)\right) d\Pi(f) \right\} \\
 & \leq \sum_{j=1}^s E_{f_0} \left\{ \int_{A'_{n2}} \|f - f_0\|^a \prod_{i \in I_j} (p_f/p_{f_0})(Z_i) \exp\left(-\frac{n\lambda}{2} J(f)\right) d\Pi(f) \right\} \\
 & = s \int_{A'_{n2}} \|f - f_0\|^a \exp\left(-\frac{n\lambda}{2} J(f)\right) d\Pi(f) \\
 & \leq s \exp(-(M - J(f_0)^{1/2})^2 nr_n^2/2) C(a, \Pi),
 \end{aligned}$$

which leads to that

$$\begin{aligned}
 & \max_{1 \leq j \leq s} \int_{A'_{n2}} \|f - f_0\|^a \prod_{i \in I_j} (p_f/p_{f_0})(Z_i) \exp\left(-\frac{n\lambda}{2} J(f)\right) d\Pi(f) \\
 & = O_{P_{f_0}}(s \exp(-(M - J(f_0)^{1/2})^2 nr_n^2/2)). \tag{S.33}
 \end{aligned}$$

It follows from (S.31) and (S.33) that

$$\begin{aligned}
 & \max_{1 \leq j \leq s} \frac{1}{I_{j1}} \int_{A'_{n2}} \|f - f_0\|^a \prod_{i \in I_j} (p_f/p_{f_0})(Z_i) \exp\left(-\frac{n\lambda}{2} J(f)\right) d\Pi(f) \\
 & = O_{P_{f_0}} \left( s \exp(-(M - J(f_0)^{1/2})^2 nr_n^2/2 + c_2 nr_n^2) \right) = O_{P_{f_0}}(s \exp(-nr_n^2)), \tag{S.34}
 \end{aligned}$$

where the last inequality follows by  $(M - J(f_0)^{1/2})^2 > 2(c_2 + 1)$ .

To continue, we need to build uniformly consistent test. Let  $d_H^2(P_f, P_g) = \frac{1}{2} \int (\sqrt{dP_f} - \sqrt{dP_g})^2$  be the squared Hellinger distance between the two probability measures  $P_f(z)$  and  $P_g(z)$ . Recall that their corresponding probability density functions are  $p_f$  and  $p_g$ , respectively. Next we present a lemma showing the local equivalence of  $V$  and  $d_H^2$ .

**Lemma 14** *Let  $\varepsilon \in (0, 1)$  satisfy  $\varepsilon^2 + 32\varepsilon \exp(1/2)C_\varepsilon \leq 2$ , where  $C_\varepsilon = E\{\exp(|\varepsilon|)\}$ . Then for any  $f, g \in S^m(\mathbb{I})$  satisfying  $\|f - g\|_\infty \leq \varepsilon$ ,  $V(f - g)/16 \leq d_H^2(P_f, P_g) \leq 3V(f - g)/16$ .*

Let  $\varepsilon$  satisfy the conditions in Lemma 14. Define  $\mathcal{F}_n = \{f \in S^m(\mathbb{I}) : \|f - f_0\|_\infty \leq \varepsilon/2, J(f) \leq (M + J(f_0)^{1/2})^2 r_n^2 \lambda^{-1}\}$ . Let  $\mathcal{P}_n = \{P_f : f \in \mathcal{F}_n\}$  and  $D(\delta, \mathcal{P}_n, d_H)$  be the  $\delta$ -packing number in terms of  $d_H$ . Since  $r_n^2 \geq \lambda$  which leads to  $(M + J(f_0)^{1/2})r_n h^{-m} > M + J(f_0)^{1/2} > \varepsilon + \|f_0\|_\infty$ , it can be easily checked that  $\mathcal{F}_n \subset (M + J(f_0)^{1/2})r_n h^{-m} \mathcal{T}$ , where  $\mathcal{T} = \{f \in S^m(\mathbb{I}) : \|f\|_\infty \leq 1, J(f) \leq 1\}$ .

For any  $f, g \in \mathcal{F}_n$  with  $\|f - g\|_\infty \leq \varepsilon$ , it follows by Lemma 14 that  $D(\delta, \mathcal{P}_n, d_H) \leq D(4\delta/\sqrt{3}, \mathcal{F}_n, d_V)$ , where  $d_V$  is the distance induced by  $V$ , i.e.,  $d_V(f, g) = V^{1/2}(f - g)$ . And hence, it follows by (Kosorok, 2008, Theorem 9.21) that

$$\begin{aligned}
 \log D(\delta, \mathcal{P}_n, d_H) & \leq \log D(4\delta/\sqrt{3}, \mathcal{F}_n, d_V) \\
 & \leq \log D(4\delta/\sqrt{3}, (M + J(f_0)^{1/2})r_n h^{-m} \mathcal{T}, d_V) \\
 & \leq c_V \left( \frac{\delta}{(M + J(f_0)^{1/2})r_n h^{-m}} \right)^{-1/m},
 \end{aligned}$$

where  $c_V$  is a universal constant only depending on the regularity level  $m$ . This implies that for any  $\delta > 2r_n$ ,

$$\begin{aligned}\log D(\delta/2, \mathcal{P}_n, d_H) &\leq \log D(r_n, \mathcal{P}_n, d_H) \\ &\leq c_V(M + J(f_0)^{1/2})^{1/m} h^{-1} \\ &\leq c_V(M + J(f_0)^{1/2})^{1/m} n r_n^2,\end{aligned}$$

where the last inequality follows by the fact  $r_n^2 \geq (nh)^{-1}$ . Thus, the right side of the above inequality is constant in  $\delta$ . By (Ghosal et al., 2000, Theorem 7.1), with  $\delta = Mr_n/4$ , there exists test  $\tilde{\phi}_{j,n}$  and a universal constant  $k_0 > 0$  satisfying

$$\begin{aligned}E_{f_0}\{\tilde{\phi}_{j,n}\} &= P_{f_0}\tilde{\phi}_{j,n} \\ &\leq \frac{\exp(c_V(M + J(f_0)^{1/2})^{1/m} n r_n^2) \exp(-k_0 n \delta^2)}{1 - \exp(-k_0 n \delta^2)} \\ &= \frac{\exp(c_V(M + J(f_0)^{1/2}) n r_n^2 - k_0 M^2 n r_n^2 / 16)}{1 - \exp(-k_0 M^2 n r_n^2 / 16)},\end{aligned}$$

and, combined with Lemma 14,

$$\begin{aligned}\sup_{\substack{f \in \mathcal{F}_n \\ d_V(f, f_0) \geq 4\delta}} E_f\{1 - \tilde{\phi}_{j,n}\} &= \sup_{\substack{f \in \mathcal{F}_n \\ d_V(f, f_0) \geq 4\delta}} P_f\{1 - \tilde{\phi}_{j,n}\} \\ &\leq \sup_{\substack{f \in \mathcal{F}_n \\ d_H(P_f, P_{f_0}) \geq \delta}} P_f\{1 - \tilde{\phi}_{j,n}\} \\ &\leq \exp(-k_0 n \delta^2) = \exp(-k_0 M^2 n r_n^2 / 16).\end{aligned}$$

