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► **To cite this version:**

William Kengne, Pierre Alquier. Minimax optimality of deep neural networks on dependent data via PAC-Bayes bounds. 2024. hal-04785234

**HAL Id: hal-04785234**

**<https://hal.science/hal-04785234v1>**

Preprint submitted on 15 Nov 2024

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# Minimax optimality of deep neural networks on dependent data via PAC-Bayes bounds

October 30, 2024

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**Abstract:** In a groundbreaking work, [34] proved the minimax optimality of deep neural networks with ReLU activation for least-square regression estimation over a large class of functions defined by composition. In this paper, we extend these results in many directions. First, we remove the i.i.d. assumption on the observations, to allow some time dependence. The observations are assumed to be a Markov chain with a non-null pseudo-spectral gap. Then, we study a more general class of machine learning problems, which includes least-square and logistic regression as special cases. Leveraging on PAC-Bayes oracle inequalities and a version of Bernstein inequality due to [31], we derive upper bounds on the estimation risk for a generalized Bayesian estimator. In the case of least-square regression, this bound matches (up to a logarithmic factor) the lower bound in [34]. We establish a similar lower bound for classification with the logistic loss, and prove that the proposed DNN estimator is optimal in the minimax sense.

*Keywords:* Deep neural networks, minimax-optimality, Bayesian neural network, PAC-Bayes bounds, oracle inequality.

## 1 Introduction

Since almost 20 years, deep neural networks (DNN) are the most efficient predictors for most large-scale applications of machine learning, including images, sound and video processing, high-dimensional time-series prediction, etc. [6]. However, a complete theory of deep learning is still missing. In particular, until recently, it was not understood why deep networks perform better than other nonparametric methods in classification or regression problems. In a groundbreaking work, [34] defined a set of functions that are composition of dimension-reducing smooth functions. He derived the minimax rate of estimation for this class of functions. A very important fact is that this rate can be reached by deep ReLU networks, but not by more classical methods such as wavelets. Since then, these results were extended in many directions. The smoothness of the function was defined in terms of Hölder spaces, this was extended to Besov spaces by [37]. Also, while the estimator

used in [34] is frequentist, similar results were proven for Bayesian deep networks by [33, 36, 7, 8, 9], from independent observations. For deep learning from non-i.i.d. data, we refer to [25, 24] for some recent advances on nonparametric regression and for [19, 20, 21, 22], for some recent results on classification and regression, and where the optimality of the bounds established is unclear. In this new contribution, we perform the PAC-Bayes approach for deep learning from Markov chains and deal with a setting that includes classification and nonparametric regression.

More precisely, we extend the results of [34] in two directions. First, we relax the independence assumption on the observations. Instead, the observations can be sampled from a Markov chain with a positive pseudo-spectral gap. Then, we study a more general class of learning problems, that includes least-square regression but also classification with the logistic loss. We propose a generalized Bayesian estimator for which, we derive an upper bound on the excess risk. In the case of least-square regression, this bound matches (up to a logarithmic factor) the lower bound in [34]. We are not aware of similar lower bounds on the excess risk in the logistic regression case, so we derive such a bound, which matches (up to a logarithmic factor), our upper bound.

Generalized Bayesian methods are an extension of Bayesian estimation available when no likelihood is available (or, when we do not want to assume that the likelihood is actually connected to the true, unknown data-generating process). In this case, we replace the negative log-likelihood by a loss function similar to the ones used in machine learning. This approach is discussed in depth by [23]. It can be motivated by the fact that such estimators are obtained by minimizing upper bounds on the generalization error known as PAC-Bayes bounds [28]. It was actually observed empirically that the minimization of PAC-Bayes bounds for neural networks lead to good results in practice [15, 32, 13, 12]. It appears that, PAC-Bayes bounds can also be used to derive oracle inequalities and rates of convergence in statistics [10, 17]. In the i.i.d. setting, PAC-Bayes oracle bounds were actually proven to lead to minimax rates for least-square regression in various nonparametric classes of functions, including the class of compositions structured Hölder functions studied in [34], see, for instance, [11, 35, 27]. We refer the reader to [1] for a comprehensive review on PAC-Bayes bounds, oracle inequalities and applications to neural networks.

PAC-Bayes bounds were extended to non-i.i.d. settings under various assumptions: mixing, weak-dependence, Markov property, among others. The PAC-Bayes oracle inequalities in [3] lead to slow rates of convergence for weakly-dependent time series. It is to be noted that one of the applications covered in the paper are (shallow) neural networks. Faster rates were proven in [2], under more restrictive mixing assumptions. More recently, [4] derived PAC-Bayes bounds for Markov chains via  $\alpha$ -mixing coefficients. Here, we prove a new PAC-Bayes oracle inequality for Markov chains. It is based on a version of Bernstein inequality due to [31] that turned out to be very useful in machine learning [16]. We then apply it on the class of compositions based on Hölder functions to derive our rates of convergence for the DNN estimators. Note that, the generalized-Bayes estimators in [3, 2, 4] require some prior knowledge on the strength of the dependence between the observations to be calibrated optimally. Our results are no different, in the sense that we need to know a lower bound *a priori* on the pseudo-spectral gap of the observations to calibrate our estimator properly. However, thanks to some recent advances on the estimation of the mixing time of Markov chains [26, 18, 39], which itself provides bounds on the pseudo-spectral gap, we can actually get rid of this assumption in some specific cases.

The paper is organized as follows. In a first time, we describe the setting of our general learning problem, and the main assumptions: Section 2. The generalized Bayesian estimator is described in Section 3. Section 4

established our PAC-Bayesian oracle inequalities as well as the excess risk of the Bayesian DNN estimator on the class of Hölder functions and the compositions structured class. Applications to nonparametric regression and classification are carried out in Section 5. All the proofs are gathered in Section 6.

## 2 Setting and notations

Let us first introduce a few notations and conventions used in the paper. We let  $\mathbb{N}$  denote the set of natural integers. Give a set  $A$ , we let  $|A|$  denote its cardinality. For all  $x \in \mathbb{R}$ ,  $\lceil x \rceil$  denotes the smallest integer  $\geq x$  and  $\lfloor x \rfloor$  denotes the largest integer  $\leq x$ . For any vector  $x = (x_1, \dots, x_d)^T \in \mathbb{R}^d$ ,  $\|x\| = \max_{1 \leq i \leq d} |x_i|$ ,  $|x|_0 = \sum_{i=1}^d \mathbf{1}(x_i \neq 0)$ . We let  $M_{p,q}(\mathbb{R})$  denote the set of matrices of dimension  $p \times q$  with coefficients in  $\mathbb{R}$ . For any  $x = (x_{i,j}) \in M_{p,q}(\mathbb{R})$ , we put  $\|x\| = \max_{1 \leq i \leq p} \sum_{j=1}^q |x_{i,j}|$ . For all  $x = (x_1, \dots, x_d) \in \mathbb{R}^d$  and  $\beta = (\beta_1, \dots, \beta_d) \in \mathbb{N}_0^d$ ,  $x^\beta = x_1^{\beta_1} \cdot \dots \cdot x_d^{\beta_d}$ . For  $(a_n)$  and  $(b_n)$  two sequences of real numbers, we write  $a_n \lesssim b_n$  if there exists a constant  $C > 0$  such that  $a_n \leq b_n$  for all  $n \in \mathbb{N}$ . Also, we set  $a_n \asymp b_n$  if  $a_n \lesssim b_n$  and  $b_n \lesssim a_n$ .

Given  $d \in \mathbb{N}$ , and  $E_1, E_2$  two subsets of separable Banach spaces equipped with norms  $\|\cdot\|_{E_1}$  and  $\|\cdot\|_{E_2}$  respectively,  $\mathcal{F}(E_1, E_2)$  denotes the set of measurable functions from  $E_1$  to  $E_2$ . For any function  $h : E_1 \rightarrow E_2$  and  $U \subseteq E_1$ ,

$$\|h\|_\infty = \sup_{x \in E_1} \|h(x)\|_{E_2}, \quad \|h\|_{\infty, U} = \sup_{x \in U} \|h(x)\|_{E_2} \text{ and}$$

$$\text{Lip}_\alpha(h) := \sup_{x_1, x_2 \in E_1, x_1 \neq x_2} \frac{\|h(x_1) - h(x_2)\|_{E_2}}{\|x_1 - x_2\|_{E_1}^\alpha} \text{ for any } \alpha \in [0, 1].$$

For any  $\mathcal{K} > 0$  and  $\alpha \in [0, 1]$ ,  $\Lambda_{\alpha, \mathcal{K}}(E_1, E_2)$  (simply  $\Lambda_{\alpha, \mathcal{K}}(E_1)$  when  $E_2 \subseteq \mathbb{R}$ ) denotes the set of functions  $h : E_1 \rightarrow E_2$  for some  $u \in \mathbb{N}$ , such that  $\|h\|_\infty < \infty$  and  $\text{Lip}_\alpha(h) \leq \mathcal{K}$ . When  $\alpha = 1$ , we set  $\text{Lip}_1(h) = \text{Lip}(h)$  and  $\Lambda_1(E_1) = \Lambda_{1,1}(E_1, \mathbb{R})$ .

### 2.1 Setting

Let us consider the supervised learning framework with training sample  $D_n = \{Z_1 = (X_1, Y_1), \dots, Z_n = (X_n, Y_n)\}$ .  $D_n$  is a trajectory of a stationary and ergodic process  $\{Z_t = (X_t, Y_t), t \in \mathbb{N}\}$ , with values in  $\mathcal{Z} = \mathcal{X} \times \mathcal{Y}$ , where  $\mathcal{X}$  is the input space and  $\mathcal{Y}$  the output space. We let  $P_n$  denote the probability distribution of  $D_n$ . In the sequel, we will deal with the case where  $\{Z_t = (X_t, Y_t), t \in \mathbb{Z}\}$  is a Markov process. Also, assume that  $\mathcal{X} \subset \mathbb{R}^{d_x}$  and  $\mathcal{Y} \subset \mathbb{R}^{d_y}$ , with  $d_x, d_y \in \mathbb{N}$ .

Let  $\ell : \mathbb{R}^{d_y} \times \mathcal{Y} \rightarrow [0, \infty)$  a loss function. For any  $h \in \mathcal{F}(\mathcal{X}, \mathcal{Y})$ , define the risk,

$$R(h) = \mathbb{E}_{Z_0} [\ell(h(X_0), Y_0)]. \quad (2.1)$$

Denote by  $h^* \in \mathcal{F}(\mathcal{X}, \mathcal{Y})$ , a target predictor (assumed to exist), satisfying,

$$R(h^*) = \inf_{h \in \mathcal{F}(\mathcal{X}, \mathcal{Y})} R(h). \quad (2.2)$$

Define for all  $h \in \mathcal{F}(\mathcal{X}, \mathcal{Y})$ , the empirical risk,

$$\widehat{R}_n(h) = \frac{1}{n} \sum_{i=1}^n \ell(h(X_i), Y_i). \quad (2.3)$$

The aim is to build from the training sample  $D_n$ , a learner  $\widehat{h}_n$ , that achieves the smallest excess risk, given by

$$\mathcal{E}(\widehat{h}_n) = R(\widehat{h}_n) - R(h^*). \quad (2.4)$$

Also denotes for all  $h \in \mathcal{F}(\mathcal{X}, \mathcal{Y})$ ,

$$\widehat{\mathcal{E}}_n(h) = \widehat{R}_n(h) - \widehat{R}_n(h^*). \quad (2.5)$$

In the following, we set  $\ell(h, z) = \ell(h(x), y)$  for all  $z = (x, y) \in \mathcal{X} \times \mathcal{Y}$  and  $h \in \mathcal{F}(\mathcal{X}, \mathcal{Y})$ .

We focus on deep neural networks (DNN) predictors, with activation function  $\sigma : \mathbb{R} \rightarrow \mathbb{R}$ . Let  $L \in \mathbb{N}$ ,  $\mathbf{p} = (p_0, p_1, \dots, p_{L+1}) \in \mathbb{N}^{L+2}$ . A DNN, with network architecture  $(L, \mathbf{p})$  is any function of the form,

$$h_\theta : \mathbb{R}^{p_0} \rightarrow \mathbb{R}^{p_{L+1}}, \quad x \mapsto h_\theta(x) = A_{L+1} \circ \sigma_L \circ A_L \circ \sigma_{L-1} \circ A_{L-1} \circ \dots \circ \sigma_1 \circ A_1(x), \quad (2.6)$$

where for any  $\ell = 1, \dots, L+1$ ,  $A_\ell : \mathbb{R}^{p_{\ell-1}} \rightarrow \mathbb{R}^{p_\ell}$  is an affine application defined by  $A_\ell(x) := W_\ell x + b_\ell$  for given weight matrix  $W_\ell \in M_{p_{\ell-1}, p_\ell}(\mathbb{R})$ , a shift vector  $b_\ell \in \mathbb{R}^{p_\ell}$  and  $\sigma_\ell : \mathbb{R}^{p_\ell} \rightarrow \mathbb{R}^{p_\ell}$  is an element-wise activation map defined as  $\sigma_\ell(z) = (\sigma(z_1), \dots, \sigma(z_{p_\ell}))^T$  for all  $z = (z_1, \dots, z_{p_\ell})^T \in \mathbb{R}^{p_\ell}$ , and

$$\theta = (\text{vec}(W_1)^T, b_1^T, \dots, \text{vec}(W_{L+1})^T, b_{L+1}^T), \quad (2.7)$$

is the network parameters (weights), where  $\text{vec}(W)$  is obtained by concatenating the column vectors of the matrix  $W$  and  $^T$  denotes the transpose. In our setting here,  $p_0 = d_x$  (input dimension) and  $p_{L+1} = d_y$  (output dimension). So, the total number of network parameters is

$$n_{L, \mathbf{p}} = \sum_{\ell=1}^{L+1} p_\ell \times p_{\ell-1} + \sum_{\ell=1}^{L+1} p_\ell. \quad (2.8)$$

