A PAC-Bayes oracle inequality for sparse neural networks

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Abstract

We study the Gibbs posterior distribution for sparse deep neural nets in a nonparametric regression setting. The posterior can be accessed via Metropolis-adjusted Langevin algorithms. Using a mixture over uniform priors on sparse sets of network weights, we prove an oracle inequality which shows that the method adapts to the unknown regularity and hierarchical structure of the regression function. The estimator achieves the minimax-optimal rate of convergence (up to a logarithmic factor).

Keywords: Adaptive nonparametric estimation, stochastic neural network, optimal contraction rate, oracle inequality

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1 Introduction

Driven by the enormous success of neural networks in a broad spectrum of machine learning applications, see Goodfellow et al. [16] and Schmidhuber [29] for an introduction, the theoretical understanding of network based methods is a dynamic and flourishing research area at the intersection of mathematical statistics, optimization and approximation theory. In addition to theoretical guarantees, uncertainty quantification is an important and challenging problem for neural networks and has motivated the introduction of Bayesian neural networks, where for each network weight a distribution is learned, see Graves [17] and Blundell et al. [8] and numerous subsequent articles. In this work we study the Gibbs posterior distribution for a stochastic neural network. In a nonparametric regression problem, we show that the corresponding estimator achieves a minimax-optimal prediction risk bound up to a logarithmic factor. Moreover, the method is adaptive with respect to the unknown regularity and structure of the regression function.

While early theoretical foundations for neural nets are summarized by Anthony & Bartlett [4], the excellent approximation properties of deep neural nets, especially with the ReLU activation function, have been discovered in the last years, see e.g. Yarotsky [35], the review paper DeVore et al. [13] and Bolcskei et al. [9] for sparse deep neural networks. In addition to these approximation properties, an essential explanation of the empirical capabilities of neural networks has recently been given by Schmidt-Hieber [30] as well as Bauer & Kohler [5]. While classical regression methods suffer from the curse of dimensionality, sparse neural network estimators can profit from a hierarchical structure of the regression function and a possibly much smaller intrinsic dimension. In particular, Schmidt-Hieber [30] has analyzed sparse deep neural networks with ReLU activation function which is the network class considered subsequently. To achieve a sparse neural network, a standard approach is to use penalized empirical risk minimization which has been analyzed for neural nets by Taheri et al. [33].

Instead of penalized empirical risk minimization, we train a neural network by learning the Gibbs posterior distribution. The resulting stochastic neural network satisfies an oracle inequality which implies an adaptive version of the upper bound by Schmidt-Hieber [30], i.e., the network estimator achieves this

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upper bound without prior knowledge of the hierarchical structure and the regularity of the regression function.

The PAC-Bayes approach goes back to Shawe-Taylor & Williamson [51] and McAllester [22, 23]. In a quite general setting it is possible to derive upper bounds for the prediction error either in terms of the empirical risk or in terms of an oracle inequality. We refer to the review papers by Guedj [19] and Alquier [2] as well as Alquier & Biau [3] and Steffen [32] for applications in sparse nonparametric regression. Empirical PAC-Bayes bounds are intensively studied for (deep) neural nets, see Dziugaite & Roy [13], Pérez-Ortiz et al. [24] and further references in Alquier [2, Section 3.3]. PAC-Bayes oracle inequalities are less well studied. Exceptions are Chérief-Abdellatif [12], who has proved a (non-adaptive) oracle inequality for the variational approximation of the PAC-Bayes procedure based on the theory by Catoni [11], and Tsinis & Dalalyan [34] who have used the PAC-Bayes bound for an aggregation of (shallow) neural networks. Further, Franssen & Szabó [15] have studied an empirical Bayes-type approach in the last layer leading to Bayesian credible sets with frequentist coverage guarantees.

In order to sample from the Gibbs posterior, a Metropolis-adjusted Langevin algorithm (MALA) can be applied, see Besag [6], Roberts & Tweedie [22]. This approach can exploit the well-established and efficient gradient descent algorithms. More precisely, MALA relies on a Metropolis-Hastings algorithm where the proposal density is centered around a gradient descent step. This yields an efficient MCMC approach that is different from the majority of literature on Bayesian neural networks which mainly focuses on variational Bayesian inference, see Blundell et al. [8] for a review on variational inference and Graves & Blundell et al. [5] for early applications to neural networks. A main reason is that with a growing sample size the calculation of the acceptance probability in the Metropolis-Hastings step becomes expensive. To adapt to sparsity, we can choose a prior that prefers networks with sparse weights.

It should be noted that due to the non-convex dependence on the network weights, the computational analysis of such an MCMC algorithm is as challenging as the convergence analysis of gradient based methods towards a global risk minimizer.

The paper is organized as follows: In Section 2 we introduce our estimation method and discuss its implementation. In Section 3 we state and discuss our main results for the proposed method. All proofs have been postponed to Section 4 and some further details on algorithmic aspects are contained in Section 5.

2 Estimation method

We consider a training sample \( D_n := \{(X_i, Y_i)\}_{i=1,...,n} \subseteq \mathbb{R}^p \times \mathbb{R} \) given by \( n \in \mathbb{N} \) i.i.d. copies of generic random variables \( (X, Y) \in \mathbb{R}^p \times \mathbb{R} \) on some probability space \( (\Omega, \mathcal{A}, \mathbb{P}) \) and the aim to estimate the regression function \( f: \mathbb{R}^p \to \mathbb{R} \) given by \( Y = f(X) + \varepsilon \) with observation error \( \varepsilon \) satisfying \( \mathbb{E}[\varepsilon | X] = 0 \) almost surely (a.s.). Equivalently, \( f(X) = \mathbb{E}[Y | X] \) a.s. For any estimator \( \hat{f} \), the prediction risk and its empirical counterpart are given by

\[
R(\hat{f}) := \mathbb{E}_{(X,Y)}[(Y - \hat{f}(X))^2] \quad \text{and} \quad R_n(\hat{f}) = \frac{1}{n} \sum_{i=1}^{n} (Y_i - \hat{f}(X_i))^2,
\]

(2.1)

respectively, where \( \mathbb{E} \) denotes the expectation under \( \mathbb{P} \) and \( \mathbb{E}_Z \) is the (conditional) expectation only with respect to a random variable \( Z \). The accuracy of the estimation procedure will be quantified in terms of the excess risk

\[
\mathcal{E}(\hat{f}) := R(\hat{f}) - R(f) = \mathbb{E}_X[(\hat{f}(X) - f(X))^2] = \|\hat{f} - f\|_{L^2(\mathbb{P} | X)}^2.
\]

In the following we first introduce the considered class of sparse neural networks. Afterwards, we introduce the estimation method and discuss its implementation. Throughout, \( |x|_q \) denotes the \( \ell^q \)-norm of a vector \( x \in \mathbb{R}^p \), \( q \in [1, \infty] \). In particular, \( |\cdot| := |\cdot|_2 \) is the Euclidean norm. For \( a, b \in \mathbb{R} \) we write \( a \vee b := \max\{a, b\} \) and \( a \wedge b := \min\{a, b\} \). The cardinality of a set \( I \) is denoted by \( |I| \).
2.1 Sparse neural networks