This implies that

$$\begin{aligned}E_{f_0}\{\max_{1 \leq j \leq s} \int_{d_V(f, f_0) \geq 4\delta} \|f - f_0\|^a \prod_{i \in I_j} (p_f/p_{f_0})(Z_i) \exp(-n\lambda J(f)/2) d\Pi(f) (1 - \tilde{\phi}_{j,n})\} \\ &\leq \sum_{j=1}^s \int_{d_V(f, f_0) \geq 4\delta} \|f - f_0\|^a E_{f_0}\{\prod_{i \in I_j} (p_f/p_{f_0})(Z_i) (1 - \tilde{\phi}_{j,n})\} d\Pi(f) \\ &= \sum_{j=1}^s \int_{d_V(f, f_0) \geq 4\delta} \|f - f_0\|^a E_f\{1 - \tilde{\phi}_{j,n}\} d\Pi(f) \\ &\leq s \exp(-k_0 M^2 n r_n^2 / 16) C(a, \Pi).\end{aligned}$$

Therefore,

$$\begin{aligned}\max_{1 \leq j \leq s} \int_{d_V(f, f_0) \geq 4\delta} \|f - f_0\|^a \prod_{i \in I_j} (p_f/p_{f_0})(Z_i) \exp(-n\lambda J(f)/2) d\Pi(f) (1 - \tilde{\phi}_{j,n}) \\ = O_{P_{f_0}}(s \exp(-k_0 M^2 n r_n^2 / 16)).\end{aligned}\tag{S.35}$$

Meanwhile, it follows by (S.31) and (S.35) that

$$\begin{aligned}
 & \max_{1 \leq j \leq s} \int_{A'_{n1}, \|f-f_0\|_\infty \leq \varepsilon/2} \|f-f_0\|^a dP(f|\mathbf{D}_j) (1 - \tilde{\phi}_{j,n}) \\
 & \leq \max_{1 \leq j \leq s} \int_{\mathcal{F}_n, d_V(f, f_0) \geq 4\delta} \|f-f_0\|^a dP(f|\mathbf{D}_j) (1 - \tilde{\phi}_{j,n}) \\
 & \leq \frac{\max_{1 \leq j \leq s} \int_{\mathcal{F}_n, d_V(f, f_0) \geq 4\delta} \|f-f_0\|^a \prod_{i \in I_j} (p_f/p_{f_0})(Z_i) \exp(-n\lambda J(f)/2) d\Pi(f) (1 - \tilde{\phi}_{j,n})}{\min_{1 \leq j \leq s} I_{j1}} \\
 & = O_{P_{f_0}}(s \exp(-k_0 M^2 nr_n^2/16 + c_2 nr_n^2)) = O_{P_{f_0}}(s \exp(-nr_n^2)).
 \end{aligned}$$

Choose the constant  $M$  to be even bigger so that  $c_V(M + J(f_0)^{1/2}) + 1 + c_2 < k_0 M^2/16$ . Similar to (S.32) we get

$$\max_{1 \leq j \leq s} \int_{A'_{n1}, \|f-f_0\|_\infty \leq \varepsilon/2} \|f-f_0\|^a dP(f|\mathbf{D}_j) \tilde{\phi}_{j,n} = O_{P_{f_0}}(s^2 \exp(-nr_n^2)).$$

Therefore,

$$\max_{1 \leq j \leq s} \int_{A'_{n1}, \|f-f_0\|_\infty \leq \varepsilon/2} \|f-f_0\|^a dP(f|\mathbf{D}_j) = O_{P_{f_0}}(s^2 \exp(-nr_n^2)). \quad (\text{S.36})$$

Together with (S.25), (S.32) and (S.36), we get

$$\begin{aligned}
 & \max_{1 \leq j \leq s} \int_{A'_n} \|f-f_0\|^a dP(f|\mathbf{D}_j) \\
 & \leq \max_{1 \leq j \leq s} \int_{A'_{n1}} \|f-f_0\|^a dP(f|\mathbf{D}_j) + \max_{1 \leq j \leq s} \int_{A'_{n2}} \|f-f_0\|^a dP(f|\mathbf{D}_j) \\
 & \leq \max_{1 \leq j \leq s} \int_{A'_{n1}, \|f-f_0\|_\infty \leq \varepsilon/2} \|f-f_0\|^a dP(f|\mathbf{D}_j) + \max_{1 \leq j \leq s} \int_{\|f-f_0\|_\infty > \varepsilon/2} \|f-f_0\|^a dP(f|\mathbf{D}_j) \\
 & \quad + \max_{1 \leq j \leq s} \int_{A'_{n2}} \|f-f_0\|^a dP(f|\mathbf{D}_j) \\
 & = O_{P_{f_0}}(s^2 \exp(-nr_n^2)).
 \end{aligned}$$

This completes the proof. ■

**Proof** [Proof of Lemma 14] For any  $f, g \in S^m(\mathbb{I})$  with  $\|f-g\|_\infty \leq \varepsilon$ , define  $\Delta_Z(f, g) = \frac{1}{2}[Y(f(X) - g(X)) - f(X)^2/2 + g(X)^2/2]$ , where recall and  $Z = (Y, X)$ . It is easy to see by direct calculations that  $d_H^2(P_f, P_g) = 1 - E_g\{\exp(\Delta_Z(f, g))\}$ . By Taylor's expansion, for some random  $t \in [0, 1]$ ,

$$\begin{aligned}
 & 1 - E_g\{\exp(\Delta_Z(f, g))\} \\
 & = -E_g\{\Delta_Z(f, g)\} - \frac{1}{2}E_g\{\Delta_Z(f, g)^2\} - \frac{1}{6}E_g\{\exp(t\Delta_Z(f, g))\Delta_Z(f, g)^3\}.
 \end{aligned}$$

We will analyze the terms on the right side of the equation.

Define  $\xi = Y - \dot{A}(g(X))$ . By Morris et al. (1983) we get  $E_g\{\xi|X\} = 0$  and  $E_g\{\xi^2|X\} = 1$ . By Taylor's expansion,  $\Delta_Z(f, g) = \frac{1}{2}[\xi(f(X) - g(X)) - \frac{1}{2}(f(X) - g(X))^2]$ . Then we get that  $-E_g\{\Delta_Z(f, g)\} = \frac{1}{4}V(f - g)$  and

$$\begin{aligned} E_g\{\Delta_Z(f, g)^2\} &= E_g\left\{\left(\frac{1}{2}\xi(f(X) - g(X)) - \frac{1}{4}(f(X) - g(X))^2\right)^2\right\} \\ &= \frac{1}{4}E_g\{\xi^2(f(X) - g(X))^2\} - \frac{1}{4}E_g\{\xi(f(X) - g(X))^3\} + \frac{1}{16}E_g\{(f(X) - g(X))^4\} \\ &= \frac{1}{4}V(f - g) + \frac{1}{16}E_g\{(f(X) - g(X))^4\}. \end{aligned}$$