Let  $\mathcal{H}_{\sigma, d_x, d_y}$  denotes the set of DNNs of the form (2.6) with  $d_x$  dimensional input,  $d_y$  dimensional output, with activation function  $\sigma$ . For any  $h \in \mathcal{H}_{\sigma, d_x, d_y}$  with a neural network architecture  $(L, \mathbf{p})$ , denote  $\text{depth}(h) = L$  and  $\text{width}(h) = \max_{1 \leq \ell \leq L} p_\ell$ , respectively the depth and width of  $h$ . For any  $L, N, S, B, F > 0$ , consider the sets,

$$\mathcal{H}_{\sigma, d_x, d_y}(L, N) = \{h_\theta \in \mathcal{H}_{\sigma, d_x, d_y}, \text{depth}(h) \leq L, \text{width}(h) \leq N\},$$

$$\mathcal{H}_{\sigma, d_x, d_y}(L, N, S, B) = \{h_\theta \in \mathcal{H}_{\sigma, d_x, d_y}(L, N), |\theta|_0 \leq S, \|\theta\| \leq B\}, \quad (2.9)$$

$$\mathcal{H}_{\sigma, d_x, d_y}(L, N, S, B, F) = \{h_\theta \mathbf{1}_{\mathcal{X}}, h \in \mathcal{H}_{\sigma, d_x, d_y}(L, N, S, B), \|h\|_{\infty, \mathcal{X}} \leq F\}. \quad (2.10)$$

Let  $L, N > 0$ . For any  $h \in \mathcal{H}_{\sigma, d_x, d_y}(L, N)$ , the maximum number of parameter of  $h$  is,

$$n_{L, N} := N(N+1)(L+1). \quad (2.11)$$

For any  $h \in \mathcal{H}_{\sigma, d_x, d_y}(L, N)$ , we will consider in the sequel,  $\theta(h)$  as a  $n_{L, N}$ -dimensional vector by adding 0 if not. For any active set  $\mathcal{I} \subseteq \{1, 2, \dots, n_{L, N}\}$ , define the corresponding class of sparse DNNs by,

$$\mathcal{H}_{\sigma, d_x, d_y}(L, N, \mathcal{I}) = \{h_\theta \in \mathcal{H}_{\sigma, d_x, d_y}(L, N), \theta_i = 0 \text{ if } i \notin \mathcal{I}\}, \quad (2.12)$$

$$\mathcal{H}_{\sigma, d_x, d_y}(L, N, B, \mathcal{I}) = \{h_\theta \in \mathcal{H}_{\sigma, d_x, d_y}(L, N, \mathcal{I}), \|\theta\| \leq B\}, \quad (2.13)$$

$$\mathcal{H}_{\sigma, d_x, d_y}(L, N, B, F, \mathcal{I}) = \{h_\theta \in \mathcal{H}_{\sigma, d_x, d_y}(L, N, B, \mathcal{I}), \|h\|_{\infty, \mathcal{X}} \leq F\}, \quad (2.14)$$

where  $\theta := (\theta_1, \dots, \theta_{n_{L, N}})^T$ . In the sequel, for a DNN  $h_\theta$ , denote,

$$R(\theta) = R(h_\theta), \quad \widehat{R}_n(\theta) = \widehat{R}_n(h_\theta), \quad \mathcal{E}(\theta) = R(\theta) - R(h^*) \text{ and } \widehat{\mathcal{E}}_n(\theta) = \widehat{R}_n(\theta) - \widehat{R}_n(h^*). \quad (2.15)$$

## 2.2 Markov chains and pseudo-spectral gap

We assume that  $Z = \{Z_t = (X_t, Y_t), t \in \mathbb{N}\}$  is a stationary and ergodic Markov process with transition kernel  $K$  and stationary distribution  $\pi$ .  $K$  can be then viewed as a linear operator  $\mathbf{K}$  on  $L^2(\pi)$  defined as  $(\mathbf{K}f)(z) := \mathbb{E}_{K(z, \cdot)}(f)$  for all  $f \in L^2(\pi)$ . For any such operator  $\mathbf{F}$  on  $L^2(\pi)$ , we can define

$$S_2(\mathbf{F}) := \{\lambda \in \mathbb{C} : (\lambda I - \mathbf{F}) \text{ is not invertible on } L^2(\pi)\}, \quad (2.16)$$

where  $I$  denotes the identity operator on  $L^2(\pi)$ . The spectral gap of  $\mathbf{F}$  is given by,

$$\gamma(\mathbf{F}) := \begin{cases} 1 - \sup\{\lambda \in S_2(\mathbf{F}) : \lambda \neq 1\} & \text{if eigenvalue 1 has multiplicity 1} \\ 0 & \text{otherwise.} \end{cases} \quad (2.17)$$

We will refer to  $\gamma(\mathbf{K})$  simply as the spectral gap of the chain  $Z$ . Now, define the time reversal of the kernel  $K$  by,

$$K^*(z, du) := \frac{K(u, dz)}{\pi(dz)}\pi(du). \quad (2.18)$$

Therefore, the linear operator  $\mathbf{K}^*$  is the adjoint of the linear operator  $\mathbf{K}$  on  $L^2(\pi)$ . Define  $\gamma_{ps}$ , called the pseudo spectral gap of  $\mathbf{K}$  see [31], as

$$\gamma_{ps} = \max_{k \geq 1} \left\{ \frac{1}{k} \gamma((\mathbf{K}^*)^k \mathbf{K}^k) \right\}. \quad (2.19)$$

The exact assumptions for our theorem will be discussed below in detail. However, the main assumption on  $K$  will be that  $\gamma_{ps} > 0$ . This condition is weaker than the assumption  $\gamma(\mathbf{K}) > 0$ , as discussed in Remark 3.2 of [31]. Let us now briefly discuss examples where this assumption is satisfied. In order to do so, we introduce the more classical notion of mixing time.

For the process  $Z = \{Z_t = (X_t, Y_t), t \in \mathbb{N}\}$ , the mixing time for some  $\epsilon > 0$  is defined as,

$$t_{\text{mix}}(\epsilon) := \min \left\{ t \in \mathbb{N}, \sup_{z \in \mathcal{Z}} \|K^t(z, \cdot) - \pi\|_{TV} \leq \epsilon \right\}, \text{ and } t_{\text{mix}} := t_{\text{mix}}(1/4), \quad (2.20)$$

where  $K^t(z, \cdot)$  is the  $t$ -step transition kernel (i.e. the distribution of  $Z_t | Z_0 = z$ ), and  $\|\cdot\|_{TV}$  denotes the total variation distance between two probability measures  $Q_1, Q_2$  defined on the same state space  $(\Omega, \mathcal{F})$  and is given by,

$$\|Q_1 - Q_2\|_{TV} := \sup_{A \in \mathcal{F}} |Q_1(A) - Q_2(A)|. \quad (2.21)$$

[31] derived relations between mixing time and pseudo spectral gap (Propositions 3.3 and 3.4).

**Exemple 2.1.** *Assume that the chain  $(Z_t)$  is uniformly ergodic, that is, there are constants  $C > 0$  and  $\rho < 1$  such that*

$$\sup_{z \in \mathcal{Z}} \|K^t(z, \cdot) - \pi\|_{TV} \leq C\rho^t.$$

*In this case, Proposition 3.4 in [31] shows that  $\gamma_{ps} \geq 1/2t_{\text{mix}}$ . Thus, we have  $t_{\text{mix}}(\epsilon) \leq \lceil \log(C/\epsilon)/\log(\rho) \rceil$  and in particular,  $\gamma_{ps} \geq 1/2t_{\text{mix}} = \lceil \log(4C)/\log(\rho) \rceil > 0$ .*

*When the set  $\mathcal{Z}$  is finite, any irreducible and aperiodic Markov chain is immediately uniformly ergodic [14]. Examples of uniformly ergodic chains on infinite state-space are also well known [14].*

### 3 Prior distribution and Gibbs estimator

Let  $L, N, B > 0$ . For a given active set  $\mathcal{I} \subseteq \{1, 2, \dots, n_{L,N}\}$ , the prior  $\Pi_{\mathcal{I}}$  on the networks parameter of the DNNs class  $\mathcal{H}_{\sigma, d_x, d_y}(L, N, B, \mathcal{I})$  is set as the uniform distribution on

$$\mathcal{S}_{\mathcal{I}} = \{\theta = (\theta_1, \dots, \theta_{n_{L,N}})^T \in [-B, B]^{n_{L,N}}, \theta_i = 0 \text{ if } i \notin \mathcal{I}\}. \quad (3.1)$$

Let us define the mixture of the uniform priors  $\mathcal{S}_{\mathcal{I}}$  as,

$$\Pi = \sum_{i=1}^{n_{L,N}} s^{-i} \sum_{\substack{\mathcal{I} \subseteq \{1, 2, \dots, n_{L,N}\}, \\ |\mathcal{I}|=i}} \binom{n_{L,N}}{i}^{-1} \Pi_{\mathcal{I}} / C_s \quad \text{with } C_s := (1 - s^{-n_{L,N}}) / (s - 1), \quad (3.2)$$

where  $s \geq 2$  is a sparsity parameter. The Gibbs posterior probability distribution  $\Pi_{\lambda}(\cdot | D_n)$  based on  $\Pi$  is defined via,

$$\Pi_{\lambda}(d\theta | D_n) \propto \exp(-\widehat{R}_n(\theta)) \Pi(d\theta), \quad (3.3)$$

where  $\lambda > 0$  is the so-called temperature parameter and the empirical risk defined in (2.3). For any  $\lambda > 0$ , the corresponding weight  $\widehat{\theta}_{\lambda}$  and predictor  $\widehat{h}_{\lambda}$  are drawing from the posterior distribution, that is,

$$\widehat{\theta}_{\lambda} \sim \Pi_{\lambda}(\cdot | D_n), \quad \text{and } \widehat{h}_{\lambda} := h_{\widehat{\theta}_{\lambda}}. \quad (3.4)$$

For  $L, N, B, F, S > 0$ , if we consider the DNN class  $\mathcal{H}_{\sigma, d_x, d_y}(L, N, B, F)$  or  $\mathcal{H}_{\sigma, d_x, d_y}(L, N, B, S, F)$ ,  $\widehat{\theta}_{\lambda}$  is defined as above, where for any  $\mathcal{I} \subseteq \{1, 2, \dots, n_{L,N}\}$ , the prior  $\Pi_{\mathcal{I}}$  on the networks parameter of  $\mathcal{H}_{\sigma, d_x, d_y}(L, N, B, F, \mathcal{I})$  or  $\mathcal{H}_{\sigma, d_x, d_y}(L, N, S, B, F, \mathcal{I})$ , is set as the uniform distribution on  $\mathcal{S}_{\mathcal{I}}$  (given in (3.1)).

## 4 Oracle inequality and excess risk bounds

### 4.1 Oracle inequality

We consider the process  $Z = (Z_t)_{t \in \mathbb{N}}$  (with  $Z_t = (X_t, Y_t)$ ) with values in  $\mathcal{Z} = \mathcal{X} \times \mathcal{Y} \subset \mathbb{R}^{d_x} \times \mathbb{R}^{d_y}$ , and assume:

**(A1):**  $Z = (Z_t)_{t \in \mathbb{N}}$  is a stationary and ergodic Markov process with transition kernel  $K$ , stationary distribution  $\pi$  and pseudo spectral gap  $\gamma_{ps} > 0$ .

Consider the learning problem of  $Y_t$  from  $X_t$  based on the observations  $D_n = \{Z_1 = (X_1, Y_1), \dots, Z_n = (X_n, Y_n)\}$ . We carry out the PAC-Bayes approach on the class of DNNs predictor in (2.10) and set the following assumptions on the input space, the loss and the activation.

**(A2):**  $\mathcal{X} \subset \mathbb{R}^{d_x}$  is a compact set.

Under **(A2)**, we set,

$$\mathcal{K}_{\mathcal{X}} = \sup_{x \in \mathcal{X}} \|x\|. \quad (4.1)$$

**(A3):** There exists  $\mathcal{K}_{\ell} > 0$ , such that, for the DNN class  $\mathcal{H}_{\sigma, d_x, d_y}(L, N, B, F)$ , for  $L, N, B, F > 0$ , we have for all  $h \in \mathcal{H}_{\sigma, d_x, d_y}(L, N, B, F)$  and  $(x, y) \in \mathcal{Z}$ ,  $|\ell(h(x), y) - \ell(h^*(x), y)| \leq \mathcal{K}_{\ell} |h(x) - h^*(x)|$ .

**(A4):** There exists  $\mathcal{K}_{\sigma} > 0$ , such that  $\sigma \in \Lambda_{1, \mathcal{K}_{\sigma}}(\mathbb{R})$ . Moreover,  $\sigma$  is either piecewise linear or locally quadratic and fixes a segment  $I \subseteq [0, 1]$ .

**(A5):** There exists  $\mathcal{K} > 0$ , such that the target function defined in (2.2), satisfied  $h^* \in \Lambda_{1,\mathcal{K}}(\mathcal{X})$ .

Let us recall that, a function  $g : \mathbb{R} \rightarrow \mathbb{R}$  is locally quadratic (see also [29], [30]) if there exists an interval  $(a, b)$  on which  $g$  is three times continuously differentiable with bounded derivatives and there exists  $t \in (a, b)$  such that  $g'(t) \neq 0$  and  $g''(t) \neq 0$ . **(A4)** is satisfied by the ReLU activation and several other activation functions, see, for instance [19].

For all  $L, N, B, F > 0$  and  $\mathcal{I} \subseteq \{1, 2, \dots, n_{L,N}\}$ , define,

$$\theta_{\mathcal{I}}^* \in \underset{\theta \in \mathcal{S}_{\mathcal{I}}}{\operatorname{argmin}} R(\theta), \quad (4.2)$$

where  $\mathcal{S}_{\mathcal{I}}$  is defined in (3.1). Also, let us set the Bernstein's condition:

**(A6):** The Bernstein's condition for some  $K > 0$  and  $\kappa \in [0, 1]$  : For all  $\theta \in \mathcal{S}_{\mathcal{I}}$ ,

$$\mathbb{E}_{\pi} \left[ \left( \ell(h_{\theta}(X_i), Y_i) - \ell(h^*(X_i), Y_i) \right)^2 \right] \leq K (R(\theta) - R(h^*))^{\kappa}. \quad (4.3)$$

**(A7):** Local quadratic structure of the excess risk: There exists two constants  $\mathcal{K}_0 := \mathcal{K}_0(Z_0, \ell, h^*)$ ,  $\varepsilon_0 := \varepsilon_0(Z_0, \ell, h^*) > 0$  such that,

$$R(h) - R(h^*) \leq \mathcal{K}_0 \|h - h^*\|_{2, P_{X_0}}^2, \quad (4.4)$$

for any measurable function  $h : \mathbb{R}^{d_x} \rightarrow \mathbb{R}^{d_y}$  satisfying  $\|h - h^*\|_{\infty, \mathcal{X}} \leq \varepsilon_0$ ; where  $P_{X_0}$  denotes the distribution of  $X_0$  and

$$\|h - h^*\|_{q, P_{X_0}}^q := \int \|h(x) - h^*(x)\|^q dP_{X_0}(x),$$

for all  $q \geq 1$ .