We consider a feedforward multilayer perceptron with $L \in \mathbb{N}$ hidden layers of constant width $r \in \mathbb{N}$. The latter restriction is purely to simplify the notation. The rectified linear unit (ReLU) $\sigma(x) := x \vee 0$, $x \in \mathbb{R}$, is used as activation function. We write $\sigma_v x := (\sigma(x_i + v_i))_{i=1,\ldots,d}$ for vectors $x, v \in \mathbb{R}^d$. With this notation we can represent such neural networks as

$$g_\vartheta(x) := W^{(L+1)} \sigma_{\vartheta(L)} W^{(L)} \sigma_{\vartheta(L-1)} \cdots W^{(2)} \sigma_{\vartheta(1)} W^{(1)} x + v^{(L+1)}, \quad x \in \mathbb{R}^p,$$

where the entries of the weight matrices $W^{(1)} \in \mathbb{R}^{r \times p}$, $W^{(2)}, \ldots, W^{(L)} \in \mathbb{R}^{r \times r}$, $W^{(L+1)} \in \mathbb{R}^{1 \times r}$ and shift vectors $v^{(1)}, \ldots, v^{(L)} \in \mathbb{R}^r, v^{(L+1)} \in \mathbb{R}$ are all collected in one parameter vector $\vartheta$. The total number of network parameters is

$$P := (p+1)r + (L-1)(r+1)r + r + 1.$$

A possibly more intuitive layer-wise representation of $g_\vartheta$ is given by

$$x^{(0)} := x \in \mathbb{R}^p,$$

$$x^{(l)} := \sigma(W^{(l)} x^{(l-1)} + v^{(l)}), \quad l = 1, \ldots, L,$$

$$g_\vartheta(x) := x^{(L+1)} := W^{(L+1)} x^{(L)} + v^{(L+1)},$$

where the activation function is applied coordinate-wise. We denote the class of all such functions $g_\vartheta$ by $\mathcal{G}(p, L, r)$. A network is sparse, or more precisely connection sparse, if many weights in the network are zero and thus some links between nodes are inactive. For some active set $\mathcal{I} \subseteq \{1, \ldots, P\}$, the corresponding class of sparse networks is defined by

$$\mathcal{G}(p, L, r, \mathcal{I}) := \{g_\vartheta \in \mathcal{G}(p, L, r) : \vartheta_i = 0 \text{ if } i \notin \mathcal{I}\}.$$

For some $C \geq 1$, we also introduce the class of clipped networks

$$\mathcal{F}(p, L, r, C) := \{f_\vartheta := (-C) \vee (g_\vartheta \wedge C) \mid g_\vartheta \in \mathcal{G}(p, L, r)\}$$

and similarly we denote clipped networks with active set $\mathcal{I}$ by $\mathcal{F}(p, L, r, \mathcal{I}, C)$. We abbreviate $R(\vartheta) := R(f_\vartheta)$ and $R_n(\vartheta) := R_n(f_\vartheta)$.

2.2 Prior and posterior distribution

In order to adopt the PAC-Bayes approach to neural networks, we first choose a prior on the weights in the network class $\mathcal{G}(p, L, r)$. For a given active set $\mathcal{I}$ the prior $\Pi_{\mathcal{I}}$ on the parameter set of the class $\mathcal{G}(p, L, r, \mathcal{I})$ is defined as the uniform distribution on

$$\mathcal{S}_{\mathcal{I}} := \{\vartheta \in [-B, B]^P \mid \vartheta_i = 0 \text{ if } i \notin \mathcal{I}\}$$

for some $B \geq 1$. In the special case $\mathcal{I}^* := \{1, \ldots, P\}$ we obtain a prior $\Pi^* := \Pi_{\mathcal{I}^*}$ on the non-sparse network class $\mathcal{G}(p, L, r)$. To allow for a data-driven choice of the active set, we define the prior $\Pi$ as a mixture of the uniform priors $\Pi_{\mathcal{I}}$:

$$\Pi := \sum_{i=1}^P 2^{-i} \sum_{\mathcal{I} \subseteq \{1, \ldots, P\}, |\mathcal{I}|=i} \left(\begin{array}{c} P \\ i \end{array}\right)^{-1} \Pi_{\mathcal{I}} \big/ C_P \quad \text{with} \quad C_P := (1 - 2^{-P}).$$

The basis 2 of the geometric weights is arbitrary and can be replaced by a larger constant leading to a stronger preference of sparse networks. The theoretical results remain unchanged up to constants. The prior $\Pi$ can be understood as a hierarchical prior, where we first draw a geometrically distributed sparsity $i$, given $i$ we uniformly choose an active set $\mathcal{I} \subseteq \{1, \ldots, P\}$ with $|\mathcal{I}| = i$ and on $\mathcal{I}$ the uniform prior $\Pi_{\mathcal{I}}$ is applied.
Based on II, the Gibbs posterior probability distribution $\Pi_{\lambda}(\cdot | D_n)$ is defined via

$$\Pi_{\lambda}(d\theta | D_n) \propto \exp(-\lambda R_n(\theta))\Pi(d\theta)$$

(2.5)

with the so-called inverse temperature parameter $\lambda > 0$ and empirical prediction risk from (2.1). While (2.5) coincides with the classical Bayesian posterior distribution if $Y_i = f_\theta(X_i) + \varepsilon_i$ with i.i.d. $\varepsilon_i \sim \mathcal{N}(0, n/(2\lambda))$, the so-called tempered likelihood $\exp(-\lambda R_n(\theta))$ serves as a proxy for the unknown distribution of the observations given $\theta$. As we will see, the method is indeed applicable under quite general assumptions on the regression model. The Gibbs posterior distribution weights each $\theta$ based on its empirical performance on the data, where the inverse temperature parameter $\lambda$ determines the impact of $R_n(\theta)$ in comparison to the prior beliefs.

An estimator for $f$ can be obtained by drawing from the posterior distribution, i.e.,

$$\hat{f}_\lambda := f_{\hat{\theta}_\lambda} \quad \text{for} \quad \hat{\theta}_\lambda | D_n \sim \Pi_{\lambda}(\cdot | D_n)$$

(2.6)

or in the form of the posterior mean

$$f_{\lambda} := \mathbb{E}[f_{\hat{\theta}_\lambda} | D_n] = \int f_\theta \Pi_{\lambda}(d\theta | D_n).$$

(2.7)

The maximum a posteriori (MAP) estimator could be used as well, but we will focus on the previous two estimators.

### 2.3 MCMC algorithm

Since the normalizing constant of the posterior distribution is unknown, the posterior distribution itself is not accessible in practice. Popular Bayesian networks rely on a variational Bayes approach, cf. Blei et al. [7], and approximate the posterior by some easier distribution. For instance, the Bayes by backprop method by Blundell et al. [8] uses independent normal distributions for the weights such that the training of the Bayesian network reduces to the calibration of the means and variances for all weights. In contrast, the classical approach in Bayesian statistics is to sample $\hat{\theta}_\lambda$ by constructing a Markov-chain $(\hat{\theta}(k))_{k \in \mathbb{N}_0}$ with stationary distribution $\Pi_{\lambda}(\cdot | D_n)$ with a Markov chain Monte Carlo (MCMC) method, see Robert & Casella [24]. MCMC methods aim for the exact posterior distribution and have been successfully applied to neural networks, see e.g. Zhang et al. [36], Alexos et al. [1].

For ease of presentation, we will discuss MALA for the prior $\Pi^\bullet$ on the non-sparse network class $\mathcal{G}(p, L, r)$, i.e. $\Pi^\bullet$ is the uniform distribution on $[-B, B]^P$. The corresponding posterior distribution is denoted by $\Pi^\bullet_{\lambda}(d\theta | D_n) \propto \exp(-\lambda R_n(\theta))\Pi^\bullet(d\theta)$.