Since  $\|f - g\|_\infty \leq \varepsilon < 1$  and  $|\Delta_Z(f, g)| \leq \frac{1}{2}(|\xi| + 1/2)|f(X) - g(X)|$ , we get

$$\begin{aligned} &|E_g\{\exp(t\Delta_Z(f, g))\Delta_Z(f, g)^3\}| \\ &\leq E_g\{\exp(|\Delta_Z(f, g)|)|\Delta_Z(f, g)|^3\} \\ &\leq E_g\{\exp(\varepsilon|\xi|/2 + \varepsilon/4)(|\xi|/2 + 1/4)^3|f(X) - g(X)|^3\} \\ &= 6E_g\left\{\exp(\varepsilon|\xi|/2 + \varepsilon/4) \times \frac{1}{3!}(|\xi|/2 + 1/4)^3|f(X) - g(X)|^3\right\} \\ &\leq 6E_g\{\exp(\varepsilon|\xi|/2 + \varepsilon/4)\exp(|\xi|/2 + 1/4)|f(X) - g(X)|^3\} \\ &\leq 6\exp(\varepsilon/4 + 1/4)E_g\{\exp(|\xi|)|f(X) - g(X)|^3\} \\ &\leq 6\varepsilon\exp(1/2)C_\varepsilon V(f - g). \end{aligned}$$

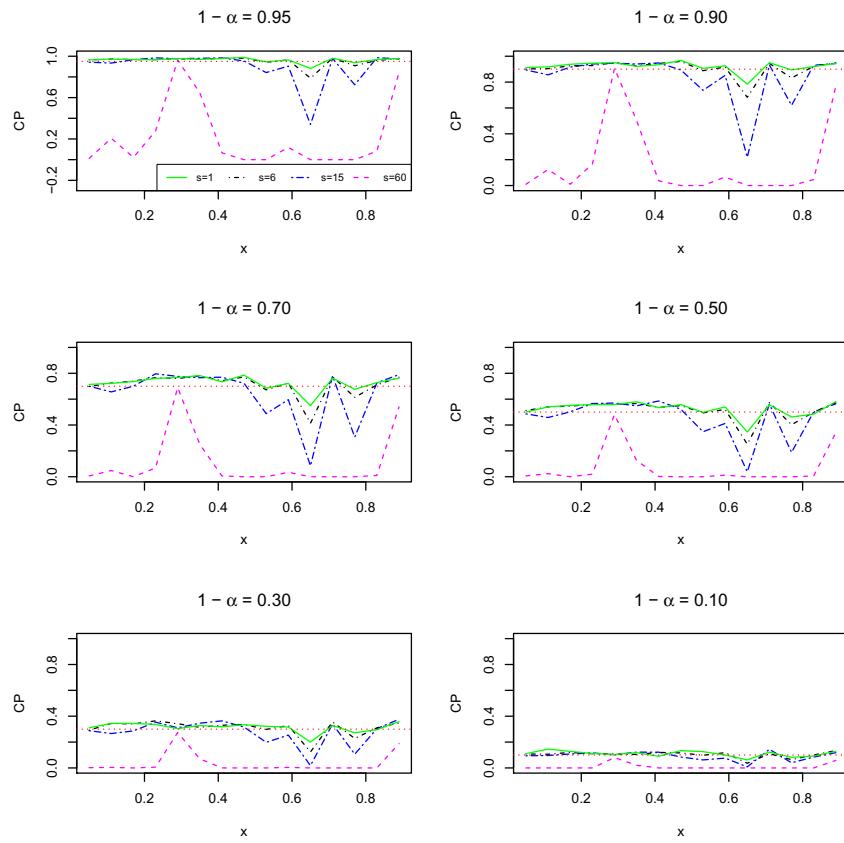
It also holds that  $|E_g\{(f(X) - g(X))^4\}| \leq \varepsilon^2V(f - g)$ . Therefore, for any  $f, g \in S^m(\mathbb{I})$  with  $\|f - g\|_\infty \leq \varepsilon$ ,

$$\begin{aligned} &|d_H^2(P_f, P_g) - V(f - g)/8| \\ &= \left|\frac{1}{32}E_g\{(f(X) - g(X))^4\} + \frac{1}{6}E_g\{\exp(t\Delta_Z(f, g))\Delta_Z(f, g)^3\}\right| \\ &\leq (\varepsilon C_\varepsilon \exp(1/2) + \varepsilon^2/32)V(f - g) < V(f - g)/16, \end{aligned}$$

which implies  $V(f - g)/16 \leq d_H^2(P_f, P_g) \leq 3V(f - g)/16$ . This proves Lemma 14.  $\blacksquare$

### S.8.6. Additional Plots in Section 5

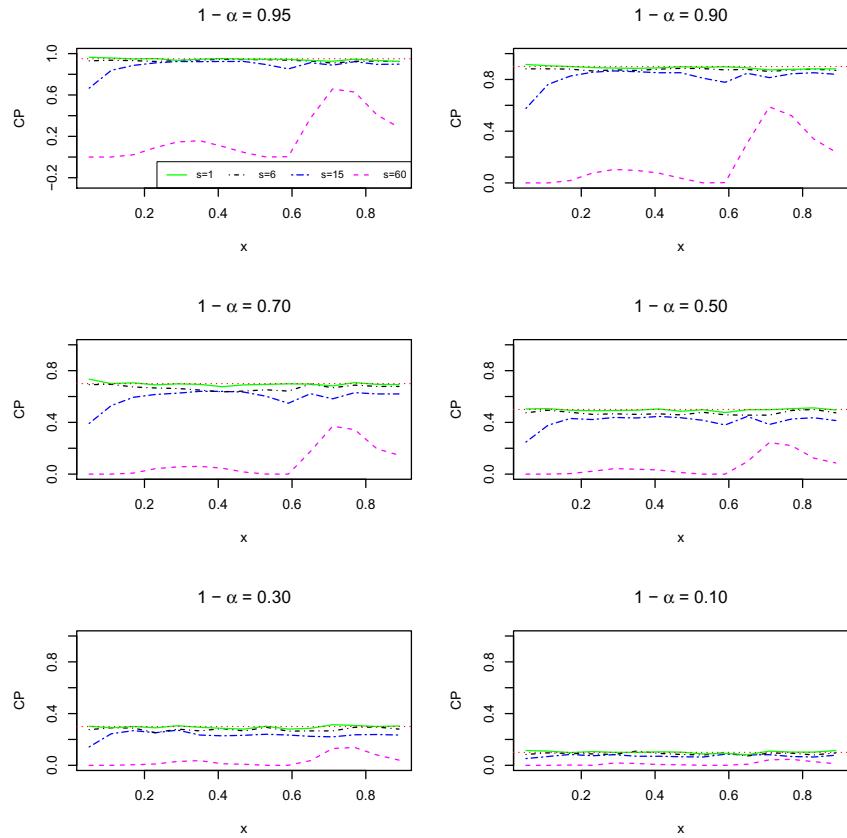
#### RADIUS OF THE CREDIBLE SETS/INTERVALS



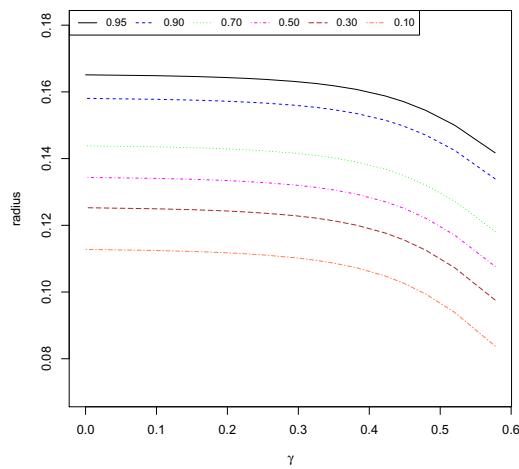
**Figure 11.**  $CP$  of  $F_x(f) = f(x)$  against  $x$  based on asymptotic theory.