$\theta_{\mathcal{I}}^*$  in (4.2) is well defined, since  $\mathcal{S}_{\mathcal{I}}$  is compact and the function  $\theta \mapsto R(\theta)$  is continuous. The following theorem provides a non-asymptotic oracle inequality of the excess risk. It is essentially an extension of Corollary 3 from [35] to the case of Markov chains. The proof relies on Paulin's version of Bernstein's inequality [31] together with standard PAC-Bayes tools [10, 1].

**Theorem 4.1.** *Assume that **(A1)**-**(A5)** and **(A6)** with  $\kappa = 1$  hold and take*

$$\lambda = \frac{n\gamma_{ps}}{32K + 10}, \quad (4.5)$$

where  $K$  is given in (4.3). Consider the DNNs class  $\mathcal{H}_{\sigma, d_x, d_y}(L, N, B, F)$  for  $L, N, B, F > 0$ , and  $\widehat{\theta}_{\lambda}$  defined as in (3.4). Then, for all  $\delta \in (0, 1)$ , with  $P_n \otimes \Pi_{\lambda}$ -probability at least  $1 - \delta$ , we have

$$\mathcal{E}(\widehat{\theta}_{\lambda}) \leq \min_{\mathcal{I} \subseteq \{1, 2, \dots, n_{L,N}\}} \left( 3\mathcal{E}(\theta_{\mathcal{I}}^*) + \frac{\Xi_1}{n\gamma_{ps}} \left[ |\mathcal{I}|L \log(\max(n, B, n_{L,N})) + \log(1/\delta) \right] \right) + \frac{3\mathcal{K}_{\ell}}{n}$$

for some constant  $\Xi_1$  independent of  $n, L, N, B, F, \gamma_{ps}$  and  $\mathcal{K}_{\ell}$ .

Note that, to compute the estimator that depends on  $\lambda$ , we need to know the spectral gap  $\gamma_{ps}$ , or an upper bound on it. This is not always a realistic assumption. However, recent stream of work to estimate this quantity on a single trajectory [26, 18, 39], when the state space is finite. Using Theorem 2.1 in [39], we obtain the following result.



**Corollary 4.2.** *Under the same assumptions as in Theorem 4.1, assume that  $\mathcal{X} \times \mathcal{Y}$  is finite, and let  $\pi$  denote the stationary distribution of the data, and  $\pi_* = \min_{z \in \mathcal{X} \times \mathcal{Y}} \pi(z)$ . Assume  $\pi_* > 0$ . Take*

$$\lambda = \frac{n\hat{\gamma}_{ps}}{32K + 10}, \quad (4.6)$$

where  $K$  is given in (4.3) and  $\hat{\gamma}_{ps}$  is the estimator of  $\gamma_{ps}$  in [39]. Then, there is a constant  $c > 0$  such that, as soon as

$$n \geq \frac{4c}{\gamma_{ps}^3 \pi_*} \log \frac{1}{\pi_*} \log \frac{2}{\pi_* \gamma_{ps} \delta} \log \frac{2}{\pi_* \gamma_{ps}^2 \delta},$$

for all  $\delta \in (0, 1)$ , with  $P_n \otimes \Pi_\lambda$ -probability at least  $1 - 2\delta$ , we have

$$\mathcal{E}(\hat{\theta}_\lambda) \leq \min_{\mathcal{I} \subseteq \{1, 2, \dots, n_{L, N}\}} \left( 3\mathcal{E}(\theta_{\mathcal{I}}^*) + \frac{2\Xi_1}{n\gamma_{ps}} \left[ |\mathcal{I}|L \log(\max(n, B, n_{L, N})) + \log(1/\delta) \right] \right) + \frac{3\mathcal{K}_\ell}{n}$$

for  $\Xi_1$  as in Theorem 4.1.

## 4.2 Excess risk bound on the Hölder class

In the sequel, we consider a class of Hölder smooth functions. Let  $U \subset \mathbb{R}^d$  (with  $d \in \mathbb{N}$ ),  $\beta = (\beta_1, \dots, \beta_d)^T \in \mathbb{N}^d$ ,  $x = (x_1, \dots, x_d)^T \in U$ , set

$$|\beta| = \sum_{i=1}^d \beta_i \text{ and } \partial^\beta = \frac{\partial^{|\beta|}}{\partial^{\beta_1} x_1 \dots \partial^{\beta_d} x_d}.$$

For any  $s > 0$ , the Hölder space  $\mathcal{C}^s(U)$  is the set of functions  $h : U \rightarrow \mathbb{R}$  such that, for any  $\beta \in \mathbb{N}^d$  with  $|\beta| \leq \lfloor s \rfloor$ ,  $\|\partial^\beta h\|_\infty < \infty$  and for any  $\beta \in \mathbb{N}^d$  with  $|\beta| = \lfloor s \rfloor$ ,  $\text{Lip}_{s-\lfloor s \rfloor}(\partial^\beta h) < \infty$ . This space is equipped with the norm

$$\|h\|_{\mathcal{C}^s(U)} = \sum_{0 \leq |\beta| \leq \lfloor s \rfloor} \|\partial^\beta h\|_\infty + \sum_{|\beta| = \lfloor s \rfloor} \text{Lip}_{s-\lfloor s \rfloor}(\partial^\beta h). \quad (4.7)$$

For any  $s > 0$ ,  $U \subset \mathbb{R}^d$  and  $\mathcal{K} > 0$ , consider the set,

$$\mathcal{C}^{s, \mathcal{K}}(U) = \{h \in \mathcal{C}^s(U), \|h\|_{\mathcal{C}^s(U)} \leq \mathcal{K}\}. \quad (4.8)$$

Now, we deal with the network architecture parameters  $L_n, N_n, B_n, F_n$  that depend on the sample size  $n$ . An application of Theorem 4.1 together with a tight control of  $\mathcal{E}(\theta_{\mathcal{I}}^*)$  on the Hölder's class leads to the following result.

**Theorem 4.3.** *Assume that (A1)-(A5), (A6) with  $\kappa = 1$ , (A7) hold and that there exists  $s, \mathcal{K} > 0$ , such that  $h^* \in \mathcal{C}^{s, \mathcal{K}}(\mathcal{X})$ . Take  $\lambda$  as in (4.5). Consider the DNNs class  $\mathcal{H}_{\sigma, d_x, d_y}(L_n, N_n, S_n, B_n, F_n)$  with  $L_n \asymp \log n$ ,  $N_n \asymp n^{\frac{d_x}{2s+d_x}}$ ,  $S_n \asymp n^{\frac{d_x}{2s+d_x}} \log n$ ,  $B_n \asymp n^{\frac{4(s+d_x)}{2s+d_x}}$  and  $F_n > 0$ . Then, for all  $\delta \in (0, 1)$ , with  $P_n \otimes \Pi_\lambda$ -probability at least  $1 - \delta$ , we have for  $n \geq \varepsilon_0^{-(2+d_x/s)}$ ,*

$$\mathcal{E}(\hat{\theta}_\lambda) \leq \Xi_2 \left( \frac{\log^3 n}{n^{\frac{2s}{2s+d_x}}} + \frac{\mathcal{K}_\ell + \log(1/\delta)}{n} \right),$$

for some constant  $\Xi_2$  independent of  $n$  and  $\mathcal{K}_\ell$ , and where  $\varepsilon_0$  is given in the assumption (A7).

Therefore, the rate of the excess risk of  $\hat{h}_\lambda = h_{\hat{\theta}_\lambda}$  is of order  $\mathcal{O}(n^{-\frac{2s}{2s+d_x}} (\log n)^3)$ .

### 4.3 Excess risk bound on a compositions structured Hölder class

For this purpose, we assume that the target function  $h^*$  belongs to a class of composition structured functions, defined by [34].

Let  $d, r \in \mathbb{N}$  with  $d \geq r$ ,  $s, \mathcal{K} > 0$  and  $a, b \in \mathbb{R}$  with  $a < b$ . Denote by  $\mathcal{C}_r^{s, \mathcal{K}}([a, b]^d)$  the set of functions  $f : [a, b]^d \rightarrow \mathbb{R}$  satisfying:

- $f$  is a  $r$ -variate function i.e.  $f$  depends on at most  $r$  coordinates;
- $f \in \mathcal{C}^{s, \mathcal{K}}([a, b]^d)$ , defined in (4.8).

Let  $q \in \mathbb{N}$ ,  $\mathbf{d} = (d_0, \dots, d_{q+1}) \in \mathbb{N}^{q+2}$  with  $d_0 = d_x$  and  $d_{q+1} = d_y$ ,  $\mathbf{t} = (t_0, \dots, t_q) \in \mathbb{N}^{q+1}$  with  $t_i \leq d_i$  for all  $i = 0, \dots, q$ ,  $\mathbf{s} = (s_0, \dots, s_q) \in (0, \infty)^{q+1}$  and  $\mathcal{K} > 0$ . Following [34], define the class of functions:

$$\mathcal{G}(q, \mathbf{d}, \mathbf{t}, \mathbf{s}, \mathcal{K}) := \left\{ h = g_q \circ \dots \circ g_0, \quad g_i = (g_{i,j})_{j=1, \dots, d_{i+1}} : [a_i, b_i]^{d_i} \rightarrow [a_{i+1}, b_{i+1}]^{d_{i+1}}, \text{ with} \right. \\ \left. g_{i,j} \in \mathcal{C}_{t_i}^{s_i, \mathcal{K}}([a_i, b_i]^{d_i}), \text{ for some } a_i, b_i \in \mathbb{R} \text{ such that } |a_i|, |b_i| \leq \mathcal{K}, \forall i = 1, \dots, q \right\}. \quad (4.9)$$

For the class  $\mathcal{G}(q, \mathbf{d}, \mathbf{t}, \mathbf{s}, \mathcal{K})$ , define:

$$\beta_i^* := \beta_i \prod_{k=i+1}^q \min(\beta_k, 1) \text{ for all } i = 0, \dots, q; \text{ and } \phi_n := \max_{i=0, \dots, q} n^{-\frac{2\beta_i^*}{2\beta_i^* + t_i}}. \quad (4.10)$$

The next theorem provides a bound of the excess risk of the estimator  $\widehat{h}_\lambda$ , for structured composite target function, in the case  $\mathcal{X} = [0, 1]^{d_x}$ . Here again this is obtained by an application of Theorem 4.1.

**Theorem 4.4.** *Set  $\mathcal{X} = [0, 1]^{d_x}$ . Assume that (A1)-(A3), (A6) with  $\kappa = 1$ , (A7) hold and that  $h^* \in \mathcal{G}(q, \mathbf{d}, \mathbf{t}, \mathbf{s}, \mathcal{K})$  for some composition structured class, and take  $\lambda$  as in (4.5). Consider the DNNs class  $\mathcal{H}_{\sigma, d_x, d_y}(L_n, N_n, S_n, B_n, F_n)$  where  $\sigma$  is the ReLU activation function and with:*

$$L_n = C_0 \log n, N_n \asymp n\phi_n, S_n \asymp n\phi_n \log n, B_n = B \geq 1, F_n > \max(\mathcal{K}, 1), \quad (4.11)$$

for some constant  $C_0 \geq \sum_{i=0}^q \log_4(4 \max(t_i, s_i))$  and where  $\phi_n$  is defined in (4.10). Then, for all  $\delta \in (0, 1)$ , with  $P_n \otimes \Pi_\lambda$ -probability at least  $1 - \delta$ , we have

$$\mathcal{E}(\widehat{\theta}_\lambda) \leq \Xi_3 \left( \phi_n (\log n)^3 + \frac{\mathcal{K}_\ell + \log(1/\delta)}{n} \right),$$

for some constant  $\Xi_3$  independent of  $n$  and  $\mathcal{K}_\ell$ .

So, when  $h^*$  belongs to a class of Hölder compositions functions, the rate of the excess risk of  $\widehat{h}_\lambda = h_{\widehat{\theta}_\lambda}$  is of order  $\mathcal{O}(\phi_n (\log n)^3)$ .

## 5 Examples of nonparametric regression and classification

### 5.1 Nonparametric regression

Consider the nonparametric time series regression,

$$Y_t = h^*(X_t) + \varepsilon_t, \quad t \in \mathbb{N}, \quad (5.1)$$

with  $(X_t, Y_t) \in \mathcal{X} \times \mathcal{Y} \subset \mathbb{R}^{d_x} \times \mathbb{R}$  ( $d_y = 1$ ), where  $h^* : \mathbb{R}^{d_x} \rightarrow \mathbb{R}$  is the unknown regression function and  $(\varepsilon_t)_{t \in \mathbb{N}}$  is a sequence of i.i.d. centered random variable and for all  $t \in \mathbb{N}$ ,  $\varepsilon_t$  is independent of the input variable  $X_t$ . The goal is the estimation of  $h^*$ , based on the observations  $\{(X_i, Y_i)\}_{1 \leq i \leq n}$ , generated from (5.1). We perform the quasi-Bayesian DNN estimator proposed above, with a DNNs class  $\mathcal{H}_{\sigma, d_x, d_y}(L_n, N_n, S_n, B_n, F_n)$  and the square loss function.

In this subsection, assume that  $\{(X_t, Y_t)\}_{t \in \mathbb{N}}$  is a stationary and ergodic Markov process and that  $\mathcal{X}$  and  $\mathcal{Y}$  are compact sets. Hence, the assumptions **(A1)**-**(A3)** hold. Also, **(A6)** with  $\kappa = 1$  holds if we deal with a network architecture parameters  $L_n, N_n, B_n, F_n$  with  $F_n = F > \max(\mathcal{K}, 1)$ . Note that, in this framework with the square loss, **(A7)** holds automatically. Therefore:

- If the activation function  $\sigma$  satisfies **(A4)** and  $h^* \in \mathcal{C}^{s, \mathcal{K}}(\mathcal{X})$  for some  $s, \mathcal{K} > 0$ , then, the result of Theorem 4.3 holds.
- For  $\mathcal{X} = [0, 1]^{d_x}$ , if  $h^* \in \mathcal{G}(q, \mathbf{d}, \mathbf{t}, \mathbf{s}, \mathcal{K})$  for some composition structured class, then the result of Theorem 4.4 is applied with the ReLU deep neural networks.

