

# Posterior contraction rates for constrained deep Gaussian processes in density estimation and classification

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## Abstract

We provide posterior contraction rates for constrained deep Gaussian processes in non-parametric density estimation and classification. The constraints are in the form of bounds on the values and on the derivatives of the Gaussian processes in the layers of the composition structure. The contraction rates are first given in a general framework, in terms of a new concentration function that we introduce and that takes the constraints into account. Then, the general framework is applied to integrated Brownian motions, Riemann-Liouville processes, and Matérn processes and to standard smoothness classes of functions. In each of these examples, we can recover known minimax rates.

*Keywords:* Gaussian priors, deep Gaussian priors, Bayesian inference, nonparametric density estimation, classification, posterior contraction, smoothness classes, Matérn covariance functions.

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## 1 Introduction

Gaussian processes are widely used in statistics and machine learning to model a wide range of data [37]. They have become a popular method for a large range of applications, such

as geostatistics [7, 32, 35], numerical code approximation [39, 41, 2], calibration [34, 3], and global optimization [23]. In particular, they have been adopted in nonparametric Bayesian methods for constructing prior distributions for infinite-dimensional statistical models in several settings. Many related theoretical contributions were obtained since the late 2000's [45] and practical contributions have been developed even before [26]. We refer to the following books on the topic [37, 18] and the references therein. For instance, when considering the nonparametric estimation of a density relative to some measure  $\mu$  from a sample  $(X_1, \dots, X_n)$ , one may consider as prior distribution the random density

$$p_Z(x) = \frac{e^{Z(x)}}{\int e^{Z(y)} d\mu(y)},$$

where  $(Z(x))_{x \in \mathcal{X}}$  is a Gaussian process indexed by the space  $\mathcal{X}$  of the observations. Here the exponential form forces the prior to weight only nonnegative functions and the renormalization permits to integrate to unity. We refer to Section 3.1 for more details on this context and also to, e.g., [37, 27, 42, 17]. Dealing with classification is also of interest and can be handled again using Gaussian processes. Here the estimation of the binary regression function  $\mathbb{P}(Y = 1|X = x)$  can be done from a bivariate sample  $((X_1, Y_1), \dots, (X_n, Y_n))$  and using priors of the form

$$f_Z(x) = \Psi(Z(x)),$$

where  $\Psi$  is a fixed measurable function from  $\mathbb{R}$  to  $(0, 1)$ . We refer to Section 3.2 and [11, 48] for more details on this context. Other settings have also been considered in the literature as regression with fixed covariates [45, 10], and white noise models [45] to name a few. In the literature, several examples of Gaussian priors have been considered as the integrated Brownian motion [45], the Riemann-Liouville process [45, 8], the Matérn process [44], and the exponential process [49].

Now given a prior as illustrated in the previous paragraph and the observations, Bayes' rule leads to a posterior distribution on the function of interest defining the unknown data distribution. One is then typically interested in proving posterior consistency, meaning that the posterior distribution converges to this function of interest as the sample size goes to infinity (see, e.g., [4]). Another question of interest is the one of rates of contraction of posterior distributions based on Gaussian process priors. In a nutshell, the rate of contraction of the posterior corresponds to an  $\varepsilon_n$  as small as possible such that the posterior probability of the ball centered at the function of interest and of radius  $\varepsilon_n$  still converges to one in probability. Other directions have been investigated. In particular, while upper bounds are available and express in terms of a concentration function involving the reproducing kernel Hilbert space (RKHS) associated to the Gaussian prior, the author of [8] exhibits lower bound counterparts. More recently, more flexibility has been allowed considering a randomly rescaled smooth Gaussian field as a prior that adapts to smoothness [47].

In this article, we consider deep Gaussian priors to reach further generality, similarly as deep neural networks are exploited to go beyond standard shallow neural networks. The reader is referred to [25, 16, 33, 14] for some references on both deep Gaussian processes

and deep neural networks. Deep Gaussian processes, introduced in [12], are non-Gaussian stochastic processes, constructed from a network of Gaussian processes, similarly as neural networks. A deep Gaussian process is then a stochastic process from  $\mathbb{R}^d$  to  $\mathbb{R}$  of the form

$$Z_H \circ Z_{H-1} \circ \cdots \circ Z_1, \tag{1}$$

where, for  $h = 1, \dots, H$ ,  $Z_h$  is a (multivariate) Gaussian process from  $\mathbb{R}^{d_h}$  to  $\mathbb{R}^{d_{h+1}}$ , with the convention  $d_1 = d$  and  $d_{H+1} = 1$ . In analogy to neural networks,  $Z_2, \dots, Z_{H-1}$  may be interpreted as hidden layer processes and  $H$  may be called the number of layers. In particular, since deep Gaussian processes are based on composing Gaussian processes, their mathematical analysis becomes challenging.

Deep Gaussian processes are commonly used as a prior for a function that is observed exactly. For instance, [21] tackles optimization and [36] deals with surrogate modeling of computer models with applications to nuclear engineering. Deep Gaussian processes are exploited as well with noisy/indirect function observations [13, 40]. From a methodological point of view, deep Gaussian processes are also an efficient way to obtain more non-stationarity than simple Gaussian processes. This need for non-stationarity is largely acknowledged in the Gaussian process literature (see e.g. [20, 31]). Hence, because of its practical impact, the theoretical analysis of deep Gaussian processes is beneficial.

In this work, several Gaussian processes are constrained (in terms of bounded norms for the processes themselves and their first derivatives) and then composed to form constrained deep Gaussian processes. The constraints are necessary for our theoretical analysis (see more details in Section 2.1 in the discussion of (2) and (3)) and may be useful in practice to exclude very irregular realizations from the Bayesian model. Note that these bounds and derivative constraints may also be enforced to standard Gaussian processes, for a better modeling in some situations, especially with additional available expertise [19, 29, 30]. In the same vein of previous works, we investigate posterior contraction for density estimation and classification. We establish original general rates of contraction extending those available for classical Gaussian processes (see Theorems 3.1 and 3.2). The proofs are original and exploit the results established in [45]. In [45], the authors consider a single Gaussian process defined on a compact space and valued in  $\mathbb{R}$ . A prior step before proving our results is then the construction of a single global Gaussian process from the collection of the Gaussian processes involved in the deep Gaussian process prior (see Appendix B). In addition, we study several examples of deep Gaussian priors: integrated Brownian motions (Section 4.1) and Riemann-Liouville processes (Section 4.2) in dimension one, and Matérn processes in general dimension (Section 4.3). It appears that the optimal rates are recovered in these examples for standard classes of functions. The proofs of these results rely on the proofs of the analog results in the context of classical (single) Gaussian processes [45, 44].

We would like to mention that, while preparing this article, we have been aware of the independent work of Finocchio and Schmidt-Hieber [15] on the same topic. Their paper presents many interesting results. In contrast to our work, they consider the problem of regression rather than density estimation and classification. They address adaptivity with

respect to the smoothness and structure of the function of interest, which we do not. Their proofs are independent of the proofs of the present paper and the techniques used are also different. To our knowledge, [15] is the only already existing work providing posterior contraction results for deep Gaussian processes.

The paper is organized as follows. In Section 2, we present the setting and some notation. Section 3 is dedicated to posterior contraction for both density estimation and classification. Examples of rates of contraction for specific function classes and priors are given in Section 4. Appendix A explains how to allow for more flexibility on the constraints considered in Section 2 using linear transformations of inputs and outputs. In Appendix B, we transform our deep Gaussian process into a single global real-valued Gaussian process defined on a compact space in order to apply the results of [45]. The proofs of the results of Sections 3 and 4, and of Appendix B are postponed to Appendix C.

## 2 Setting and preliminary notation

### 2.1 Gaussian and deep Gaussian priors with constraints

Here  $\mathbb{N}$  denotes the set of natural numbers (including zero) and  $\mathbb{N}^*$  denotes the set of nonzero natural numbers. For  $k \in \mathbb{N}^*$  and  $A \subset \mathbb{R}^k$ , let  $\mathcal{C}_0(A, \mathbb{R})$  be the set of continuous functions from  $A$  to  $\mathbb{R}$ , endowed with the Borel sigma algebra of the uniform norm  $\|\cdot\|_\infty$ . Let  $H \in \mathbb{N}^* \setminus \{1\}$  and  $d \in \mathbb{N}^*$  be fixed. Let also  $d_1 = d$  and  $d_{H+1} = 1$  by convention. For  $h = 1, \dots, H$ , consider a centered multivariate Gaussian process  $Z_h = (Z_{h,1}, \dots, Z_{h,d_{h+1}}) : \mathbb{R}^{d_h} \rightarrow \mathbb{R}^{d_{h+1}}$ . Assume that  $Z_1, \dots, Z_H$  are independent, with independent components and with continuous realizations. Assume moreover that  $Z_2, \dots, Z_H$  have continuously differentiable realizations.

This paper deals with a deep Gaussian process obtained by composing the previous Gaussian processes  $Z_h$ , for  $h = 1, \dots, H$ :

$$Z_H \circ \dots \circ Z_1.$$

Such a process gives a prior on the continuous functions from  $\mathbb{R}^d$  to  $\mathbb{R}$ . An illustration is provided in Figure 1.

We consider the input space  $[-1, 1]^d$  for the deep Gaussian process prior  $Z_H \circ \dots \circ Z_1$ . For our proof techniques, we constrain the process  $Z_h$ ,  $h = 2, \dots, H$ , to also have the fixed input domain  $[-1, 1]^{d_h}$ . The reader is referred to Appendix B for more details. To do so, we condition  $Z_1, \dots, Z_{H-1}$  by the following constraints, that we call *value constraints*: for all  $h = 1, \dots, H - 1$ ,

$$\|Z_h\|_{\infty, [-1, 1]^{d_h}} \leq 1, \tag{2}$$

where we define for any  $k_1, k_2 \in \mathbb{N}^*$ , for any  $A \subset \mathbb{R}^{k_1}$ , and for any  $f = (f_1, \dots, f_{k_2}) : A \rightarrow \mathbb{R}^{k_2}$ ,

$$\|f\|_{\infty, A} = \sup_{t \in A} \max_{\ell=1, \dots, k_2} |f_\ell(t)|.$$

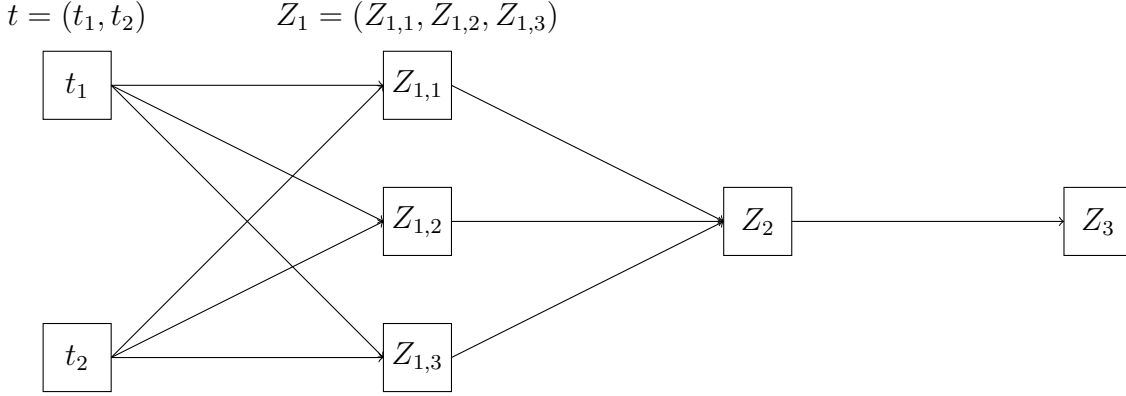


Figure 1: Example of a deep Gaussian process from  $\mathbb{R}^2$  to  $\mathbb{R}$ . Here  $H = 3$ ,  $d_1 = d = 2$ ,  $d_2 = 3$ ,  $d_3 = 1$ , and  $d_{H+1} = d_4 = 1$ .

This set of constraints has strictly positive probability (see Lemma C.3). In addition, for technical reasons again (in particular for the proof of Lemma C.7), we consider a second set of constraints, that we call *derivative constraints*: for  $h = 2, \dots, H$ , for  $i = 1, \dots, d_{h+1}$ , and for  $j = 1, \dots, d_h$ , there exists a fixed deterministic constant  $K_{h,i,j}$  such that

$$\left\| \frac{\partial Z_{h,i}}{\partial x_j} \right\|_{\infty, [-1,1]^{d_h}} \leq K_{h,i,j}. \quad (3)$$

This second set of constraints has again strictly positive probability (see Lemma C.3 applied to the derivatives of  $Z_{h,i}$  for  $h = 2, \dots, H$  and for  $i = 1, \dots, d_{h+1}$ ). As explained, the previous constraints are necessary for our theoretical analysis and may also be useful in practice to exclude very irregular realizations from the Bayesian model. Observe that the form of the constraints in (2) can be extended to more flexible bounds on the values of the components of  $Z_1, \dots, Z_{H-1}$  (see Appendix A). Outside of Appendix A, we consider the constraints (2) for convenience of exposition.

Now we index all the univariate components of  $Z_1, \dots, Z_H$ , defining the finite set

$$\mathcal{I} = \{(h, i); h \in \{1, \dots, H\}, i \in \{1, \dots, d_{h+1}\}\}.$$

In the sequel, for  $(h, i) \in \mathcal{I}$ , we denote by  $Z_{c,h,i}$  a stochastic process from  $[-1, 1]^{d_h}$  to  $\mathbb{R}$  which law is that of the process  $Z_{h,i}$  conditioned by (2) and/or (3). More precisely, for any Borel set  $B$ , for  $h = 2, \dots, H - 1$ , and for  $i = 1, \dots, d_{h+1}$ ,

$$\begin{aligned} & \mathbb{P}(Z_{c,h,i} \in B) \\ &= \mathbb{P}\left(Z_{h,i} \in B \mid \|Z_{h,i}\|_{\infty, [-1,1]^{d_h}} \leq 1, \|\partial Z_{h,i}/\partial x_j\|_{\infty, [-1,1]^{d_h}} \leq K_{h,i,j}, j = 1, \dots, d_h\right) \end{aligned} \quad (4)$$

and

$$\begin{cases} \mathbb{P}(Z_{c,1,i} \in B) = \mathbb{P}\left(Z_{1,i} \in B \mid \|Z_{1,i}\|_{\infty, [-1,1]^{d_1}} \leq 1\right) & \text{for } i = 1, \dots, d_2, \\ \mathbb{P}(Z_{c,H} \in B) = \mathbb{P}\left(Z_H \in B \mid \|\partial Z_H/\partial x_j\|_{\infty, [-1,1]^{d_H}} \leq K_{H,1,j}, j = 1, \dots, d_H\right). \end{cases} \quad (5)$$

For  $h = 1, \dots, H$ , we let  $Z_{c,h} = (Z_{c,h,1}, \dots, Z_{c,h,d_{h+1}})$ . Note that the independence of the processes  $Z_{h,i}$ , for  $(h, i) \in \mathcal{I}$ , yields that, for any Borel sets  $B_1, \dots, B_H$ ,

$$\begin{aligned} & \mathbb{P}(Z_{c,h} \in B_h, h = 1, \dots, H) \\ = & \mathbb{P}(Z_h \in B_h, h = 1, \dots, H \mid \|Z_{h,i}\|_{\infty, [-1,1]^{d_h}} \leq 1, h = 1, \dots, H-1, i = 1 \dots, d_{h+1}, \\ & \|\partial Z_{h,i}/\partial x_j\|_{\infty, [-1,1]^{d_h}} \leq K_{h,i,j} h = 2, \dots, H, i = 1 \dots, d_{h+1}, j = 1 \dots, d_h). \end{aligned}$$

For  $h = 1, \dots, H$ , let  $\mathbb{B}_h$  be the Banach space of the continuous functions from  $[-1, 1]^{d_h}$  to  $\mathbb{R}$  endowed with the uniform norm. In addition, for any  $h = 2, \dots, H-1$  and for any  $i = 1, \dots, d_{h+1}$ , we define the subset  $\mathbb{B}_{c,h,i}$  of  $\mathbb{B}_h$  composed by the continuously differentiable functions  $z \in \mathbb{B}_h$  satisfying (2) and (3) (with  $Z$  replaced by  $z$ ). Similarly, for  $i = 1, \dots, d_2$ ,  $\mathbb{B}_{c,1,i}$  stands for the subset of the functions  $z \in \mathbb{B}_1$  satisfying (2) only and  $\mathbb{B}_{c,H,1}$  stands for the subset of the continuously differentiable functions  $z \in \mathbb{B}_H$  satisfying (3) only. Hence (4) and (5) simply rewrite, for any Borel set  $B \subset \mathbb{B}_h$  and for any  $(h, i) \in \mathcal{I}$ ,

$$\mathbb{P}(Z_{c,h,i} \in B) = \mathbb{P}(Z_{h,i} \in B \mid Z_{h,i} \in \mathbb{B}_{c,h,i}).$$

The constrained deep Gaussian process prior is then given by

$$Z_{c,H} \circ \dots \circ Z_{c,1}.$$

## 2.2 A concentration function for constrained deep Gaussian processes

For a centered Gaussian process  $X$  on a space  $E$ , we define its RKHS  $\mathbb{H}_X$  on  $E$  from the covariance function of  $X$ , on  $E \times E$ , as in [46, Section 2.1]. Then let  $\|\cdot\|_{\mathbb{H}_X}$  be the Hilbertian norm in this RKHS. In particular, for  $(h, i) \in \mathcal{I}$ , we let  $k_{h,i}$  be the covariance function of  $Z_{h,i}$  on  $[-1, 1]^{d_h}$  and  $\mathbb{H}_{h,i}$  be the corresponding RKHS (that is thus defined as in [46, Section 2.1]) with RKHS-norm  $\|\cdot\|_{\mathbb{H}_{h,i}}$ . We also write  $\mathcal{C}^1([-1, 1]^\ell, \mathbb{R})$  for the Banach space of continuously differentiable functions  $f$  from  $[-1, 1]^\ell$  to  $\mathbb{R}$ , equipped with the norm  $\|\cdot\|_{\infty,1}$  defined by

$$\|f\|_{\infty,1} = \|f\|_{\infty} + \sum_{j=1}^{\ell} \left\| \frac{\partial f}{\partial x_j} \right\|_{\infty}. \quad (6)$$

In [45], the rates of contraction for classical Gaussian processes are given in terms of a concentration function involving the RKHS associated to the Gaussian process prior. More precisely, the concentration function for a single Gaussian process  $X$  from a compact space  $E$  to  $\mathbb{R}$ , with a continuous function  $x_0$  on  $E$ , and  $\varepsilon > 0$ , is given by

$$\phi_{x_0}(\varepsilon) = \inf_{\substack{h \in \mathbb{H}_X \\ \|h - x_0\|_{\infty} < \varepsilon}} \|h\|_{\mathbb{H}_X}^2 - \log \mathbb{P}(\|X\|_{\infty} < \varepsilon) \quad (7)$$

where  $\|\cdot\|_\infty$  is the uniform norm for continuous functions from  $E$  to  $\mathbb{R}$ . This function is interpreted as measuring the concentration around the fixed function  $x_0$ .