#### RESULTS ON LARGER $N$

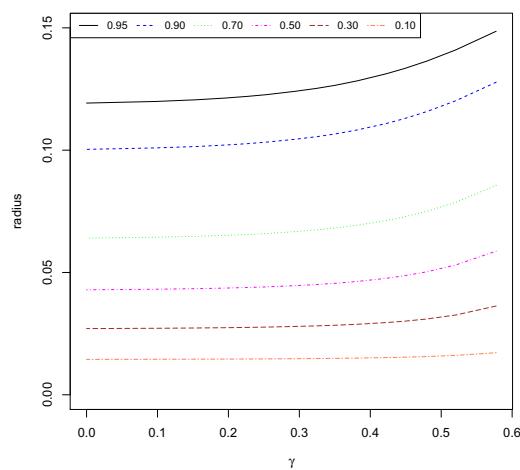
Simulation results about credible regions/intervals in Section 5 are based on  $N = 1200$ . This section repeated the same study for  $N = 1800, 2400$ . Results are summarized in following plots.



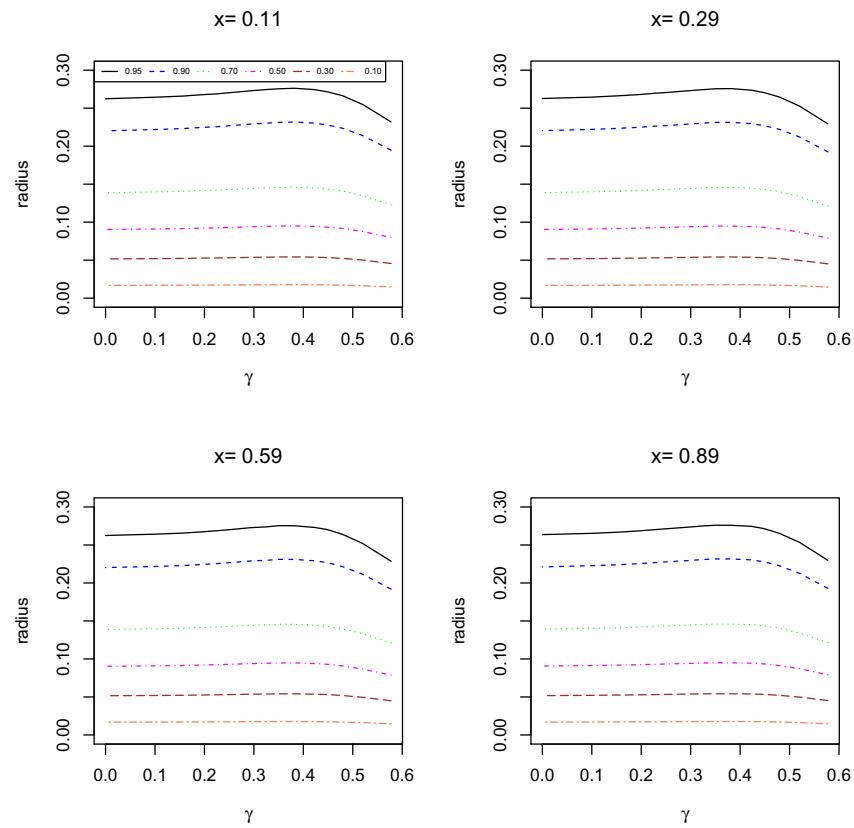
**Figure 12.**  $CP$  of  $F_x(f) = \int_0^x f(z)dz$  against  $x$  based on asymptotic theory.



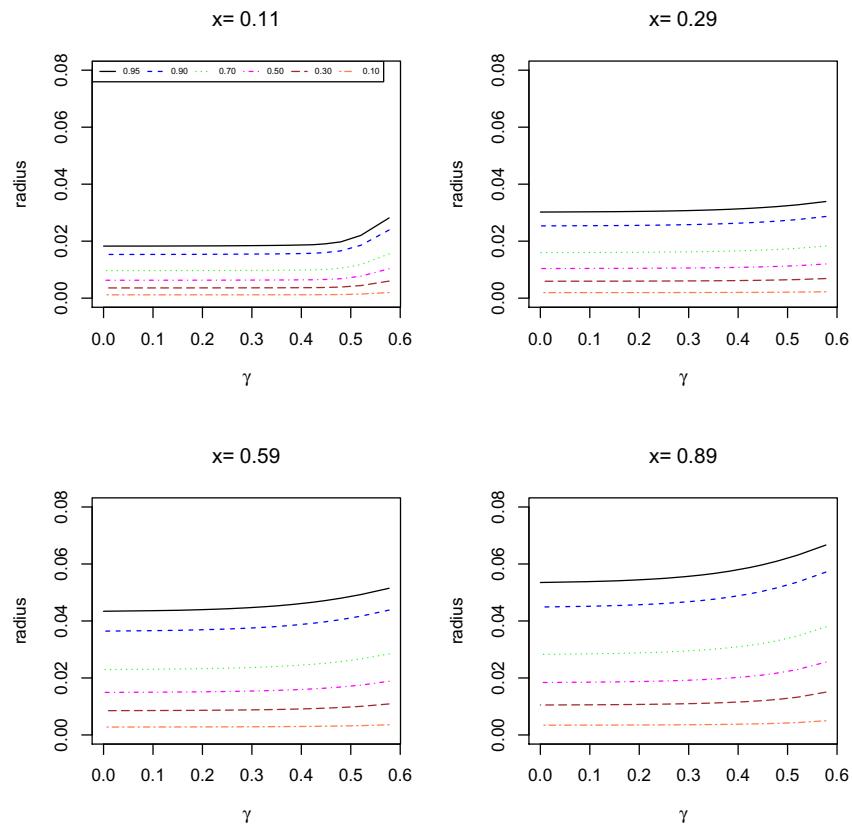
**Figure 13.** Radius of credible region (32) against  $\gamma$ . Legend indicates the credibility levels  $1 - \alpha$ .



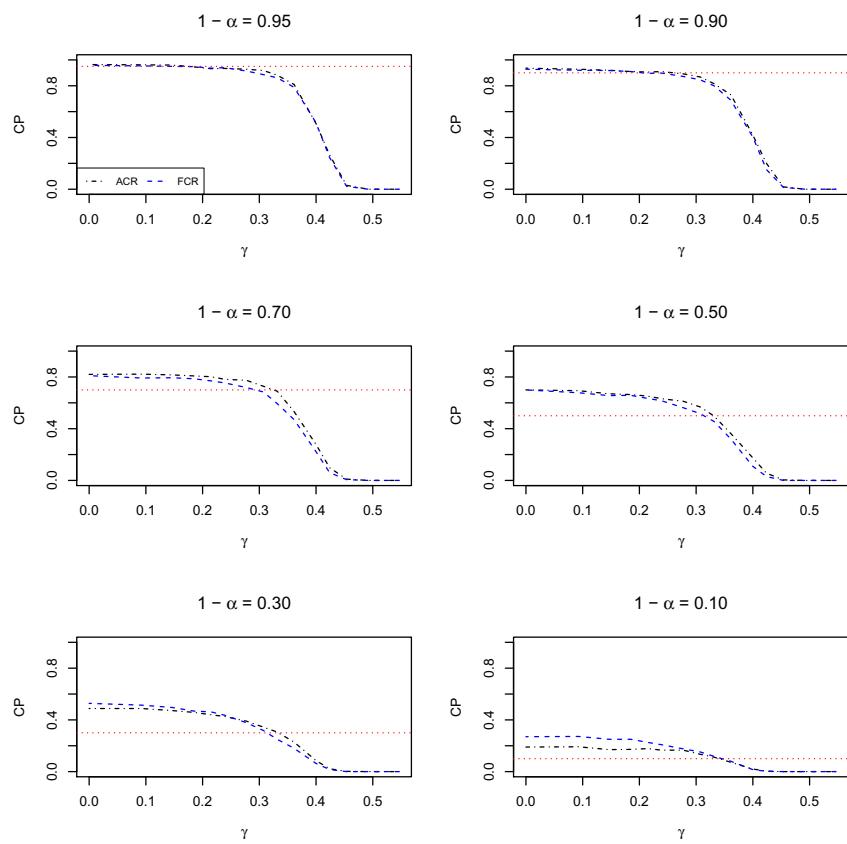
**Figure 14.** Radius of credible region (33) against  $\gamma$ . Legend indicates the credibility levels  $1 - \alpha$ .