Applying the generic Metropolis-Hastings algorithm to $\Pi^\bullet_{\lambda}(d\theta | D_n)$ and taking into account that the prior $\Pi^\bullet$ is uniform, we obtain the following iterative method: Starting with some initial choice $\theta(0) \in \mathbb{R}^P$, we successively generate $\theta(k+1)$ given $\theta(k)$, $k \in \mathbb{N}_0$, by

$$\theta(k+1) = \begin{cases} \tau(k) \quad \text{with probability } \alpha(\tau(k) | \theta(k)) \\ \theta(k) \quad \text{with probability } 1 - \alpha(\tau(k) | \theta(k)) \end{cases},$$

where $\tau(k)$ is a random variable drawn from some conditional proposal density $q(\cdot | \theta(k))$ and the acceptance probability is given by

$$\alpha(\tau(k) | \theta(k)) = \min\left\{1, \exp\left(-\lambda R_n(\tau(k)) + \lambda R_n(\theta(k))\right) \mathbb{I}_{[-B,B]}(\tau(k)) \frac{q(\theta(k) | \tau(k))}{q(\tau(k) | \theta(k))}\right\}.$$

The Metropolis-Hastings acceptance step ensures that $(\theta(k))_{k \in \mathbb{N}_0}$ is a Markov chain with invariant distribution $\Pi^\bullet_{\lambda}(\cdot | D_n)$. The convergence to the invariant distribution follows from Roberts & Tweedie [28, Theorem 2.2].
The practical success of the Metropolis-Hastings algorithm fundamentally depends on the choice of the proposal distribution. In the construction of \( q(\tau \mid \vartheta) \), MALA exploits the well-known gradient approach for an empirical risk minimizer

\[
\vartheta^* \in \arg \min_{\vartheta} R_n(\vartheta)
\]

with the empirical risk \( R_n(\vartheta) = R_n(f_\vartheta) \) from \([2.1]\). The gradient \( \nabla_\vartheta R_n(\vartheta) \) of \( R_n(\vartheta) \) with respect to \( \vartheta \) can be computed efficiently using backpropagation. The gradient descent method commonly used to train neural networks would suggest to tweak a given \( \vartheta^{(k)} \) in the direction of the gradient, that is

\[
\tilde{\vartheta}^{(k+1)} = \vartheta^{(k)} - \gamma \nabla_\vartheta R_n(\vartheta^{(k)})
\]

with a learning rate \( \gamma > 0 \). Therefore, MALA proposes a normal distribution around \( \tilde{\vartheta}^{(k+1)} \) with some standard deviation \( s > 0 \). This standard deviation should not be too large as otherwise the acceptance probability might be too small. As a result the proposal would rarely be accepted, the chain might not be sufficiently randomized and the convergence to the invariant target distribution would be too slow in practice. On the other hand, \( s \) should not be smaller than the shift \( \gamma \nabla_\vartheta R_n(\vartheta^{(k)}) \) in the mean, since otherwise \( q(\vartheta^{(k)} \mid \tau^{(k)}) \) might be too small. Therefore, the probability density \( q \) of the proposal distribution is given by the density

\[
q(\tau \mid \vartheta) = \frac{1}{(2\pi s^2)^{d/2}} \exp \left( -\frac{1}{2s^2} |\tau - \vartheta + \gamma \nabla_\vartheta R_n(\vartheta)|^2 \right).
\]

(2.8)

To calculate the estimators \( \hat{f}_\lambda \) and \( \hat{f}_\Lambda \) from \([2.6]\) and \([2.7]\) respectively, one chooses a burn-in time \( b \in \mathbb{N} \) to let the distribution of the Markov chain stabilize at its invariant distribution and then sets

\[
\hat{f}_\lambda := f_{\vartheta^{(b)}} \quad \text{and} \quad \hat{f}_\Lambda := \frac{1}{N} \sum_{k=1}^{N} f_{\vartheta^{(b+ck)}}.
\]

A sufficiently large gap length \( c \in \mathbb{N} \) ensures the necessary variability and an approximate independence between \( \vartheta^{(b+ck)} \) and \( \vartheta^{(b+c(k+1))} \), whereas \( N \in \mathbb{N} \) has to be large enough for a good approximation of the expectation by the empirical mean.

Note that the gradient has to be calculated only once in each MCMC iteration. While we use the standard gradient, the calculation of \( \nabla_\vartheta R_n \) could be realized and combined with state-of-art gradient based methods such as mini-batch stochastic gradient descent or Adam \([24]\). Compared to the training of a non-stochastic network, the additional computational price of MALA is determined by the computation of the acceptance probability \( \alpha(\tau^{(k)} \mid \vartheta^{(k)}) \) and a larger number of necessary iterations due to the potential rejection of proposals.

In order to extend the Metropolis-Hastings algorithm from the full prior \( \Pi^* \) to the mixing prior \( \Pi \) from \([2.4]\), we have to take into account the hierarchical structure of \( \Pi \). Hence, we use the reversible-jump Markov chain Monte Carlo (RJMCMC) algorithm first proposed by Green \([18]\). In the context of a PAC-Bayes method it has been discussed in Guedj \([19]\). In particular, the RJMCMC algorithm has been successfully applied by Alquier & Biau \([3]\) in a high-dimensional regression setting. Some further details on the of neural networks with the RJMCMC algorithm are given in Section 5.

### 3 Oracle inequality

In this section we state the theoretical guarantees for the Gibbs posterior distribution. As a benchmark for the performance of the method, we define the oracle choice on \( S_I \) from \([2.3]\) for some active set \( I \) as

\[
\vartheta^*_I \in \arg \min_{\vartheta \in S_I} R(\vartheta).
\]

(3.1)

The oracle is not accessible to the practitioner because \( R(\vartheta) \) depends on the unknown distribution of \((X, Y)\). A solution to the minimization problem in \((3.1)\) always exists since \( S_I \) is compact and
Assumption A.

1. For \( K, C \geq 1 \) we have \( \mathbb{E}[\|X\|^2] \leq pK \) and \( \|f\|_{\infty} \leq C \).

2. \( \varepsilon \) is conditionally on \( X \) sub-Gaussian. More precisely, there are constants \( \sigma, \Gamma > 0 \) such that

\[
\mathbb{E}[|\varepsilon|^k \mid X] \leq \frac{k^4}{2}\sigma^2\Gamma^{k-2} \text{a.s., \ for all } k \geq 2.
\]

Note that neither the loss function nor the data are assumed to be bounded. We obtain the following non-asymptotic oracle inequality:

**Theorem 1** (PAC-Bayes oracle inequality). Under Assumption A there are constants \( \Xi_0, \Xi_1 > 0 \) only depending on \( C, \Gamma, \sigma \) such that for \( \lambda = n/\Xi_0 \) and sufficiently large \( n \), we have with probability of at least \( 1 - \delta \), that

\[
\mathcal{E}(\hat{f}_\lambda) \leq \min_{\lambda} \left( 4\mathcal{E}(f_\lambda) + \frac{\Xi_1}{n} |I| L \log(p \lor n) + \log(2/\delta) \right).
\]

**Remark 2.** \( \Xi_0 \) can explicitly be chosen as \( \Xi_0 = 16(C^2 + \sigma^2) + 16C(\Gamma \lor (2C)) \), the dependence of \( \Xi_1 \) on \( C, \Gamma, \sigma \) is at most quadratic and \( n \geq n_0 := 2 \lor r \lor b \lor K \) is sufficiently large.

The right-hand side of (3.2) can be interpreted similarly to the classical bias-variance decomposition in nonparametric statistics. The first term \( \mathcal{E}(f_\lambda) = \mathbb{E}((f_\lambda(X) - f(X))^2) \) quantifies the approximation error while second term is an upper bound for the stochastic error. In particular, we recover \( \frac{|I|}{n} \log p \) as the typical error term for estimating high-dimensional vectors with sparsity \( |I| \). The factor 4 in the upper bound can be improved to \( (1 + \eta) \) for any \( \eta > 0 \) at the cost of a larger constant \( \Xi_1 \).

**Theorem 1** is in line with classical PAC-Bayes oracle inequalities, see Alquier [2]. Chérief-Abdellatif [12] has obtained a similar oracle inequality for a variational approximation of the Gibbs posterior distribution, but without the minimum over the active sets. For penalized empirical risk minimization, Taheri et al. [33] have obtained another oracle inequality with a different dependence on the depth \( L \).

