Statistical Guarantees for Regularized Neural Networks

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Abstract

Neural networks have become standard tools in the analysis of data, but they lack comprehensive mathematical theories. For example, there are very few statistical guarantees for learning neural networks from data, especially for classes of estimators that are used in practice or at least similar to such. In this paper, we develop a general statistical guarantee for estimators that consist of a least-squares term and a regularizer. We then exemplify this guarantee with ℓ_1 -regularization, showing that the corresponding prediction error increases at most logarithmically in the total number of parameters and can even decrease in the number of layers. Our results establish a mathematical basis for regularized estimation of neural networks, and they deepen our mathematical understanding of neural networks and deep learning more generally.

Keywords: neural networks, deep learning, prediction guarantees, regularization

1. Introduction

Neural networks have proved extremely useful across a variety of applications, including speech recognition (Hinton et al., 2012; Graves et al., 2013; Chorowski et al., 2015), natural language processing (Jozefowicz et al., 2016), object categorization (Girshick et al., 2014; Szegedy et al., 2015), and image segmentation (Long et al., 2015; Badrinarayanan et al., 2017). But our mathematical understanding of neural networks and deep learning has not developed at the same speed.

A central objective is to equip methods for learning neural networks with statistical guarantees. Some guarantees are available for unconstrained estimators (Anthony and Bartlett, 2009), but these bounds are linear in the number of parameters, which conflicts with the large sizes of typical networks. The focus has thus shifted to estimators that in-

volve constraints or regularizers. Recently surged in popularity have estimators with ℓ_1 -regularizers (Bartlett, 1998; Bartlett and Mendelson, 2002; Anthony and Bartlett, 2009; Barron and Klusowski, 2018, 2019; Liu and Ye, 2019), motivated by the success of this type of regularization in linear regression (Tibshirani, 1996), compressed sensing (Candès et al., 2006; Donoho, 2006), and many other parts of data science. A key feature of ℓ_1 -regularization is that it is easy to include into optimization schemes and, at the same time, induces sparsity, which has a number of favorable effects in deep learning (Glorot et al., 2011). There has been some progress on guarantees for least-squares with constraints based on the sparsity of the networks (Schmidt-Hieber, 2017) or group-type norms on the weights (Neyshabur et al., 2015). These developments have provided valuable intuition, for example, about the role of network widths and depths, but important problems remain: for example, the combinatorial constraints in the first paper render the corresponding estimators infeasible in practice, the exponential dependence of the bounds in the second paper are contrary to the trend toward very deep networks. More generally, many questions about the statistical properties of constraint and regularized estimation of neural networks remain open.

In this paper, we introduce a general class of regularized least-squares estimators. Our strategy is to disentangle the parameters into a "scale" and a "direction"—similarly to introducing polar coordinates—which allows us to focus the regularization on a one-dimensional parameter. We call our approach scale regularization. We then equip the scale regularized least-squares estimators with a general statistical guarantee for prediction. A main feature of this guarantee is that it connects neural networks to standard empirical process theory through a quantity that we call the effective noise. This connection facilitates the specification of the bound to different types of regularization.

In a second step, we exemplify the general bound for ℓ_1 -regularization. We find a guarantee for the squared prediction error of the order of

$$(L/2)^{1/2-L}\sqrt{\log(P)}\,\frac{\log(n)}{\sqrt{n}},$$

which decreases essentially as $1/\sqrt{n}$ in the number of samples n, increases only logarithmically in the total number of parameters P, and—everything else fixed—decreases in the number of hidden layers L. This result suggests that ℓ_1 -regularization can ensure accurate prediction even of very wide and deep networks.

In Section 2, we introduce our regularization scheme and establish a general prediction bound that allows for different types of regularization. In Section 3, we specify this bound to ℓ_1 -regularization. In Section 4, we establish Lipschitz and complexity properties of neural networks. Section 5, we give detailed proofs. In Section 6, we conclude our paper and discuss some limitations.

2. Scale regularization for neural networks

We first establish an alternative parametrization of neural networks and use this parameterization to define our regularization strategy. We then provide a prediction guarantee for the corresponding estimators.

2.1 Alternative parametrization

Consider data $(x_1, y_1), \dots, (x_n, y_n) \in \mathbb{R}^d \times \mathbb{R}$ that follow a regression model

$$y_i = g_*(\boldsymbol{x}_i) + u_i \qquad \text{for } i \in \{1, \dots, n\}$$

for some function $g_*: \mathbb{R}^d \to \mathbb{R}$. We are interested in approximating g_* based on neural networks. Following first standard approaches, we consider feedforward neural networks of the form

$$g_{\Theta} : \mathbb{R}^d \to \mathbb{R}$$

 $\boldsymbol{x} \mapsto g_{\Theta}(\boldsymbol{x}) := W^L \boldsymbol{f}^L (\dots W^1 \boldsymbol{f}^1 (W^0 \boldsymbol{x}))$ (2)