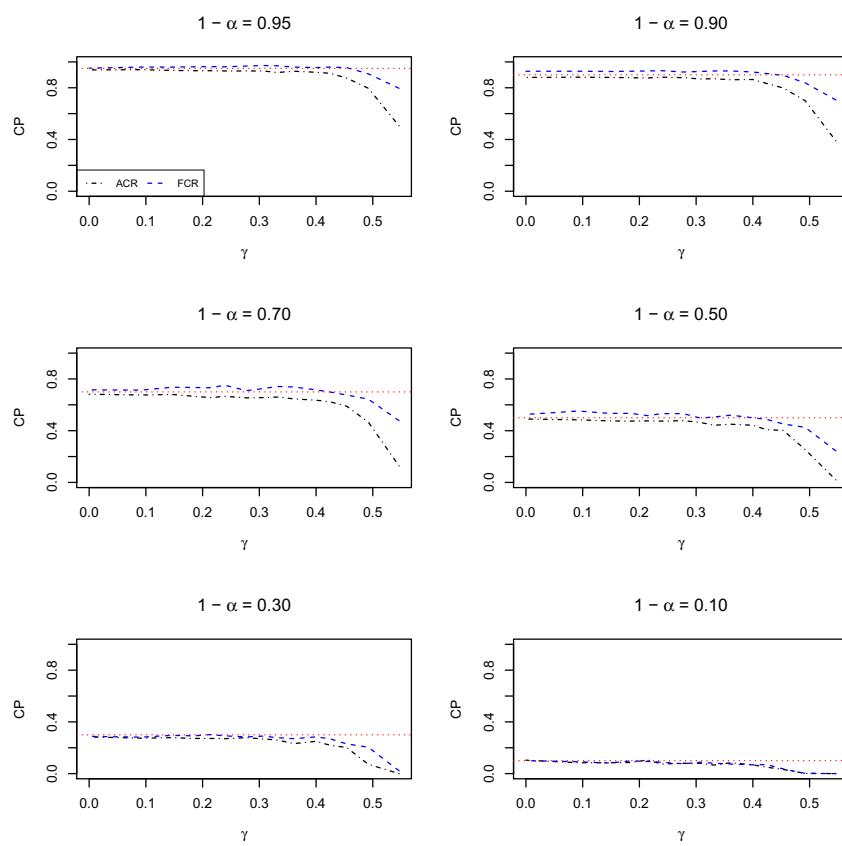
**Figure 15.** Radius of credible interval (36) for pointwise functional  $F_x(f) = f(x)$  against  $\gamma$ . Legend indicates the credibility levels  $1 - \alpha$ . Four values of  $x$  are considered.



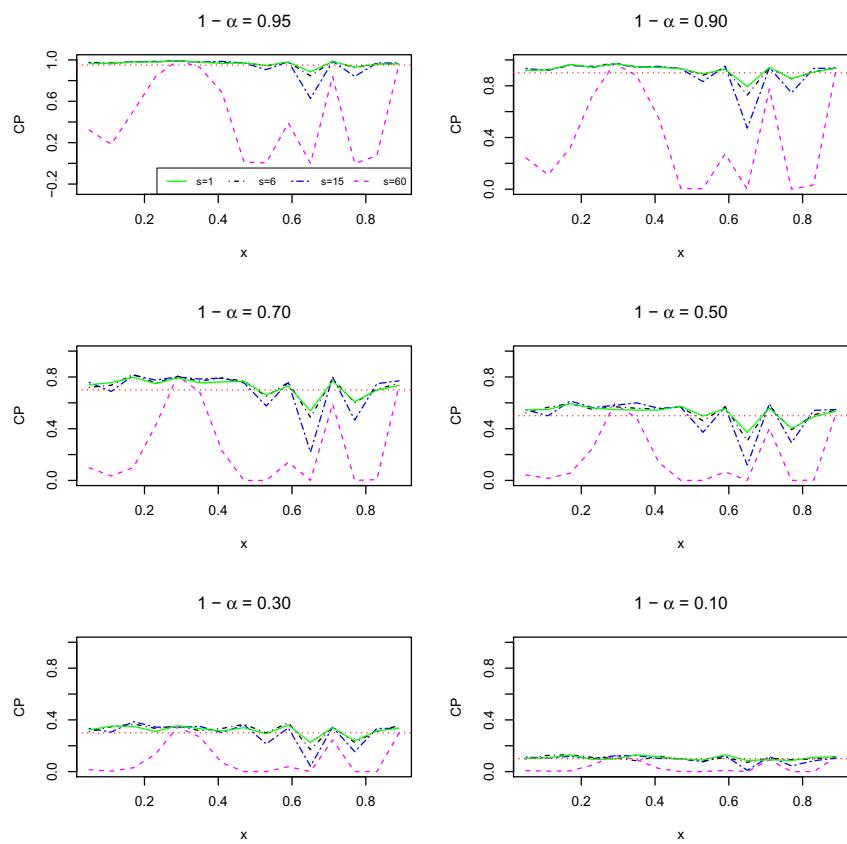
**Figure 16.** Radius of credible interval (36) for integral functional  $F_x(f) = \int_0^x f(z)dz$  against  $\gamma$ . Legend indicates the credibility levels  $1 - \alpha$ . Four values of  $x$  are considered.