The \( 1 - \delta \) probability takes into account the randomness of the data and of the estimate. Denoting

\[
r_{n,p}^2 = \min_{\lambda} \left( 4\|f_\lambda - f\|_{L^2(pX)}^2 + \frac{\Xi_1}{n} |I| L \log(p \lor n) \right),
\]

we can rewrite (3.2) as

\[
\mathbb{E}[\Pi_\lambda(\|f_\lambda - f\|_{L^2(pX)}^2 > r_{n,p}^2 + t^2 \mid D_n)] \leq 2e^{-nt^2/\Xi_1}, \quad t > 0,
\]

which is a contraction rate result in terms of a frequentist analysis of the nonparametric Bayes method.

An immediate consequence of the previous theorem is an analogous oracle inequality of the posterior mean \( f_\lambda \) from (2.7):

**Corollary 3** (Posterior mean). Under the conditions of **Theorem 1** we have with probability of at least \( 1 - \delta \) that

\[
\mathcal{E}(\hat{f}_\lambda) \leq \min_{\lambda} \left( 4\mathcal{E}(f_\lambda) + \frac{\Xi_2}{n} |I| L \log(p \lor n) + \log(2/\delta) \right)
\]

with a constant \( \Xi_2 \) only depending on \( C, \Gamma, \sigma \).

The infimum over all \( I \) in the oracle inequalities shows that the estimator may choose a sparse neural network for approximating \( f \) in a data-driven way. In particular, \( f_\lambda \) as well as \( f_\lambda \) adapt to the unknown regularity and a potentially lower dimensional structure of \( f \). Using the approximation properties of
neural networks, the oracle inequality yields the optimal rate of convergence (up to a logarithmic factor) over the following class of hierarchical functions:

\[
\mathcal{H}(q, d, t, \beta, C_0) := \left\{ g_q \circ \cdots \circ g_0 : [0,1]^p \to \mathbb{R} \left\vert g_i = (g_{ij})^\top : [a_i, b_i]^{t_i} \to [a_{i+1}, b_{i+1}]^{t_{i+1}}, \right. \\
g_{ij} \text{ depends on at most } t_i \text{ arguments,} \\
g_{ij} \in C^{\beta_i}_{t_i}([a_i, b_i]^{t_i}, C_0), \text{ for some } |a_i|, |b_i| \leq C_0 \right\},
\]

where \(d := (p, d_1, \ldots, d_q, 1) \in \mathbb{N}^{q+2}, t := (t_0, \ldots, t_q) \in \mathbb{N}^{q+1}, \beta := (\beta_0, \ldots, \beta_q) \in (0, \infty)^{q+1}\) and where \(C^{\beta_i}_{t_i}([a_i, b_i]^{t_i}, C_0)\) denote classical Hölder balls with Hölder regularity \(\beta_i > 0\) and radius \(C_0 \geq 1\). Theorem 1 reveals the following adaptive version of the upper bound by Schmidt-Hieber [30]:

**Proposition 4** (Rates of convergence). Let \(\log p \leq n/(\log^2 n)\) and \(X \in [0,1]^p\). In the situation of Theorem 1 there exists a network architecture \((L,r) = (C_1[\log_2 n],C_2 n)\) with \(C_1\) and \(C_2\) only depending on upper bounds for \(q,((d_1,\ldots,d_q)|_\infty,|t|_\infty,|\beta|_\infty\) and \(C_0\) such that the estimators \(\hat{f}_\lambda\) and \(\hat{f}_\hat{\lambda}\) yield an excess risk for sufficiently large \(n\) uniformly over all hierarchical functions \(\lambda \in \mathcal{H}(q,d,t,\beta,C_0)\) of at most

\[
\mathcal{E}(\hat{f}_\lambda) \leq \Xi_3\left(\frac{\log(p \vee n) \log^2(n)}{n}\right)^{2\beta^*/(2\beta^* + t^*)} + \Xi_4\frac{\log(2/\delta)}{n} \quad \text{and}
\]

\[
\mathcal{E}(\hat{f}_{\hat{\lambda}}) \leq \Xi_4\left(\frac{\log(p \vee n) \log^2(n)}{n}\right)^{2\beta^*/(2\beta^* + t^*)} + \Xi_4\frac{\log(2/\delta)}{n}
\]

with probability of at least \(1 - \delta\), respectively, where \(\beta^*\) and \(t^*\) are given by

\[
\beta^* := \beta_i^*, \quad t^* := t_i^*, \quad \text{for } \quad \beta_i^* := \arg \min_{\lambda \in [0,1]} \frac{2\beta_i}{2\beta_i + t_i}
\]

and \(\beta_0 \equiv 1\).

The constants \(\Xi_3\) and \(\Xi_4\) only depend on \(q,((d_1,\ldots,d_q),t,\beta,C_0\) and \(C,\Gamma,\sigma\).

For a fixed dimension \(p\) it has been proved by Schmidt-Hieber [30] that this rate is indeed optimal in a minimax sense up to a logarithmic factor in \(n\). Studying classical Hölder balls \(C^{\beta}_{t}([0,1]^p,C_0)\), a contraction rate of order \(n^{-2\beta^*/(2\beta^* + p)}\) has been derived by Polson & Ročková [25] and Chérief-Abdellatif [12], where Polson & Ročková [25] have used a hierarchical prior to obtain adaptivity with respect to \(\beta\) and the result by Chérief-Abdellatif [12] is non-adaptive, but incorporates a variational Bayes method.

### 4 Proofs

We first provide some preliminary results in Section 4.1 before we prove the oracle inequality in Section 4.2. All remaining proofs can be found in the last two subsections.

#### 4.1 A PAC-Bayes bound

Let \(\mu, \nu\) be probability measures on a measurable space \((E, \mathcal{E})\). The **Kullback-Leibler divergence** of \(\mu\) with respect to \(\nu\) is defined via

\[
\text{KL}(\mu \mid \nu) := \int \log \left( \frac{d\mu}{d\nu} \right) d\mu, \quad \text{if } \mu \ll \nu
\]

\[
\infty, \quad \text{otherwise}.
\]

The following classical lemma is a key ingredient for PAC-Bayes bounds. A proof can be found in Catoni [10, p. 159] or Alquier [2].
Lemma 5. Let \( h : E \to \mathbb{R} \) be a measurable function such that \( \int \exp h \, d\mu < \infty \). With the convention \( \infty - \infty = -\infty \), it then holds that

\[
\log \left( \int \exp h \, d\mu \right) = \sup_{\nu} \left( \int h \, d\nu - \text{KL}(\nu \mid \mu) \right),
\]

where the supremum is taken over all probability measures \( \nu \) on \( (E, \mathcal{A}) \). If additionally, \( h \) is bounded from above on the support of \( \mu \), then the supremum in (4.1) is attained for \( \nu = g \) with the Gibbs distribution \( g \), i.e. \( \frac{dg}{d\mu} \propto \exp h \).

Note that no generality is lost by considering only those probability measures \( \nu \) on \( (E, \mathcal{A}) \) such that \( \nu \ll \mu \) and thus

\[
\log \left( \int \exp h \, d\mu \right) = -\inf_{\nu \ll \mu} \left( \text{KL}(\nu \mid \mu) - \int h \, d\nu \right).
\]

Next we state a Bernstein type inequality for the excess risk \( \mathcal{E}(\vartheta) := \mathcal{E}(f_0) = R(\vartheta) - \mathbb{E}_{X,Y}[ (Y - f(X))^2 ] \). Its proof is given in Section 4.3.