Note that, for regression problem with the Gaussian error  $\varepsilon_t$ , square loss and  $\mathcal{X} = [0, 1]^{d_x}$ , [34] proved that, the lower bound for the minimax estimation risk over a class  $\mathcal{G}(q, \mathbf{d}, \mathbf{t}, \mathbf{s}, \mathcal{K})$  is  $\phi_n$  (up to a constant). Unfortunately, Theorem 4.3 does not cover the Gaussian error case as they would require  $\mathcal{Y} = \mathbb{R}$  to be not compact, a setting in which the quadratic loss is not Lipschitz. This can however be fixed.

**Lemma 5.1.** *Assume (5.1) with  $h^* \in \mathcal{C}^{s, \mathcal{K}}(\mathcal{X})$  for some  $s, \mathcal{K} > 0$ ,  $(\varepsilon_t)_{t \in \mathbb{N}}$  is i.i.d.  $\mathcal{N}(0, \sigma^2)$  distributed. For any  $\delta > 0$ , define the event*

$$\tilde{\Omega}_\delta = \left\{ \sup_{1 \leq t \leq n} |Y_t| \leq \mathcal{K} + \sigma \sqrt{2 \log \frac{2n}{\delta}} \right\}.$$

Then  $\mathbb{P}(\tilde{\Omega}_\delta) \geq 1 - \delta$ .

*Proof.* Fix  $\alpha > 0$  and  $\epsilon > 0$ . By using the Markov's inequality, we have,

$$\begin{aligned} \mathbb{P} \left( \sup_{1 \leq t \leq n} |\varepsilon_t| \geq \epsilon \right) &\leq \sum_{t=1}^n \mathbb{P}(|\varepsilon_t| \geq \epsilon) \leq 2 \sum_{t=1}^n \mathbb{P}(\varepsilon_t \geq \epsilon) = 2 \sum_{t=1}^n \mathbb{P}(\exp(\alpha \varepsilon_t) \geq \exp(\alpha \epsilon)) \\ &\leq 2 \sum_{t=1}^n \mathbb{E}[\exp(\alpha \varepsilon_t - \alpha \epsilon)] = 2 \sum_{t=1}^n \exp(\alpha^2 \sigma^2 / 2 - \alpha \epsilon). \end{aligned}$$

For a fixed  $\epsilon$ , the function  $\alpha \mapsto \alpha^2 \sigma^2 / 2 - \alpha \epsilon$  reaches its minimum when  $\alpha = \epsilon / \sigma^2$  and thus,

$$\mathbb{P} \left( \sup_{1 \leq t \leq n} |\varepsilon_t| \geq \epsilon \right) \leq 2n \exp \left( - \frac{\epsilon^2}{2\sigma^2} \right). \quad (5.2)$$

Putting  $\delta = 2n \exp(-\epsilon^2 / 2\sigma^2)$ , (5.2) gives

$$\mathbb{P} \left( \sup_{1 \leq t \leq n} |\varepsilon_t| \geq \sigma \sqrt{2 \log \frac{2n}{\delta}} \right) \leq \delta. \quad (5.3)$$

Finally, since  $h^* \in \mathcal{C}^{s, \mathcal{K}}(\mathcal{X})$ , it holds a.s. that,  $|Y_t| \leq |h^*(X_t)| + |\varepsilon_t| \leq \|h^*\|_{\infty, \mathcal{X}} + |\varepsilon_t| \leq \mathcal{K} + |\varepsilon_t|$ . Thus, the result follows from (5.3).  $\blacksquare$

Therefore, consider a DNN class  $\mathcal{H}_{\sigma, d_x, d_y}(L_n, N_n, B_n, F_n)$  for  $L_n, N_n, B_n > 0$  and  $F_n = F > \max(\mathcal{K}, 1)$ . From Lemma 5.1, it holds on  $\tilde{\Omega}_\delta$  that, all the variables  $Y_t$  ( $t \in \mathbb{N}$ ) belong to the compact set  $[-\mathcal{K} - \sigma\sqrt{2\log\frac{2n}{\delta}}, \mathcal{K} + \sigma\sqrt{2\log\frac{2n}{\delta}}]$  and thus, for  $h \in \mathcal{H}_{\sigma, d_x, d_y}(L_n, N_n, B_n, F_n)$  and  $y \in [-\mathcal{K} - \sigma\sqrt{2\log\frac{2n}{\delta}}, \mathcal{K} + \sigma\sqrt{2\log\frac{2n}{\delta}}]$ ,

$$\begin{aligned} |\ell(h(x), y) - \ell(h^*(x), y)| &= |(h(x) - y)^2 - (h^*(x) - y)^2| \\ &\leq |(2y - h(x) - h^*(x))(h(x) - h^*(x))| \\ &\leq (2\mathcal{K} + 2\sigma\sqrt{2\log\frac{2n}{\delta}} + F + \mathcal{K})|h(x) - h^*(x)|, \end{aligned}$$

that is, we have Assumption **(A3)** with  $\mathcal{K}_\ell = 3\mathcal{K} + 2\sigma\sqrt{2\log\frac{2n}{\delta}} + F$ . Thus, on this set, we can apply Theorem 4.4 with  $F_n = F > \max(\mathcal{K}, 1)$ . Thus, in this setting, we obtain, with probability at least  $1 - 2\delta$ ,

$$\mathcal{E}(\hat{\theta}_\lambda) \leq \Xi_3 \left( \phi_n(\log n)^3 + \frac{3\mathcal{K} + 2\sigma\sqrt{2\log\frac{2n}{\delta}} + F + \log(1/\delta)}{n} \right) \leq \Xi_4 \left( \phi_n(\log n)^3 + \frac{\log(1/\delta)}{n} \right),$$

for some  $\Xi_4 > 0$  independent of  $n$ . Thus, the convergence rate of  $\mathcal{E}(\hat{\theta}_\lambda)$  matches (up to a  $\log^3 n$  factor) with the lower bound of [34]. Which shows that, the Bayesian DNN estimator  $\hat{h}_\lambda = h_{\hat{\theta}_\lambda}$  for the least squares nonparametric regression is optimal in the minimax sense.

## 5.2 Classification with the logistic Loss

Consider a stationary and ergodic Markov process  $(X_t, Y_t)_{t \in \mathbb{N}}$  with distribution  $P_{Z_0}$  ( $Z_0 = (X_0, Y_0)$ ) and with values in  $\mathcal{X} \times \{-1, 1\} \subset \mathbb{R}^{d_x} \times \mathbb{R}$  (that is,  $d_y = 1$ ) satisfying for all  $x \in \mathcal{X}$ ,

$$Y_t | X_t = x \sim 2\mathcal{B}(\eta(x)) - 1, \quad \text{with } \eta(x) = P(Y_t = 1 | X_t = x), \quad (5.4)$$

where  $\mathcal{B}(\eta(x))$  denotes the Bernoulli distribution with parameter  $\eta(x)$ . We focus on the margin-based logistic loss function given by,  $\ell(y, u) = \phi(yu)$  for all  $(y, u) \in \{-1, 1\} \times \mathbb{R}$  and with  $\phi(v) = \log(1 + e^{-v})$ ,  $\forall v \in \mathbb{R}$ . For any predictor  $h : \mathbb{R}^{d_x} \rightarrow \mathbb{R}$ , we have,

$$R(h) = \mathbb{E}[\phi(Y_0 h(X_0))] = \int_{\mathcal{X} \times \{-1, 1\}} \phi(yh(x)) dP_{Z_0}(x, y).$$

Here, we assume that  $\mathcal{X}$  is a compact set and deal with a class of bounded deep neural networks  $\mathcal{H}_{\sigma, d_x, d_y}(L_n, N_n, S_n, B_n, F_n)$  with  $F_n = F > \max(\mathcal{K}, 1)$ . So, the assumptions **(A1)**-**(A3)** and **(A6)** with  $\kappa = 1$  are satisfied; see for instance [5] in the case of **(A6)**.

Let us check **(A7)**. The target function, with respect to the  $\phi$ -loss is given by (see also Lemma **C.2** in [40]) is the function  $h^* : \mathcal{X} \rightarrow [-\infty, \infty]$ , defined by:

$$h^*(x) = \begin{cases} \infty & \text{if } \eta(x) = 1, \\ \log \frac{\eta(x)}{1-\eta(x)} & \text{if } \eta(x) \in (0, 1), \\ -\infty & \text{if } \eta(x) = 0. \end{cases} \quad (5.5)$$

Let  $x \in \mathcal{X}$  such that  $\eta(x) \in (0, 1)$ . For any measurable function  $h : \mathbb{R}^{d_x} \rightarrow \mathbb{R}$ , we have,

$$\begin{aligned}
& \mathbb{E}[\phi(Y_0 h(X_0)) | X_0 = x] - \mathbb{E}[\phi(Y_0 h^*(X_0)) | X_0 = x] \\
&= \eta(x)\phi(h(x)) + (1 - \eta(x))\phi(-h(x)) - \eta(x)\phi(h^*(x)) - (1 - \eta(x))\phi(-h^*(x)) \\
&= \eta(x)\phi(h(x)) + (1 - \eta(x))\phi(-h(x)) - \eta(x) \log \frac{1}{\eta(x)} - (1 - \eta(x)) \log \frac{1}{1 - \eta(x)} \\
&\leq \frac{1}{8} \left| h(x) - \log \frac{\eta(x)}{1 - \eta(x)} \right|^2 \leq \frac{1}{8} |h(x) - h^*(x)|^2,
\end{aligned} \tag{5.6}$$

where the inequality (5.6) holds from the Lemma C.6 in [40]. With the convention  $0 \times \infty = 0$ , the inequality (5.6) holds for  $\eta(x) = 1$  or  $\eta(x) = 0$ . Hence,

$$R(h) - R(h^*) = \mathbb{E}[\phi(Y_0 h(X_0))] - \mathbb{E}[\phi(Y_0 h^*(X_0))] \leq \frac{1}{8} \mathbb{E}[|h(X_0) - h^*(X_0)|^2] = \frac{1}{8} \|h - h^*\|_{2, P_{X_0}}^2.$$

Thus, (A7) holds with  $\mathcal{K}_0 = \frac{1}{8}$ . Therefore:

- If (A4) holds and  $h^* \in \mathcal{C}^{s, \mathcal{K}}(\mathcal{X})$  for some  $s, \mathcal{K} > 0$ , then, the result of Theorem 4.3 is applied.
- For  $\mathcal{X} = [0, 1]^{d_x}$ , if  $h^* \in \mathcal{G}(q, \mathbf{d}, \mathbf{t}, \mathbf{s}, \mathcal{K})$  for some composition structured class, then the result of Theorem 4.4 is applicable with the ReLU deep neural networks.

The next theorem provides a lower bound of the excess risk on a class of composition structured functions.

**Theorem 5.2** (Lower bound for classification). *Set  $\mathcal{X} = [0, 1]^{d_x}$  and assume that  $(X_t, Y_t)_{t \in \mathbb{N}}$  satisfying (5.4) is a stationary and ergodic Markov process. Consider a class of composition structured functions  $\mathcal{G}(q, \mathbf{d}, \mathbf{t}, \mathbf{\beta}, \mathcal{K})$  with  $t_i \leq \min(d_0, \dots, d_{i-1})$  for all  $i$ . Then, for sufficiently large  $\mathcal{K}$ , there exist a constant  $C > 0$  such that*

$$\inf_{\hat{h}_n} \sup_{h^* \in \mathcal{G}(q, \mathbf{d}, \mathbf{t}, \mathbf{\beta}, \mathcal{K})} \mathbb{E}[R(\hat{h}_n) - R(h^*)] \geq C\phi_n, \tag{5.7}$$

where the infimum is taken over all estimator  $\hat{h}_n$ , based on  $(X_1, Y_1), \dots, (X_n, Y_n)$  generated from (5.4) and  $\phi_n$  is defined in (4.10).

Theorem 4.4 and 5.2 show that, for the classification problem of Markov processes with the logistic loss, the quasi-Bayesian DNN predictor is optimal (up to a  $\log^3 n$  factor) in the minimax sense, on the class of composition structured functions.

## 6 Proofs of the main results

### 6.1 Some technical lemmas

The following lemmas are useful in the proofs of the main results.

**Lemma 6.1.** (Paulin [31]). *Consider a trajectory  $(Z_1, \dots, Z_n)$  of a process  $Z = (Z_t)_{t \in \mathbb{N}}$  with values in  $\mathcal{Z}$  and assume that (A1) holds. Let  $f \in L^2(\pi)$  such that, there exists  $C > 0$  satisfying  $|f(z) - \mathbb{E}_\pi(f)| \leq C$  for all  $z \in \mathcal{Z}$ . Set  $V_f := \text{Var}_\pi(f)$  and  $S = \sum_{i=1}^n f(Z_i)$ . Then, for all  $\vartheta \in (0, \gamma_{ps}/10)$ , we have,*

$$\mathbb{E}_\pi(\exp(\vartheta S)) \leq \exp\left(\frac{2(n+1)V_f}{\gamma_{ps}} \cdot \vartheta^2 \cdot \left(1 - \frac{10\vartheta}{\gamma_{ps}}\right)^{-1}\right). \tag{6.1}$$

**Lemma 6.2.** *Assume that (A1), (A3), (A5) and (A6) hold. Consider the DNNs class  $\mathcal{H}_{\sigma, d_x, d_y}(L, N, B, F, \mathcal{I})$  for  $L, N, B, F > 0$ ,  $\mathcal{I} \subseteq \{1, 2, \dots, n_{L,N}\}$ . For all  $\lambda \in (0, n \cdot \gamma_{ps}/10)$  and  $\theta \in \mathcal{S}_{\mathcal{I}}$  we have,*

$$\max\left(\mathbb{E}\left[\exp\left(\lambda\left(\widehat{\mathcal{E}}_n(\theta) - \mathcal{E}(\theta)\right)\right)\right], \mathbb{E}\left[\exp\left(\lambda\left(\mathcal{E}(\theta) - \widehat{\mathcal{E}}_n(\theta)\right)\right)\right]\right) \leq \exp\left(\frac{16K\lambda^2\mathcal{E}(\theta)^\kappa}{n\gamma_{ps}}\left(1 - \frac{10\lambda}{n\gamma_{ps}}\right)^{-1}\right), \quad (6.2)$$

where  $K, \kappa$  are given in assumption (A6).