Here, we propose a novel concentration function adapted to the deep context and to the constraints. First, for  $h = 2, \dots, H$  and for  $i = 1, \dots, d_{h+1}$ , we consider  $z_{0,h,i}$  in the closure of  $\mathbb{H}_{h,i}$  in  $(\mathcal{C}^1([-1, 1]^{d_h}, \mathbb{R}), \|\cdot\|_{\infty,1})$  and for  $i = 1, \dots, d_2$ , we consider  $z_{0,1,i}$  in the closure of  $\mathbb{H}_{1,i}$  in  $(\mathcal{C}^0([-1, 1]^{d_1}, \mathbb{R}), \|\cdot\|_\infty)$ . Second, we define, for  $\varepsilon > 0$ ,

$$\begin{aligned} \Phi_{c,z_0}(\varepsilon) := & \sum_{i=1}^{d_2} \left( \frac{3}{2} \inf_{\substack{g \in \mathbb{H}_{1,i} \\ \|g - z_{0,1,i}\|_\infty < \varepsilon}} \|g\|_{\mathbb{H}_{1,i}}^2 - 2 \log \mathbb{P}(\|Z_{1,i}\|_\infty < \varepsilon) \right) \\ & + \sum_{\substack{(h,i) \in \mathcal{I} \\ h \geq 2}} \left( \frac{3}{2} \inf_{\substack{g \in \mathbb{H}_{h,i} \\ \|g - z_{0,h,i}\|_\infty < \frac{\varepsilon}{2} \\ \|\partial g / \partial x_j - \partial z_{0,h,i} / \partial x_j\|_\infty < \frac{K_{\min}}{4}, \\ j=1, \dots, d_h}} \|g\|_{\mathbb{H}_{h,i}}^2 \right. \\ & \left. - 2 \log \mathbb{P}\left(\|Z_{h,i}\|_\infty \leq \frac{\varepsilon}{2}\right) - 2 \sum_{j=1}^{d_h} \log \mathbb{P}\left(\|\partial Z_{h,i} / \partial x_j\|_\infty \leq \frac{K_{\min}}{4}\right) \right), \end{aligned} \quad (8)$$

where

$$K_{\min} = \min_{h=2, \dots, H} \min_{i=1, \dots, d_{h+1}} \min_{j=1, \dots, d_h} K_{h,i,j}. \quad (9)$$

This function is interpreted as evaluating the concentration of the processes  $Z_{h,i}$  around the fixed functions  $z_{0,h,i}$  for  $(h, i) \in \mathcal{I}$ , taking the constraints into account.

## 3 Posterior contraction in density estimation and classification

### 3.1 Density estimation

Consider the observation of an i.i.d. sample  $X_1, \dots, X_n$  from a fixed unknown probability density function  $p_0: [-1, 1]^d \rightarrow (0, +\infty)$  (such that  $\int_{[-1, 1]^d} p_0(t) dt = 1$ ). For  $z: [-1, 1]^d \rightarrow \mathbb{R}$ , let  $p_z: [-1, 1]^d \rightarrow (0, +\infty)$  be given by

$$p_z(t) = \frac{e^{z(t)}}{\int_{[-1, 1]^d} e^{z(s)} ds}, \quad \text{for } t \in [-1, 1]^d. \quad (10)$$

Suppose that  $p_0$  can be written as  $p_{z_{0,H} \circ \dots \circ z_{0,1}}$  where  $z_{0,h} = (z_{0,h,1}, \dots, z_{0,h,d_{h+1}})$  for  $h = 1, \dots, H$  and such that  $z_{0,h,i} \in \mathbb{B}_{c,h,i}$  for  $(h, i) \in \mathcal{I}$ . As above, assume that, for  $h = 2, \dots, H$  and for  $i = 1, \dots, d_{h+1}$ ,  $z_{0,h,i}$  is in the closure of  $\mathbb{H}_{h,i}$  in  $(\mathcal{C}^1([-1, 1]^{d_h}, \mathbb{R}), \|\cdot\|_{\infty,1})$  and for  $i = 1, \dots, d_2$ ,  $z_{0,1,i}$  is in the closure of  $\mathbb{H}_{1,i}$  in  $(\mathcal{C}^0([-1, 1]^d, \mathbb{R}), \|\cdot\|_\infty)$ .

We consider the prior  $p_{Z_{c,H} \circ \dots \circ Z_{c,1}}$  on  $p_0$ , where, for any  $h = 1, \dots, H$ ,  $Z_{c,h}$  has been defined in Section 2.1. Then the posterior is given by

$$\mathbb{P}(p_{Z_{c,H} \circ \dots \circ Z_{c,1}} \in \cdot | X_1, \dots, X_n).$$

The posterior is a random measure on  $(\mathcal{C}^0([-1, 1]^d, \mathbb{R}))$  that depends on the observations  $X_1, \dots, X_n$  and we are interested in its convergence to  $p_0$  as  $n \rightarrow \infty$ .

Before stating the main result of this section, we recall the definition of the Hellinger distance  $h$ : for  $f, g : [-1, 1]^d \rightarrow [0, \infty)$  with  $\int_{[-1, 1]^d} f(t) dt = \int_{[-1, 1]^d} g(t) dt = 1$ ,

$$h(f, g) = \sqrt{\int_{[-1, 1]^d} \left( \sqrt{f(t)} - \sqrt{g(t)} \right)^2 dt}. \quad (11)$$

The next theorem is an extension of [45, Theorem 3.1] to constrained deep Gaussian priors.

**Theorem 3.1.** *Let  $\Phi_{c,z_0}$  be the function defined in (8) and recall  $K_{\min}$  in (9). Assume that, for  $h = 1, \dots, H - 1$  and for  $i = 1, \dots, d_{h+1}$ ,  $\|z_{0,h,i}\|_\infty < 1$  and for  $h = 2, \dots, H$ , for  $i = 1, \dots, d_{h+1}$ , and for  $j = 1, \dots, d_h$ ,  $\|\partial z_{0,h,i}/\partial x_j\|_\infty \leq K_{\min}/2$ . Then, for a sequence  $(\varepsilon_{c,n})_{n \in \mathbb{N}}$  satisfying  $\varepsilon_{c,n} > 0$ ,  $\varepsilon_{c,n} \rightarrow 0$ ,  $n\varepsilon_{c,n}^2 \rightarrow \infty$ , and  $\Phi_{c,z_0}(\varepsilon_{c,n}) \leq n\varepsilon_{c,n}^2$ , the posterior distribution satisfies*

$$\mathbb{P}(h(p_{Z_{c,H} \circ \dots \circ Z_{c,1}}, p_0) > M_n \varepsilon_{c,n} | X_1, \dots, X_n) \xrightarrow[n \rightarrow \infty]{} 0 \quad (12)$$

in probability, for any sequence  $(M_n)$  such that  $M_n \rightarrow \infty$ .

Remark that in Theorem 3.1, the conditions  $\|z_{0,h,i}\|_\infty < 1$  and  $\|\partial z_{0,h,i}/\partial x_j\|_\infty \leq K_{\min}/2$  are not restrictive since, for a given  $p_0$ ,  $z_{0,H}$  can be taken with large enough values and derivatives values, to compensate for the bounded values of  $z_{0,1}, \dots, z_{0,H-1}$ , and then the  $K_{h,i,j}$  in (9) can be taken large enough. Recall also that Appendix A shows that the value bound 1 can be replaced by arbitrary large bounds, up to linear changes of inputs and outputs of the Gaussian processes.

## 3.2 Classification

Consider the observation of an i.i.d. sample  $(U_1, V_1), \dots, (U_n, V_n)$  distributed as  $(U, V)$  where  $U$  is a random variable in  $[-1, 1]^d$  and  $V$  is a binary random variable ( $V \in \{0, 1\}$ ) such that  $\mathbb{P}(V = 1 | U) = f_0(U)$ , with a fixed unknown function  $f_0 : [-1, 1]^d \rightarrow (0, 1)$ . Consider a function  $\Psi : \mathbb{R} \rightarrow (0, 1)$  such that  $\Psi$  has a bounded derivative  $\Psi'$  on  $\mathbb{R}$  and such that  $\Psi' / (\Psi(1 - \Psi))$  is bounded on  $\mathbb{R}$ . For instance, one may use the standard logistic function  $\Psi(x) = e^x / (1 + e^x)$ . For  $z : [-1, 1]^d \rightarrow \mathbb{R}$ , let  $f_z : [-1, 1]^d \rightarrow (0, 1)$  be given by

$$f_z(t) = \Psi(z(t)), \quad \text{for } t \in [-1, 1]^d. \quad (13)$$

Suppose that  $f_0$  can be written as  $f_{z_{0,H} \circ \dots \circ z_{0,1}}$  where  $z_{0,h} = (z_{0,h,1}, \dots, z_{0,h,d_{h+1}})$  for  $h = 1, \dots, H$  and such that  $z_{0,h,i} \in \mathbb{B}_{c,h,i}$  for  $(h, i) \in \mathcal{I}$ . Further, as above, assume that, for  $h =$



$2, \dots, H$  and for  $i = 1, \dots, d_{h+1}$ ,  $z_{0,h,i}$  is in the closure of  $\mathbb{H}_{h,i}$  in  $(\mathcal{C}^1([-1, 1]^{d_h}, \mathbb{R}), \|\cdot\|_{\infty,1})$  and for  $i = 1, \dots, d_2$ ,  $z_{0,1,i}$  is in the closure of  $\mathbb{H}_{1,i}$  in  $(\mathcal{C}^0([-1, 1]^d, \mathbb{R}), \|\cdot\|_{\infty})$ .

We consider the prior  $f_{Z_{c,H} \circ \dots \circ Z_{c,1}}$ , where, for  $h = 1, \dots, H$ ,  $Z_{c,h}$  has been defined in Section 2.1. Then the posterior is given by

$$\mathbb{P}(f_{Z_{c,H} \circ \dots \circ Z_{c,1}} \in \cdot | (U_1, V_1), \dots, (U_n, V_n)).$$

Again, the posterior is a random measure on  $(\mathcal{C}^0([-1, 1]^d, \mathbb{R}))$  that depends on the observations  $(U_1, V_1), \dots, (U_n, V_n)$  and we are interested in its convergence to  $f_0$  as  $n \rightarrow \infty$ .

We let  $\|g\|_{2,U}$  be the  $L^2$  norm of a function  $g : [-1, 1]^d \rightarrow \mathbb{R}$  with respect to the law of  $U$ . The next theorem is an extension of [45, Theorem 3.2] (see also [18, Theorem 11.22]) to constrained deep Gaussian priors.

**Theorem 3.2.** *Consider the same setting and the same assumptions as in Theorem 3.1 for  $\Phi_{c,z_0}$ ,  $K_{\min}$ , and  $(z_{0,h,i})_{(h,i) \in \mathcal{I}}$ . Then, for a sequence  $(\varepsilon_{c,n})_{n \in \mathbb{N}}$  satisfying  $\varepsilon_{c,n} > 0$ ,  $\varepsilon_{c,n} \rightarrow 0$ ,  $n\varepsilon_{c,n}^2 \rightarrow \infty$ , and  $\Phi_{c,z_0}(\varepsilon_{c,n}) \leq n\varepsilon_{c,n}^2$ , the posterior distribution satisfies*

$$\mathbb{P}\left(\|f_{Z_{c,H} \circ \dots \circ Z_{c,1}} - f_0\|_{2,U} > M_n \varepsilon_{c,n} | (U_1, V_1), \dots, (U_n, V_n)\right) \xrightarrow{n \rightarrow \infty} 0 \quad (14)$$

in probability, for any sequence  $(M_n)$  such that  $M_n \rightarrow \infty$ .

## 4 Examples of rates of contraction for specific function classes and specific priors

In this section, we apply Theorems 3.1 and 3.2 to classical examples of Gaussian processes for  $Z_1, \dots, Z_H$  and to classical examples of function classes for  $z_{0,1}, \dots, z_{0,H}$ . These examples are by no means exhaustive, and Theorems 3.1 and 3.2 would enable to obtain contraction rates in other settings as well.

### 4.1 Integrated Brownian motion processes in dimension one

First consider independent Brownian motions as studied in [45] for standard (non deep) Gaussian processes. Here, we let  $d_1 = \dots = d_{H+1} = 1$ , that is we consider the composition of univariate processes. Thus we simply have  $Z_h = Z_{h,1}$  for  $h = 1, \dots, H$  and the constants  $K_{h,i,j}$  involved in the constraints (3) will simply be denoted by  $K_h$ . For  $x \in \mathbb{R}$ , let  $\lfloor x \rfloor$  be the largest integer strictly smaller than  $x$ . For  $\beta > 0$ , let  $\mathcal{F}^\beta([-1, 1], \mathbb{R})$  be the set of functions from  $[-1, 1]$  to  $\mathbb{R}$  that have derivatives up to order  $\lfloor \beta \rfloor$  and which derivative of order  $\lfloor \beta \rfloor$  is  $\beta - \lfloor \beta \rfloor$ -Hölder. The space  $\mathcal{F}^\beta([-1, 1], \mathbb{R})$  is called the Hölder space of order  $\beta$ .

For a continuous function  $g : [0, \infty) \rightarrow \mathbb{R}$ , we let  $I^0 g = g$  and, for  $\ell \in \mathbb{N}^*$ , we define by induction  $I^\ell g : [0, \infty) \rightarrow \mathbb{R}$  by, for  $t \in [0, \infty)$ ,  $(I^\ell g)(t) = \int_0^t (I^{\ell-1} g)(s) ds$ . We let  $N_1 \in \mathbb{N}$

and, for  $h = 2, \dots, H$ ,  $N_h \in \mathbb{N}^*$ . We also let  $Z_h$  be the Gaussian process defined by

$$Z_h(t) = (I^{N_h} B_h)(t+1) + \sum_{\ell=0}^{N_h} X_{h,\ell} \frac{(t+1)^\ell}{\ell!}, \quad \text{for } t \in (-1, \infty),$$

where  $B_h$  is a standard Brownian motion on  $[0, \infty)$  and where  $X_{h,0}, \dots, X_{h,N_h}$  are independent standard Gaussian variables that are also independent of  $B_h$ . Remark that  $Z_h$  is then defined on  $(-1, \infty)$ , is  $N_h$ -times differentiable, and has value and derivatives values at  $t = -1$  given by  $X_{h,0}, \dots, X_{h,N_h}$ .

In order to fit with the formalism of Sections 2 and 3, we now extend  $Z_1, \dots, Z_h$  to the real line. This extension is done simply with a constant or a linear function. This choice is arbitrary and has no impact on the constrained deep Gaussian process priors constructed as in Sections 2 and 3. If  $N_1 = 0$ , we extend the definition of  $Z_1(t)$  for  $t \in (-\infty, -1)$  by taking the value at  $t = -1$ . If  $N_h \geq 1$ , we extend the definition of  $Z_h(t)$  for  $t \in (-\infty, -1)$  by a linear function based on the values of  $Z_h$  and its derivative at  $t = -1$ . After this,  $Z_h$  is a continuous Gaussian process on  $\mathbb{R}$  (continuously differentiable if  $N_h \geq 1$ ).

As in Sections 2 and 3, we let  $Z_1, \dots, Z_H$  be independent. The next theorem then provides the rates of contraction given by Theorems 3.1 and 3.2.

**Theorem 4.1.** *First consider the setting of Theorem 3.1. Assume that  $p_0$  is strictly positive and belongs to  $\mathcal{F}^\beta([-1, 1], \mathbb{R})$  for a fixed  $\beta > 0$ . Assume that  $\beta \leq N_1 + 1/2$  and that  $\beta \leq N_h$  for  $h = 2, \dots, H$ . Then the fixed constants  $K_1, \dots, K_H$  in (3) can be chosen large enough so that the conclusion of Theorem 3.1 holds with*

$$\varepsilon_{c,n} = C_{\text{sup}} n^{-\beta/(2N_1+2)}$$

for some constant  $C_{\text{sup}}$  that does not depend on  $n$ . Second, consider the setting of Theorem 3.2, with  $f_0 = f_{g_0}$  where  $g_0$  belongs to  $\mathcal{F}^\beta([-1, 1], \mathbb{R})$ , with the same conditions on  $\beta, N_1, \dots, N_H$ . Then the first conclusion again holds, with the same expression for  $\varepsilon_{c,n}$ .