indexed by the network parameter $\Theta = (W^L, \dots, W^0)$ that summarizes the weight matrices $W^l \in \mathbb{R}^{p_{l+1} \times p_l}$. The \boldsymbol{x}_i and y_i are the network's inputs and outputs, respectively, and the u_i are the noise variables. For ease of notation, the \boldsymbol{x}_i are fixed except in the generalization bounds. The network's architecture is specified by the number of hidden layers or depth $L \in \{1, 2, \dots\}$ and by the number of neurons in each layer or width $p_0, \dots, p_{L+1} \in \{1, 2, \dots\}$. The 0th layer is the input layer with $p_0 = d$, and the (L+1)th layer is the output layer with $p_{L+1} = 1$. The total number of parameters is $P := \sum_{l=0}^{L} p_{l+1} p_l$. The functions $\boldsymbol{f}^l : \mathbb{R}^{p_l} \to \mathbb{R}^{p_l}$ are called activation functions. We omit shifts in the activation functions for notational simplicity, but such can often be incorporated as additional neurons (Barron and Klusowski, 2018).

The parameter space in the above formulation is

$$\mathcal{A} := \{ \Theta = (W^L, \dots, W^0) : W^l \in \mathbb{R}^{p_{l+1} \times p_l} \}.$$

In the following, however, we propose an alternative parametrization. We say that a function $q: \mathbb{R}^s \to \mathbb{R}^t$ is nonnegative homogeneous of degree $k \in (0, \infty)$ if

$$q(az) = a^k q(z)$$
 for all $a \in [0, \infty)$ and $z \in \mathbb{R}^s$

and we say that a function $q: \mathbb{R}^s \to [0, \infty)$ is positive definite if

$$q(z) = 0 \Leftrightarrow z = \mathbf{0}_s.$$

The corresponding properties for functions on \mathcal{A} are defined accordingly. For example, every norm on \mathbb{R}^s or \mathcal{A} is nonnegative homogeneous of degree 1 and positive definite. We then find the following:

Proposition 1 (Equivalence between neural networks) Assume that the activation functions f^1, \ldots, f^L are nonnegative homogeneous of degree 1. Consider a function $h: A \to [0, \infty)$ that is nonnegative homogeneous of degree $k \in (0, \infty)$ and positive definite, and denote the corresponding unit ball by

$$\mathcal{A}_h := \{ \Theta \in \mathcal{A} : h(\Theta) \le 1 \}.$$

Then, for every $\Theta \in \mathcal{A}$, there exists a pair of $\kappa \in [0, \infty)$ and $\Omega \in \mathcal{A}_h$ such that

$$g_{\Theta}(\boldsymbol{x}) = \kappa g_{\Omega}(\boldsymbol{x})$$
 for all $\boldsymbol{x} \in \mathbb{R}^d$;

and vice versa, for every pair of $\kappa \in [0, \infty)$ and $\Omega \in \mathcal{A}_h$, there exists a $\Theta \in \mathcal{A}$ such that the above equality holds.

Proposition 1 is just a formulation of the known fact that weights can be rescaled across layers that have nonnegative-homogeneous activations (Du et al., 2018; Hebiri and Lederer, 2020; Neyshabur et al., 2014). The interesting part of this section is not Proposition 1 itself but the observation that this rescaling can lead to a reparameterization that is particularly suitable for regularization. Motivated by Proposition 1, we change the parameter space for estimating the true data generating function g_* to $[0, \infty) \times \mathcal{A}_h$ and the corresponding space of networks to $\{\kappa g_{\Omega} : \kappa \in [0, \infty), \Omega \in \mathcal{A}_h\}$. In other words, we study the neural networks

$$\kappa g_{\Omega} : \mathbb{R}^{d} \to \mathbb{R}$$

$$\boldsymbol{x} \mapsto \kappa g_{\Omega}(\boldsymbol{x}) := \kappa U^{L} \boldsymbol{f}^{L} (\dots U^{1} \boldsymbol{f}^{1} (U^{0} \boldsymbol{x}))$$
(3)

indexed by the parameters $\kappa \in [0, \infty)$ and $\Omega = (U^L, \dots, U^0) \in \mathcal{A}_h$. We can interpret κ as the network's "scale" and Ω as the network's "orientation." Proposition 1 ensures equivalence to the original set of networks if the activations are nonnegative homogeneous (ReLU activations are popular examples), but we can use the proposed parametrization more generally. We now argue that the scale parameter is particularly suitable for regularizing the "overall size" of the network and the orientation parameter for specifying the desired "type" of the network. In particular, rather than naively transferring standard regularization schemes from other parts of machine learning, we propose to tailor these regularization schemes to the characteristics of neural networks as captured by the above parameterization. We detail this argument in the following sections, where we introduce concrete regularization schemes and develop statistical guarantees. These statistical guarantees are the main result of this paper.