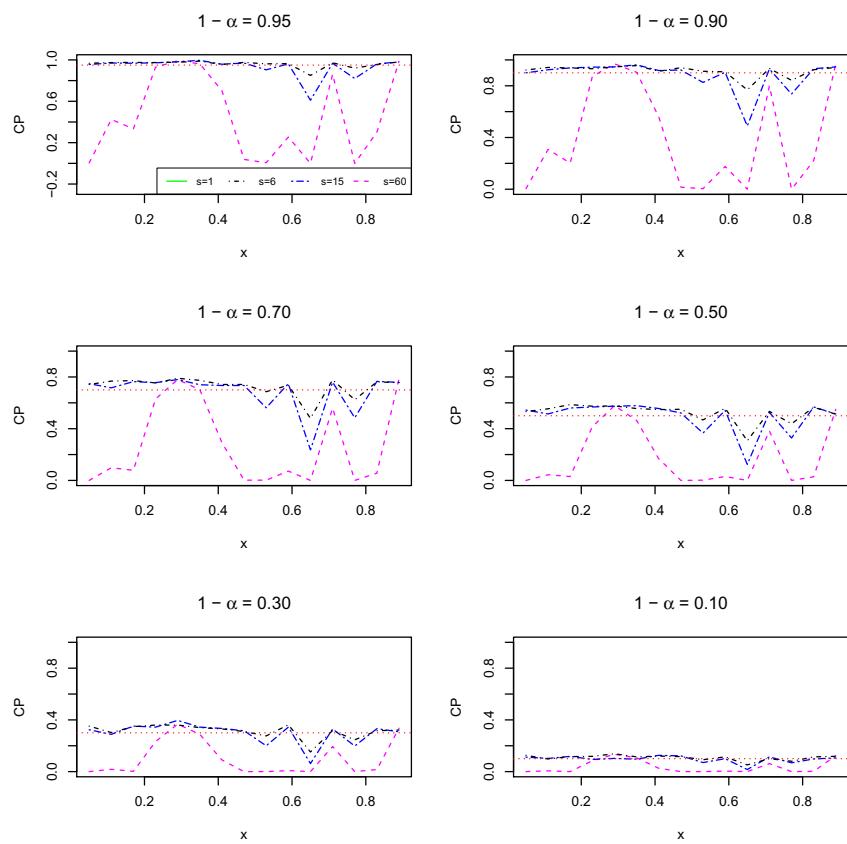
**Figure 17.**  $N = 1800$ : CP of ACR and FCR based on strong topology.



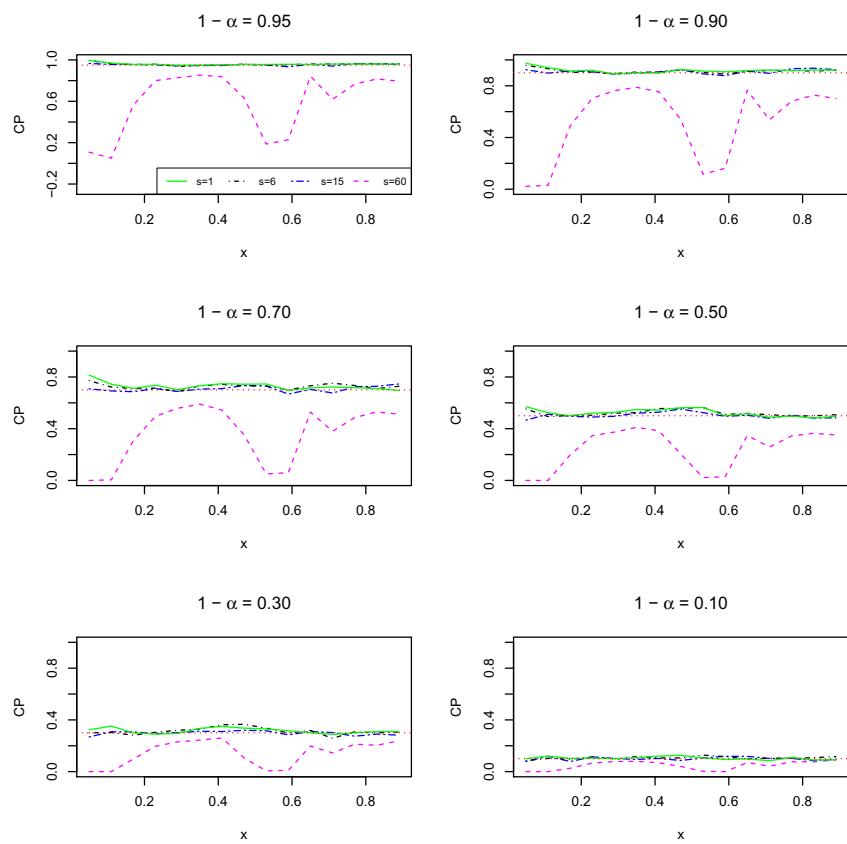
**Figure 18.**  $N = 1800$ : CP of ACR and FCR based on weak topology.



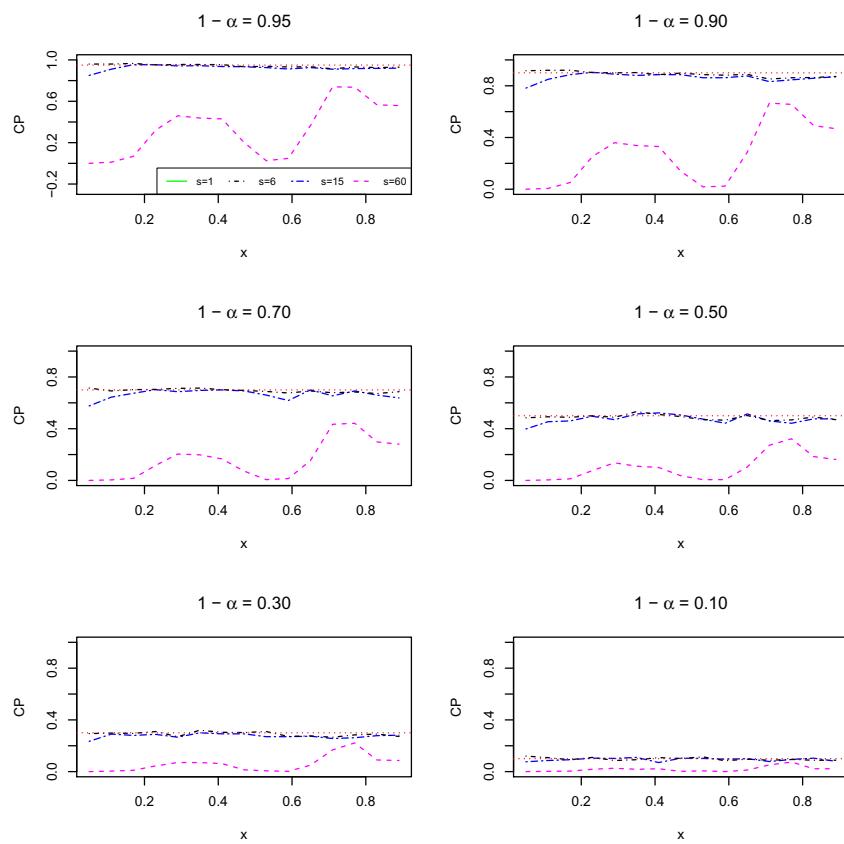
**Figure 19.**  $N = 1800$ : CP of  $F_x(f) = f(x)$  against  $x$  based on posterior samples of  $f$ .