From Theorem 4.1 with the condition  $\beta \leq N_1 + 1/2$ , the rate of contraction is fastest when  $N_1 + 1/2 = \beta$  (which is possible when  $\beta = k + 1/2, k \in \mathbb{N}$ , and means that the smoothness of  $Z_1$  matches that of the fixed unknown function), in which case we recover the classical minimax rate  $n^{-\beta/(2\beta+1)}$  (see [45, Theorem 4.1 and below]). For a larger  $N_1$ , the rate deteriorates (oversmooth prior). Note that the processes  $Z_2, \dots, Z_H$  are chosen smoother than the fixed unknown function from the condition  $N_h \geq \beta$  for  $h = 2, \dots, H$ .

## 4.2 Riemann-Liouville processes in dimension one

While the smoothness index of the Brownian motion is necessarily of the form integer  $+ 1/2$ , any smoothness index can be reached with the Riemann-Liouville process as explained in [45]. As in Section 4.1, in the sequel, we let  $d_1 = \dots = d_{H+1} = 1$ , we simply have  $Z_h Z_{h,1}$ , and we simply denote  $K_h$  for  $K_{h,1,1}$  in (3),  $h = 1, \dots, H$ .

For  $x \in \mathbb{R}$ , let  $\underline{x}$  be the largest integer smaller or equal to  $x$ . For  $h = 1, \dots, H$ , we set  $\alpha_1 > 0$  and for  $h = 2, \dots, H$ ,  $\alpha_h > 1$ . We let  $B_h$  be a standard Brownian motion on  $[0, \infty)$ .

We define  $R_h$  as the Gaussian process on  $[0, \infty)$  defined by  $R_h(t) = \int_0^t (t-s)^{\alpha_h-1/2} dB_h(s)$  and then the Gaussian process  $Z_h$  on  $[-1, \infty)$  by

$$Z_h(t) = R_h(t+1) + \sum_{\ell=0}^{\alpha_h+1} X_{h,\ell} \frac{(t+1)^\ell}{\ell!},$$

for  $t \in [-1, \infty)$  and where  $X_{h,1}, \dots, X_{h,\alpha_h+1}$  are independent standard Gaussian variables. We then extend  $Z_h$  on  $(-\infty, 1)$  as in Section 4.1.

Again as in Section 4.1, we let  $Z_1, \dots, Z_H$  be independent. The next theorem then provides the rates of contraction given by Theorems 3.1 and 3.2.

**Theorem 4.2.** *First consider the setting of Theorem 3.1. Assume that  $p_0$  is strictly positive and belongs to  $\mathcal{F}^{\alpha_1}([-1, 1], \mathbb{R})$ . Assume that for  $h = 2, \dots, H$ ,  $\alpha_h \geq \alpha_1$ . Then the fixed constants  $K_1, \dots, K_H$  in (3) can be chosen large enough so that the conclusion of Theorem 3.1 holds with*

$$\varepsilon_{c,n} = C_{\text{sup}} n^{-\alpha_1/(2\alpha_1+1)}$$

for some constant  $C_{\text{sup}}$  that does not depend on  $n$ . Second, consider the setting of Theorem 3.2, with  $f_0 = f_{g_0}$  where  $g_0$  belongs to  $\mathcal{F}^{\alpha_1}([-1, 1], \mathbb{R})$ , with the same conditions on  $\alpha_1, \dots, \alpha_H$ . Then the first conclusion again holds, with the same expression for  $\varepsilon_{c,n}$ .

Note that the smoothness of  $Z_1$  exactly matches that of the fixed unknown function and the processes  $Z_2, \dots, Z_H$  have a smoothness that is larger than or equal to that of the fixed unknown function. This enables to recover the standard minimax rate  $n^{-\alpha_1/(2\alpha_1+1)}$  (see [45, Theorem 4.3 and below]).

### 4.3 Matérn processes in general dimension

Here we consider Gaussian processes with Matérn covariance functions, which allows for both arbitrary input dimension and arbitrary smoothness. These processes were studied in [44, Section 3.1] for standard (non deep) Gaussian processes.

Let us first extend the definition of  $\mathcal{F}^\beta([-1, 1], \mathbb{R})$  to larger dimensions. For  $\beta > 0$  and  $\ell \in \mathbb{N}^*$ , we let  $\mathcal{F}^\beta([-1, 1]^\ell, \mathbb{R})$  be the set of functions from  $[-1, 1]^\ell$  to  $\mathbb{R}$  for which all the partial derivatives of order  $(a_1, \dots, a_\ell)$  exist for all  $a_1, \dots, a_\ell \in \mathbb{N}$  with  $a_1 + \dots + a_\ell \leq \lfloor \beta \rfloor$  and which partial derivatives of order  $\lfloor \beta \rfloor$  are  $\beta - \lfloor \beta \rfloor$ -Hölder.

For  $(h, i) \in \mathcal{I}$ , we let  $Z_{h,i}$  have Matérn covariance function, that is, for  $u, v \in \mathbb{R}^{d_h}$ ,

$$\text{Cov}(Z_{h,i}(u), Z_{h,i}(v)) = \int_{\mathbb{R}^{d_h}} e^{i\lambda^\top(u-v)} m_{h,i}(\lambda) d\lambda,$$

where

$$m_{h,i}(\lambda) = \frac{1}{(1 + \|\lambda\|^2)^{\alpha_{h,i}+d/2}} \quad (15)$$

is called the spectral density and  $\alpha_{h,i} > 0$  is called the smoothness parameter. A Gaussian process on  $[-1, 1]^\ell$  ( $\ell \in \mathbb{N}^*$ ) with Matérn covariance function with  $\alpha_{h,i} = \alpha$  in (15) has sample paths in  $\mathcal{F}^\beta([-1, 1]^\ell, \mathbb{R})$  for any  $\beta < \alpha$ .

Then, as in [44], we define the Sobolev space  $\mathcal{H}^\beta([-1, 1]^\ell, \mathbb{R})$  as the set of functions  $f$  from  $[-1, 1]^\ell$  to  $\mathbb{R}$  that are restrictions of functions  $f$  from  $\mathbb{R}^\ell \rightarrow \mathbb{R}$  with Fourier transform  $\hat{f}(\lambda) = (2\pi)^{-\ell} \int e^{i\lambda^\top t} f(t) dt$  such that, defining

$$\|f\|_\beta^2 := \int_{\mathbb{R}^d} (1 + \|\lambda\|^2)^\beta |\hat{f}(\lambda)|^2 d\lambda < \infty.$$

The next theorem provides the rates of contraction given by Theorems 3.1 and 3.2.

**Theorem 4.3.** *First consider the setting of Theorem 3.1. Assume that  $p_0$  is strictly positive and belongs to  $\mathcal{F}^\beta([-1, 1]^d, \mathbb{R}) \cap \mathcal{H}^\beta([-1, 1]^d, \mathbb{R})$  for some  $\beta > 0$ . Assume that, for  $(h, i) \in \mathcal{I}$ ,  $\beta \leq \alpha_{h,i}$ . Then the fixed constants  $K_{h,i,j}$  for  $h = 2, \dots, H$ , for  $i = 1, \dots, d_{h+1}$ , and for  $j = 1, \dots, d_h$  in (3) can be chosen large enough such that the conclusion of Theorem 3.1 holds with*

$$\varepsilon_{c,n} = C_{\text{sup}} n^{-\beta/(2\alpha_{1,\min}+d)},$$

where  $\alpha_{1,\min} = \min(\alpha_{1,1}, \dots, \alpha_{1,d_2})$  and  $C_{\text{sup}}$  is some constant that does not depend on  $n$ . Second, consider the setting of Theorem 3.2, with  $f_0 = f_{g_0}$  where  $g_0$  belongs to  $\mathcal{F}^\beta([-1, 1]^d, \mathbb{R}) \cap \mathcal{H}^\beta([-1, 1]^d, \mathbb{R})$ , with the same conditions on  $\beta, K_{h,i,j}, \alpha_{h,i}$  for  $h = 1, \dots, H$ , for  $i = 1, \dots, d_{h+1}$ , and for  $j = 1, \dots, d_h$ . Then the first conclusion again holds, with the same expression for  $\varepsilon_{c,n}$ .

Above, the Gaussian process priors are taken smoother than the fixed unknown function. With the appropriate smoothness  $\alpha_{1,\min} = \beta$  for the first layer, we recover the classic optimal rate  $n^{-\beta/(2\beta+d)}$  as pointed out in [44, Theorem 5].

## 5 Conclusion

In this paper, we have provided rates of contraction for the posterior distribution of a deep Gaussian process prior, with constraints on the values and the derivatives. These results are the first to address density estimation and classification, to the best of our knowledge. Recently, [15] addressed contraction rates for deep Gaussian processes in regression. These general rates (Theorems 3.1 and 3.2) measure in terms of a new concentration function, that takes the constraints into account. The proofs of these general rates are based on constructing a single global Gaussian process prior in order to exploit existing results for standard Gaussian processes [45]. Some of the techniques for taking the constraints into account could be considered of independent interest (in particular the proofs in Section C.1).

We show in three examples how the general rates enable to recover existing minimax rates for standard function classes and Gaussian processes. These examples are not exhaustive. In future work, it would be beneficial to exploit Theorems 3.1 and 3.2 in other settings, with more involved function classes based on composition structures, in the aim of obtaining contraction rates that are out of reach for a single Gaussian process prior, thus further illustrating the flexibility benefit brought by deep Gaussian processes. Finally, adaptivity to function smoothness is an important topic for future work as well.

## A More flexibility on the constraints by linear transformations of inputs and outputs

Here, we consider that  $Z_1, \dots, Z_H$  satisfy constraints of the form (3) but the constraints  $\|Z_h\|_{\infty, [-1, 1]^{d_h}} \leq 1$  are replaced by more general constraints: for  $h = 1, \dots, H - 1$  and for  $i = 1, \dots, d_{h+1}$ , we assume

$$\|Z_{h,i}\|_{\infty, \prod_{\ell=1, \dots, d_h} [-L_{h,\ell}, L_{h,\ell}]} \leq L_{h+1,i} \quad (16)$$

where the constants  $L_{h+1,i} > 0$  (for  $h = 1, \dots, H - 1$  and for  $i = 1, \dots, d_{h+1}$ ) are arbitrary and  $L_{1,1} = \dots = L_{1,d_1} = 1$ .

We show that we can construct processes  $Y_1, \dots, Y_H$  that provide the same composition

$$Y_H \circ \dots \circ Y_1 = Z_H \circ \dots \circ Z_1,$$

that have constraints of the form (2) and (3), and that are obtained from linear transformations of inputs and outputs. Indeed, define the Gaussian processes  $Y_1, \dots, Y_H$  as follows. For  $h = 1, \dots, H - 1$ , for  $t_1, \dots, t_{d_h} \in \mathbb{R}$ , and for  $i = 1, \dots, d_{h+1}$ , let

$$Y_{h,i}(t_1, \dots, t_{d_h}) = \frac{1}{L_{h+1,i}} Z_{h,i}(L_{h,1}t_1, \dots, L_{h,d_h}t_{d_h}). \quad (17)$$

Recall that  $d_{H+1} = 1$  and let

$$Y_H(t_1, \dots, t_{d_H}) = Z_H(L_{H,1}t_1, \dots, L_{H,d_H}t_{d_H}), \quad \text{for } t_1, \dots, t_{d_H} \in \mathbb{R}. \quad (18)$$

The next lemma then shows the composition equality.

**Lemma A.1.** *For any  $t_1, \dots, t_d \in \mathbb{R}$ , we have*

$$Y_H \circ \dots \circ Y_1(t_1, \dots, t_d) = Z_H \circ \dots \circ Z_1(t_1, \dots, t_d)$$

recalling the convention  $d_1 = d$ .

*Proof of Lemma A.1.* First let us prove by induction that, for  $h = 1, \dots, H - 1$ , for  $i = 1, \dots, d_{h+1}$ , and for  $t_1, \dots, t_d \in \mathbb{R}$ ,

$$Y_{h,i} \circ Y_{h-1} \circ \dots \circ Y_1(t_1, \dots, t_d) = \frac{1}{L_{h+1,i}} Z_{h,i} \circ Z_{h-1} \circ \dots \circ Z_1(t_1, \dots, t_d). \quad (19)$$

For  $h = 1$ , this is true from (17) with  $L_{1,1} = \dots = L_{1,d_1} = 1$  and  $d_1 = d$ . Assume that this is true for some  $h \in \{1, \dots, H - 2\}$ . Thus by (19) and then by (17), for  $i = 1, \dots, d_{h+1}$ ,

$$\begin{aligned} & Y_{h+1,i} \circ \dots \circ Y_1(t_1, \dots, t_d) \\ &= Y_{h+1,i}(Y_{h,1} \circ Y_{h-1} \circ \dots \circ Y_1(t_1, \dots, t_d), \dots, Y_{h,d_{h+1}} \circ Y_{h-1} \circ \dots \circ Y_1(t_1, \dots, t_d)) \\ &= Y_{h+1,i}\left(\frac{1}{L_{h+1,1}} Z_{h,1} \circ Z_{h-1} \circ \dots \circ Z_1(t_1, \dots, t_d), \dots, \frac{1}{L_{h+1,d_{h+1}}} Z_{h,d_{h+1}} \circ Z_{h-1} \circ \dots \circ Z_1(t_1, \dots, t_d)\right) \\ &= \frac{1}{L_{h+2,i}} Z_{h+1,i}(Z_{h,1} \circ Z_{h-1} \circ \dots \circ Z_1(t_1, \dots, t_d), \dots, Z_{h,d_{h+1}} \circ Z_{h-1} \circ \dots \circ Z_1(t_1, \dots, t_d)) \\ &= \frac{1}{L_{h+2,i}} Z_{h+1,i} \circ Z_h \circ \dots \circ Z_1(t_1, \dots, t_d). \end{aligned}$$

This concludes the proof of (19) by induction. Finally, from (19) and (18), we obtain, for  $t_1, \dots, t_d \in \mathbb{R}$ ,

$$\begin{aligned}
& Y_H \circ \dots \circ Y_1(t_1, \dots, t_d) \\
&= Y_H(Y_{H-1,1} \circ Y_{H-2} \circ \dots \circ Y_1(t_1, \dots, t_d), \dots, Y_{H-1,d_H} \circ Y_{H-2} \circ \dots \circ Y_1(t_1, \dots, t_d)) \\
&= Y_H\left(\frac{1}{L_{H,1}} Z_{H-1,1} \circ Z_{H-2} \circ \dots \circ Z_1(t_1, \dots, t_d), \dots, \frac{1}{L_{H,d_H}} Z_{H-1,d_H} \circ Z_{H-2} \circ \dots \circ Z_1(t_1, \dots, t_d)\right) \\
&= Z_H(Z_{H-1,1} \circ Z_{H-2} \circ \dots \circ Z_1(t_1, \dots, t_d), \dots, Z_{H-1,d_H} \circ Z_{H-2} \circ \dots \circ Z_1(t_1, \dots, t_d)) \\
&= Z_H \circ Z_{H-1} \circ \dots \circ Z_1(t_1, \dots, t_d). \quad \square
\end{aligned}$$

The next lemma shows that  $Y_1, \dots, Y_H$  satisfy constraints of the form (2) when  $Z_1, \dots, Z_H$  satisfy the more general ones given in (16).

**Lemma A.2.** *The two following assertions are equivalent.*

1. For  $h = 1, \dots, H - 1$  and for  $i = 1, \dots, d_{h+1}$ ,

$$\|Z_{h,i}\|_{\infty, \prod_{\ell=1, \dots, d_h} [-L_{h,\ell}, L_{h,\ell}]} \leq L_{h+1,i}.$$

2. For  $h = 1, \dots, H - 1$  and for  $t \in [-1, 1]^{d_h}$ ,  $Y_h(t) \in [-1, 1]^{d_{h+1}}$ .

*Proof of Lemma A.2.* The second assertion can be written as: for  $h = 1, \dots, H - 1$  and  $i = 1, \dots, d_{h+1}$ ,

$$\|Y_{h,i}\|_{\infty, [-1, 1]^{d_h}} \leq 1.$$

Hence, to prove the lemma, it is sufficient to show that, for  $h = 1, \dots, H - 1$  and  $i = 1, \dots, d_{h+1}$ ,

$$\|Z_{h,i}\|_{\infty, \prod_{\ell=1, \dots, d_h} [-L_{h,\ell}, L_{h,\ell}]} \leq L_{h+1,i} \Leftrightarrow \|Y_{h,i}\|_{\infty, [-1, 1]^{d_h}} \leq 1.$$

The latter equivalence follows from (17). □

Finally, the next lemma shows that  $Y_1, \dots, Y_H$  and  $Z_1, \dots, Z_H$  equivalently satisfy constraints of the form (3).