**Proof.** Let  $\theta \in \mathcal{S}_{\mathcal{I}}$ . We have,

$$\begin{aligned} \widehat{\mathcal{E}}_n(\theta) - \mathcal{E}(\theta) &= \widehat{R}_n(\theta) - \widehat{R}_n(h^*) - R(\theta) + R(h^*) \\ &= \frac{1}{n} \sum_{i=1}^n \left( \ell(h_\theta(X_i), Y_i) - \ell(h^*(X_i), Y_i) - \mathbb{E}_\pi[\ell(h_\theta(X_1), Y_1)] + \mathbb{E}_\pi[\ell(h^*(X_1), Y_1)] \right) = \frac{1}{n} \sum_{i=1}^n g_\theta(Z_i), \end{aligned}$$

with  $Z_i = (X_i, Y_i)$ ,  $g_\theta(z) = \ell(h_\theta(x), y) - \ell(h^*(x), y) - \mathbb{E}_\pi[\ell(h_\theta(X_1), Y_1)] + \mathbb{E}_\pi[\ell(h^*(X_1), Y_1)]$  for all  $z = (x, y) \in \mathcal{Z} = \mathcal{X} \times \mathcal{Y}$ . We will apply Lemma 6.1 to the process  $(Z_t)_{t \in \mathbb{N}}$  with the function  $g_\theta$ , satisfying  $\mathbb{E}_\pi(g_\theta) = 0$ . According to the Bernstein's condition, we have,

$$\begin{aligned} \text{Var}_\pi[g_\theta(Z_1)] &= \mathbb{E}_\pi[(g_\theta(Z_1))^2] \\ &\leq 2\left(\mathbb{E}_\pi[(\ell(h_\theta(X_1), Y_1) - \ell(h^*(X_1), Y_1))^2] + (\mathbb{E}_\pi[\ell(h_\theta(X_1), Y_1)] - \mathbb{E}_\pi[\ell(h^*(X_1), Y_1)])^2\right) \\ &\leq 4\mathbb{E}_\pi[(\ell(h_\theta(X_1), Y_1) - \ell(h^*(X_1), Y_1))^2] \leq 4K\mathcal{E}(\theta)^\kappa. \end{aligned}$$

So, for any  $\vartheta \in (0, \gamma_{ps}/10)$ , it holds from Lemma 6.1 that,

$$\mathbb{E}_\pi\left[\exp\left(\vartheta \sum_{i=1}^n g_\theta(Z_i)\right)\right] \leq \exp\left(\frac{16Kn\mathcal{E}(\theta)^\kappa}{\gamma_{ps}} \cdot \vartheta^2 \cdot \left(1 - \frac{10\vartheta}{\gamma_{ps}}\right)^{-1}\right). \quad (6.3)$$

Hence, for any  $\lambda \in (0, n \cdot \gamma_{ps}/10)$ , we get,

$$\mathbb{E}_\pi\left[\exp\left(\lambda\left(\widehat{\mathcal{E}}_n(\theta) - \mathcal{E}(\theta)\right)\right)\right] = \mathbb{E}_\pi\left[\exp\left(\frac{\lambda}{n} \sum_{i=1}^n g_\theta(Z_i)\right)\right] \leq \exp\left(\frac{16\lambda^2K\mathcal{E}(\theta)^\kappa}{n\gamma_{ps}}\left(1 - \frac{10\lambda}{n\gamma_{ps}}\right)^{-1}\right). \quad (6.4)$$

Similar arguments yield,

$$\mathbb{E}_\pi\left[\exp\left(\lambda\left(\mathcal{E}(\theta) - \widehat{\mathcal{E}}_n(\theta)\right)\right)\right] \leq \exp\left(\frac{16\lambda^2K\mathcal{E}(\theta)^\kappa}{n\gamma_{ps}}\left(1 - \frac{10\lambda}{n\gamma_{ps}}\right)^{-1}\right),$$

for all  $\lambda \in (0, n \cdot \gamma_{ps}/10)$ ; which completes the proof of the lemma.  $\blacksquare$

Let  $(E, \mathcal{A})$  be a measurable space and  $\mu_1, \mu_2$  two probability measures on this space. Define the Kullback-Leibler divergence of  $\mu_1$  with respect to  $\mu_2$  by,

$$\text{KL}(\mu_1, \mu_2) = \begin{cases} \int \log\left(\frac{d\mu_1}{d\mu_2}\right) d\mu_1 & \text{if } \mu_1 \ll \mu_2, \\ \infty & \text{otherwise,} \end{cases}$$

where the notation  $\mu_1 \ll \mu_2$  means "  $\mu_1$  is absolutely continuous with respect to  $\mu_2$ ". The following lemma is classical for PAC-Bayes bounds, the proof can be found in [10].

**Lemma 6.3.** *Let  $(E, \mathcal{A})$  be a measurable space,  $\mu$  a probability measure on  $(E, \mathcal{A})$  and  $h : E \rightarrow \mathbb{R}$  a measurable function such that  $\int \exp \circ h \, d\mu < \infty$ . With the convention  $\infty - \infty = -\infty$ , we have,*

$$\log \left( \int \exp \circ h \, d\mu \right) = \sup_{\nu} \left( \int h \, d\nu - KL(\nu, \mu) \right), \quad (6.5)$$

where the supremum is taken over all probability measures  $\nu$  on  $(E, \mathcal{A})$ . In addition, if  $h$  is bounded from above on the support of  $\mu$ , the supremum in (6.5) is reached for the Gibbs distribution  $\nu = g$ , with  $\frac{dg}{d\mu} \propto \exp \circ h$ .

The following lemmas are also needed.

**Lemma 6.4.** *Assume that (A1), (A3), (A5) and (A6) with  $\kappa = 1$  hold and consider the DNNs class  $\mathcal{H}_{\sigma, d_x, d_y}(L, N, B, F, \mathcal{I})$  for  $L, N, B, F > 0$ ,  $\mathcal{I} \subseteq \{1, 2, \dots, n_{L, N}\}$ . Let  $\rho$  be a  $D_n$ -dependent probability measure on  $\mathcal{S}_{\mathcal{I}}$  such that  $\rho \ll \Pi$ . For any  $\lambda \in \left(0, \frac{n\gamma_{ps}}{16K + 10}\right)$  and  $\delta \in (0, 1)$ , we have with probability at least  $1 - \delta$ ,*

$$\mathcal{E}(\hat{\theta}) \leq \frac{1}{1 - \frac{16K\lambda}{n\gamma_{ps} - 10\lambda}} \left[ \hat{\mathcal{E}}_n(\hat{\theta}) + \frac{1}{\lambda} \left( \log(1/\delta) + \log \left( \frac{d\rho}{d\Pi}(\hat{\theta}) \right) \right) \right]. \quad (6.6)$$

where  $\hat{\theta}$  is distributed according to  $\rho$ .

**Proof.** Let  $\theta \in \mathcal{S}_{\mathcal{I}}$ ,  $\lambda \in (0, n \cdot \gamma_{ps}/10)$  and  $\delta \in ]0, 1[$ . We have from Lemma 6.2,

$$\mathbb{E} \left\{ \exp \left[ \lambda (\mathcal{E}(\theta) - \hat{\mathcal{E}}_n(\theta)) \right] \right\} \leq \exp \left( \frac{16\lambda^2 K \mathcal{E}(\theta)}{n\gamma_{ps}} \left( 1 - \frac{10\lambda}{n\gamma_{ps}} \right)^{-1} \right).$$

Therefore,

$$\mathbb{E} \left\{ \exp \left[ \left( \lambda - \frac{16K\lambda^2}{n\gamma_{ps} \left( 1 - \frac{10\lambda}{n\gamma_{ps}} \right)} \right) \mathcal{E}(\theta) - \lambda \hat{\mathcal{E}}_n(\theta) - \log(1/\delta) \right] \right\} \leq \delta. \quad (6.7)$$

Let us recall that  $\Pi$  is a prior probability measure on  $\mathcal{S}_{\mathcal{I}}$ . From (6.7), we have

$$\int \mathbb{E} \left\{ \exp \left[ \left( \lambda - \frac{16K\lambda^2}{n\gamma_{ps} \left( 1 - \frac{10\lambda}{n\gamma_{ps}} \right)} \right) \mathcal{E}(\theta) - \lambda \hat{\mathcal{E}}_n(\theta) - \log(1/\delta) \right] \right\} d\Pi(\theta) \leq \delta,$$

and by the Fubini's theorem,

$$\mathbb{E} \left\{ \int \exp \left[ \left( \lambda - \frac{16K\lambda^2}{n\gamma_{ps} \left( 1 - \frac{10\lambda}{n\gamma_{ps}} \right)} \right) \mathcal{E}(\theta) - \lambda \hat{\mathcal{E}}_n(\theta) - \log(1/\delta) \right] d\Pi(\theta) \right\} \leq \delta.$$

Hence, for any data-dependent probability measure  $\rho$  absolutely continuous with respect to  $\Pi$ , we have

$$\mathbb{E} \left\{ \int \exp \left[ \left( \lambda - \frac{16K\lambda^2}{n\gamma_{ps} \left( 1 - \frac{10\lambda}{n\gamma_{ps}} \right)} \right) \mathcal{E}(\theta) - \lambda \hat{\mathcal{E}}_n(\theta) - \log(1/\delta) - \log \left( \frac{d\rho}{d\Pi}(\theta) \right) \right] d\rho(\theta) \right\} \leq \delta, \quad (6.8)$$

with the convention  $\infty \times 0 = 0$ . Recall that,  $P_n$  denotes the distribution of the sample  $D_n$ . The inequality (6.8) can also be written as,

$$\mathbb{E}_{D_n \sim P_n} \mathbb{E}_{\hat{\theta} \sim \rho} \left\{ \exp \left[ \left( \lambda - \frac{16K\lambda^2}{n\gamma_{ps} \left( 1 - \frac{10\lambda}{n\gamma_{ps}} \right)} \right) \mathcal{E}(\hat{\theta}) - \lambda \hat{\mathcal{E}}_n(\hat{\theta}) - \log(1/\delta) - \log \left( \frac{d\rho}{d\Pi}(\hat{\theta}) \right) \right] \right\} \leq \delta,$$

Therefore, from the inequality  $\exp(\lambda x) \geq \mathbf{1}_{x \geq 0}$ , we get with  $P_n \otimes \rho$ -probability at most  $\delta$ ,

$$\left(1 - \frac{16K\lambda}{n\gamma_{ps}\left(1 - \frac{10\lambda}{n\gamma_{ps}}\right)}\right) \mathcal{E}(\hat{\theta}) \geq \hat{\mathcal{E}}_n(\hat{\theta}) + \frac{1}{\lambda} \left( \log(1/\delta) + \log\left(\frac{d\rho}{d\Pi}(\hat{\theta})\right) \right).$$

Since  $\lambda \in \left(0, \frac{n\gamma_{ps}}{16K+10}\right)$ , we have with  $P_n \otimes \rho$ -probability at least  $1 - \delta$ ,

$$\mathcal{E}(\hat{\theta}) \leq \frac{1}{1 - \frac{16K\lambda}{n\gamma_{ps} - 10\lambda}} \left[ \hat{\mathcal{E}}_n(\hat{\theta}) + \frac{1}{\lambda} \left( \log(1/\delta) + \log\left(\frac{d\rho}{d\Pi}(\hat{\theta})\right) \right) \right]. \quad (6.9)$$

This completes the proof of the lemma. ■

**Lemma 6.5.** *Assume that (A1), (A3), (A5) and (A6) with  $\kappa = 1$  hold and consider the DNNs class  $\mathcal{H}_{\sigma, d_x, d_y}(L, N, B, F, \mathcal{I})$  for  $L, N, B, F > 0$ ,  $\mathcal{I} \subseteq \{1, 2, \dots, n_{L, N}\}$ . Let  $\rho$  be a  $D_n$ -dependent probability measure on  $\mathcal{S}_{\mathcal{I}}$  such that  $\rho \ll \Pi$ . For any  $\lambda \in \left(0, \frac{n\gamma_{ps}}{16K+10}\right)$  and  $\delta \in (0, 1)$ , we have with probability at least  $1 - \delta$ ,*

$$\mathcal{E}(\hat{\theta}_\lambda) \leq \frac{1}{1 - \frac{16K\lambda}{n\gamma_{ps} - 10\lambda}} \left[ \left(1 + \frac{16K\lambda}{n\gamma_{ps} - 10\lambda}\right) \int \mathcal{E}(\theta) d\rho(\theta) + \frac{2}{\lambda} (KL(\rho, \Pi) + \log(1/\delta)) \right], \quad (6.10)$$

where  $\hat{\theta}_\lambda \sim \Pi_\lambda(\cdot | D_n)$ .