Lemma 6. Set \( \mathcal{E}(\vartheta) := R(\vartheta) - R(f) \) and \( \mathcal{E}_n(\vartheta) := R_n(\vartheta) - R_n(f) \). For \( C_{n,\lambda} := \frac{8(C^2 + \sigma^2)}{\lambda^2 \Sigma_n} \) and \( w := 16C(\Gamma \vee 2C) \), we have for all \( \lambda \in [0, n/w] \) that

\[
\max \left\{ \mathbb{E}[\exp(\lambda(\mathcal{E}(\vartheta) - \mathcal{E}_n(\vartheta)))], \mathbb{E}[\exp(\lambda(\mathcal{E}_n(\vartheta) - \mathcal{E}(\vartheta)))] \right\} \leq \mathbb{E}(C_{n,\lambda} \lambda \mathcal{E}(\vartheta)).
\]

Based on these two lemmas, we can verify a PAC-Bayes bound for the excess risk. The basic proof strategy is standard in the PAC-Bayes literature, see e.g. Alquier & Biau [3].

Proposition 7 (PAC-Bayes bound). For any \( \mathcal{D}_n \)-dependent (in a measurable way) probability measure \( \rho \ll \Pi \) and any \( \lambda \in (0, n/w] \) such that \( C_{n,\lambda} \leq 1/2 \), we have

\[
\mathcal{E}(\hat{\vartheta}_\lambda) \leq 3 \int \mathcal{E} \, d\rho + \frac{4}{\lambda} (\text{KL}(\rho \mid \Pi) + \log(2/\delta))
\]

with probability of at least \( 1 - \delta \).

Proof. Lemma 6 yields

\[
\max \left\{ \mathbb{E}[\exp(\lambda(1 - C_{n,\lambda})\mathcal{E}(\vartheta) - \mathcal{E}_n(\vartheta) - \log \delta^{-1})], \mathbb{E}[\exp(\lambda C_{n,\lambda}\mathcal{E}(\vartheta) - \log \delta^{-1})] \right\} \leq \delta.
\]

Integrating in \( \vartheta \) with respect to the prior probability measure \( \Pi \) and applying Fubini’s theorem, we conclude

\[
\mathbb{E}\left[ \int \exp \left( \lambda(1 - C_{n,\lambda})\mathcal{E}(\vartheta) - \mathcal{E}_n(\vartheta) - \log \delta^{-1} \right) \, d\Pi(\vartheta) \right] \leq \delta \quad \text{and}
\]

\[
\mathbb{E}\left[ \int \exp \left( \lambda \mathcal{E}_n(\vartheta) - \lambda(1 + C_{n,\lambda})\mathcal{E}(\vartheta) - \log \delta^{-1} \right) \, d\Pi(\vartheta) \right] \leq \delta.
\]

For the posterior distribution \( \Pi_\lambda(\cdot \mid \mathcal{D}_n) \ll \Pi \) with corresponding Radon-Nikodým density

\[
\frac{d\Pi_\lambda(\vartheta \mid \mathcal{D}_n)}{d\Pi} = D_{\lambda}^{-1} \exp(-\lambda R_n(\vartheta)), \quad D_{\lambda} := \int \exp(-\lambda R_n(\vartheta)) \, d\Pi(\vartheta)
\]

with respect to \( \Pi \), we obtain

\[
\mathbb{E}_{\mathcal{D}_n, \tilde{\vartheta} \sim \Pi_\lambda(\cdot \mid \mathcal{D}_n)} \left[ \exp \left( \lambda(1 - C_{n,\lambda})\mathcal{E}(\tilde{\vartheta}) - \mathcal{E}_n(\tilde{\vartheta}) - \log \delta^{-1} + \lambda R_n(\tilde{\vartheta}) + \log D_{\lambda} \right) \right]
\]

\[
= \mathbb{E}_{\mathcal{D}_n, \tilde{\vartheta} \sim \Pi_\lambda(\cdot \mid \mathcal{D}_n)} \left[ \exp \left( \lambda(1 - C_{n,\lambda})\mathcal{E}(\tilde{\vartheta}) - \mathcal{E}_n(\tilde{\vartheta}) - \log \delta^{-1} - \log \left( \frac{d\Pi_\lambda(\tilde{\vartheta} \mid \mathcal{D}_n)}{d\Pi} \right) \right) \right]
\]

\[
= \mathbb{E}_{\mathcal{D}_n} \left[ \int \exp \left( \lambda(1 - C_{n,\lambda})\mathcal{E}(\vartheta) - \mathcal{E}_n(\vartheta) - \log \delta^{-1} \right) \, d\Pi(\vartheta) \right] \leq \delta.
\]
Therefore, we conclude with probability of at least \(1\) that
\[
(1 - C_{n,\lambda})\mathcal{E}(\hat{\theta}) - \mathcal{E}_n(\hat{\theta}) + R_n(\hat{\theta}) - \lambda^{-1}(\log \delta^{-1} - \log D_\lambda) \geq 0.
\]
Provided \((1 - C_{n,\lambda}) > 0\), we thus have with probability of at least \(1 - \delta\):
\[
\mathcal{E}(\hat{\theta}) \leq \frac{1}{1 - C_{n,\lambda}}( - R_n(f) + \lambda^{-1}(\log \delta^{-1} - \log D_\lambda)).
\]

Lemma 5 yields
\[-\log D_\lambda = -\log \left( \int \exp(-\lambda R_n(\theta)) d\Pi(\theta) \right) = \inf_{\rho \in \Pi} \left( KL(\rho \mid \Pi) + \int \lambda R_n(\theta) d\rho(\theta) \right).
\]
Therefore, we have with probability of at least \(1 - \delta\):
\[
\mathcal{E}(\hat{\theta}) \leq \frac{1}{1 - C_{n,\lambda}} \inf_{\rho \in \Pi} \left( \int \mathcal{E}_n(\theta) d\rho(\theta) + \lambda^{-1}(\log \delta^{-1} + KL(\rho \mid \Pi)) \right).
\]
In order to reduce the integral \(\int \mathcal{E}_n(\theta) d\rho(\theta)\) we use Jensen’s inequality and [4.3] to obtain for any probability measure \(\rho \ll \Pi\) (which may depend on \(\mathcal{D}_n\))
\[
\mathbb{E}_{\mathcal{D}_n} \left[ \exp \left( \int \lambda \mathcal{E}_n(\theta) - \lambda(1 + C_{n,\lambda}) \mathcal{E}(\theta) d\rho(\theta) - KL(\rho \mid \Pi) - \log \delta^{-1} \right) \right] \\
= \mathbb{E}_{\mathcal{D}_n} \left[ \exp \left( \int \lambda \mathcal{E}_n(\theta) - \lambda(1 + C_{n,\lambda}) \mathcal{E}(\theta) - \log \left( \frac{d\rho}{d\Pi} \right) - \log \delta^{-1} d\rho(\theta) \right) \right] \\
\leq \mathbb{E}_{\mathcal{D}_n, \rho \ll \Pi} \left[ \exp \left( \lambda \mathcal{E}_n(\theta) - \lambda(1 + C_{n,\lambda}) \mathcal{E}(\theta) - \log \left( \frac{d\rho}{d\Pi} \right) - \log \delta^{-1} \right) \right] \\
= \mathbb{E}_{\mathcal{D}_n} \left[ \int \exp \left( \lambda \mathcal{E}_n(\theta) - \lambda(1 + C_{n,\lambda}) \mathcal{E}(\theta) - \log \delta^{-1} \right) d\Pi(\theta) \right] \leq \delta.
\]
Using \(\mathbbm{1}_{[0,\infty)}(x) \leq e^{\lambda x}\) again, we conclude with probability of at least \(1 - \delta\):
\[
\int \mathcal{E}_n(\theta) d\rho(\theta) \leq (1 + C_{n,\lambda}) \int \mathcal{E}(\theta) d\rho(\theta) + \lambda^{-1}(KL(\rho \mid \Pi) + \log \delta^{-1}).
\]
Therefore, we conclude with probability of at least \(1 - 2\delta\)
\[
\mathcal{E}(\hat{\theta}) \leq \frac{1}{1 - C_{n,\lambda}} \inf_{\rho \in \Pi} \left( (1 + C_{n,\lambda}) \int \mathcal{E}(\theta) d\rho(\theta) + \frac{2}{\lambda}(\log \delta^{-1} + KL(\rho \mid \Pi)) \right)
\]
which yields the claimed bound if \(C_{n,\lambda} \leq 1/2\).