**Lemma A.3.** *For  $h = 2, \dots, H$ , for  $i = 1, \dots, d_{h+1}$ , and for  $j = 1, \dots, d_h$ ,*

$$\left\| \frac{\partial Z_{h,i}}{\partial x_j} \right\|_{\infty, \prod_{\ell=1, \dots, d_h} [-L_{h,\ell}, L_{h,\ell}]} \leq K_{h,i,j} \Leftrightarrow \left\| \frac{\partial Y_{h,i}}{\partial x_j} \right\|_{\infty, [-1, 1]^{d_h}} \leq \frac{L_{h,j}}{L_{h+1,i}} K_{h,i,j}.$$

*Proof of Lemma A.3.* Let  $L_{H+1,1} = 1$  by convention. From (17) and (18), we have, for  $h = 2, \dots, H$ , for  $i = 1, \dots, d_{h+1}$ ,  $j = 1, \dots, d_h$ , and for  $t_1, \dots, t_{d_h} \in \mathbb{R}$ ,

$$\begin{aligned}
\left( \frac{\partial}{\partial x_j} Y_{h,i} \right) (t_1, \dots, t_{d_h}) &= \frac{\partial}{\partial t_j} \left( \frac{1}{L_{h+1,i}} Z_{h,i}(L_{h,1}t_1, \dots, L_{h,d_h}t_{d_h}) \right) \\
&= \frac{L_{h,j}}{L_{h+1,i}} \left( \frac{\partial}{\partial x_j} Z_{h,i} \right) (L_{h,1}t_1, \dots, L_{h,d_h}t_{d_h}).
\end{aligned}$$

Hence we have

$$\left\| \frac{\partial Z_{h,i}}{\partial x_j} \right\|_{\infty, \prod_{\ell=1, \dots, d_h} [-L_{h,\ell}, L_{h,\ell}]} \leq K_{h,i,j} \iff \left\| \frac{\partial Y_{h,i}}{\partial x_j} \right\|_{\infty, [-1,1]^{d_h}} \leq \frac{L_{h,j}}{L_{h+1,i}} K_{h,i,j}.$$

which concludes the proof.  $\square$

## B Preliminary notation and intermediate results

The proofs will exploit the results established in [45] for a single Gaussian process. Thus we will consider the setting of a single Gaussian process defined on a compact space and valued in  $\mathbb{R}$ . The following section is dedicated to the construction of this process.

### B.1 Introduction of a single global Gaussian prior

Let  $d_{\max} = \max(d_1, \dots, d_H)$  and let  $\mathcal{X}$  be the compact subspace  $[-1, 1]^{d_{\max}} \times \mathcal{I}$  with the distance  $d$  defined by

$$d((t, h, i), (t', h', i')) = \|(t, \sigma(h, i)) - (t', \sigma(h', i'))\|, \quad \text{for } (t, h, i) \text{ and } (t', h', i') \text{ in } \mathcal{X}$$

where the norm is the Euclidean norm in dimension  $d_{\max} + 1$  and  $\sigma$  is any fixed bijection from  $\mathcal{I}$  to  $\{1, \dots, |\mathcal{I}|\}$  with  $|\mathcal{I}|$  the cardinality of  $\mathcal{I}$ . We introduce the centered Gaussian process  $W$ , defined by

$$W(t, h, i) = Z_{h,i}(T_h(t)), \quad \text{for } (t, h, i) \in \mathcal{X}, \quad (20)$$

where  $T_h(t)$  is the vector of length  $d_h$  obtained from the  $d_h$  first coordinates of  $t$ . Then  $W$  has continuous trajectories from  $\mathcal{X}$  to  $\mathbb{R}$ .

Let  $\mathbb{B}$  be the Banach space of the continuous functions from  $\mathcal{X}$  to  $\mathbb{R}$  endowed with the uniform norm given by

$$\|w\|_{\infty, \mathcal{X}} := \vee_{(h,i) \in \mathcal{I}} \|w(\cdot, h, i)\|_{\infty, [-1,1]^{d_{\max}}}$$

for any  $w \in \mathbb{B}$ . Here  $t \vee s$  stands for  $\max(t, s)$  between  $t, s \in \mathbb{R}$ . From now on, we simply denote  $\|\cdot\|_{\infty, \mathcal{X}}$  by  $\|\cdot\|_{\infty}$ . For  $w \in \mathbb{B}$  and  $(h, i) \in \mathcal{I}$ , we define  $P_{h,i}(w)$  as the real-valued function on  $[-1, 1]^{d_h}$ , defined by

$$P_{h,i}(w)(t) = w((t, 0), h, i), \quad \text{for } t \in [-1, 1]^{d_h},$$

where the vector  $(t, 0)$  has dimension  $d_{\max}$ . Consequently, for  $(h, i) \in \mathcal{I}$  and for  $t \in [-1, 1]^{d_h}$ ,

$$P_{h,i}(W)(t) = Z_{h,i}(t).$$

Now we define the subset  $\mathbb{B}_c$  of  $\mathbb{B}$  composed by the functions  $w \in \mathbb{B}$  such that the three following conditions (corresponding to (2) and (3)) hold.

- For  $h = 1, \dots, H - 1, i = 1, \dots, d_{h+1}$ ,  $\|P_{h,i}(w)\|_{\infty, [-1, 1]^{d_h}} \leq 1$ .
- For  $h = 2, \dots, H, i = 1, \dots, d_{h+1}$ ,  $P_{h,i}(w)$  is continuously differentiable on  $[-1, 1]^{d_h}$ .
- For  $h = 2, \dots, H, i = 1, \dots, d_{h+1}, j = 1, \dots, d_h$ ,  $\|\partial P_{h,i}(w)/\partial x_j\|_{\infty, [-1, 1]^{d_h}} \leq K_{h,i,j}$ .

Then we consider a process  $W_c$  valued in  $\mathbb{B}$  with distribution defined by

$$\mathbb{P}(W_c \in B) = \mathbb{P}(W \in B \mid W \in \mathbb{B}_c), \quad (21)$$

for any Borel set  $B \subset \mathbb{B}$ . Hence  $W_c$  corresponds to the Gaussian process  $W$  conditioned by the constraints (2) and/or (3).

For any function  $\psi \in \mathbb{B}_c$ , let  $C_\psi$  be the function from  $[-1, 1]^d$  to  $\mathbb{R}$  defined by the following. For  $h = 1, \dots, H$ , we let the function  $C_{\psi,h} = (P_{h,1}(\psi), \dots, P_{h,d_{h+1}}(\psi))$  be defined on  $[-1, 1]^{d_h}$  and valued in  $[-1, 1]^{d_{h+1}}$ . Then we let, for  $t \in [-1, 1]^d$ ,

$$C_\psi(t) = C_{\psi,H} \circ \dots \circ C_{\psi,1}(t). \quad (22)$$

Remark that, for  $t \in [-1, 1]^d$ , when  $W \in \mathbb{B}_c$ ,

$$C_W(t) = Z_H \circ \dots \circ Z_1(t). \quad (23)$$

Hence, considering the conditioned version  $W_c$  of  $W$  (as defined in (21)),  $C_{W_c}$  has the distribution of the deep Gaussian process  $Z_H \circ \dots \circ Z_1$  where the univariate Gaussian processes  $Z_{h,i}$  are conditioned to (2) and/or (3).

Finally, we let  $k$  be the covariance function of  $W$  on  $\mathcal{X} \times \mathcal{X}$  and  $\mathbb{H}$  be the RKHS of  $W$  (that is defined as in [46, Section 2.1]) with RKHS-norm  $\|\cdot\|_{\mathbb{H}}$ .

## B.2 The global concentration function is upper bounded

For  $w_0$  in the closure of  $\mathbb{H}$  in  $\mathbb{B}$  (with respect to  $\|\cdot\|_{\infty}$ ), we define, for  $\varepsilon > 0$ ,

$$\phi_{c,w_0}(\varepsilon) = \inf_{\substack{h \in \mathbb{H} \\ \|h - w_0\|_{\infty} < \varepsilon}} \|h\|_{\mathbb{H}}^2 - \log \mathbb{P}(\|W_c\|_{\infty} < \varepsilon) - \log \mathbb{P}(\|W - w_0\|_{\infty} < 2\varepsilon, W \in \mathbb{B}_c). \quad (24)$$

The function  $\phi_{c,w_0}$  is interpreted as the concentration function of  $W$  around  $w_0$  and is an extension of the function  $\phi_{x_0}$  already defined in (7) and in [45, Equation (1.2)], that takes the bound constraints in  $W_c$  into account. The next lemma shows that the presence of the constraints increases the concentration function.

**Lemma B.1.** *Let  $\phi_{w_0}(\varepsilon)$  be as in (7) with  $x_0 = w_0$ ,  $X = W$  and  $E = \mathcal{X}$ . One has  $\phi_{w_0}(\varepsilon) \leq \phi_{c,w_0}(\varepsilon)$  for any  $\varepsilon > 0$ .*



*Proof of Lemma B.1.* For any  $\varepsilon > 0$ , let us consider the difference between the two concentration functions

$$\begin{aligned} \phi_{c,w_0}(\varepsilon) - \phi_{w_0}(\varepsilon) &= -\log \mathbb{P}(\|W_c\|_\infty < \varepsilon) - \log \mathbb{P}(\|W - w_0\|_\infty < 2\varepsilon, W \in \mathbb{B}_c) \\ &\quad + \log \mathbb{P}(\|W\|_\infty < \varepsilon). \end{aligned}$$

Since  $\mathbb{P}(\|W_c\|_\infty < \varepsilon) = \mathbb{P}(\|W\|_\infty < \varepsilon, W \in \mathbb{B}_c) / \mathbb{P}(W \in \mathbb{B}_c)$ ,

$\mathbb{P}(\|W\|_\infty < \varepsilon) \geq \mathbb{P}(\|W\|_\infty < \varepsilon, W \in \mathbb{B}_c)$  and  $\mathbb{P}(W \in \mathbb{B}_c) \geq \mathbb{P}(\|W - w_0\|_\infty < 2\varepsilon, W \in \mathbb{B}_c)$ ,

the latter difference is non-negative.  $\square$

The next theorem shows that the global  $\phi_{c,w_0}$  defined in (24) is upper bounded by  $\Phi_{c,w_0}$  defined in (8).

**Theorem B.2.** *Let  $w_0$  in  $\mathbb{B}$ . For  $(h, i) \in \mathcal{I}$ , assume that  $w_0(\cdot, h, i) = P_{h,i}(w_0)(T_h(\cdot))$ . For  $h = 2, \dots, H$  and for  $i = 1, \dots, d_{h+1}$ , assume that  $P_{h,i}(w_0)$  is in the closure of  $\mathbb{H}_{h,i}$  in  $(\mathcal{C}^1([-1, 1]^{d_h}, \mathbb{R}), \|\cdot\|_{\infty,1})$ . Recall that  $\|\cdot\|_{\infty,1}$  is defined in (6). For  $i = 1, \dots, d_2$ , assume that  $P_{1,i}(w_0)$  is in the closure of  $\mathbb{H}_{1,i}$  in  $(\mathcal{C}^0([-1, 1]^{d_1}, \mathbb{R}), \|\cdot\|_\infty)$ . Then  $w_0$  is in the closure of  $\mathbb{H}$  in  $(\mathbb{B}, \|\cdot\|_\infty)$ .*

Now consider  $\varepsilon \in (0, 1]$  and assume that, for  $h = 1, \dots, H - 1$ , for  $i = 1, \dots, d_{h+1}$ ,

$$\|P_{h,i}(w_0)\|_\infty + 2\varepsilon \leq 1 \quad (25)$$

and, for  $h = 2, \dots, H$ , for  $i = 1, \dots, d_{h+1}$ , and for  $j = 1, \dots, d_h$ ,

$$\left\| \frac{\partial P_{h,i}(w_0)}{\partial x_j} \right\|_\infty \leq \frac{K_{\min}}{2} \quad (26)$$

where  $K_{\min}$  is defined in (9). Then we have

$$\phi_{c,w_0}(\varepsilon) \leq \Phi_{c,w_0}(\varepsilon)$$

where  $\Phi_{c,w_0}$  is as in (8) with  $z_{0,h,i} = P_{h,i}(w_0)$  for  $(h, i) \in \mathcal{I}$ .

### B.3 Contraction rates with the global concentration function

The next theorem is an adaptation of [45, Theorem 2.1]. For a metric space  $(E, d)$ , any subset  $A \subset E$ , and any  $\varepsilon > 0$ , we let  $N(\varepsilon, A, d)$  be the minimum number of balls of radius  $\varepsilon$  needed to cover  $A$ .

**Theorem B.3.** *Consider any sequence  $(\varepsilon_{c,n})_{n \in \mathbb{N}}$ , satisfying  $n\varepsilon_{c,n}^2 \rightarrow \infty$  and  $\phi_{c,w_0}(\varepsilon_{c,n}) \leq n\varepsilon_{c,n}^2$  for  $\phi_{c,w_0}$  defined in (24), and any  $C > 1$  with  $e^{-Cn\varepsilon_{c,n}^2} < 1/2$ . Then there exists an integer  $n_C \geq 0$  and a sequence of measurable sets  $(B_{c,n})_{n \in \mathbb{N}}$  with  $B_{c,n} \subset \mathbb{B}_c$  such that, for  $n \geq n_C$ ,*

$$\log N(6\sqrt{C}\varepsilon_{c,n}, B_{c,n}, \|\cdot\|_\infty) \leq n(12\sqrt{C}\varepsilon_{c,n})^2, \quad (27)$$

$$\mathbb{P}(W_c \notin B_{c,n}) \leq e^{-Cn\varepsilon_{c,n}^2}, \quad (28)$$

$$\mathbb{P}(\|W_c - w_0\|_\infty < 2\varepsilon_{c,n}) \geq e^{-n\varepsilon_{c,n}^2}. \quad (29)$$

Theorem B.3 enables to obtain posterior contraction rates at speed  $\varepsilon_{c,n}$  satisfying  $\phi_{c,w_0}(\varepsilon_{c,n}) \leq n\varepsilon_{c,n}^2$  similarly as done in [45]. This directly allows to prove Theorems 3.1 and 3.2, that is contraction rates at speed  $\varepsilon_{c,n}$  satisfying  $\Phi_{c,z_0}(\varepsilon_{c,n}) \leq n\varepsilon_{c,n}^2$  from the bound  $\phi_{c,w_0} \leq \Phi_{c,z_0}$  of Theorem B.2.

## C Proofs

In the rest of the appendix, we write  $C_{\text{sup}}$  for a finite constant which value is allowed to change between occurrences.

### C.1 Proof of Theorem B.2

Before proving Theorem B.2, let us establish several useful lemmas. We do not exclude that results similar to Lemma C.1 could be known by the experts, but we have not found any reference. We prove Lemma C.1 after its statement for self-sufficiency.

**Lemma C.1.** *The RKHS  $\mathbb{H}$  of the covariance function  $k$  is equal to the set of functions  $g : \mathcal{X} \rightarrow \mathbb{R}$  such that, for  $(h, i) \in \mathcal{I}$ ,*

$$g(\cdot, h, i) = P_{h,i}(g)(T_h(\cdot)) \quad \text{and} \quad P_{h,i}(g) \in \mathbb{H}_{h,i}. \quad (30)$$

Furthermore, for  $g \in \mathbb{H}$ , one has

$$\|g\|_{\mathbb{H}}^2 = \sum_{(h,i) \in \mathcal{I}} \|P_{h,i}(g)\|_{\mathbb{H}_{h,i}}^2. \quad (31)$$

*Proof of Lemma C.1.* For  $h = 1, \dots, H$  and for  $t \in [-1, 1]^{d_{\max}}$ , recall that  $T_h(t) \in [-1, 1]^{d_h}$  is composed of the  $d_h$  first coordinates of  $t$ . For  $(h, i) \in \mathcal{I}$ , let  $\mathbb{H}_{0,h,i}$  be the set of functions of the form

$$t \in [-1, 1]^{d_h} \mapsto \sum_{a=1}^{N_{h,i}} \alpha_{h,i,a} k_{h,i}(t_{h,i,a}, t), \quad (32)$$

for  $N_{h,i} \in \mathbb{N}^*$ , for  $t_{h,i,1}, \dots, t_{h,i,N_{h,i}} \in [-1, 1]^{d_h}$ , and for  $\alpha_{h,i,1}, \dots, \alpha_{h,i,N_{h,i}} \in \mathbb{R}$ . Also, let  $\mathbb{H}_0$  be the set of functions of the form

$$(t, h, i) \in \mathcal{X} \mapsto \sum_{a=1}^N \gamma_a k((t_a, h_a, i_a), (t, h, i)), \quad (33)$$

for  $N \in \mathbb{N}^*$ , for  $(t_1, h_1, i_1), \dots, (t_N, h_N, i_N) \in \mathcal{X}$ , and for  $\gamma_1, \dots, \gamma_N \in \mathbb{R}$ . Then, from Moore-Aronszajn theorem (see [6, Theorem 3]), we have  $\mathbb{H}_{0,h,i} \subset \mathbb{H}_{h,i}$  for  $(h, i) \in \mathcal{I}$  and  $\mathbb{H}_0 \subset \mathbb{H}$ .

We have, for any function  $g_0 \in \mathbb{H}_0$  of the form (33), using the independence of the  $Z_{h,i}$  for  $(h, i) \in \mathcal{I}$ , that  $P_{h,i}(g_0)$  is the function

$$t \in [-1, 1]^{d_h} \mapsto \sum_{\substack{a=1 \\ (h_a, i_a)=(h,i)}}^N \gamma_a k_{h,i}(T_{h,i}(t_a), t)$$

and thus belongs to  $\mathbb{H}_{0,h,i}$ .

Hence we have, using the independence of the  $Z_{h,i}$  for  $(h, i) \in \mathcal{I}$ , again,

$$\begin{aligned} \|g_0\|_{\mathbb{H}}^2 &= \sum_{a,b=1}^N \gamma_a \gamma_b k((t_a, h_a, i_a), (t_b, h_b, i_b)) \\ &= \sum_{(h,i) \in \mathcal{I}} \sum_{\substack{a,b=1 \\ (h_a, i_a)=(h_b, i_b)=(h,i)}}^N \gamma_a \gamma_b k_{h,i}(T_{h_a}(t_a), T_{h_b}(t_b)) \\ &= \sum_{(h,i) \in \mathcal{I}} \|P_{h,i}(g_0)\|_{\mathbb{H}_{h,i}}^2. \end{aligned} \tag{34}$$

Now let  $g \in \mathbb{H}$ . Again from Moore-Aronszajn theorem, there exists a sequence  $(g_N)_{N \in \mathbb{N}^*}$  of elements of  $\mathbb{H}_0$ , that is a Cauchy sequence with  $\|\cdot\|_{\mathbb{H}}$  converging pointwise to  $g$ . This implies that the first property in (30) holds for  $g$  since it holds for  $g_N$  of the form (33). For  $(h, i) \in \mathcal{I}$ , let  $g_{N,h,i} = P_{h,i}(g_N)$ . From (34) and the linearity of  $P_{h,i}$ ,  $(g_{N,h,i})_{N \in \mathbb{N}^*}$  is a Cauchy sequence of elements of  $\mathbb{H}_{0,h,i}$  with the norm  $\|\cdot\|_{\mathbb{H}_{h,i}}$ . Hence, by completeness, as  $N \rightarrow \infty$ ,  $g_{N,h,i}$  converges (with the norm  $\|\cdot\|_{\mathbb{H}_{h,i}}$ ) to a function  $g_{h,i} \in \mathbb{H}_{h,i}$ .