**Proof.** Let  $\lambda \in \left(0, \frac{n\gamma_{ps}}{16K+10}\right)$  and  $\delta \in (0, 1)$ . Apply Lemma 6.4 for the posterior distribution  $\Pi_\lambda(\cdot | D_n) \ll \Pi$  with the corresponding Radon-Nikodym density

$$\frac{d\Pi_\lambda(\theta | D_n)}{d\Pi(\theta)} = \frac{\exp(-\lambda \hat{R}_n(\theta))}{\int \exp(-\lambda \hat{R}_n(\theta)) d\Pi(\theta)}. \quad (6.11)$$

So, in addition to Lemma 6.3, we have with probability at least  $1 - \delta$ ,

$$\begin{aligned} \mathcal{E}(\hat{\theta}_\lambda) &\leq \frac{1}{1 - \frac{16K\lambda}{n\gamma_{ps} - 10\lambda}} \left[ \hat{\mathcal{E}}_n(\hat{\theta}_\lambda) + \frac{1}{\lambda} \left( \log(1/\delta) - \lambda \hat{R}_n(\hat{\theta}_\lambda) - \log \int \exp(-\lambda \hat{R}_n(\theta)) d\Pi(\theta) \right) \right] \\ &\leq \frac{1}{1 - \frac{16K\lambda}{n\gamma_{ps} - 10\lambda}} \left[ \hat{R}_n(h^*) + \frac{1}{\lambda} \left( \log(1/\delta) - \log \int \exp(-\lambda \hat{R}_n(\theta)) d\Pi(\theta) \right) \right] \\ &\leq \frac{1}{1 - \frac{16K\lambda}{n\gamma_{ps} - 10\lambda}} \left[ \hat{R}_n(h^*) + \frac{1}{\lambda} \left( \log(1/\delta) - \sup_{\rho, \rho \ll \Pi} \left[ -\lambda \int \hat{R}_n(\theta) d\rho(\theta) - KL(\rho, \Pi) \right] \right) \right] \\ &\leq \frac{1}{1 - \frac{16K\lambda}{n\gamma_{ps} - 10\lambda}} \inf_{\rho, \rho \ll \Pi} \left[ \hat{R}_n(h^*) + \frac{1}{\lambda} \left( \log(1/\delta) + \lambda \int \hat{R}_n(\theta) d\rho(\theta) + KL(\rho, \Pi) \right) \right] \\ &\leq \frac{1}{1 - \frac{16K\lambda}{n\gamma_{ps} - 10\lambda}} \inf_{\rho, \rho \ll \Pi} \left[ \int \hat{\mathcal{E}}_n(\theta) d\rho(\theta) + \frac{1}{\lambda} \left( \log(1/\delta) + KL(\rho, \Pi) \right) \right] \end{aligned} \quad (6.12)$$



Let  $\rho$  a probability measure on  $\mathcal{S}_{\mathcal{I}}$  such that  $\rho \ll \Pi$ . From Lemma 6.2, we have

$$\mathbb{E}\left\{\exp\left[\lambda\left(\widehat{\mathcal{E}}_n(\theta) - \mathcal{E}(\theta)\right)\right]\right\} \leq \exp\left(\frac{16K\lambda^2\mathcal{E}(\theta)}{n\gamma_{ps}}\left(1 - \frac{10\lambda}{n\gamma_{ps}}\right)^{-1}\right).$$

Therefore,

$$\mathbb{E}\left\{\exp\left[\lambda\widehat{\mathcal{E}}_n(\theta) - \lambda\left(1 + \frac{16K\lambda}{n\gamma_{ps} - 10\lambda}\right)\mathcal{E}(\theta) - \log(1/\delta)\right]\right\} \leq \delta, \quad (6.13)$$

and from the Fubini's theorem,

$$\mathbb{E}\left\{\int \exp\left[\lambda\widehat{\mathcal{E}}_n(\theta) - \lambda\left(1 + \frac{16K\lambda}{n\gamma_{ps} - 10\lambda}\right)\mathcal{E}(\theta) - \log(1/\delta)\right]d\Pi(\theta)\right\} \leq \delta. \quad (6.14)$$

Hence, in addition to the Jensen's inequality,

$$\begin{aligned} & \mathbb{E}_{D_n}\left[\exp\left(\int\left[\lambda\widehat{\mathcal{E}}_n(\theta) - \lambda\left(1 + \frac{16K\lambda}{n\gamma_{ps} - 10\lambda}\right)\mathcal{E}(\theta)\right]d\rho(\theta) - \text{KL}(\rho, \Pi) - \log(1/\delta)\right)\right] \\ &= \mathbb{E}_{D_n}\left[\exp\left(\int\left[\lambda\widehat{\mathcal{E}}_n(\theta) - \lambda\left(1 + \frac{16K\lambda}{n\gamma_{ps} - 10\lambda}\right)\mathcal{E}(\theta) - \frac{d\rho(\theta)}{d\Pi(\theta)} - \log(1/\delta)\right]d\rho(\theta)\right)\right] \\ &\leq \mathbb{E}_{D_n, \theta \sim \rho}\left[\exp\left(\lambda\widehat{\mathcal{E}}_n(\theta) - \lambda\left(1 + \frac{16K\lambda}{n\gamma_{ps} - 10\lambda}\right)\mathcal{E}(\theta) - \frac{d\rho(\theta)}{d\Pi(\theta)} - \log(1/\delta)\right)\right] \\ &\leq \mathbb{E}_{D_n}\left[\int \exp\left(\lambda\widehat{\mathcal{E}}_n(\theta) - \lambda\left(1 + \frac{16K\lambda}{n\gamma_{ps} - 10\lambda}\right)\mathcal{E}(\theta) - \log(1/\delta)\right)d\Pi(\theta)\right] \leq \delta. \end{aligned}$$

Therefore, from the inequality  $\exp(\lambda x) \geq \mathbb{1}_{x \geq 0}$ , we get with probability at least  $1 - \delta$ ,

$$\int \widehat{\mathcal{E}}_n(\theta)d\rho(\theta) \leq \left(1 + \frac{16K\lambda}{n\gamma_{ps} - 10\lambda}\right) \int \mathcal{E}(\theta)d\rho(\theta) + \frac{1}{\lambda}(\text{KL}(\rho, \Pi) + \log(1/\delta)). \quad (6.15)$$

According to (6.12) and (6.15), we get we with probability at least  $1 - 2\delta$ ,

$$\begin{aligned} \mathcal{E}(\widehat{\theta}_\lambda) &\leq \frac{1}{1 - \frac{16K\lambda}{n\gamma_{ps} - 10\lambda}} \inf_{\rho, \rho \ll \Pi} \left[ \left(1 + \frac{16K\lambda}{n\gamma_{ps} - 10\lambda}\right) \int \mathcal{E}(\theta)d\rho(\theta) + \frac{2}{\lambda}(\text{KL}(\rho, \Pi) + \log(1/\delta)) \right] \\ &= \frac{1}{1 - \frac{16K\lambda}{n\gamma_{ps} - 10\lambda}} \inf_{\rho, \rho \ll \Pi} \left[ \left(1 + \frac{16K\lambda}{n\gamma_{ps} - 10\lambda}\right) \int \mathcal{E}(\theta)d\rho(\theta) + \frac{2}{\lambda}(\text{KL}(\rho, \Pi) + \log(1/\delta)) \right] \end{aligned}$$

■

**Lemma 6.6.** Assume that (A4) and consider the DNNs class  $\mathcal{H}_{\sigma, d_x, d_y}(L, N, B, F, \mathcal{I})$  for  $L, N, B, F > 0$ ,  $\mathcal{I} \subseteq \{1, 2, \dots, n_{L, N}\}$ . For all  $x \in \mathbb{R}^{d_x}$ ,  $\theta, \tilde{\theta} \in \mathcal{S}_{\mathcal{I}}$ , we have,

$$|h_\theta(x) - h_{\tilde{\theta}}(x)| \leq 2L^2(|\sigma(0)| + \|x\| + 1)(1 + \mathcal{K}_\sigma B) \max(1, (\mathcal{K}_\sigma B)^{2L})\|\theta - \tilde{\theta}\|.$$

**Proof.** In the sequel, we use the following elementary result: Let  $a \geq 0$  and  $(b_m)_{m \in \mathbb{N}}, (u_m)_{m \in \mathbb{N}}$  two sequences of non negative numbers such that  $u_m \leq au_{m-1} + b_{m-1}$  for all  $m \geq 1$ . Then, for all  $m \geq 1$ ,

$$u_m \leq a^m u_0 + \sum_{k=1}^m b_{m-k} a^{k-1}. \quad (6.16)$$

Consider two neural networks  $h_\theta, h_{\tilde{\theta}}$  as in (2.6) with  $A_\ell(x) = W_\ell x + b_\ell$ ,  $\tilde{A}_\ell(x) = \tilde{W}_\ell x + \tilde{b}_\ell$  for all  $\ell = 1, \dots, L+1$  and  $\theta = (\text{vec}(W_1)^T, b_1^T, \dots, \text{vec}(W_{L+1})^T, b_{L+1}^T)$ ,  $\tilde{\theta} = (\text{vec}(\tilde{W}_1)^T, \tilde{b}_1^T, \dots, \text{vec}(\tilde{W}_{L+1})^T, \tilde{b}_{L+1}^T) \in \mathcal{S}_{\mathcal{I}}$  (see also (2.7)). Let  $x \in \mathbb{R}^{d_x}$ . Set,

$$x^{(0)} = \tilde{x}^{(0)} = x, \quad x^{(\ell)} = \sigma_\ell \circ A_\ell(x^{(\ell-1)}) \text{ and } \tilde{x}^{(\ell)} = \sigma_\ell \circ \tilde{A}_\ell(\tilde{x}^{(\ell-1)}) \text{ for any } \ell = 1, \dots, L+1. \quad (6.17)$$

According to assumption **(A4)**, we have for  $\ell = 1, \dots, L$ ,

$$\begin{aligned} \|x^{(\ell)}\| &= \|\sigma_1 \circ A_\ell(x^{(\ell-1)})\| \leq |\sigma(0)| + \mathcal{K}_\sigma \|A_\ell(x^{(\ell-1)})\| \\ &\leq |\sigma(0)| + \mathcal{K}_\sigma (\|W_\ell\| \|x^{(\ell-1)}\| + \|b_\ell\|) \leq |\sigma(0)| + \mathcal{K}_\sigma B + \mathcal{K}_\sigma B \|x^{(\ell-1)}\|. \end{aligned}$$

Therefore, in addition to (6.16), we have for all  $\ell = 1, \dots, L$ ,

$$\begin{aligned} \|x^{(\ell)}\| &\leq (\mathcal{K}_\sigma B)^\ell \|x\| + (|\sigma(0)| + \mathcal{K}_\sigma B) \sum_{k=1}^{\ell} (\mathcal{K}_\sigma B)^{k-1} \\ &\leq (\|x\| + 1) \sum_{k=1}^{\ell} (\mathcal{K}_\sigma B)^k + |\sigma(0)| \sum_{k=1}^{\ell} (\mathcal{K}_\sigma B)^{k-1} \\ &\leq (\|x\| + 1) \sum_{k=1}^L (\mathcal{K}_\sigma B)^k + |\sigma(0)| \sum_{k=1}^L (\mathcal{K}_\sigma B)^{k-1} \\ &\leq L(|\sigma(0)| + \|x\| + 1) \max(1, (\mathcal{K}_\sigma B)^L). \end{aligned} \quad (6.18)$$

Similarly, we have for all  $\ell = 1, \dots, L$ ,

$$\begin{aligned} \|x^{(1)} - \tilde{x}^{(1)}\| &= \|\sigma_1 \circ A_1(x) - \sigma_1 \circ \tilde{A}_1(x)\| \leq \mathcal{K}_\sigma \|A_1(x) - \tilde{A}_1(x)\| \\ &\leq \mathcal{K}_\sigma (\|W_1 - \tilde{W}_1\| \|x\| + \|b_1 - \tilde{b}_1\|) \leq \mathcal{K}_\sigma (\|x\| + 1) \|\theta - \tilde{\theta}\|. \end{aligned}$$

$$\begin{aligned} |x^{(\ell)} - \tilde{x}^{(\ell)}| &= |\sigma_\ell \circ A_\ell(x^{(\ell-1)}) - \sigma_\ell \circ \tilde{A}_\ell(\tilde{x}^{(\ell-1)})| \leq \mathcal{K}_\sigma \|A_\ell(x^{(\ell-1)}) - \tilde{A}_\ell(\tilde{x}^{(\ell-1)})\| \\ &\leq \mathcal{K}_\sigma \|(W_\ell - \tilde{W}_\ell)x^{(\ell-1)} + \tilde{W}_\ell(x^{(\ell-1)} - \tilde{x}^{(\ell-1)}) + (b_\ell - \tilde{b}_\ell)\| \\ &\leq \mathcal{K}_\sigma (\|W_\ell - \tilde{W}_\ell\| \|x^{(\ell-1)}\| + \|\tilde{W}_\ell\| \|x^{(\ell-1)} - \tilde{x}^{(\ell-1)}\| + \|b_\ell - \tilde{b}_\ell\|) \\ &\leq \mathcal{K}_\sigma (\|x^{(\ell-1)}\| + 1) \|\theta - \tilde{\theta}\| + \mathcal{K}_\sigma B \|x^{(\ell-1)} - \tilde{x}^{(\ell-1)}\| \\ &\leq 2\mathcal{K}_\sigma L (|\sigma(0)| + \|x\| + 1) \max(1, (\mathcal{K}_\sigma B)^L) \|\theta - \tilde{\theta}\| + \mathcal{K}_\sigma B \|x^{(\ell-1)} - \tilde{x}^{(\ell-1)}\|, \end{aligned} \quad (6.19)$$

where (6.18) is used in (6.19). This recurrence relation is also satisfied with  $\ell = 1$ . Hence, from (6.16), we get for all  $\ell = 1, \dots, L$ ,

$$\begin{aligned} |x^{(\ell)} - \tilde{x}^{(\ell)}| &\leq 2\mathcal{K}_\sigma L (|\sigma(0)| + \|x\| + 1) \max(1, (\mathcal{K}_\sigma B)^L) \|\theta - \tilde{\theta}\| \sum_{k=1}^{\ell} (\mathcal{K}_\sigma B)^{k-1} \\ &\leq 2\mathcal{K}_\sigma L (|\sigma(0)| + \|x\| + 1) \max(1, (\mathcal{K}_\sigma B)^L) \|\theta - \tilde{\theta}\| \sum_{k=1}^L (\mathcal{K}_\sigma B)^{k-1} \\ &\leq 2\mathcal{K}_\sigma L^2 (|\sigma(0)| + \|x\| + 1) \max(1, (\mathcal{K}_\sigma B)^{2L}) \|\theta - \tilde{\theta}\|. \end{aligned} \quad (6.20)$$