\(\square\)

### 4.2 Proof of Theorem 1
We fix some index set \(\mathcal{I}\), a radius \(\eta \in (0,1]\) and apply Proposition 7 with \(\rho = \rho_{\mathcal{I},\eta}\) defined via
\[
\frac{d\rho_{\mathcal{I},\eta}}{dH_{\mathcal{I}}}(\theta) \propto \mathbbm{1}_{\{\theta - \theta_{2}\|_{\infty} \leq \eta\}}
\]
with \(\theta_{2}\) from [3.1]. Note that indeed \(C_{n,\lambda} \leq 1/2\) for the given choice of \(\lambda\). In order to control the integral term, we decompose
\[
\int \mathcal{E} d\rho = \mathcal{E}(\theta_{2}) + \int \mathbb{E}[(f_\theta(X) - f(X))^2 - (f_\theta(X) - f(X))^2] d\rho(\theta) \\
= \mathcal{E}(\theta_{2}) + \int \mathbb{E}[(f_{\theta_2}(X) - f_\theta(X))^2] d\rho(\theta) + 2 \int \mathbb{E}[(f(X) - f_\theta(X))(f_{\theta_2}(X) - f_\theta(X))] d\rho(\theta)
\]

\[
\]

9
\[
\begin{align*}
&\leq \mathcal{E}(\vartheta_2^\ast) + \int \mathbb{E}[(f_{\vartheta_2}(X) - f_\vartheta(X))^2] \, d\rho(\vartheta) \\
&+ 2 \int \mathbb{E}[(f(X) - f_{\vartheta_2}(X))^2]^{1/2} \mathbb{E}[(f_{\vartheta_2}(X) - f_\vartheta(X))^2]^{1/2} \, d\rho(\vartheta) \\
&\leq \frac{4}{3} \mathcal{E}(\vartheta_2^\ast) + 4 \int \mathbb{E}[(f_{\vartheta_2}(X) - f_\vartheta(X))^2] \, d\rho(\vartheta),
\end{align*}
\]

using \(2a^2 \leq \frac{a^3}{3} + 3b^2\) in the last step. To bound the remainder, we use the Lipschitz continuity of the map \(\vartheta \mapsto f_\vartheta(x)\) for fixed \(x\):

**Lemma 8.** Let \(\vartheta, \tilde{\vartheta} \in [-B, B]^P\). Then we have for \(x \in \mathbb{R}^p\) that

\[
|f_\vartheta(x) - f_{\tilde{\vartheta}}(x)| \leq 4(2rB)^C(|x|_1 \lor 1) \cdot |\vartheta - \tilde{\vartheta}|_\infty.
\]

Due to the support of \(\rho = \rho^{\mathcal{I}, \eta}\), we obtain

\[
\int \mathcal{E} \, d\rho \leq \frac{4}{3} \mathcal{E}(\vartheta_2^\ast) + \frac{4}{n^2} \quad \text{for } \eta = \frac{1}{8(2rB)^C pKn}.
\]

(4.4)

It remains to bound the Kullback-Leibler term in (4.2) which can be done with the following lemma:

**Lemma 9.** We have

\(i\) \ KL(\rho^{\mathcal{I}, \eta} \mid \Pi) = KL(\rho^{\mathcal{I}, \eta} \mid \Pi_{\mathcal{I}}) + \log(C_\mathcal{I})\) where \(C_\mathcal{I} := C_P 2^{\mathcal{I}}(P/|\mathcal{I}|)\).

\(ii\) \ KL(\rho^{\mathcal{I}, \eta} \mid \Pi_{\mathcal{I}}) \leq |\mathcal{I}| \log(2B/\eta).

In particular,

\[
\text{KL}(\rho \mid \Pi) \leq |\mathcal{I}| \log(2B/\eta) + \log(C_\mathcal{I}).
\]

Plugging (4.4) and (4.5) into the PAC-Bayes bound (4.2) we conclude

\[
\mathcal{E}(\tilde{\vartheta}_\lambda) \leq \frac{4}{3} \mathcal{E}(\vartheta_2^\ast) + \frac{4}{n^2} + \frac{4}{\lambda} (|\mathcal{I}| \log(32BP e^{BP} pKn) + \log(2/\delta)) \\
\leq \frac{4}{3} \mathcal{E}(\vartheta_2^\ast) + \frac{\Xi_1}{n} (|\mathcal{I}| \log(p \lor n) + \log(2/\delta))
\]

(4.6)

for \(n \geq n_0 := 2 \lor r \lor B \lor K\) and some constant \(\Xi_1\) only depending on \(C, \Gamma, \sigma\). Note that the upper bound in (4.6) is deterministic and \(\mathcal{I}\) is arbitrary. Therefore, we can choose \(\mathcal{I}\) such that this bound is minimized, which completes the proof.

\(\square\)

### 4.3 Remaining proofs for Section 3

#### 4.3.1 Proof of Corollary 3

Jensen’s and Markov’s inequality yield for \(r_{n,p}^2\) from (3.3) that

\[
\mathbb{P} \left( \mathcal{E}(\tilde{f}_\lambda) > r_{n,p}^2 + \frac{\Xi_1}{n} + \frac{\Xi_2}{n} \log(2/\delta) \right) = \mathbb{P} \left( \|f_{\tilde{\vartheta}_\lambda} \mid \mathcal{D}_n\|_2^2 - f_{\tilde{\vartheta}_\lambda}^2(X) > r_{n,p}^2 + \frac{\Xi_1}{n} + \frac{\Xi_2}{n} \log(2/\delta) \right) \\
\leq \mathbb{P} \left( \|f_{\tilde{\vartheta}_\lambda} - f_{\vartheta}^2(X) \mid \mathcal{D}_n\|_2^2 > r_{n,p}^2 + \frac{\Xi_1}{n} + \frac{\Xi_2}{n} \log(2/\delta) \right) \\
= \mathbb{P} \left( \int_{\Xi_2}^\infty \Pi_\lambda \left( \|f_{\tilde{\vartheta}_\lambda} - f_{\vartheta}^2(X) \mid \mathcal{D}_n\|_2^2 > r_{n,p}^2 + t \mid \mathcal{D}_n \right) dt > \frac{\Xi_1}{n} \right)
\]
additional layers after the last hidden layer, instead of right after the input to preserve the order of the sparsity.

Using Theorem 1, we conclude
\[ \mathbb{P}(\mathcal{E}(\tilde{\alpha}) > r_{n,p}^2 + \frac{E}{n} + \frac{1}{n} \log(2/\delta)) \leq \frac{2n}{\Xi_1} \int_{-\Delta}^{\Delta} e^{-nt/\Xi_1} dt = \delta. \]

4.3.2 Proof of Proposition 4

Throughout, denote by $C_i, i = 1, 2, \ldots$ constants only depending on upper bounds for $q, \|\{d_1, \ldots, d_q\}\|_{\infty}$, $|t|_{\infty}$, $|\beta|_{\infty}$ and $C_0$.