Since RKHS convergence implies pointwise convergence [6, Lemma 8], we have, for  $t \in [-1, 1]^{d_h}$ ,

$$P_{h,i}(g)(t) = \lim_{N \rightarrow \infty} P_{h,i}(g_N)(t) = \lim_{N \rightarrow \infty} g_{N,h,i}(t) = g_{h,i}(t).$$

Hence the second property in (30) holds and  $g$  can be written as in (30). Conversely, let a function  $g : \mathcal{X} \rightarrow \mathbb{R}$  that satisfies (30). For  $(h, i) \in \mathcal{I}$ , from Moore-Aronszajn theorem, there exist  $(g_{N,h,i})_{N \in \mathbb{N}^*}$  as in (32) that is a Cauchy sequence of elements of  $\mathbb{H}_{0,h,i}$  with the norm  $\|\cdot\|_{\mathbb{H}_{h,i}}$  and such that, as  $N \rightarrow \infty$ ,  $g_{N,h,i} \rightarrow P_{h,i}(g)$  pointwise on  $[-1, 1]^{d_h}$ . Then let us show that the function  $g_N : \mathcal{X} \rightarrow \mathbb{R}$  defined by, for  $(t, h, i) \in \mathcal{X}$ ,

$$g_N(t, h, i) = g_{N,h,i}(T_h(t)), \tag{35}$$

belongs to  $\mathbb{H}_0$ . We have

$$\begin{aligned}
g_N(t, h, i) &= \sum_{a=1}^{N_{h,i}} \alpha_{h,i,a} k_{h,i}(t_{h,i,a}, T_h(t)) \\
&= \sum_{a=1}^{N_{h,i}} \alpha_{h,i,a} k((t_{h,i,a}, 0), h, i), (t, h, i)) \\
&= \sum_{(h',i') \in \mathcal{I}} \sum_{a=1}^{N_{h',i'}} \alpha_{h',i',a} k((t_{h',i',a}, 0), h', i'), (t, h, i)),
\end{aligned}$$

using the independence of the  $P_{h,i}(W)$  for  $(h, i) \in \mathcal{I}$ . Hence,  $g_N$  belongs to  $\mathbb{H}_{0,N}$  and thus to  $\mathbb{H}_0$ .

Observe that we have, for  $(h, i) \in \mathcal{I}$ ,  $P_{h,i}(g_N) = g_{N,h,i}$  and thus from (34), as  $N \rightarrow \infty$ ,  $g_N$  is a Cauchy sequence of elements in  $\mathbb{H}_0$  with the norm  $\|\cdot\|_{\mathbb{H}}$ . Hence  $g_N$  also converges pointwise on  $\mathcal{X}$  and the pointwise limit function  $\lim_{N \rightarrow \infty} g_N$  belongs to  $\mathbb{H}$  from Moore-Aronszajn theorem. We also have, for fixed  $(t, h, i) \in \mathcal{X}$ ,

$$\begin{aligned}
\lim_{N \rightarrow \infty} g_N(t, h, i) &= \lim_{N \rightarrow \infty} g_{N,h,i}(T_h(t)) \\
&= P_{h,i}(g)(T_h(t)) = g(t, h, i),
\end{aligned}$$

using at the end the first equality in (30). Hence, any  $g : \mathcal{X} \rightarrow \mathbb{R}$  satisfying (30) does belong to  $\mathbb{H}$ . This shows that the RKHS  $\mathbb{H}$  is as indicated in the lemma.

Finally, let us prove (31). Let  $g : \mathcal{X} \rightarrow \mathbb{R}$  in  $\mathbb{H}$  and thus satisfying (30). Then, for  $(h, i) \in \mathcal{I}$ , there exists a sequence  $(g_{N,h,i})_{N \in \mathbb{N}^*}$  of functions in  $\mathbb{H}_{0,h,i}$  that converges to  $P_{h,i}(g)$  with the norm  $\|\cdot\|_{\mathbb{H}_{h,i}}$ . Define  $g_N$  as in (35). We have shown that  $(g_N)_{N \in \mathbb{N}^*}$  is a Cauchy sequence of elements in  $\mathbb{H}_0$  with the norm  $\|\cdot\|_{\mathbb{H}}$  that converges pointwise to  $g$ . Hence  $g_N$  also converges with the norm  $\|\cdot\|_{\mathbb{H}}$  to  $g$  and we have, using (34),

$$\|g\|_{\mathbb{H}}^2 = \lim_{N \rightarrow \infty} \|g_N\|_{\mathbb{H}}^2 = \lim_{N \rightarrow \infty} \sum_{(h,i) \in \mathcal{I}} \|P_{h,i}(g_N)\|_{\mathbb{H}_{h,i}}^2.$$

Because of (35), we have  $P_{h,i}(g_N) = g_{N,h,i}$  and thus

$$\|g\|_{\mathbb{H}}^2 = \lim_{N \rightarrow \infty} \sum_{(h,i) \in \mathcal{I}} \|g_{N,h,i}\|_{\mathbb{H}_{h,i}}^2 = \sum_{(h,i) \in \mathcal{I}} \|P_{h,i}(g)\|_{\mathbb{H}_{h,i}}^2.$$

This concludes the proof.  $\square$

**Lemma C.2.** *Consider a centered Gaussian process  $X$ , valued in a Banach space  $(E, \|\cdot\|)$  composed of functions from a set  $T$  to  $\mathbb{R}$ . Let  $\mathbb{H}_X$  be the RKHS of  $X$ , with RKHS-norm  $\|\cdot\|_{\mathbb{H}_X}$ . Let  $f \in E$ . Then we have, for any  $\varepsilon > 0$ ,*

$$-\log \mathbb{P}(\|X - f\| < 2\varepsilon) \leq \frac{1}{2} \inf_{\substack{g \in \mathbb{H}_X \\ \|g-f\| < \varepsilon}} \|g\|_{\mathbb{H}_X}^2 - \log \mathbb{P}(\|X\| \leq \varepsilon),$$

with the convention that the infimum above is equal to  $+\infty$  if there are no  $g \in \mathbb{H}_X$  such that  $\|g - f\| < \varepsilon$ .

*Proof of Lemma C.2.* If there is no  $g \in \mathbb{H}_X$  such that  $\|g - f\| < \varepsilon$ , then the inequality of the lemma is trivially true. If there exists one  $g \in \mathbb{H}_X$  with  $\|g - f\| < \varepsilon$ , we have, for such a  $g$ , using first the triangle inequality and then [28, Theorem 3.1],

$$-\log \mathbb{P}(\|X - f\| < 2\varepsilon) \leq -\log \mathbb{P}(\|X - g\| \leq \varepsilon) \leq \frac{1}{2} \|g\|_{H_X}^2 - \log \mathbb{P}(\|X\| < \varepsilon).$$

This concludes the proof.  $\square$

**Lemma C.3.** *Let  $T$  be a compact metric set and let  $X$  be a continuous centered univariate Gaussian process indexed by  $T$ . Then, for  $u > 0$ ,*

$$\mathbb{P}\left(\sup_{t \in T} |X(t)| \leq u\right) > 0.$$

*Proof of Lemma C.3.* This result is often stated implicitly in the literature (for instance in [28]) but we are not aware of an explicit statement. Here is a proof.

Let  $u > 0$  and let  $(t_i)_{i \in \mathbb{N}^*}$  be a sequence of elements in  $T$  that is dense in  $T$ . For  $n \in \mathbb{N}^*$ , let  $\mathcal{F}_n$  be the  $\sigma$ -algebra generated by  $X(t_1), \dots, X(t_n)$ . Then, from [5, Proposition 2.9] for instance,  $\mathbb{E}[X(\cdot)|\mathcal{F}_n] \rightarrow X$  uniformly on  $T$  and almost surely. Hence, one has

$$\mathbb{P}\left(\sup_{t \in T} |X(t) - \mathbb{E}[X(t)|\mathcal{F}_n]| \leq \frac{u}{2}\right) \rightarrow 1$$

as  $n \rightarrow \infty$ . Using the triangular inequality and from the independence between  $X - \mathbb{E}[X(\cdot)|\mathcal{F}_n]$  and  $\mathbb{E}[X(\cdot)|\mathcal{F}_n]$  (as the conditional distribution of the first process given  $\mathcal{F}_n$  is deterministic), we obtain

$$\begin{aligned} \mathbb{P}\left(\sup_{t \in T} |X(t)| \leq u\right) &\geq \mathbb{P}\left(\sup_{t \in T} |X(t) - \mathbb{E}(X(t)|\mathcal{F}_n)| \leq \frac{u}{2}, \sup_{t \in T} |\mathbb{E}(X(t)|\mathcal{F}_n)| \leq \frac{u}{2}\right) \\ &= \mathbb{P}\left(\sup_{t \in T} |X(t) - \mathbb{E}(X(t)|\mathcal{F}_n)| \leq \frac{u}{2}\right) \mathbb{P}\left(\sup_{t \in T} |\mathbb{E}(X(t)|\mathcal{F}_n)| \leq \frac{u}{2}\right). \end{aligned}$$

The first probability above is non-zero for  $n$  large enough, as seen before. The second probability is non-zero for any  $n \in \mathbb{N}^*$ , because  $\sup_{t \in T} |\mathbb{E}(X(t)|\mathcal{F}_n)|$  is a continuous function of the Gaussian vector  $(X(t_1), \dots, X(t_n))$ , since the covariance function of  $X$  is continuous [22, Lemma 1].  $\square$

**Lemma C.4.** *Let  $X$  be a centered univariate Gaussian process with continuous realizations, indexed by a compact metric set  $T$ . Then, for all  $u > 0$ ,*

$$\mathbb{P}\left(\sup_{t \in T} |X(t)| = u\right) = 0.$$

*In other words, the random variable  $\sup_{t \in T} |X(t)|$  is absolutely continuous on the half-line  $(0, +\infty)$ .*

*Proof of Lemma C.4.* Let  $T'$  be a dense countable subset of  $T$ . By density, since  $T'$  is dense, and  $X$  has continuous realizations, we have, for  $u > 0$ ,

$$\begin{aligned} \mathbb{P}(\sup_{t \in T} |X(t)| = u) &= \mathbb{P}(\sup_{t \in T'} |X(t)| = u) \\ &\leq \mathbb{P}(\sup_{t \in T'} X(t) = u) + \mathbb{P}(\inf_{t \in T'} X(t) = -u) \\ &= \mathbb{P}(\sup_{t \in T'} X(t) = u) + \mathbb{P}(\sup_{t \in T'} (-X(t)) = u) \\ &= 2\mathbb{P}(\sup_{t \in T'} X(t) = u), \end{aligned}$$

where we have used the symmetry of the law of a centered Gaussian process. This last probability is zero from Tsirelson's theorem ([43], see also [1, Theorem 7.1]), together with Lemma C.3.  $\square$

**Lemma C.5.** *Let  $X$  be a centered univariate Gaussian process indexed by  $[-1, 1]^\ell$  for some  $\ell \in \mathbb{N}^*$  with continuously differentiable realizations. Then, for  $a > 0$  and for  $b_1, \dots, b_\ell > 0$ , we have*

$$\begin{aligned} &\mathbb{P}\left(\sup_{t \in [-1, 1]^\ell} |X(t)| \leq a, \sup_{t \in [-1, 1]^\ell} |\partial X(t)/\partial x_i| \leq b_i \text{ for } i = 1, \dots, \ell\right) \\ &\geq \mathbb{P}\left(\sup_{t \in [-1, 1]^\ell} |X(t)| \leq a\right) \prod_{i=1}^{\ell} \mathbb{P}\left(\sup_{t \in [-1, 1]^\ell} |\partial X(t)/\partial x_i| \leq b_i\right). \end{aligned}$$

*Proof of Lemma C.5.* Let  $T = [-1, 1]^\ell$  and  $(t_j)_{j \in \mathbb{N}^*}$  be a sequence of elements of  $T$  that is dense in  $T$ . From the dominated convergence theorem and Lemma C.4, as  $n \rightarrow \infty$ ,

$$\begin{aligned} &\mathbb{P}\left(\max_{j=1, \dots, n} |X(t_j)| \leq a, \max_{j=1, \dots, n} |\partial X(t_j)/\partial x_i| \leq b_i \text{ for } i = 1, \dots, \ell\right) \\ &\rightarrow \mathbb{P}\left(\sup_{t \in T} |X(t)| \leq a, \sup_{t \in T} |\partial X(t)/\partial x_i| \leq b_i \text{ for } i = 1, \dots, \ell\right). \end{aligned}$$

Let

$$A = \left\{ (z_1, \dots, z_n, z_1^{(1)}, \dots, z_n^{(1)}, \dots, z_1^{(\ell)}, \dots, z_n^{(\ell)}) \in \mathbb{R}^{n+\ell n}; \max_{j=1, \dots, n} |z_j| \leq a \right\}$$

and, for  $i = 1, \dots, \ell$

$$B_i = \left\{ (z_1, \dots, z_n, z_1^{(1)}, \dots, z_n^{(1)}, \dots, z_1^{(\ell)}, \dots, z_n^{(\ell)}) \in \mathbb{R}^{n+\ell n}; \max_{j=1, \dots, n} |z_j^{(i)}| \leq b_i \right\}.$$

Then  $A$  and  $B$  are convex symmetric subsets of  $\mathbb{R}^{2n}$ . Hence, from the Gaussian correlation

inequality ([38], see also [24]), we obtain

$$\begin{aligned}
& \mathbb{P} \left( \max_{j=1, \dots, n} |X(t_j)| \leq a, \max_{j=1, \dots, n} |\partial X(t_j)/\partial x_i| \leq b_i, i = 1, \dots, \ell \right) \\
&= \mathbb{P} \left( (X(t_1), \dots, X(t_n), \partial X(t_1)/\partial x_1, \dots, \partial X(t_n)/\partial x_1, \dots, \partial X(t_1)/\partial x_\ell, \dots, \partial X(t_n)/\partial x_\ell) \right. \\
&\quad \left. \in A \cap \bigcap_{i=1}^\ell B_i \right) \\
&\geq \mathbb{P} \left( (X(t_1), \dots, X(t_n), \partial X(t_1)/\partial x_1, \dots, \partial X(t_n)/\partial x_1, \dots, \partial X(t_1)/\partial x_\ell, \dots, \partial X(t_n)/\partial x_\ell) \in A \right) \\
&\quad \times \prod_{i=1}^\ell \mathbb{P} \left( (X(t_1), \dots, X(t_n), \partial X(t_1)/\partial x_1, \dots, \partial X(t_n)/\partial x_1, \dots, \partial X(t_1)/\partial x_\ell, \dots, \partial X(t_n)/\partial x_\ell) \in B_i \right) \\
&= \mathbb{P} \left( \max_{j=1, \dots, n} |X(t_j)| \leq a \right) \times \prod_{i=1}^\ell \mathbb{P} \left( \max_{j=1, \dots, n} |\partial X(t_j)/\partial x_i| \leq b_i \right) \\
&\rightarrow \mathbb{P} \left( \sup_{t \in T} |X(t)| \leq a \right) \times \prod_{i=1}^\ell \mathbb{P} \left( \sup_{t \in T} |\partial X(t)/\partial x_i| \leq b_i \right),
\end{aligned}$$

as  $n \rightarrow \infty$ , again from the dominated convergence theorem and Lemma C.4. This concludes the proof.  $\square$

Now we are able to prove Theorem B.2.