Therefore, in addition to (6.18), we have,

$$\begin{aligned}
|h_\theta(x) - h_{\tilde{\theta}}(x)| &= |A_{L+1} \circ \sigma_L \circ A_L \circ \sigma_{L-1} \circ A_{L-1} \circ \cdots \circ \sigma_1 \circ A_1(x) - \tilde{A}_{L+1} \circ \sigma_L \circ \tilde{A}_L \circ \sigma_{L-1} \circ \tilde{A}_{L-1} \circ \cdots \circ \sigma_1 \circ \tilde{A}_1(x)| \\
&= |A_{L+1}(x^{(L)}) - \tilde{A}_{L+1}(\tilde{x}^{(L)})| = |W_{L+1}(x^{(L)}) - \tilde{W}_{L+1}(\tilde{x}^{(L)}) + b_{L+1} - \tilde{b}_{L+1}| \\
&\leq \|W_{L+1} - \tilde{W}_{L+1}\| \|x^{(L)}\| + \|\tilde{W}_{L+1}\| \|x^{(L)} - \tilde{x}^{(L)}\| + \|b_{L+1} - \tilde{b}_{L+1}\| \\
&\leq (\|x^{(L)}\| + 1) \|\theta - \tilde{\theta}\| + B \|x^{(L)} - \tilde{x}^{(L)}\| \\
&\leq 2L(|\sigma(0)| + \|x\| + 1) \max(1, (\mathcal{K}_\sigma B)^L) \|\theta - \tilde{\theta}\| + 2\mathcal{K}_\sigma B L^2 (|\sigma(0)| + \|x\| + 1) \max(1, (\mathcal{K}_\sigma B)^{2L}) \|\theta - \tilde{\theta}\| \\
&\leq 2L^2 (|\sigma(0)| + \|x\| + 1) (1 + \mathcal{K}_\sigma B) \max(1, (\mathcal{K}_\sigma B)^{2L}) \|\theta - \tilde{\theta}\|.
\end{aligned}$$

■

## 6.2 Proof of Theorem 4.1

Let  $\mathcal{I} \subseteq \{1, 2, \dots, n_{L,N}\}$  and  $\eta \in (0, 1]$ . Consider the probability measure  $\rho := \rho_{\mathcal{I}, \eta}$  on  $\mathcal{S}_{\mathcal{I}}$  defined such that,

$$\frac{d\rho_{\mathcal{I}, \eta}}{d\Pi_{\mathcal{I}}(\theta)} \propto \mathbf{1}_{\|\theta - \theta_{\mathcal{I}}^*\| \leq \eta},$$

where  $\theta_{\mathcal{I}}^*$  is defined in (4.2). According to Lemma 6.6, **(A2)**, **(A3)** and the support of  $\rho = \rho_{\mathcal{I}, \eta}$ , we have,

$$\begin{aligned}
\int \mathcal{E}(\theta) d\rho(\theta) &= \mathcal{E}(\theta_{\mathcal{I}}^*) + \int \mathbb{E}_\pi[\ell(h_\theta(X_1), Y_1) - \ell(h_{\theta_{\mathcal{I}}^*}(X_1), Y_1)] d\rho(\theta) \\
&= \mathcal{E}(\theta_{\mathcal{I}}^*) + \mathcal{K}_\ell \int \mathbb{E}_\pi |h_\theta(X_1) - h_{\theta_{\mathcal{I}}^*}(X_1)| d\rho(\theta) \\
&\leq \mathcal{E}(\theta_{\mathcal{I}}^*) + 2L^2 \mathcal{K}_\ell (|\sigma(0)| + \mathcal{K}_{\mathcal{X}} + 1) (1 + \mathcal{K}_\sigma B) \max(1, (\mathcal{K}_\sigma B)^{2L}) \int \|\theta - \theta_{\mathcal{I}}^*\| d\rho(\theta) \\
&\leq \mathcal{E}(\theta_{\mathcal{I}}^*) + 2L^2 \mathcal{K}_\ell (|\sigma(0)| + \mathcal{K}_{\mathcal{X}} + 1) (1 + \mathcal{K}_\sigma B) \max(1, (\mathcal{K}_\sigma B)^{2L}) \eta \\
&\leq \mathcal{E}(\theta_{\mathcal{I}}^*) + \frac{\mathcal{K}_\ell}{n},
\end{aligned} \tag{6.21}$$

with

$$\eta = \frac{1}{2L^2 (|\sigma(0)| + \mathcal{K}_{\mathcal{X}} + 1) (1 + \mathcal{K}_\sigma B) \max(1, (\mathcal{K}_\sigma B)^{2L}) n}.$$

Now, consider the Kullback-Leibler term in (6.10). From Lemma 10 in [35], we have,

$$\text{KL}(\rho, \Pi) = \text{KL}(\rho_{\mathcal{I}, \eta}, \Pi) \leq |\mathcal{I}| \log \left( \frac{2sC_s B n_{L, N} e}{\eta} \right), \tag{6.22}$$

where  $s \geq 2$  denotes sparsity parameter and  $C_s$  is defined in (3.2). So, from (6.10), (6.21) and (6.22), we get with probability at least  $1 - \delta$ ,

$$\mathcal{E}(\hat{\theta}_\lambda) \leq \frac{1}{1 - \frac{16K\lambda}{n\gamma_{ps} - 10\lambda}} \left[ \left(1 + \frac{16K\lambda}{n\gamma_{ps} - 10\lambda}\right) \left(\mathcal{E}(\theta_{\mathcal{I}}^*) + \frac{\mathcal{K}_\ell}{n}\right) + \frac{2}{\lambda} \left[ |\mathcal{I}| \log \left( \frac{2sC_s B n_{L, N} e}{\eta} \right) + \log(1/\delta) \right] \right],$$

By choosing,

$$\lambda = \frac{n\gamma_{ps}}{32K + 10},$$

we have with probability at least  $1 - \delta$ ,

$$\begin{aligned} \mathcal{E}(\hat{\theta}_\lambda) &\leq 3\mathcal{E}(\theta_{\mathcal{I}}^*) + \frac{3\mathcal{K}_\ell}{n} + \frac{4(32K + 10)}{n\gamma_{ps}} \left[ |\mathcal{I}| \log \left( \frac{2sC_s B n_{L,N} \epsilon}{\eta} \right) + \log(1/\delta) \right] \\ &\leq 3\mathcal{E}(\theta_{\mathcal{I}}^*) + \frac{\Xi_1}{n\gamma_{ps}} \left[ |\mathcal{I}| L \log(\max(n, B, n_{L,N})) + \log(1/\delta) \right] + \frac{3\mathcal{K}_\ell}{n}, \end{aligned} \quad (6.23)$$

where  $\Xi_1$  is a constant which is independent of  $n, L, N, B, F, \gamma_{ps}, \mathcal{K}_\ell$ . This completes the proof of the theorem, since the bound in (6.23) holds for all  $\mathcal{I} \subseteq \{1, 2, \dots, n_{L,N}\}$ .

### 6.3 Proof of Corollary 4.2

Follow the previous proof, but use  $\lambda = \frac{n\hat{\gamma}_{ps}}{32K + 10}$ . We obtain, with probability  $1 - \delta$ ,

$$\mathcal{E}(\hat{\theta}_\lambda) \leq 3\mathcal{E}(\theta_{\mathcal{I}}^*) + \frac{\Xi_1}{n\hat{\gamma}_{ps}} \left[ |\mathcal{I}| L \log(\max(n, B, n_{L,N})) + \log(1/\delta) \right] + \frac{3\mathcal{K}_\ell}{n}.$$

Now, Theorem 2.1 in [39] states there is a  $c > 0$  such that, for any  $\varepsilon > 0$ , when

$$n \geq \frac{c}{\gamma_{ps}\varepsilon^2\pi_*} \log \frac{1}{\pi_*} \log \frac{1}{\pi_*\varepsilon\delta} \log \frac{1}{\pi_*\gamma_{ps}\varepsilon\delta},$$

we have with probability at least  $1 - \delta$

$$|\gamma_{ps} - \hat{\gamma}_{ps}| \leq \varepsilon.$$

Putting  $\varepsilon = \gamma_{ps}/2$ , we obtain, for

$$n \geq \frac{4c}{\gamma_{ps}^3\pi_*} \log \frac{1}{\pi_*} \log \frac{2}{\pi_*\gamma_{ps}\delta} \log \frac{2}{\pi_*\gamma_{ps}^2\delta}$$

with probability at least  $1 - \delta$ ,

$$\hat{\gamma}_{ps} \leq \frac{\gamma_{ps}}{2}. \quad (6.24)$$

Thanks to a union bound, (6.24) and (6.24) hold simultaneously with probability at least  $1 - 2\delta$ . In this case, plugging (6.24) into (6.23) gives

$$\mathcal{E}(\hat{\theta}_\lambda) \leq 3\mathcal{E}(\theta_{\mathcal{I}}^*) + \frac{2\Xi_1}{n\gamma_{ps}} \left[ |\mathcal{I}| L \log(\max(n, B, n_{L,N})) + \log(1/\delta) \right] + \frac{3\mathcal{K}_\ell}{n}.$$

### 6.4 Proof of Theorem 4.3

We have,

$$\begin{aligned} &\min_{\mathcal{I} \subseteq \{1, 2, \dots, n_{L_n, N_n}\}} \left( 3\mathcal{E}(\theta_{\mathcal{I}}^*) + \frac{\Xi_1}{n} \left[ |\mathcal{I}| L_n \log(\max(n, B_n, n_{L_n, N_n})) + \log(1/\delta) \right] \right) \\ &= \min_{\mathcal{I} \subseteq \{1, 2, \dots, n_{L_n, N_n}\}} \left( 3 \inf_{\theta \in \mathcal{S}_{\mathcal{I}}} (R(h_\theta) - R(h^*)) + \frac{\Xi_1}{n} \left[ |\mathcal{I}| L_n \log(\max(n, B_n, n_{L_n, N_n})) + \log(1/\delta) \right] \right), \end{aligned}$$

where the constant  $\Xi_1$  is given in Theorem 4.1. In the sequel, we set:

$$\mathcal{H}_{\sigma, d_x, d_y, n} := \mathcal{H}_{\sigma, d_x, d_y}(L_n, N_n, S_n, B_n, F_n). \quad (6.25)$$

Let  $h \in \mathcal{H}_{\sigma, d_x, d_y, n}$ . Set  $\theta(h) = (\theta_1, \dots, \theta_{n_{L_n, N_n}})$  and  $\mathcal{J} = \{i \in \{1, \dots, n_{L_n, N_n}\}, \theta_i \neq 0\}$ . We have,  $\mathcal{J} \subset \{1, 2, \dots, n_{L_n, N_n}\}$ ,  $\theta(h) \in \mathcal{S}_{\mathcal{J}}$  and  $|\mathcal{J}| = |\theta(h)|_0 \leq S_n$ . Hence,

$$\begin{aligned} & \min_{\mathcal{I} \subset \{1, 2, \dots, n_{L_n, N_n}\}} \left( 3 \inf_{\theta \in \mathcal{S}_{\mathcal{I}}} (R(h_\theta) - R(h^*)) + \frac{\Xi_1}{n} \left[ |\mathcal{I}| L_n \log(\max(n, B_n, n_{L_n, N_n})) + \log(1/\delta) \right] \right) \\ & \leq 3 \inf_{\theta \in \mathcal{S}_{\mathcal{J}}} (R(h_\theta) - R(h^*)) + \frac{\Xi_1}{n} \left[ |\mathcal{J}| L_n \log(\max(n, B_n, n_{L_n, N_n})) + \log(1/\delta) \right] \\ & \leq 3(R(h) - R(h^*)) + \frac{\Xi_1}{n} \left[ S_n L_n \log(\max(n, B_n, n_{L_n, N_n})) + \log(1/\delta) \right] \end{aligned} \quad (6.26)$$

Since (6.26) is satisfied for all  $h \in \mathcal{H}_{\sigma, d_x, d_y, n}$ , we get,

$$\begin{aligned} & \min_{\mathcal{I} \subset \{1, 2, \dots, n_{L_n, N_n}\}} \left( 3 \inf_{\theta \in \mathcal{S}_{\mathcal{I}}} (R(h_\theta) - R(h^*)) + \frac{\Xi_1}{n} \left[ |\mathcal{I}| L_n \log(\max(n, B_n, n_{L_n, N_n})) + \log(1/\delta) \right] \right) \\ & \leq \inf_{h \in \mathcal{H}_{\sigma, d_x, d_y, n}} \left( 3(R(h) - R(h^*)) + \frac{\Xi_1}{n} \left[ S_n L_n \log(\max(n, B_n, n_{L_n, N_n})) + \log(1/\delta) \right] \right) \\ & \leq 3 \inf_{h \in \mathcal{H}_{\sigma, d_x, d_y, n}} (R(h) - R(h^*)) + \frac{\Xi_1}{n} \left[ S_n L_n \log(\max(n, B_n, n_{L_n, N_n})) + \log(1/\delta) \right]. \end{aligned}$$

Therefore, from Theorem 4.1, it holds with  $P_n \otimes \Pi_\lambda$ -probability at least  $1 - \delta$  that,

$$\mathcal{E}(\hat{\theta}_\lambda) \leq 3 \inf_{h \in \mathcal{H}_{\sigma, d_x, d_y, n}} (R(h) - R(h^*)) + \frac{\Xi_1}{n} \left[ S_n L_n \log(\max(n, B_n, n_{L_n, N_n})) + \log(1/\delta) + 3\mathcal{K}_\ell \right]. \quad (6.27)$$

Set  $\varepsilon_n = \frac{1}{n^{\frac{\varepsilon}{2s+d_x}}}$ . Since  $h^* \in \mathcal{C}^{s, \mathcal{K}}(\mathcal{X})$  for some  $s, \mathcal{K} > 0$ , then from [19], there exists constants  $L_0, N_0, S_0, B_0 > 0$  such that with

$$L_n = \frac{sL_0}{s+d_x} \log n, \quad N_n = N_0 n^{\frac{d_x}{2s+d_x}}, \quad S_n = \frac{sS_0}{2s+d_x} n^{\frac{d_x}{2s+d_x}} \log n, \quad B_n = B_0 n^{\frac{4(s+d_x)}{2s+d_x}}, \quad (6.28)$$

there is a neural network  $h_n \in \mathcal{H}_{\sigma, d_x, d_y, n}$  that satisfies,

$$\|h_n - h^*\|_{\infty, \mathcal{X}} \leq \varepsilon_n.$$

Set,

$$\tilde{\mathcal{H}}_{\sigma, d_x, d_y, n} := \{h \in \mathcal{H}_{\sigma, d_x, d_y, n}, \|h - h^*\|_{\infty, \mathcal{X}} \leq \varepsilon_n\}.$$