We will verify that for any sufficiently large $n, M \in \mathbb{N}$ there exists a sparse ReLU neural network $g = g_\theta \in \mathcal{G}(p, C_1 \log_2 n, C_2 M, \mathcal{T})$ with $|\mathcal{T}| \leq C_3 M \log_2 n$ and $|\theta|_{\infty} \leq 1 \leq B$ such that
\[ \|g - f\|_{L^\infty([0,1]^p)} \leq C_4 M^{-\beta^*/\tau^*}. \] (4.7)

Careful inspection of the proof of Schmidt-Hieber [30, Theorem 1] reveals that there exists a sparse ReLU neural network $g \in \mathcal{G}(p, L, r, \mathcal{J})$ with weights and shifts absolutely bounded by 1 and
\[
L = 3(q - 1) + \sum_{i=0}^{q} (8 + (\log_2 n) + 5)(1 + \log_2(t_i \lor \beta_i)) \quad \text{and} \quad r = 6M \max_{i=0,\ldots,q} d_i + 1 \quad \text{and} \quad |\mathcal{J}| \leq \sum_{i=0}^{q} d_i + 1 (141(t_i + \beta_i + 1)^{3+t_i} M (\log_2 n + 6) + 4)
\]
such that (4.7) holds with
\[
M = \left[\left(\frac{n}{\log^2(n) \log(p \lor n)}\right)^{\tau^*/(2\beta^* + \tau^*)}\right] \leq n,
\]
provided $M \geq \max_{i=0,\ldots,q}(\beta_i + 1)^{t_i} \lor (C_0(2C_0)^{\beta_i} + 1) e^{t_i}$. Hence, it remains to show that $g$ can also be represented as a ReLU neural network in
\[ \mathcal{G}(p, C_1 \log_2 n, C_2 n, \mathcal{T}). \] (4.8)

To do this, we employ the embedding properties of network function classes from Schmidt-Hieber [30, Section 7.1].

Note that $L$, $r$ and the upper bound for $|\mathcal{J}|$ are independent of $d_0 = p$ and monotonically increasing in $q, \|\{d_1, \ldots, d_q\}\|_{\infty}, |t|_{\infty}$ and $|\beta|_{\infty}$. Also, $r$ is of order $M$, $L$ is of order $\log_2 n$ and the upper bound for $|\mathcal{J}|$ is of order $M \log_2 n$. Using the enlarging and the depth synchronisation properties, $g$ can indeed be written as a ReLU neural network in (4.8). Note that to ensure the depth of the network, we added additional layers after the last hidden layer, instead of right after the input to preserve the order of the sparsity.

Theorem 1 together with $\mathcal{E}(f_{\tilde{\alpha}}) \leq \|g_\theta - f\|_{L^\infty([0,1]^p)}$ now yields
\[
\mathcal{E}(\tilde{\alpha}) \leq 4C_4 M^{-2\beta^*/\tau^*} + \frac{\Xi_1 C_3}{n} M \log_2 n \log(p \lor n) + \Xi_1 \frac{\log(2/\delta)}{n}
\]
with probability at least $1 - \delta$.

The convergence rate for the posterior mean is obtained analogously using Corollary 3.
4.4 Proofs of the auxiliary results

4.4.1 Proof of Lemma 6

We write $E_n(\theta) = \frac{1}{n} \sum_{i=1}^{n} Z_i$ with centered and independent random variables

$$Z_i := (Y_i - f_\theta(X_i))^2 - (Y_i - f(X_i))^2 = - (2\varepsilon_i + f(X_i) - f_\theta(X_i))(f_\theta(X_i) - f(X_i))$$

Since $f$ and $f_\theta$ are bounded by $C$ and $\varepsilon_i$ is sub-Gaussian we have

$$E[Z_i^2] = E[(2\varepsilon_i + f(X_i) - f_\theta(X_i))^2(f_\theta(X_i) - f(X_i))^2] \leq 2(4\sigma^2 + 4C^2)E(\theta) = U$$

and for $k \geq 3$

$$\mathbb{E}[Z_i^k] \leq \mathbb{E}[2\varepsilon_i + f(X_i) - f_\theta(X_i)]^k|f_\theta(X_i) - f(X_i)|^{k-2}(f_\theta(X_i) - f(X_i))^2$$

$$\leq (2C)^{k-2}\mathbb{E}[2\varepsilon_i + f(X_i) - f_\theta(X_i))^k(f_\theta(X) - f(X))^2]$$

$$\leq (2C)^{k-2}(2k-1)!2^{k-1}\sigma^2\Gamma^{k-2} + (2C)^k)\mathcal{E}(\theta)$$

$$\leq (2C)^{k-2}(2k-1)!8k-2(\Gamma^{k-2} + (2C)^k)v = kUw^{k-2}.$$ 

In view of $\mathbb{E}[E_n(\theta)] = \mathcal{E}(\theta)$, Bernstein’s inequality [21, inequality (2.21)] yields

$$\mathbb{E}[\exp(\lambda(E_n(\theta) - \mathcal{E}(\theta)))] \leq \exp(\frac{U\lambda^2}{n(1 - \lambda/\nu)})$$

The same bound remains true if we replace $Z_i$ by $-Z_i$. \hfill \Box

4.4.2 Proof of Lemma 8

Set $\eta := |\theta - \tilde{\theta}|_\infty$ and let $W^{(1)}, \ldots, W^{(L+1)}, v^{(1)}, \ldots, v^{(L+1)}$ and $\tilde{W}^{(1)}, \ldots, \tilde{W}^{(L+1)}, \tilde{v}^{(1)}, \ldots, \tilde{v}^{(L+1)}$ be the weights and shifts associated with $\theta$ and $\tilde{\theta}$, respectively. Define $\tilde{x}^{(l)}$, $l = 0, \ldots, L+1$, analogously to [2,2]. We can recursively deduce from the Lipschitz-continuity of $\sigma$ that for $l = 2, \ldots, L$:

$$|x^{(l)}|_1 \leq |W^{(1)}|_1 + |v^{(l)}|_1$$

$$|x^{(l)}|_1 \leq 2rB(|x^{(l)}|_1 \lor 1),$$

$$|\tilde{x}^{(l)}|_1 \leq |W^{(1)}|_1 |x^{(0)}|_1 + |v^{(l)}|_1 - \tilde{W}^{(l)}(\tilde{x}^{(0)} - \tilde{v}^{(l)})|_1$$

$$\leq \eta 2r(|x^{(l)}|_1 \lor 1),$$

$$|x^{(l)}|_1 \leq |W^{(1)}|_1 |x^{(l-1)}|_1 + |v^{(l)}|_1$$

$$\leq 2rB(|x^{(l-1)}|_1 \lor 1)$$

and

$$|x^{(l)}|_1 - \tilde{x}^{(l)}|_1 \leq |W^{(1)}|_1 |x^{(l-1)}|_1 + |v^{(l)}|_1 - \tilde{W}^{(l)}(\tilde{x}^{(l-1)} - \tilde{v}^{(l)})|_1$$

$$\leq |W^{(1)}|_1 |x^{(l-1)}|_1 + |v^{(l)}|_1 - \tilde{W}^{(l)}|x^{(l-1)}|_1 + |v^{(l)}|_1 - \tilde{v}^{(l)}|_1$$

$$\leq \eta 2r(|x^{(l-1)}|_1 \lor 1) + rB|x^{(l-1)}|_1 - \tilde{x}^{(l-1)}|_1.$$ 

Therefore,

$$|x^{(L)}|_1 \leq (2rB)^L - 1(|x^{(1)}|_1 \lor 1)$$

$$\leq (2rB)^L(|x^{(l)}|_1 \lor 1)$$

and

$$|x^{(L)}|_1 - \tilde{x}^{(l)}|_1 \leq \eta 2r \sum_{k=1}^{L-1} (rB)^{k-1}(|x^{(L-k)}|_1 \lor 1) + (rB)^L|x^{(1)}|_1 - \tilde{x}^{(l)}|_1$$

$$\leq \eta 2(L+1)r(|x^{(l)}|_1 \lor 1)(rB)^{L-1}$$

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Since the clipping function \( y \mapsto (-C) \lor (y \land C) \) has Lipschitz constant 1, we conclude
\[
|f_\vartheta(x) - f_\vartheta(x)| \leq |g_\vartheta(x) - g_\vartheta(x)| = |\mathcal{X}^{(L+1)} - \mathcal{X}^{(L+1)}|\]
\[
= |W^{(L+1)} x^{(L)}(L) + v^{(L+1)} - \tilde{W}^{(L+1)} x^{(L)}(L) - \tilde{v}^{(L+1)}|\]
\[
\leq |W^{(L+1)} x^{(L)} - \tilde{W}^{(L+1)} x^{(L)}| + |\tilde{W}^{(L+1)} x^{(L)} - \tilde{v}^{(L+1)}| + |v^{(L+1)} - \tilde{v}^{(L+1)}|\]
\[
\leq \eta(2rB)^L(|x|_1 \lor 1) + \eta(2rB)^L 2^{L+1} (|x|_1 \lor 1) + \eta\]
\[
\leq \eta(2rB)^L (|x|_1 \lor 1). \quad \blacksquare
\]