*Proof of Theorem B.2.* From the assumptions of the theorem and Lemma C.1, we obtain that  $w_0$  is indeed in the closure of  $\mathbb{H}$  in  $\mathbb{B}$  (with respect to  $\|\cdot\|_\infty$ ). Then, using Lemma C.1,  $\varepsilon \in (0, 1]$  and (25), we obtain

$$\begin{aligned}
\phi_{c, w_0}(\varepsilon) &= \inf_{\substack{g \in \mathbb{H} \\ \|g - w_0\|_\infty < \varepsilon}} \|g\|_{\mathbb{H}}^2 - \log \mathbb{P}(\|W_c\|_\infty < \varepsilon) - \log \mathbb{P}(\|W - w_0\|_\infty < 2\varepsilon, W \in \mathbb{B}_c) \\
&\leq \inf_{\substack{\{g_{h,i}; (h,i) \in \mathcal{I}\} \\ \text{for all } (h,i), g_{h,i} \in \mathbb{H}_{h,i}, \\ \|g_{h,i} - P_{h,i}(w_0)\|_\infty < \varepsilon}} \left( \sum_{(h,i) \in \mathcal{I}} \|g_{h,i}\|_{\mathbb{H}_{h,i}}^2 \right) \\
&\quad - \log \mathbb{P} \left( \|Z_{h,i}\|_\infty < \varepsilon \text{ for } (h,i) \in \mathcal{I} \text{ and} \right. \\
&\quad \quad \left. \|\partial Z_{h,i}/\partial x_j\|_\infty \leq K_{h,i,j} \text{ for } h = 2, \dots, H, \text{ for } i = 1, \dots, d_{h+1}, \text{ for } j = 1, \dots, d_h \right) \\
&\quad - \log \mathbb{P} \left( \|Z_{h,i} - P_{h,i}(w_0)\|_\infty < 2\varepsilon \text{ for } (h,i) \in \mathcal{I} \text{ and} \right. \\
&\quad \quad \left. \|\partial Z_{h,i}/\partial x_j\|_\infty \leq K_{h,i,j} \text{ for } h = 2, \dots, H, \text{ for } i = 1, \dots, d_{h+1}, \text{ for } j = 1, \dots, d_h \right).
\end{aligned}$$

Using now the independence between the  $Z_{h,i}$ 's for  $(h,i) \in \mathcal{I}$ , we obtain

$$\phi_{c, w_0}(\varepsilon) \leq \sum_{i=1}^{d_2} A_i + \sum_{\substack{(h,i) \in \mathcal{I} \\ h \geq 2}} B_{h,i}, \tag{36}$$

where we have defined

$$A_i = \inf_{\substack{g \in \mathbb{H}_{1,i} \\ \|g - P_{1,i}(w_0)\|_\infty < \varepsilon}} \|g\|_{\mathbb{H}_{1,i}}^2 - \log \mathbb{P}(\|Z_{1,i}\|_\infty < \varepsilon) - \log \mathbb{P}(\|Z_{1,i} - P_{1,i}(w_0)\|_\infty < 2\varepsilon)$$

and

$$\begin{aligned} B_{h,i} &= \inf_{\substack{g \in \mathbb{H}_{h,i} \\ \|g - P_{h,i}(w_0)\|_\infty < \varepsilon}} \|g\|_{\mathbb{H}_{h,i}}^2 \\ &\quad - \log \mathbb{P}\left(\|Z_{h,i}\|_\infty < \varepsilon, \|\partial Z_{h,i}/\partial x_j\|_\infty \leq K_{h,i,j} \text{ for } j = 1, \dots, d_h\right) \\ &\quad - \log \mathbb{P}\left(\|Z_{h,i} - P_{h,i}(w_0)\|_\infty < 2\varepsilon, \|\partial Z_{h,i}/\partial x_j\|_\infty \leq K_{h,i,j} \text{ for } j = 1, \dots, d_h\right). \end{aligned}$$

First let us bound  $A_i$ . Since  $P_{1,i}(w_0)$  is in the closure of  $H_{1,i}$  in  $(\mathcal{C}^0([-1, 1]^{d_1}), \mathbb{R}), \|\cdot\|_\infty)$ , using Lemmas C.2, C.3, and C.4, we have

$$\begin{aligned} A_i &\leq \inf_{\substack{g \in \mathbb{H}_{1,i} \\ \|g - P_{1,i}(w_0)\|_\infty < \varepsilon}} \|g\|_{\mathbb{H}_{1,i}}^2 - \log \mathbb{P}(\|Z_{1,i}\|_\infty < \varepsilon) + \frac{1}{2} \inf_{\substack{g \in \mathbb{H}_{1,i} \\ \|g - P_{1,i}(w_0)\|_\infty < \varepsilon}} \|g\|_{\mathbb{H}_{1,i}}^2 - \log \mathbb{P}(\|Z_{1,i}\|_\infty < \varepsilon) \\ &= \frac{3}{2} \inf_{\substack{g \in \mathbb{H}_{1,i} \\ \|g - P_{1,i}(w_0)\|_\infty < \varepsilon}} \|g\|_{\mathbb{H}_{1,i}}^2 - 2 \log \mathbb{P}(\|Z_{1,i}\|_\infty < \varepsilon). \end{aligned} \quad (37)$$

Second let us bound  $B_{h,i}$ . We have, from (26),

$$\begin{aligned} B_{h,i} &\leq \inf_{\substack{g \in \mathbb{H}_{h,i} \\ \|g - P_{h,i}(w_0)\|_\infty < \varepsilon}} \|g\|_{\mathbb{H}_{h,i}}^2 - \log \mathbb{P}\left(\|Z_{h,i}\|_\infty < \varepsilon, \|\partial Z_{h,i}/\partial x_j\|_\infty \leq K_{\min}, j = 1, \dots, d_h\right) \\ &\quad - \log \mathbb{P}\left(\|Z_{h,i} - P_{h,i}(w_0)\|_\infty < 2\varepsilon, \|\partial Z_{h,i}/\partial x_j - \partial P_{h,i}(w_0)/\partial x_j\|_\infty \leq K_{\min}/2, j = 1, \dots, d_h\right) \\ &\leq \inf_{\substack{g \in \mathbb{H}_{h,i} \\ \|g - P_{h,i}(w_0)\|_\infty < \varepsilon}} \|g\|_{\mathbb{H}_{h,i}}^2 - \log \mathbb{P}\left(\|Z_{h,i}\|_\infty < \varepsilon, \|\partial Z_{h,i}/\partial x_j\|_\infty \leq K_{\min}, j = 1, \dots, d_h\right) \\ &\quad - \log \mathbb{P}\left(\|Z_{h,i} - P_{h,i}(w_0)\|_\infty \leq \varepsilon, 2\varepsilon \|\partial Z_{h,i}/\partial x_j - \partial P_{h,i}(w_0)/\partial x_j\|_\infty / K_{\min} \leq \varepsilon, j = 1, \dots, d_h\right). \end{aligned} \quad (38)$$

Let us define the Banach space  $\mathbb{B}_h$  as the set of continuous functions from  $[-1, 1]^{d_h} \times \{0, 1, \dots, d_h\}$ , equipped with the norm  $\|\cdot\|_{\infty, \varepsilon}$  defined by, for  $z \in \mathbb{B}_h$ ,

$$\|z\|_{\infty, \varepsilon} = \|z(\cdot, 0)\|_\infty \vee \frac{2\varepsilon}{K_{\min}} \|z(\cdot, 1)\|_\infty \vee \dots \vee \frac{2\varepsilon}{K_{\min}} \|z(\cdot, d_h)\|_\infty.$$

We consider the map  $M$  from  $(\mathcal{C}^1([-1, 1]^{d_h}, \mathbb{R}), \|\cdot\|_{\infty, 1})$  to  $(\mathbb{B}_h, \|\cdot\|_{\infty, \varepsilon})$  defined by, for  $f \in \mathcal{C}^1([-1, 1]^{d_h}, \mathbb{R})$ ,  $(Mf)(\cdot, 0) = f$ ,  $(Mf)(\cdot, 1) = \partial f/\partial x_1, \dots, (Mf)(\cdot, d_h) = \partial f/\partial x_{d_h}$ . Let us define the Gaussian process  $\bar{Z}$  on  $\mathbb{B}_h$  by  $\bar{Z} = M(Z_{h,i})$  and similarly the function  $\bar{w}_0$  in  $\mathbb{B}_h$  by  $\bar{w}_0 = M(P_{h,i}(w_0))$ . We write  $\mathbb{H}_{\bar{Z}}$  the RKHS of the Gaussian process  $\bar{Z}$  and  $\|\cdot\|_{\mathbb{H}_{\bar{Z}}}$  its RKHS-norm.



**Lemma C.6.** Recall that  $h = 2, \dots, H$ . We have  $\mathbb{H}_{\bar{Z}} = \{M(g); g \in \mathbb{H}_{h,i}\}$  and, for  $g \in \mathbb{H}_{h,i}$ ,  $\|g\|_{\mathbb{H}_{h,i}} = \|M(g)\|_{H_{\bar{Z}}}$ .

The proof of Lemma C.6 is postponed after the proof of Theorem B.2. Then, using the previous notation and Lemmas C.2 and C.6, we obtain

$$\begin{aligned}
& -\log \mathbb{P}\left(\|Z_{h,i} - P_{h,i}(w_0)\|_\infty \leq \varepsilon, \frac{2\varepsilon}{K_{\min}} \|\partial Z_{h,i}/\partial x_j - \partial P_{h,i}(w_0)/\partial x_j\|_\infty \leq \varepsilon \text{ for } j = 1, \dots, d_h\right) \\
&= -\log \mathbb{P}\left(\|\bar{Z} - \bar{w}_0\|_{\infty, \varepsilon} \leq \varepsilon\right) \\
&\leq \frac{1}{2} \inf_{\substack{h \in \mathbb{H}_{\bar{Z}} \\ \|h - \bar{w}_0\|_{\infty, \varepsilon} < \frac{\varepsilon}{2}}} \|h\|_{\mathbb{H}_{\bar{Z}}}^2 - \log \mathbb{P}\left(\|\bar{Z}\|_{\infty, \varepsilon} \leq \frac{\varepsilon}{2}\right) \\
&= \frac{1}{2} \inf_{\substack{g \in \mathbb{H}_{h,i} \\ \|g - P_{h,i}(w_0)\|_\infty < \frac{\varepsilon}{2} \\ \|\partial g/\partial x_j - \partial P_{h,i}(w_0)/\partial x_j\|_\infty < \frac{K_{\min}}{4}, \\ j=1, \dots, d_h}} \|g\|_{\mathbb{H}_{h,i}}^2 - \log \mathbb{P}\left(\|Z_{h,i}\|_\infty \leq \frac{\varepsilon}{2}, \|\partial Z_{h,i}/\partial x_j\|_\infty \leq \frac{K_{\min}}{4} \text{ for } j = 1, \dots, d_h\right).
\end{aligned}$$

Now using the above display and (38), together with Lemmas C.4, and C.5, we obtain

$$\begin{aligned}
B_{h,i} &\leq \frac{3}{2} \inf_{\substack{g \in \mathbb{H}_{h,i} \\ \|g - P_{h,i}(w_0)\|_\infty < \frac{\varepsilon}{2} \\ \|\partial g/\partial x_j - \partial P_{h,i}(w_0)/\partial x_j\|_\infty < \frac{K_{\min}}{4}, \\ j=1, \dots, d_h}} \|g\|_{\mathbb{H}_{h,i}}^2 - 2 \log \mathbb{P}\left(\|Z_{h,i}\|_\infty \leq \frac{\varepsilon}{2}\right) \\
&\quad - 2 \sum_{j=1}^{d_h} \log \mathbb{P}\left(\|\partial Z_{h,i}/\partial x_j\|_\infty \leq \frac{K_{\min}}{4}\right).
\end{aligned}$$

Then the proof is concluded using (36) and (37).  $\square$

It remains to prove Lemma C.6.

*Proof of Lemma C.6.* By assumption, the Gaussian process  $Z_{h,i}$ , with input space  $[-1, 1]^{d_h}$ , has continuously differentiable realizations. Hence,  $Z_{h,i}$  can be viewed as a random element of the Banach space  $\mathcal{C}^0([-1, 1]^{d_h}, \mathbb{R})$  of continuous functions on  $[-1, 1]^{d_h}$ , equipped with the norm  $\|\cdot\|_\infty$ . The space  $(\mathbb{H}_{h,i}, \|\cdot\|_{\mathbb{H}_{h,i}})$  is defined as in [46, Section 2.1] (from the covariance function of  $Z_{h,i}$ ). From [46, Theorem 2.1],  $\mathbb{H}_{h,i}$  can be equivalently defined as in [46, Section 2.2] from the law of  $Z_{h,i}$  in  $\mathcal{C}^0([-1, 1]^{d_h}, \mathbb{R})$  and from the norm  $\|\cdot\|_\infty$ .

The identity map from  $(\mathcal{C}^1([-1, 1]^{d_h}, \mathbb{R}), \|\cdot\|_{\infty,1})$  to  $(\mathcal{C}^0([-1, 1]^{d_h}, \mathbb{R}), \|\cdot\|_\infty)$  is a one-to-one, continuous and linear application. Hence, from [46, Lemma 7.1], the RKHS  $\mathbb{H}_{h,i}$  can also be equivalently defined as in [46, Section 2.2], but this time by seeing  $Z_{h,i}$  as a random element of  $(\mathcal{C}^1([-1, 1]^{d_h}, \mathbb{R}), \|\cdot\|_{\infty,1})$ .

Now we consider the Banach space  $\mathbb{B}_h$  equipped with the norm  $\|\cdot\|_{\infty, \varepsilon}$ . We consider the map  $M$  introduced above. Then  $M$  is a one-to-one, continuous and linear application from  $(\mathcal{C}^1([-1, 1]^{d_h}, \mathbb{R}), \|\cdot\|_{\infty,1})$  to  $(\mathbb{B}_h, \|\cdot\|_{\infty, \varepsilon})$ . Also recall that we have defined  $\bar{Z} = M(Z_{h,i})$ .

Hence, from [46, Lemma 7.1], the RKHS  $\mathbb{H}_{\bar{Z}}$  of the Gaussian process  $\bar{Z}$  (defined as in [46, Section 2.2], by seeing  $\bar{Z}$  as a random element of  $(\mathbb{B}_h, \|\cdot\|_{\infty, \varepsilon})$ ), is equal to  $\{M(g); g \in \mathbb{H}_{h,i}\}$ . Furthermore, for  $g \in \mathbb{H}_{h,i}$ , we have  $\|g\|_{\mathbb{H}_{h,i}} = \|M(g)\|_{\mathbb{H}_{\bar{Z}}}$ , where we recall that  $\|\cdot\|_{\mathbb{H}_{\bar{Z}}}$  is the norm of the RKHS  $\mathbb{H}_{\bar{Z}}$ . From [46, Theorem 2.1], this latter definition of  $\mathbb{H}_{\bar{Z}}$  coincides with the definition of the RKHS  $\mathbb{H}_{\bar{Z}}$  in the statement of the lemma (from [46, Section 2.1], from the covariance function of  $\bar{Z}$ ). The two definitions of the corresponding norms also coincide (again from [46, Theorem 2.1]).  $\square$

## C.2 Proof of Theorem B.3

*Proof of Theorem B.3.* Let  $C > 1$  and let  $(\varepsilon_{c,n})_{n \in \mathbb{N}^*}$  satisfy the conditions of the theorem. We set  $\varepsilon_n^2 = \varepsilon_{c,n}^2 - \log \mathbb{P}(W \in \mathbb{B}_c)/Cn \geq \varepsilon_{c,n}^2$ . By Lemma B.1 (with the definition of  $\phi_{w_0}$  in (7)) and since  $\phi_{c,w_0}$  is non-increasing, we have

$$\phi_{w_0}(\varepsilon_n) \leq \phi_{c,w_0}(\varepsilon_n) \leq \phi_{c,w_0}(\varepsilon_{c,n}) \leq n\varepsilon_{c,n}^2 \leq n\varepsilon_n^2.$$

Furthermore, since  $\varepsilon_n^2 \geq \varepsilon_{c,n}^2$ , we have  $e^{-Cn\varepsilon_n^2} < 1/2$ . Hence we can apply [45, Theorem 2.1] to  $W$  with  $\varepsilon_n$  and  $C$ . Thus, there exists a sequence of measurable sets  $(B_n)_{n \in \mathbb{N}}$ ,  $B_n \subset \mathbb{B}$  for all  $n \in \mathbb{N}$ , such that

$$\log N(3\varepsilon_n, B_n, \|\cdot\|_{\infty}) \leq 6Cn\varepsilon_n^2, \quad (39)$$

$$\mathbb{P}(W \notin B_n) \leq e^{-Cn\varepsilon_n^2}, \quad (40)$$

$$\mathbb{P}(\|W - w_0\|_{\infty} < 2\varepsilon_n) \geq e^{-n\varepsilon_n^2}. \quad (41)$$

Now let  $B_{c,n} = B_n \cap \mathbb{B}_c$ . Clearly,  $B_{c,n} \subset B_n$ . Furthermore, since  $n\varepsilon_{c,n}^2 \rightarrow \infty$ , there exists a fixed  $n_C \in \mathbb{N}^*$  such that, for  $n \geq n_C$ ,  $\varepsilon_{c,n} \geq \varepsilon_n/2$ . Thus, for  $n \geq n_C$ ,

$$\begin{aligned} \log N(6\sqrt{C}\varepsilon_{c,n}, B_{c,n}, \|\cdot\|_{\infty}) &\leq \log N(3\sqrt{C}\varepsilon_n, B_{c,n}, \|\cdot\|_{\infty}) && \text{since } \varepsilon_{c,n} \geq \varepsilon_n/2 \\ &\leq \log N(3\varepsilon_n, B_n, \|\cdot\|_{\infty}) && \text{since } B_{c,n} \subset B_n \text{ and } C > 1 \\ &\leq 6Cn\varepsilon_n^2 && \text{from (39)} \\ &\leq 24Cn\varepsilon_{c,n}^2 && \text{since } \varepsilon_{c,n} \geq \varepsilon_n/2 \\ &\leq n(12\sqrt{C}\varepsilon_{c,n})^2. \end{aligned}$$

Hence (27) holds. As for (28), from (40), one gets

$$\mathbb{P}(W_c \notin B_{c,n}) = \mathbb{P}(W_c \notin B_n) = \mathbb{P}(W \notin B_n | W \in \mathbb{B}_c) \leq \frac{e^{-Cn\varepsilon_n^2}}{\mathbb{P}(W \in \mathbb{B}_c)} = e^{-Cn\varepsilon_{c,n}^2}$$

so that (28) holds. Last, one has

$$\mathbb{P}(\|W_c - w_0\|_{\infty} < 2\varepsilon_{c,n}) \geq \mathbb{P}(\|W - w_0\|_{\infty} < 2\varepsilon_{c,n}, W \in \mathbb{B}_c) \geq e^{-\phi_{c,w_0}(\varepsilon_{c,n})} \geq e^{-n\varepsilon_{c,n}^2}$$

so that (29) holds.  $\square$

### C.3 Proof of Theorem 3.1

Before proving Theorem 3.1, let us establish the following lemma and define

$$K_{\max} = \max_{h=2,\dots,H} \max_{i=1,\dots,d_{h+1}} \max_{j=1,\dots,d_h} K_{h,i,j}.$$

Recall the definition of  $\psi \mapsto C_\psi$  in (22).