Also, recall that  $n_{L_n, N_n} = (L_n + 1)N_n^2 + L_n N_n \leq 2(L_n + 1)N_n^2$ . Hence, from (6.27) and in addition to **(A7)**, we get for  $n \geq \varepsilon_0^{-\frac{1}{2s+d_x}}$ ,

$$\begin{aligned} \mathcal{E}(\hat{\theta}_\lambda) & \leq 3 \inf_{h \in \tilde{\mathcal{H}}_{\sigma, d_x, d_y, n}} (R(h) - R(h^*)) + \frac{\Xi_1}{n} \left[ S_n L_n \log(\max(n, B_n, n_{L_n, N_n})) + \log(1/\delta) + 3\mathcal{K}_\ell \right] \\ & \leq 3\mathcal{K}_0 \inf_{h \in \tilde{\mathcal{H}}_{\sigma, d_x, d_y, n}} \|h - h^*\|_{2, P_{X_0}}^2 + \frac{\Xi_1}{n} \left[ S_n L_n \log(\max(n, B_n, n_{L_n, N_n})) + \log(1/\delta) + 3\mathcal{K}_\ell \right] \\ & \leq 3\mathcal{K}_0 \inf_{h \in \tilde{\mathcal{H}}_{\sigma, d_x, d_y, n}} \|h_n - h^*\|_{\infty, \mathcal{X}}^2 + \frac{\Xi_1}{n} \left[ S_n L_n \log(\max(n, B_n, n_{L_n, N_n})) + \log(1/\delta) + 3\mathcal{K}_\ell \right] \\ & \leq 3\mathcal{K}_0 \varepsilon_n^2 + \frac{\Xi_1 L_0 S_0 \frac{s^2}{(s+d_x)(2s+d_x)} n^{\frac{d_x}{2s+d_x}} (\log n)^2 \log \left( \max \left[ n, B_0 n^{\frac{4(s+d_x)}{2s+d_x}} \right], 2 \left( \frac{sL_0}{s+d_x} \log n + 1 \right) N_0^2 n^{\frac{2d_x}{2s+d_x}} \right)}{n} \\ & \quad + \frac{\Xi_1 [\log(1/\delta) + 3\mathcal{K}_\ell]}{n} \\ & \leq \Xi_2 \left( \frac{\log^3 n}{n^{\frac{2s}{2s+d_x}}} + \frac{\log(1/\delta) + \mathcal{K}_\ell}{n} \right), \end{aligned} \quad (6.29)$$

for some constant  $\Xi_2 > 0$ , independent of  $n$ .

## 6.5 Proof of Theorem 4.4

Set  $\mathcal{H}_{\sigma, d_x, d_y, n} := \mathcal{H}_{\sigma, d_x, d_y}(L_n, N_n, S_n, B_n, F_n)$  and

$$\tilde{\mathcal{H}}_{\sigma, d_x, d_y, n}^{(1)} := \{h \in \mathcal{H}_{\sigma, d_x, d_y, n}, \text{ with architecture } (L_n, d_x, N_n, \dots, N_n, d_y)\}.$$

Let  $\delta > 0$ . According to (6.27), we get with  $P_n \otimes \Pi_\lambda$ -probability at least  $1 - \delta$ ,

$$\mathcal{E}(\hat{\theta}_\lambda) \leq 3 \inf_{h \in \tilde{\mathcal{H}}_{\sigma, d_x, d_y, n}^{(1)}} (R(h) - R(h^*)) + \frac{\Xi_1}{n} \left[ S_n L_n \log(\max(n, B_n, n_{L_n, N_n})) + \log(1/\delta) + 3\mathcal{K}_\ell \right]. \quad (6.30)$$

Since  $h^* \in \mathcal{G}(q, \mathbf{d}, \mathbf{t}, \mathbf{s}, \mathcal{K})$ , from the proof of Theorem 1 in [34], one can find a neural network  $h_n \in \tilde{\mathcal{H}}_{\sigma, d_x, d_y, n}^{(1)}$  satisfying

$$\|h_n - h^*\|_{\infty, \mathcal{X}}^2 \leq C_1 \max_{i=0, \dots, q} n^{-\frac{2\beta_i^*}{2\beta_i^* + t_i}} = C_1 \phi_n,$$

for some constant  $C_1 > 0$ , independent of  $n$ . Set,

$$\tilde{\mathcal{H}}_{\sigma, d_x, d_y, n}^{(2)} := \{h \in \tilde{\mathcal{H}}_{\sigma, d_x, d_y, n}^{(1)}, \|h_n - h^*\|_{\infty, \mathcal{X}} \leq \sqrt{\phi_n}\}.$$

In addition to the architecture parameter's in (4.11), (6.30) gives with  $P_n \otimes \Pi_\lambda$ -probability at least  $1 - \delta$ ,

$$\begin{aligned} \mathcal{E}(\hat{\theta}_\lambda) &\leq 3 \inf_{h \in \tilde{\mathcal{H}}_{\sigma, d_x, d_y, n}^{(2)}} (R(h) - R(h^*)) + \frac{\Xi_1}{n} \left[ S_n L_n \log(\max(n, B_n, n_{L_n, N_n})) + \log(1/\delta) + 3\mathcal{K}_\ell \right] \\ &\leq 3\mathcal{K}_0 \inf_{h \in \tilde{\mathcal{H}}_{\sigma, d_x, d_y, n}^{(2)}} \|h - h^*\|_{2, P_{X_0}}^2 + \frac{\Xi_1}{n} \left[ S_n L_n \log(\max(n, B_n, n_{L_n, N_n})) + \log(1/\delta) + 3\mathcal{K}_\ell \right] \\ &\leq 3\mathcal{K}_0 C_1 \phi_n + \frac{\Xi_1}{n} \left[ C_2 n \phi_n (\log n)^3 + \log(1/\delta) + 3\mathcal{K}_\ell \right] \\ &\leq 3\mathcal{K}_0 C_1 \phi_n + \Xi_1 C_2 \phi_n (\log n)^3 + \frac{\Xi_1 [\log(1/\delta) + 3\mathcal{K}_\ell]}{n} \\ &\leq \Xi_3 \left( \phi_n (\log n)^3 + \frac{\log(1/\delta) + \mathcal{K}_\ell}{n} \right), \end{aligned}$$

for some constants  $C_2, \Xi_3 > 0$  independent of  $n$ .

## 6.6 Proof of Theorem 5.2

Since  $\mathcal{G}(q, \mathbf{d}, \mathbf{t}, \boldsymbol{\beta}, \mathcal{K})$  is a class of bounded functions, it suffices to establish (5.7) with the infimum taken over the class of bounded estimators. Let  $\mathcal{K}_1 > 0$ . Consider a target function  $h^* \in \mathcal{G}(q, \mathbf{d}, \mathbf{t}, \boldsymbol{\beta}, \mathcal{K})$  and a predictor  $h : \mathcal{X} \rightarrow \mathbb{R}$  satisfying  $\|h\| \leq \mathcal{K}_1$ . Let  $x \in \mathcal{X}$ . We have

$$\begin{aligned} &\mathbb{E}[\phi(Y_0 h(X_0)) | X_0 = x] - \mathbb{E}[\phi(Y_0 h^*(X_0)) | X_0 = x] \\ &= \eta(x) \phi(h(x)) + (1 - \eta(x)) \phi(-h(x)) - \eta(x) \phi(h^*(x)) - (1 - \eta(x)) \phi(-h^*(x)) \\ &= \eta(x) (\phi(h(x)) - \phi(h^*(x))) + (1 - \eta(x)) (\phi(-h(x)) - \phi(-h^*(x))). \end{aligned} \quad (6.31)$$

Set  $\mathcal{K}_2 := \max(\mathcal{K}, \mathcal{K}_1)$ . Since the function  $\phi$  is strongly convex on  $[-\mathcal{K}_2, \mathcal{K}_2]$ , there exists a constant  $C_3 := C_3(\mathcal{K}_2) > 0$  such that for all  $y, y' \in [-\mathcal{K}_2, \mathcal{K}_2]$ ,

$$\phi(y) - \phi(y') \geq (y - y')\phi'(y') + C_3(y - y')^2,$$

where  $\phi'(y) = \partial\phi(y)/\partial y$ . Hence, (6.31) gives

$$\begin{aligned} & \mathbb{E}[\phi(Y_0 h(X_0)) | X_0 = x] - \mathbb{E}[\phi(Y_0 h^*(X_0)) | X_0 = x] \\ & \geq \eta(x) [(h(x) - h^*(x))\phi'(h^*(x)) + C_3(h(x) - h^*(x))^2] + (1 - \eta(x)) [-(h(x) - h^*(x))\phi'(-h^*(x)) + C_3(h(x) - h^*(x))^2] \\ & \geq (h(x) - h^*(x)) [\eta(x)\phi'(h^*(x)) - (1 - \eta(x))\phi'(-h^*(x))] + C_3(h(x) - h^*(x))^2. \end{aligned} \quad (6.32)$$

Consider the function  $\psi : [-\mathcal{K}_2, \mathcal{K}_2] \rightarrow \mathbb{R}$ , defined by,

$$\psi(\alpha) = \eta(x)\phi(\alpha) + (1 - \eta(x))\phi(-\alpha). \quad (6.33)$$

Recall that  $h^*$  is a target function. We get,

$$h^*(x) \in \underset{\alpha \in [-\mathcal{K}_2, \mathcal{K}_2]}{\operatorname{argmin}} \psi(\alpha).$$

So, since  $\psi$  is a convex function, it holds that  $\psi'(h^*(x)) = 0$ . Therefore, we have from (6.32),

$$\mathbb{E}[\phi(Y_0 h(X_0)) | X_0 = x] - \mathbb{E}[\phi(Y_0 h^*(X_0)) | X_0 = x] \geq C_3(h(x) - h^*(x))^2.$$

That is,

$$R(h) - R(h^*) \geq C_3 \|h - h^*\|_{2, P_{X_0}}^2. \quad (6.34)$$

Thus, to prove the theorem, it suffices to establish that, there exist a constant  $C > 0$  such that

$$\inf_{\hat{h}_n} \sup_{h^* \in \mathcal{G}(q, \mathbf{d}, \mathbf{t}, \boldsymbol{\beta}, \mathcal{K})} \mathbb{E}[\|\hat{h}_n - h^*\|_{2, P_{X_0}}^2] \geq C\phi_n. \quad (6.35)$$

We will establish (6.35) when the observations  $(X_1, Y_1), \dots, (X_n, Y_n)$  are i.i.d. and deduce such lower bound in the dependent case. To do so, we will apply the Theorem 2.7 in [38].

Consider a class of composition structured functions  $\mathcal{G}(q, \mathbf{d}, \mathbf{t}, \boldsymbol{\beta}, A)$ . From the proof of Theorem 3 in [34], there exists an integer  $M \geq 1$ , a constant  $\kappa > 0$  depending only on  $\mathbf{t}$  and  $\boldsymbol{\beta}$ , and functions  $h_{(0)}, \dots, h_{(M)} \in \mathcal{G}(q, \mathbf{d}, \mathbf{t}, \boldsymbol{\beta}, A)$  such that,

$$\|h_{(j)} - h_{(k)}\|_2^2 \geq \kappa^2 \phi_n, \quad \forall 0 \leq j < k \leq M. \quad (6.36)$$

Therefore, the first item of Theorem 2.7 in [38] is satisfied.

Consider model (5.4) with the target function  $h^*$  in (5.5) and denote by  $P_{h^*}^{\otimes n}$  the law of the sample  $D_n$ . For all  $j = 0, \dots, M$ , set  $P_j^{\otimes n} := P_{h_{(j)}}^{\otimes n}$  where  $h_{(j)}$  satisfies (5.5) with a parameter function,

$$\eta_j(x) = P(Y_t = 1 | X_t = x), \quad \forall x \in \mathcal{X}$$

and denote by  $P_j$  the distribution of  $(X_i, Y_i)$  (for any  $i = 1, \dots, n$ ), generated from (5.4) for  $h^* = h_{(j)}$  in (5.5). From Lemma C.19 and the proof of Lemma C.20 in [40], we get for any  $j = 1, \dots, M$ ,

$$\begin{aligned} \text{KL}(P_j, P_0) &= \int_{\mathcal{X}} \left[ \eta_j(x) \log \left( \frac{\eta_j(x)}{\eta_0(x)} \right) + (1 - \eta_j(x)) \log \left( \frac{1 - \eta_j(x)}{1 - \eta_0(x)} \right) \right] dP_{X_0}(x) \\ &= \int_{\mathcal{X}} \left[ \eta_j(x) \log \left( \frac{1}{\eta_0(x)} \right) + (1 - \eta_j(x)) \log \left( \frac{1}{1 - \eta_0(x)} \right) - \eta_j(x) \log \left( \frac{1}{\eta_j(x)} \right) - (1 - \eta_j(x)) \log \left( \frac{1}{1 - \eta_j(x)} \right) \right] dP_{X_0}(x) \\ &= \int_{\mathcal{X}} \left[ \eta_j(x) \phi(h_{(0)}(x)) + (1 - \eta_j(x)) \phi(-h_{(0)}(x)) - \eta_j(x) \log \left( \frac{1}{\eta_j(x)} \right) - (1 - \eta_j(x)) \log \left( \frac{1}{1 - \eta_j(x)} \right) \right] dP_{X_0}(x) \\ &\leq \frac{1}{8} \int_{\mathcal{X}} |h_{(0)}(x) - h_{(j)}(x)|^2 dP_{X_0}(x) \leq \frac{1}{8} \|h_{(j)} - h_{(0)}\|_2^2, \end{aligned} \quad (6.37)$$

where the inequality in (6.37) is obtained by using Lemma C.6 in [40], see also (5.6). Note that, from the proof of Theorem 3 in [34], the functions  $h_{(0)}, \dots, h_{(M)} \in \mathcal{G}(q, \mathbf{d}, \mathbf{t}, \boldsymbol{\beta}, A)$  satisfying (6.36) can be constructed so that,

$$n \sum_{j=1}^M \|h_{(j)} - h_{(0)}\|_2^2 \leq \frac{8M}{9} \log M. \quad (6.38)$$

According to (6.37) and (6.38), we have (in the i.i.d. case)

$$\frac{1}{M} \sum_{j=1}^M \text{KL}(P_j^{\otimes n}, P_0^{\otimes n}) = \frac{n}{M} \sum_{j=1}^M \text{KL}(P_j, P_0) \leq \frac{1}{9} \log M. \quad (6.39)$$

Thus, the second item of Theorem 2.7 in [38] is satisfied. Hence, one can find a constant  $C > 0$  such that (6.35) holds. This completes the proof of the theorem.

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