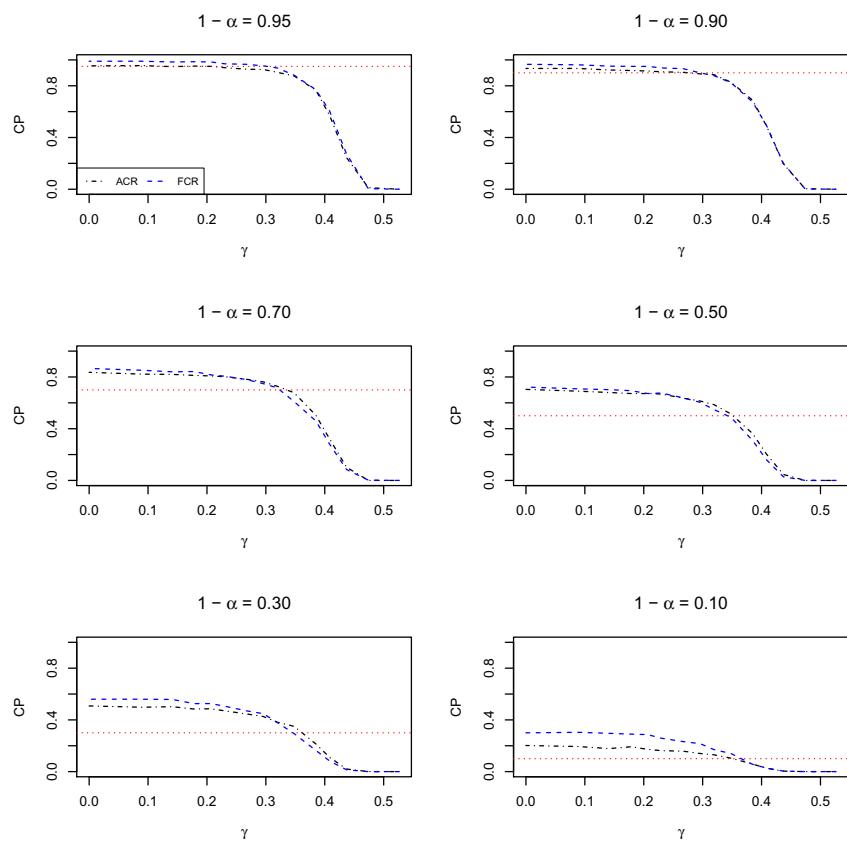
**Figure 20.**  $N = 1800$ : CP of  $F_x(f) = f(x)$  against  $x$  based on asymptotic theory.



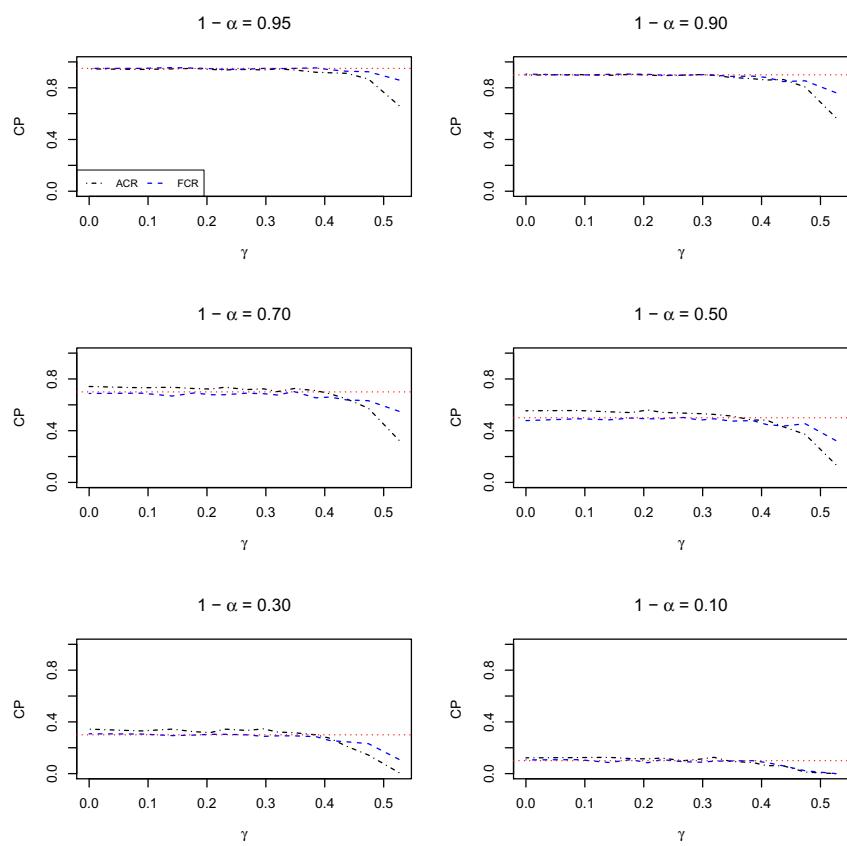
**Figure 21.**  $N = 1800$ : CP of  $F_x(f) = \int_0^x f(z)dz$  against  $x$  based on posterior samples of  $f$ .



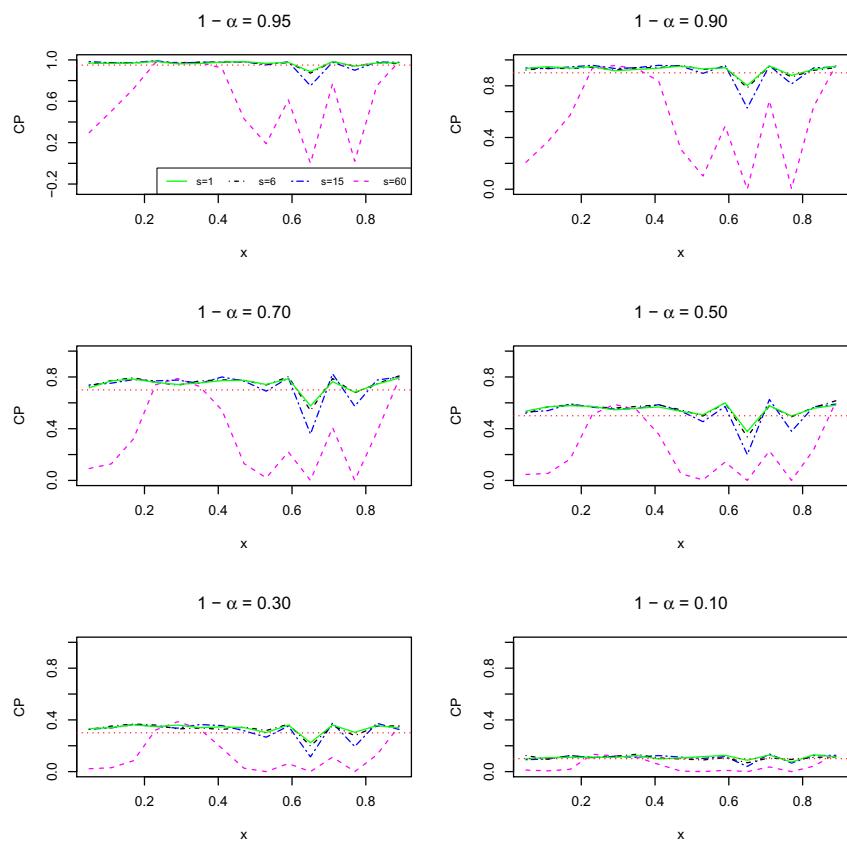
**Figure 22.**  $N = 1800$ : CP of  $F_x(f) = \int_0^x f(z)dz$  against  $x$  based on asymptotic theory.