**Lemma C.7.** *For  $w, z \in \mathbb{B}_c$ , we have*

$$\|C_w - C_z\|_\infty \leq K_H \|w - z\|_\infty$$

where  $K_H = (1 + K_{\max} d_{\max})^H$ .

*Proof of Lemma C.7.* Let, for  $h = 1, \dots, H$ ,  $C_{w,h} = (P_{h,1}(w), \dots, P_{h,d_{h+1}}(w))$  and  $C_{z,h} = (P_{h,1}(z), \dots, P_{h,d_{h+1}}(z))$ . Then we have, for  $t \in [-1, 1]^d$ , recalling that  $C_{w,H}$  is real-valued and letting  $\nabla f$  be the gradient of a function  $f$ ,

$$\begin{aligned} & |C_w(t) - C_z(t)| \\ &= |C_{w,H} \circ C_{w,H-1} \circ \dots \circ C_{w,1}(t) - C_{z,H} \circ C_{z,H-1} \circ \dots \circ C_{z,1}(t)| \\ &\leq |C_{w,H} \circ C_{w,H-1} \circ \dots \circ C_{w,1}(t) - C_{z,H} \circ C_{w,H-1} \circ \dots \circ C_{w,1}(t)| \\ &\quad + |C_{z,H} \circ C_{w,H-1} \circ \dots \circ C_{w,1}(t) - C_{z,H} \circ C_{z,H-1} \circ \dots \circ C_{z,1}(t)| \\ &\leq \|C_{w,H} - C_{z,H}\|_\infty + \sup_{x \in [-1, 1]^{d_H}} \|\nabla C_{z,H}(x)\| \times \|C_{w,H-1} \circ \dots \circ C_{w,1}(t) - C_{z,H-1} \circ \dots \circ C_{z,1}(t)\| \\ &\leq \|w - z\|_\infty + K_{\max} d_H \max_{i=1,\dots,d_H} |P_{H-1,i}(w) \circ \dots \circ C_{w,1}(t) - P_{H-1,i}(z) \circ C_{z,H-2} \circ \dots \circ C_{z,1}(t)| \\ &\leq (1 + K_{\max} d_{\max}) \times \max \left( \|w - z\|_\infty, \right. \\ &\quad \left. \max_{i=1,\dots,d_H} |P_{H-1,i}(w) \circ C_{w,H-2} \circ \dots \circ C_{w,1}(t) - P_{H-1,i}(z) \circ C_{z,H-2} \circ \dots \circ C_{z,1}(t)| \right). \end{aligned}$$

Hence, we can obtain the lemma by a descending induction from  $H$  to 1.  $\square$

Now we define the Kullback-Leibler divergence: for  $f, g : [-1, 1]^d \rightarrow (0, \infty)$  with  $\int_{[-1, 1]^d} f(t) dt = \int_{[-1, 1]^d} g(t) dt = 1$ , let

$$K(f, g) = \int_{[-1, 1]^d} \log(f(t)/g(t)) f(t) dt, \quad (42)$$

if  $\int_{[-1, 1]^d} |\log(f(t)/g(t))| f(t) dt < +\infty$  and  $K(f, g) = +\infty$  else. We also introduce

$$V(f, g) = \int_{[-1, 1]^d} (\log(f(t)/g(t)))^2 f(t) dt. \quad (43)$$

Then we have the following lemma, that follows from Lemma C.7 and [45, Lemma 3.1].

**Lemma C.8.** Recall the Hellinger distance  $h$  from (11), the function  $\psi \mapsto C_\psi$  from (22), and the function  $z \mapsto p_z$  from (10). For any functions  $v$  and  $w$  in  $\mathbb{B}_c$ , we have

$$\begin{aligned} h(p_{C_v}, p_{C_w}) &\leq K_H \|v - w\|_\infty e^{K_H \|v - w\|_\infty / 2}, \\ K(p_{C_v}, p_{C_w}) &\leq cK_H^2 \|v - w\|_\infty^2 (1 + K_H \|v - w\|_\infty) e^{K_H \|v - w\|_\infty}, \quad \text{and} \\ V(p_{C_v}, p_{C_w}) &\leq cK_H^2 \|v - w\|_\infty^2 (1 + K_H \|v - w\|_\infty)^2 e^{K_H \|v - w\|_\infty}, \end{aligned}$$

where  $K_H$  is as in Lemma C.7 and  $c \geq 1$  is a finite constant.

*Proof of Lemma C.8.* By [45, Lemma 3.1], one has, with a finite constant  $c \geq 1$ ,

$$h(p_{C_v}, p_{C_w}) \leq \|C_v - C_w\|_\infty e^{\|C_v - C_w\|_\infty / 2}, \quad (44)$$

$$K(p_{C_v}, p_{C_w}) \leq c \|C_v - C_w\|_\infty^2 (1 + \|C_v - C_w\|_\infty) e^{\|C_v - C_w\|_\infty}, \quad (45)$$

$$V(p_{C_v}, p_{C_w}) \leq c \|C_v - C_w\|_\infty^2 (1 + \|C_v - C_w\|_\infty)^2 e^{\|C_v - C_w\|_\infty}. \quad (46)$$

Thus we conclude the proof from Lemma C.7.  $\square$

Now we are able to prove Theorem 3.1.

*Proof of Theorem 3.1.* Consider a sequence  $(\varepsilon_{c,n})_{n \in \mathbb{N}}$  satisfying the conditions of the theorem. Define  $w_0 \in \mathbb{B}$  by, for  $(h, i) \in \mathcal{I}$  and for  $t \in [-1, 1]^{d_{\max}}$ ,  $w_0(t, h, i) = z_{0,h,i}(T_h(t))$ . Then, since  $\varepsilon_{c,n} \rightarrow 0$  for  $n$  large enough, from the assumptions of the theorem on the functions  $z_{0,h,i}$ , the conditions (25) and (26) of Theorem B.2 hold. Then Theorem B.2 provides  $\phi_{c,w_0}(\varepsilon_{c,n}) \leq \Phi_{c,z_0}(\varepsilon_{c,n})$  and thus

$$\phi_{c,w_0}(\varepsilon_{c,n}) \leq n\varepsilon_{c,n}^2.$$

Let, with  $c$  and  $K_H$  as in Lemma C.8,

$$t = 2cK_H^2, \quad C_c = 1 + 16t \quad \text{and} \quad C = \frac{1}{4t}.$$

Hence,

$$\frac{C_c}{4t} = C + 4. \quad (47)$$

Let  $\bar{\varepsilon}_n = 2\sqrt{t}\varepsilon_{c,n}$  and  $\varepsilon_n = 14\sqrt{C_c}K_H\varepsilon_{c,n} \geq \bar{\varepsilon}_n$ . Let us apply [18, Theorem 8.9], with the constant  $C$ , the sequences  $(\bar{\varepsilon}_n)_{n \in \mathbb{N}}$  and  $(\varepsilon_n)_{n \in \mathbb{N}}$ , and the prior  $p_{C_{w_c}}$ . Let us thus check that the assumptions of [18, Theorem 8.9] are satisfied, using Theorem B.3.

Since  $n\varepsilon_{c,n}^2 \rightarrow \infty$ , there exists  $N' \in \mathbb{N}^*$  such that, for  $n \geq N'$ ,  $e^{-C_c n \varepsilon_{c,n}^2} < 1/2$ . Hence, the assumptions of Theorem B.3 hold, with  $C$  there given by  $C_c$  and with  $(\varepsilon_{c,n})_{n \geq N'}$  as considered above. Hence, from this theorem, there exists an integer  $n_C \geq 0$  and a sequence of sets  $(B_{c,n})_{n \geq n_C}$  such that the conclusions (27), (28), and (29) hold (with  $C$  replaced by  $C_c$ ). Then, in [18, Theorem 8.9], we choose  $\mathcal{P}_{n,1} = \{p_{C_w}; w \in B_{c,n}\}$ .

• First, let  $w_1, \dots, w_N$  be a  $\|\cdot\|_\infty$ -distance covering of  $B_{c,n}$  with radius  $6\sqrt{C_c}\varepsilon_{c,n}$  with  $N = N(6\sqrt{C_c}\varepsilon_{c,n}, B_{c,n}, \|\cdot\|_\infty)$ . Now let  $x \in \mathcal{P}_{n,1}$  (so that  $x = p_{C_w}$  for some  $w \in B_{c,n}$ ). There is  $i \in \{1, \dots, N\}$  such that  $\|w - w_i\|_\infty \leq 6\sqrt{C_c}\varepsilon_{c,n}$ . Then, by Lemma C.8, one has

$$h(p_{C_w}, p_{C_{w_i}}) \leq K_H \|w - w_i\|_\infty e^{K_H \|w - w_i\|_\infty / 2} \leq 6K_H \sqrt{C_c}\varepsilon_{c,n} e^{3K_H \sqrt{C_c}\varepsilon_{c,n}} \leq 7K_H \sqrt{C_c}\varepsilon_{c,n},$$

for  $n$  large enough, since  $\varepsilon_{c,n} \rightarrow 0$ . This leads to, for  $n$  large enough,

$$\begin{aligned} \log N \left( 7\sqrt{C_c}K_H\varepsilon_{c,n}, \mathcal{P}_{n,1}, h \right) &\leq \log N \left( 6\sqrt{C_c}\varepsilon_{c,n}, B_{c,n}, \|\cdot\|_\infty \right) \\ &\leq n(12\sqrt{C_c}\varepsilon_{c,n})^2 && \text{from (27) with } C \text{ replaced by } C_c \\ &\leq n(14\sqrt{C_c}K_H\varepsilon_{c,n})^2 && \text{since } K_H > 1. \end{aligned}$$

Hence, we obtain, for  $n$  large enough,

$$\log N(\varepsilon_n/2, \mathcal{P}_{n,1}, h) \leq n\varepsilon_n^2. \quad (48)$$

• Second, using (28) in Theorem B.3 (with  $C$  replaced by  $C_c$ ) and then (47),

$$\mathbb{P}(p_{C_{W_c}} \notin \mathcal{P}_{n,1}) = \mathbb{P}(W_c \notin B_{c,n}) \leq e^{-C_c n \varepsilon_{c,n}^2} = e^{-(C+4)n\bar{\varepsilon}_n^2}. \quad (49)$$

• Third, for  $p : [-1, 1]^d \rightarrow (0, \infty)$  with  $\int_{[-1, 1]^d} p(x) dx = 1$ , let, with  $K$  and  $V$  defined in (42) and (43) respectively,

$$V_{2,0}(p_0; p) = \int_{[-1, 1]^d} \left( \log \left( \frac{p_0(t)}{p(t)} \right) - K(p_0, p) \right)^2 p_0(t) dt \leq V(p_0, p).$$

Then, using Lemma C.8 and (29) in Theorem B.3, one has, for  $n$  large enough,

$$\begin{aligned} &\mathbb{P} \left( K(p_0, p_{C_{W_c}}) < \bar{\varepsilon}_n^2, V_{2,0}(p_0; p_{C_{W_c}}) < \bar{\varepsilon}_n^2 \right) \\ &= \mathbb{P} \left( K(p_0, p_{C_{W_c}}) < 4t\varepsilon_{c,n}^2, V_{2,0}(p_0; p_{C_{W_c}}) < 4t\varepsilon_{c,n}^2 \right) \\ &\geq \mathbb{P} \left( K(p_0, p_{C_{W_c}}) < 4t\varepsilon_{c,n}^2, V(p_0, p_{C_{W_c}}) < 4t\varepsilon_{c,n}^2 \right) \\ &\geq \mathbb{P} \left( cK_H^2 \|W_c - w_0\|_\infty^2 (1 + K_H \|W_c - w_0\|_\infty) e^{K_H \|W_c - w_0\|_\infty} < 4t\varepsilon_{c,n}^2, \right. \\ &\quad \left. cK_H^2 \|W_c - w_0\|_\infty^2 (1 + K_H \|W_c - w_0\|_\infty)^2 e^{K_H \|W_c - w_0\|_\infty} < 4t\varepsilon_{c,n}^2 \right) \\ &\geq \mathbb{P} \left( 2cK_H^2 \|W_c - w_0\|_\infty^2 < 4t\varepsilon_{c,n}^2 \right) \\ &= \mathbb{P} \left( \|W_c - w_0\|_\infty < 2\varepsilon_{c,n} \right) \\ &\geq \exp\{-n\varepsilon_{c,n}^2\} = \exp\left\{-n\frac{1}{4t}\bar{\varepsilon}_n^2\right\} = \exp\{-nC\bar{\varepsilon}_n^2\}. \end{aligned} \quad (50)$$

Hence, we can apply [18, Theorem 8.9], with the sequences  $(\bar{\varepsilon}_n)$  and  $(\varepsilon_n)$  (starting at a  $n$  large enough) and the constant  $C$ . Indeed, (48) (resp. (49) and (50)) here enables to show Equation (8.5) (resp. Equation (8.6) and Equation (8.4)) in [18, Theorem 8.9]. As a consequence, [18, Theorem 8.9] implies (12).  $\square$

## C.4 Proof of Theorem 3.2

With  $\mathcal{L}_U$  the law of  $U$  and  $\mu$  the counting measure on  $\{0, 1\}$ , for any  $L: [-1, 1]^d \times \{0, 1\} \rightarrow \mathbb{R}$ , we write  $\|L\|_{2,U}$  for the  $L^2$ -norm of  $L$  with respect to the measure  $\mathcal{L}_U \otimes \mu$ . For  $w: [-1, 1]^d \rightarrow \mathbb{R}$ , we let  $L_w: [-1, 1]^d \times \{0, 1\} \rightarrow \mathbb{R}$  be defined by

$$L_w(u, v) = f_w(u)^v (1 - f_w(u))^{1-v} \quad \text{for } (u, v) \in [-1, 1]^d \times \{0, 1\}. \quad (51)$$

Notice that, if  $f_w$  (defined in (13)) is a candidate function for  $f_0$ , then  $L_w(U, V)$  is the likelihood function of  $(U, V)$  with respect to the measure  $\mathcal{L}_U \otimes \mu$ . Extend the definition of the Kullback-Liebler divergence  $K$  in (42) and that of  $V$  in (43), replacing the input space  $[-1, 1]^d$  by  $[-1, 1]^d \times \{0, 1\}$  and Lebesgue measure  $dt$  by  $\mathcal{L}_U \otimes \mu$ . For  $f: [-1, 1]^d \rightarrow \mathbb{R}$ , write also  $\|f\|_{2,U}$  for the  $L^2$  norm of  $f$  with respect to  $\mathcal{L}_U$ .

**Lemma C.9.** *For any functions  $v$  and  $w$  in  $\mathbb{B}_c$ , we have*

$$\begin{aligned} \|L_{C_v} - L_{C_w}\|_{2,U} &= \sqrt{2} \|f_{C_v} - f_{C_w}\|_{2,U} \leq \sqrt{2} K_H \|\Psi'\|_\infty \|v - w\|_\infty \\ K(L_{C_w}, L_{C_{w_0}}) &\leq K_H^2 \left( \left\| \frac{\Psi'}{\Psi(1-\Psi)} \right\|_\infty \vee 1 \right) \|w - w_0\|_\infty^2, \quad \text{and} \\ V(L_{C_w}, L_{C_{w_0}}) &\leq K_H^2 \left( \left\| \frac{\Psi'}{\Psi(1-\Psi)} \right\|_\infty \vee 1 \right)^2 \|w - w_0\|_\infty^2, \end{aligned}$$

using the definitions (22), (13), and (51) and where  $K_H$  is as in Lemma C.7.

*Proof.* Lemma 3.2 of [45], with the observation that  $S(w, w_0)$  there is bounded by

$$\left( \left\| \frac{\Psi'}{\Psi(1-\Psi)} \right\|_\infty \vee 1 \right)$$

yields

$$\begin{aligned} \|L_{C_v} - L_{C_w}\|_{2,U} &= \sqrt{2} \|f_{C_v} - f_{C_w}\|_{2,U} \leq \sqrt{2} \|\Psi'\|_\infty \|C_v - C_w\|_{2,U} \\ K(L_{C_w}, L_{C_{w_0}}) &\leq \left( \left\| \frac{\Psi'}{\Psi(1-\Psi)} \right\|_\infty \vee 1 \right) \|C_w - C_{w_0}\|_{2,U}^2, \quad \text{and} \\ V(L_{C_w}, L_{C_{w_0}}) &\leq \left( \left\| \frac{\Psi'}{\Psi(1-\Psi)} \right\|_\infty \vee 1 \right)^2 \|C_w - C_{w_0}\|_{2,U}^2. \end{aligned}$$

The proof is concluded using that  $\|\cdot\|_{2,U} \leq \|\cdot\|_\infty$  and that  $\|C_v - C_w\|_\infty \leq K_H \|v - w\|_\infty$  for  $v, w \in \mathbb{B}_c$  from Lemma C.7.  $\square$

*Proof of Theorem 3.2.* We proceed as in the proof of Theorem 3.1, using [18, Theorem 8.9], with  $d$  there given by  $d(L_{C_v}, L_{C_w}) = \|L_{C_v} - L_{C_w}\|_{2,U} / 2$  for  $v$  and  $w \in \mathbb{B}_c$ . Remark that this choice of  $d$  indeed satisfies the assumption (8.2) in [18], because of the item (vi) in [18, Lemma B.1] (see the paragraph after the assumption (8.2) in [18]). Remark that instead of using Lemma C.8 as in the proof of Theorem 3.1, we use Lemma C.9 here. This concludes the proof by also noting that  $\|L_{C_w} - L_{z_0, H^{\circ \dots \circ z_0, 1}}\|_{2,U} = \sqrt{2} \|f_{C_w} - f_{z_0, H^{\circ \dots \circ z_0, 1}}\|_{2,U} = \sqrt{2} \|f_{C_w} - f_0\|_{2,U}$  for  $w \in \mathbb{B}_c$  from Lemma C.9.  $\square$

## C.5 Proof of Theorem 4.1

Since  $Z_1, \dots, Z_H$  are univariate here, we write for simplicity, for  $h = 1, \dots, H$ ,  $z_{0,h,1} = z_{0,h}$  (when we will apply Theorems 3.1 and 3.2 below),  $Z_{h,1} = Z_h$ , and  $\mathbb{H}_{h,1} = \mathbb{H}_h$ .