4.4.3 Proof of Lemma 9

(i) We will show that
\[
\frac{d\rho_{\vartheta,\eta}}{d\Pi} = C_I \frac{d\rho_{\vartheta,\eta}}{d\Pi_I}.
\]

(4.9)

from which we can deduce
\[
\text{KL}(\rho_{\vartheta,\eta} \mid \Pi) = \int \log \left( \frac{d\rho_{\vartheta,\eta}}{d\Pi} \right) d\rho_{\vartheta,\eta} = \int \log \left( \frac{d\rho_{\vartheta,\eta}}{d\Pi}\right) d\rho_{\vartheta,\eta} + \log(C_I) = \text{KL}(\rho_{\vartheta,\eta} \mid \Pi_I) + \log(C_I).
\]

For (4.9), we need to show
\[
\rho_{\vartheta,\eta}(A) = \int_A C_I^{-1} d\rho_{\vartheta,\eta} d\Pi_I,
\]

for all \( A \in \mathcal{B}_{\mathbb{R}^r} \). Observe that for the sets
\[
\mathcal{S}_{\vartheta,\eta} := \{ \vartheta \in \mathcal{S}_{\vartheta} \mid \vartheta_i \neq 0 \Leftrightarrow i \in \mathcal{J} \}
\]

with \( \emptyset \neq \mathcal{J} \subseteq \{1, \ldots, P\} \), we have
\[
\Pi_{\vartheta}(\mathcal{S}_{\vartheta,\eta}) = 1. \quad (4.10)
\]

In particular, (4.10) holds for \( \mathcal{J} = \mathcal{I} \). Since also \( \rho_{\vartheta,\eta}(\mathcal{S}_{\vartheta,\eta}) = 1 \), no generality is lost in additionally assuming \( A \subseteq \mathcal{S}_{\vartheta,\eta} \). Note how
\[
\mathcal{S}_{\vartheta,\eta} \cap \mathcal{S}_{\vartheta,\eta} = \emptyset \quad \forall \mathcal{J} \neq \mathcal{I}. \quad (4.11)
\]

Combining (4.10) with (4.11) we see that
\[
\int_A \frac{d\rho_{\vartheta,\eta}}{d\Pi} d\Pi_{\mathcal{J}} = 0 \quad \forall \mathcal{J} \neq \mathcal{I}.
\]

Therefore,
\[
\rho_{\vartheta,\eta}(A) = \int_A \frac{d\rho_{\vartheta,\eta}}{d\Pi} d\Pi = \int_A C_I^{-1} \frac{d\rho_{\vartheta,\eta}}{d\Pi} d\Pi_{\mathcal{I}}.
\]

(ii) Since \( \rho_{\vartheta,\eta} \) and \( \Pi_{\mathcal{I}} \) are product measures, their KL-divergence is equal to the sum of the KL-divergences in each of the \( P \) factors. For factors with index \( i \notin \mathcal{I} \), this is zero, as both factors have all their mass in 0. For factors with index \( i \in \mathcal{I} \), we are comparing
\[
\mathcal{U}([(\vartheta_i^+) - \eta, (\vartheta_i^+) + \eta] \cap [-B, B]) \quad \text{with} \quad \mathcal{U}([-B, B]).
\]

The KL-divergence of these distributions is equal to
\[
\log \left( \frac{\mathcal{M}([-B, B])}{\mathcal{M}([(\vartheta_i^+) - \eta, (\vartheta_i^+) + \eta] \cap [-B, B])} \right) \leq \log \left( \frac{\mathcal{M}([-B, B])}{\mathcal{M}([0, \eta])} \right) = \log(2B/\eta).
\]

Thus,
\[
\text{KL}(\rho_{\vartheta,\eta} \mid \Pi_{\mathcal{I}}) = \sum_{i \in \mathcal{I}} \text{KL} \left( \mathcal{U}([(\vartheta_i^+) - \eta, (\vartheta_i^+) + \eta] \cap [-B, B]) \mid \mathcal{U}([-B, B]) \right) \leq |\mathcal{I}| \log(2B/\eta). \quad \blacksquare
\]
5 Implementation of the mixing prior distribution

To incorporate sparse networks, the algorithm from Section 2.3 has to be extended. The following augmentations to the proposal density are inspired by Alquier & Biau [3].

For a fixed active set $I$ we modify the proposal density from (2.8) to

$$
\psi_I(\tau) | \vartheta = \frac{1}{(2\pi s^2)^{|I|/2}} \exp \left( - \frac{1}{2s^2} \sum_{i \in I} (\tau_i - \vartheta_i + \gamma \frac{\partial}{\partial \vartheta_i} R_n(\vartheta))^2 \right)
$$

and set $\tau_i = 0$ for all $i \notin I$. The mixture over sparse active sets leads to the conditional proposal density

$$
q(\tau | \vartheta) = \frac{1}{4} q_-(\tau | \vartheta) + \frac{3}{4} q_+(\tau | \vartheta) + q_0(\tau | \vartheta) \mathbb{1}_{|I| = 1} + q_-(\tau | \vartheta) + 2q_0(\tau | \vartheta) \mathbb{1}_{|I| = P},
$$

with $I = \{i : \vartheta_i \neq 0\}$ and some $q_-$ and $q_+$ proposing to remove or add a component, respectively, while $q_0$ leaves the active set untouched. Specifically, we choose

$$
q_-(\tau | \vartheta) = \psi_{I^c}(\tau | \vartheta), \quad q_+(\tau | \vartheta) = \sum_{i \in I} w_i^- \psi_{I \cup \{i\}}(\tau | \vartheta) \quad \text{and} \quad q_0(\tau | \vartheta) = \sum_{i \in I^c} w_i^+ \psi_{I \cup \{i\}}(\tau | \vartheta)
$$

with

$$
w_i^- = \exp(-|\vartheta_i|) / \sum_{j \in I^c} \exp(-|\vartheta_j|) \quad \text{and} \quad w_i^+ = \tilde{w}_i^- / \sum_{j \in I^c} \tilde{w}_j^-,
$$

where $\tilde{w}_i^- = |\{j \in I^c : |\frac{\partial}{\partial \vartheta_j} R_n(\vartheta)| \leq |\frac{\partial}{\partial \vartheta_i} R_n(\vartheta)|\}|^2$. The weights $\tilde{w}_i^-$ are chosen such that (absolutely) smaller entries have a larger probability of being removed. On the other hand, $\tilde{w}_i^+$ are chosen such that components with a large impact (as measured by $\nabla_\vartheta R_n(\vartheta)$) on the model have a higher probability of being included. Note that this extension of the algorithm requires no additional computation of $\nabla_\vartheta R_n(\vartheta)$, as this was already done in the previous MCMC step. Finally, the mixing prior from (2.4) also has to be accounted for in the acceptance probabilities, leading to

$$
\alpha(\tau | \vartheta) = \min \left\{ 1, \exp \left( - \lambda R_n(\tau) + \lambda R_n(\vartheta) \right) \frac{\Pi(\vartheta) q(\vartheta | \tau)}{\Pi(\tau) q(\tau | \vartheta)} \right\},
$$

where some abuse of notation $\Pi(\vartheta)$ denotes the probability density of the prior.

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