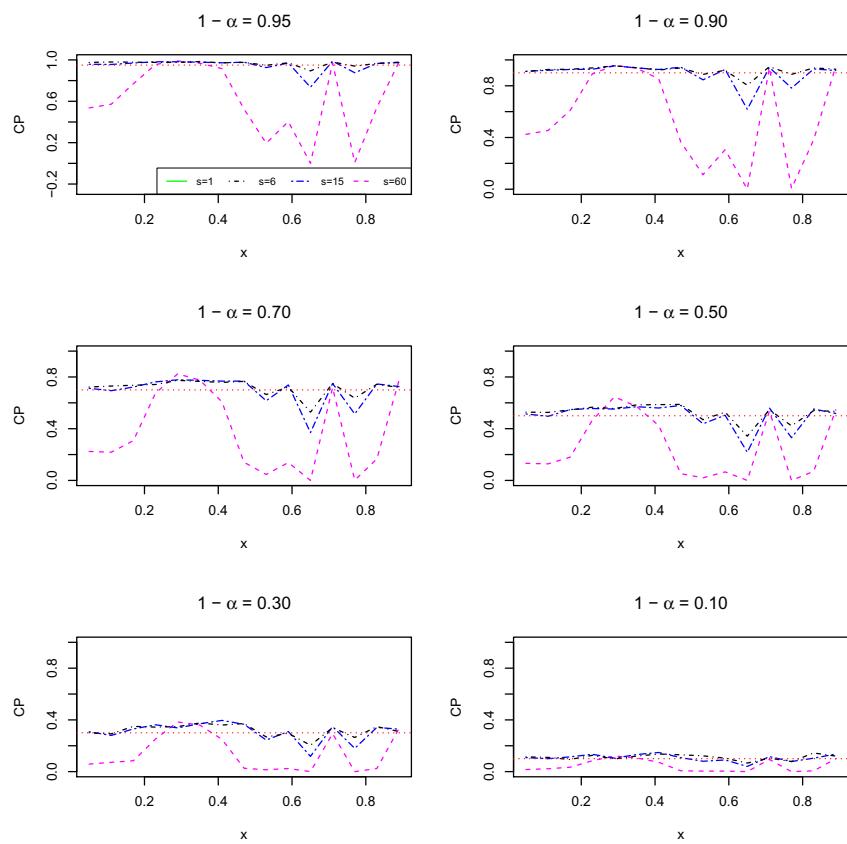
**Figure 23.**  $N = 2400$ : CP of ACR and FCR based on strong topology.



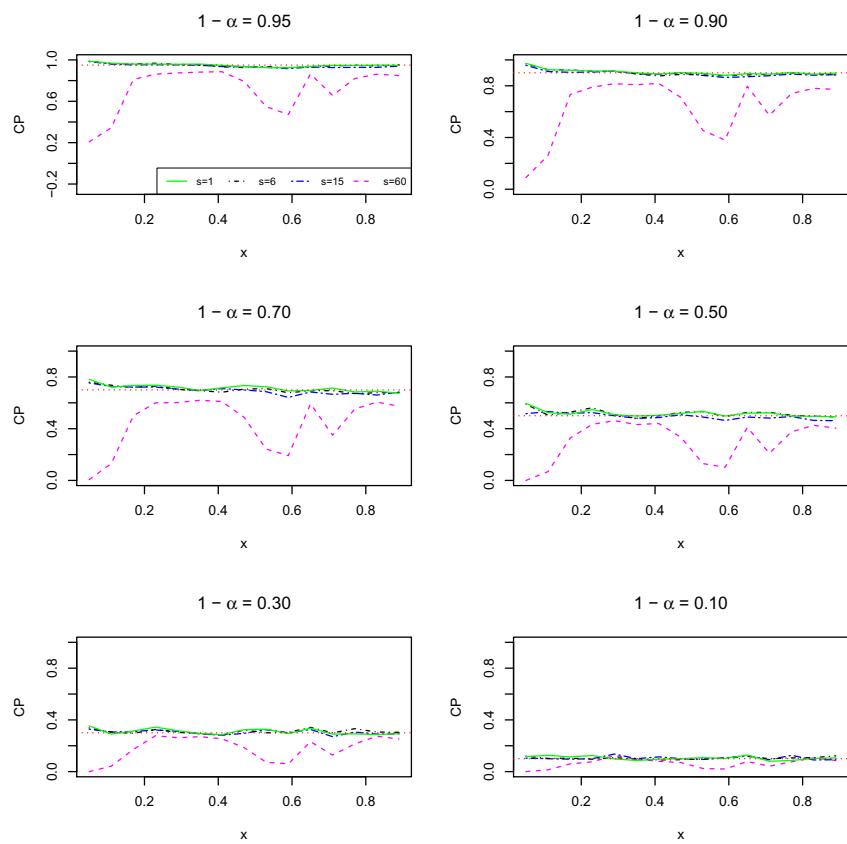
**Figure 24.**  $N = 2400$ : CP of ACR and FCR based on weak topology.



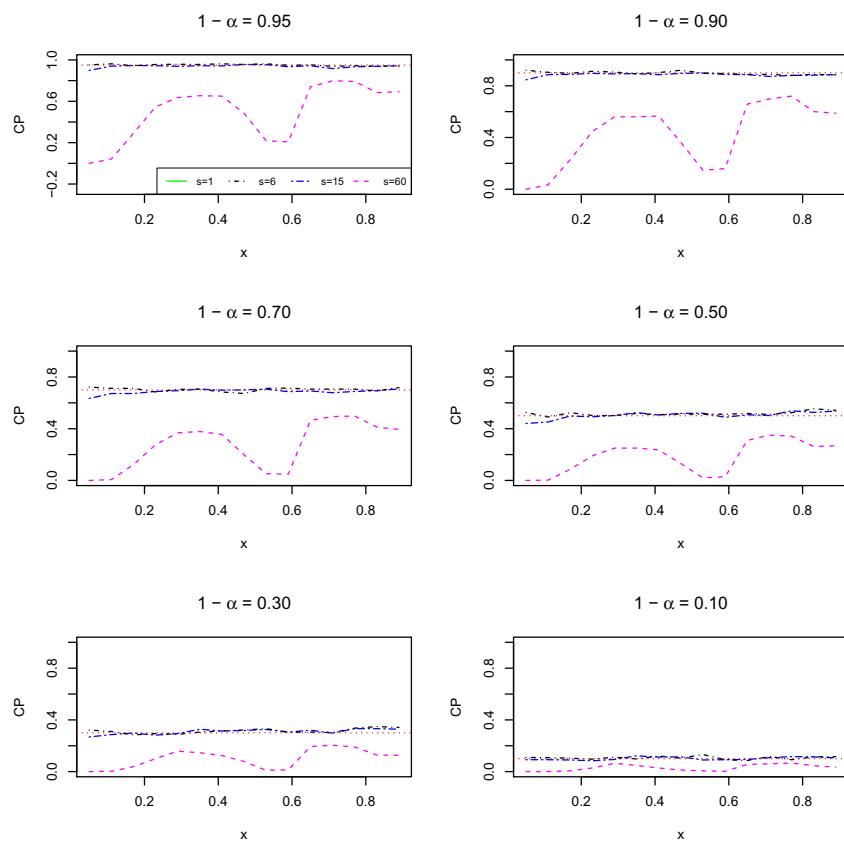
**Figure 25.**  $N = 2400$ :  $CP$  of  $F_x(f) = f(x)$  against  $x$  based on posterior samples of  $f$ .



**Figure 26.**  $N = 2400$ : CP of  $F_x(f) = f(x)$  against  $x$  based on asymptotic theory.



**Figure 27.**  $N = 2400$ : CP of  $F_x(f) = \int_0^x f(z)dz$  against  $x$  based on posterior samples of  $f$ .



**Figure 28.**  $N = 2400$ : CP of  $F_x(f) = \int_0^x f(z)dz$  against  $x$  based on asymptotic theory.