For  $\ell \in \mathbb{N}$  and for  $(a, b) \in \mathbb{R}^2$  such that  $a < b$ , let  $\mathcal{H}^{\ell+1}([a, b])$  be the Sobolev space of  $\ell$ -times continuously differentiable functions  $h$  on  $[a, b]$  with  $\ell$ -th derivative function  $h^{(\ell)}$  that is the integral of a square integrable function  $h^{(\ell+1)}$  on  $[a, b]$ :  $h^{(\ell)}(x) = \int_a^x h^{(\ell+1)}(t)dt$ , for  $x \in [a, b]$ .

For  $h = 1, \dots, H$ , as shown in [46, Section 10] and with a linear change of input variables (see [46, Lemma 7.1]), the RKHS  $\mathbb{H}_h$  of  $Z_h$  is  $\mathcal{H}^{N_h+1}([-1, 1])$  with squared RKHS-norm, for  $g \in \mathcal{H}^{N_h+1}([-1, 1])$ ,

$$\|g\|_{\mathbb{H}_h}^2 = \int_{-1}^1 (g^{(N_h+1)}(t))^2 dt + \sum_{i=0}^{N_h} g^{(i)}(-1)^2.$$

Here  $g^{(0)} = g$  and  $g^{(1)}, \dots, g^{(N_h)}$  are the derivatives of  $g$ .

First consider the setting of Theorem 3.1. Define  $z_{0,1}, \dots, z_{0,h}$  by  $z_{0,1} = \log(p_0)/2 \|\log(p_0)\|_\infty$ ,  $z_{0,h} = \text{id}$  for  $h = 2, \dots, H-1$ , and  $z_{0,H} = 2 \|\log(p_0)\|_\infty \text{id}$ . Here  $\text{id}$  is the identity function. Then  $z_{0,H} \circ \dots \circ z_{0,1} = \log(p_0)$ . Furthermore, consider that the constants  $K_1, \dots, K_H$  are selected large enough such that the functions  $z_{0,1}, \dots, z_{0,H}$  satisfy the conditions of Theorem 3.1. Recall  $K_{\min}$  defined in (9).

**Lemma C.10.** *We have, for  $\varepsilon \in (0, 1]$ ,*

$$\inf_{\substack{g \in \mathbb{H}_1 \\ \|g - z_{0,1}\| < \varepsilon}} \|g\|_{\mathbb{H}_1}^2 \leq C_{\text{sup}} \varepsilon^{-2(N_1 - \beta + 1)/\beta}$$

and, for  $h = 2, \dots, H$ ,

$$\inf_{\substack{g \in \mathbb{H}_h \\ \|g - z_{0,h}\|_\infty < \frac{\varepsilon}{2} \\ \|\partial g / \partial x_1 - \partial z_{0,h} / \partial x_1\|_\infty < \frac{K_{\min}}{4}}} \|g\|_{\mathbb{H}_h}^2 \leq C_{\text{sup}}.$$

*Proof of Lemma C.10.* The function  $z_{0,1} = \log(p_0)/2 \|\log(p_0)\|_\infty$  is a function in  $\mathcal{F}^\beta([-1, 1], \mathbb{R})$  that does not depend on  $\varepsilon$ . Hence, because  $\mathbb{H}_1 = \mathcal{H}^{N_1+1}([-1, 1])$  as seen above, from the proof of Theorem 4.1 in [45], we obtain the first inequality of the lemma.

To prove the second inequality, remark that  $z_{0,h}$  is a linear function from  $[-1, 1]$  to  $\mathbb{R}$  and thus it belongs to  $\mathbb{H}_h$ . Hence the infimum in the second inequality of the lemma is smaller than  $\|z_{0,h}\|_{\mathbb{H}_h}^2 < \infty$ .  $\square$

**Lemma C.11.** *We have, for  $\varepsilon \in (0, 1]$  and for  $h = 1, \dots, H$ ,*

$$-\log \mathbb{P}(\|Z_h\|_\infty \leq \varepsilon) \leq C_{\text{sup}} \varepsilon^{-1/(N_h+1/2)}.$$

*Proof of Lemma C.11.* We have, for  $h = 1, \dots, H$ ,

$$-\log \mathbb{P}(\|Z_h\|_\infty \leq \varepsilon) = -\log \mathbb{P}\left(\sup_{t \in [0,2]} \left| I^{N_h} B_h(t) + \sum_{\ell=0}^{N_h} X_{h,\ell} \frac{t^\ell}{\ell!} \right| \leq \varepsilon \right).$$

The right-hand side above is bounded by  $C_{\text{sup}} \varepsilon^{-1/(N_h+1/2)}$  as stated in the proof of Theorem 4.1 in [45] (this follows in particular from Theorem 1.3 in [9]).  $\square$

Recall  $\Phi_{c,z_0}$  from (8). From Lemmas C.10, C.11, and C.3 and from  $\beta \leq N_1 + 1/2$  and  $\beta \leq N_h$ , for  $h = 2, \dots, H$ , we obtain, for  $\varepsilon \in (0, 1]$ ,

$$\Phi_{c,z_0}(\varepsilon) \leq C_{\text{sup}} \varepsilon^{-2(N_1-\beta+1)/\beta}.$$

Hence, without loss of generality, one may assume that  $C_{\text{sup}} > 1$  and thus we have, for  $n$  large enough,

$$\Phi_{c,z_0}(C_{\text{sup}} n^{-\beta/(2N_1+2)}) \leq n C_{\text{sup}}^2 n^{-2\beta/(2N_1+2)}.$$

Hence, the conclusion of Theorem 3.1 holds with  $\varepsilon_{c,n} = C_{\text{sup}} n^{-\beta/(2N_1+2)}$ . The proof for the conclusion of Theorem 3.2 is the same.

## C.6 Proof of Theorem 4.2

The proof is similar to the proof of Theorem 4.1. As done previously, we write for simplicity, for  $h = 1, \dots, H$ ,  $z_{0,h,1} = z_{0,h}$ ,  $Z_{h,1} = Z_h$ , and  $\mathbb{H}_{h,1} = \mathbb{H}_h$ .

For any  $\alpha > 0$  and for any measurable function  $g$  on  $[-1, 1]$ , we define the (left-sided) Riemann-Liouville integral of  $g$  of order  $\alpha$  (if it exists) by, for  $t \in [-1, 1]$ ,

$$(I_{0+}^\alpha g)(t) = \frac{1}{\Gamma(\alpha)} \int_{-1}^t (t-s)^{\alpha-1} g(s) ds$$

where  $\Gamma$  stands for the standard Gamma function. As shown in [45, Theorem 4.2] and with a linear change of input variables (see [46, Lemma 7.1]), using the fact that the RKHS of a sum of independent Gaussian processes is the sum of their RKHS's (see [6, Theorem 5]), for  $h = 1, \dots, H$ , the RKHS  $\mathbb{H}_h$  of  $Z_h$  is the set of functions of the form

$$I_{0+}^{\alpha_h+1/2}(g) + P_{\alpha_h+1}, \tag{52}$$

where  $g$  is square integrable on  $[-1, 1]$  and where  $P_{\alpha_h+1}$  is a polynomial of degree  $\alpha_h + 1$ .

First consider the setting of Theorem 3.1. Define  $z_{0,1}, \dots, z_{0,H}$  as in the proof of Theorem 4.1 with in particular  $z_{0,H} \circ \dots \circ z_{0,1} = \log(p_0)$ . Also as in the proof of Theorem 4.1, let the constants  $K_1, \dots, K_H$  be selected large enough such that the functions  $z_{0,1}, \dots, z_{0,H}$  satisfy the conditions of Theorem 3.1.



**Lemma C.12.** *We have, for  $\varepsilon \in (0, 1]$ ,*

$$\frac{3}{2} \inf_{\substack{g \in \mathbb{H}_1 \\ \|g - z_{0,1}\|_\infty < \varepsilon}} \|g\|_{\mathbb{H}_1}^2 - 2 \log \mathbb{P}(\|Z_1\|_\infty < \varepsilon) \leq C_{\text{sup}} \varepsilon^{-1/\alpha_1}$$

and, for  $h = 2, \dots, H$ ,

$$\begin{aligned} \frac{3}{2} \inf_{\substack{g \in \mathbb{H}_h \\ \|g - z_{0,h}\|_\infty < \frac{\varepsilon}{2} \\ \|\partial g / \partial x_1 - \partial z_{0,h} / \partial x_1\|_\infty < \frac{K_{\min}}{4}}} \|g\|_{\mathbb{H}_h}^2 - 2 \log \mathbb{P}\left(\|Z_h\|_\infty \leq \frac{\varepsilon}{2}\right) \\ - 2 \log \mathbb{P}\left(\|\partial Z_h / \partial x_1\|_\infty \leq \frac{K_{\min}}{4}\right) \leq C_{\text{sup}} \varepsilon^{-1/\alpha_h}. \end{aligned}$$

*Proof of Lemma C.12.* The first part of the lemma comes with a straightforward application of [45, Theorem 4.3] (note that the arguments of its proof would be the same if the support  $[0, 1]$  there was replaced by  $[-1, 1]$ ).

Then the second infimum in the statement of the lemma is bounded because  $z_{0,h}$  (a multiple of identity) belongs to  $\mathbb{H}_h$  since  $\mathbb{H}_h$  contains the polynomials of degrees up to  $\underline{\alpha}_h + 1$ . The quantity  $-2 \log \mathbb{P}\left(\|Z_h\|_\infty \leq \varepsilon/2\right)$  is smaller than the term displayed in Lemma C.12 (with  $Z_1$  there replaced by  $Z_h$ ) and thus this quantity is bounded by  $C_{\text{sup}} \varepsilon^{-1/\alpha_h}$  from this lemma. Finally, the quantity  $-2 \log \mathbb{P}\left(\|\partial Z_h / \partial x_j\|_\infty \leq K_{\min}/4\right)$  does not depend on  $\varepsilon$ .  $\square$

Hence, we obtain from  $\alpha_h \geq \alpha_1$ , for  $h = 1, \dots, H$ , that  $\Phi_{c,z_0}(\varepsilon) \leq C_{\text{sup}} \varepsilon^{-1/\alpha_1}$ . Then, as in the proof of Theorem 4.1 and without loss of generality, one may assume that  $C_{\text{sup}} > 1$  and thus we have, for  $n$  large enough,

$$\Phi_{c,z_0}(C_{\text{sup}} n^{-\alpha_1/(2\alpha_1+1)}) \leq n C_{\text{sup}}^2 n^{-2\alpha_1/(2\alpha_1+1)}.$$

Hence, the conclusion of Theorem 3.1 holds with  $\varepsilon_{c,n} = C_{\text{sup}} n^{-\alpha_1/(2\alpha_1+1)}$ . The proof for the conclusion of Theorem 3.2 is the same.

## C.7 Proof of Theorem 4.3

The proof is similar to the proof of Theorems 4.1 and 4.2. By [47, Lemma 4.1] (as in [44, (11)]), the RKHS  $\mathbb{H}_{h,i}$  of  $Z_{h,i}$  is the set of restrictions to  $[-1, 1]^{d_h}$  of all real parts of the functions  $h : \mathbb{R}^{d_h} \rightarrow \mathbb{R}$  of the form

$$h(t) = \int_{\mathbb{R}^d} e^{i\lambda^\top t} \Psi(\lambda) m_{h,i}(\lambda) d\lambda \quad (53)$$

for  $\Psi : \mathbb{R}^d \rightarrow \mathbb{R}$  such that  $\int_{\mathbb{R}^d} \Psi^2(\lambda) m_{h,i}(\lambda) d\lambda < \infty$ , with  $m_{h,i}$  as in (15).

First consider the setting of Theorem 3.1. Define  $z_{0,h,i}$  for  $(h, i) \in \mathcal{I}$  as follows. Without loss of generality (up to swapping  $Z_{1,1}, \dots, Z_{1,d_2}$ ), we may assume that  $\alpha_{1,1} = \alpha_{1,\min}$ . Then

we let  $z_{0,1,1} = \log(p_0)/2 \|\log(p_0)\|_\infty$ ,  $z_{0,1,2} = \dots = z_{0,1,d_2} = 0$ . For  $h = 2, \dots, H-1$ , we let  $z_{0,h,1}(u_1, \dots, u_{d_h}) = u_1$  for  $(u_1, \dots, u_{d_h}) \in [-1, 1]^{d_h}$  and we let  $z_{0,h,2} = \dots = z_{0,h,d_{h+1}} = 0$ . Finally, we let  $z_{0,H,1} = (u_1, \dots, u_{d_H}) = 2u_1 \|\log(p_0)\|_\infty$  for  $(u_1, \dots, u_{d_H}) \in [-1, 1]^{d_H}$ . Then  $z_{0,H} \circ \dots \circ z_{0,1} = \log(p_0)$ . Furthermore, consider that the constants  $K_{h,i}$  for  $(h, i) \in \mathcal{I}$  are selected large enough such that the functions  $z_{0,h,i}$  for  $(h, i) \in \mathcal{I}$  satisfy the conditions of Theorem 3.1.

**Lemma C.13.** *We have, for  $\varepsilon \in (0, 1]$ ,*

$$\frac{3}{2} \inf_{\substack{g \in \mathbb{H}_{1,1} \\ \|g - z_{0,1,1}\|_\infty < \varepsilon}} \|g\|_{\mathbb{H}_{1,1}}^2 - 2 \log \mathbb{P}(\|Z_{1,1}\|_\infty < \varepsilon) \leq C_{\text{sup}} \varepsilon^{-d/\alpha_{1,1}} + C_{\text{sup}} \varepsilon^{-\frac{2\alpha_{1,1} + d - 2\beta}{\beta}}$$

and, for  $(h, i) \in \mathcal{I} \setminus \{(1, 1)\}$ , if  $h = 1$ ,

$$\frac{3}{2} \inf_{\substack{g \in \mathbb{H}_{h,i} \\ \|g - z_{0,h,i}\|_\infty < \frac{\varepsilon}{2}}} \|g\|_{\mathbb{H}_{h,i}}^2 - 2 \log \mathbb{P}\left(\|Z_{h,i}\|_\infty \leq \frac{\varepsilon}{2}\right) \leq C_{\text{sup}} \varepsilon^{-d/\alpha_{h,i}}$$

and for  $h = 2, \dots, H$ ,

$$\begin{aligned} \frac{3}{2} \inf_{\substack{g \in \mathbb{H}_{h,i} \\ \|g - z_{0,h,i}\|_\infty < \frac{\varepsilon}{2} \\ \|\partial g / \partial x_j - \partial z_{0,h,i} / \partial x_j\|_\infty < \frac{K_{\min}}{4}, \\ j=1, \dots, d_h}} \|g\|_{\mathbb{H}_{h,i}}^2 - 2 \log \mathbb{P}\left(\|Z_{h,i}\|_\infty \leq \frac{\varepsilon}{2}\right) \\ - 2 \log \mathbb{P}\left(\|\partial Z_{h,i} / \partial x_j\|_\infty \leq \frac{K_{\min}}{4}\right) \leq C_{\text{sup}} \varepsilon^{-d/\alpha_{h,i}}. \end{aligned}$$

*Proof of Lemma C.13.* A straightforward application of [44, Lemmas 3 and 4] leads to the first part of the lemma.

Then the two last infima in the statement of the lemma are bounded because  $z_{0,h,i}$  (either zero or a linear function) belongs to  $\mathbb{H}_{h,i}$ . Indeed,  $z_{0,h,i}$ , defined on  $[-1, 1]^{d_h}$  can be written as the restriction of an infinitely differentiable compactly supported function on  $\mathbb{R}^{d_h}$ , the latter function thus satisfying (53). The quantity  $-2 \log \mathbb{P}\left(\|Z_{h,i}\|_\infty \leq \varepsilon/2\right)$  is bounded by  $C_{\text{sup}} \varepsilon^{-d/\alpha_{h,i}}$  from [44, Lemma 3]. Finally, the quantity  $\log \mathbb{P}\left(\|\partial Z_{h,i} / \partial x_j\|_\infty \leq K_{\min}/4\right)$  does not depend on  $\varepsilon$ .  $\square$

Hence, we obtain from  $\alpha_{h,i} \geq \beta$  for  $(h, i) \in \mathcal{I}$  that

$$\Phi_{c,z_0}(\varepsilon) \leq C_{\text{sup}} \varepsilon^{-d/\min_{(h,i) \in \mathcal{I}} \alpha_{h,i}} + C_{\text{sup}} \varepsilon^{-(2\alpha_{1,1} + d - 2\beta)/\beta} \leq C_{\text{sup}} \varepsilon^{-(2\alpha_{1,1} + d - 2\beta)/\beta}.$$

Hence, as in the proof of Theorems 4.1 and 4.2, without loss of generality, one may assume that  $C_{\text{sup}} > 1$  and thus we have

$$\Phi_{c,z_0}(C_{\text{sup}} n^{-\beta/(2\alpha_{1,\min} + d)}) \leq n C_{\text{sup}}^2 n^{-2\beta/(2\alpha_{1,\min} + d)}.$$

Hence, the conclusion of Theorem 3.1 holds with  $\varepsilon_{c,n} = C_{\text{sup}} n^{-\beta/(2\alpha_{1,\min} + d)}$ . The proof for the conclusion of Theorem 3.2 is the same.

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