2.2 Estimation

The most basic approach to fit the model parameters of the network (2) to the model (1) is the least-squares estimator

$$\widehat{\Theta}_{\mathrm{LS}} \in \operatorname*{arg\,min}_{\Theta \in \mathcal{A}} \left\{ \frac{1}{n} \sum_{i=1}^{n} \left(y_i - g_{\Theta}(\boldsymbol{x}_i) \right)^2 \right\}.$$

But to account for the high-dimensionality of the parameter space \mathcal{A} , the least-squares estimator is often complemented with a regularizer $h: \mathcal{A} \to [0, \infty)$; popular choices for h are the ℓ_1 -norm (Zhang et al., 2016) or group versions of it (Scardapane et al., 2017). A straightforward way to incorporate such regularizers is

$$\widehat{\Theta}_{\mathrm{reg},h} \in \operatorname*{arg\,min}_{\Theta \in \mathcal{A}} \bigg\{ \frac{1}{n} \sum_{i=1}^{n} \big(y_i - g_{\Theta}(\boldsymbol{x}_i) \big)^2 + \lambda h(\Theta) \bigg\},$$

where $\lambda \in [0, \infty)$ is a tuning parameter. But in neural network frameworks, it turns out difficult to analyze such estimators statistically.

We introduce, therefore, a different way to incorporate regularizers. The approach is based on our new parametrization. The equivalent of the above least-squares estimator in the framework (3) is

$$(\hat{\kappa}_{\mathrm{LS}}, \widehat{\Omega}_{\mathrm{LS}}) \in \operatorname*{arg\,min}_{\substack{\kappa \in [0,\infty) \\ \Omega \in \mathcal{A}_{\mathrm{b}}}} \left\{ \frac{1}{n} \sum_{i=1}^{n} \left(y_{i} - \kappa g_{\Omega}(\boldsymbol{x}_{i}) \right)^{2} \right\}.$$

It holds that $g_{\widehat{\Theta}_{LS}} = \hat{\kappa}_{LS} g_{\widehat{\Omega}_{LS}}$ under the conditions of Proposition 1, but we can take this estimator as a starting point more generally. This allows us to focus the regularization on the scale-parameter κ ; in other words, we propose the estimators

$$(\hat{\kappa}_h, \widehat{\Omega}_h) \in \underset{\substack{\kappa \in [0,\infty) \\ \Omega \in \mathcal{A}_h}}{\min} \left\{ \frac{1}{n} \sum_{i=1}^n \left(y_i - \kappa g_{\Omega}(\boldsymbol{x}_i) \right)^2 + \lambda \kappa \right\}, \tag{4}$$

where $\lambda \in [0, \infty)$ is a tuning parameter. The fixed constraint $\Omega \in \mathcal{A}_h$ captures the type of regularization (such as ℓ_1), while the actual regularization concerns only on the scale $\kappa \in [0, \infty)$. We thus call our approach scale regularization.

The concentration of the regularization on a one-dimensional parameter greatly facilitates the statistical analysis. Specifically, it will allow us to focus our attention on

$$z_h := \sup_{\Omega \in \mathcal{A}_h} \left| \frac{2}{n} \sum_{i=1}^n g_{\Omega}(\boldsymbol{x}_i) u_i \right|.$$
 (5)

This quantity is related to the Gaussian and Rademacher complexities of the function class $\{g_{\Omega}: \Omega \in \mathcal{A}_h\}$. For example, the expectation of z_h is the Gaussian complexity of the function class $\{g_{\Omega}: \Omega \in \mathcal{A}_h\}$ if the u_i 's are i.i.d. standard normal random variables—cf. (Bartlett and Mendelson, 2002), for example. But while the Gaussian and Rademacher complexities are standard measures for function classes, there are two important subtleties here: first, Gaussian and Rademacher complexities require the specification of a distribution over the data, which we can avoid at this point; second, the function class at hand does not contain the entire networks κg_{Ω} but only their "orientation parts" g_{Ω} . Therefore, we should rather think of z_h as the neural-network equivalent of what high-dimensional linear regression refers to as the effective noise (Lederer and Vogt, 2020).

We need to ensure—just as in high-dimensional linear regression—that the effective noise is controlled by the tuning parameter with high probability. In this spirit, we define quantiles $\lambda_{h,t}$ of the effective noise for given level $t \in [0,1]$ through

$$\lambda_{h,t} \in \min \left\{ \delta \in [0, \infty) : \mathbb{P}(z_h \le \delta) \ge 1 - t \right\}. \tag{6}$$

In other words, $\lambda_{h,t}$ is the smallest tuning parameter that controls the effective noise z_h at level 1-t.

To measure the accuracy of the regularized estimators, we consider the (in-sample-) prediction error (also called "denoising error") with respect to the data generating function g_* :

$$\operatorname{err}(\kappa g_{\Omega}) := \sqrt{\frac{1}{n} \sum_{i=1}^{n} (\kappa g_{\Omega}(\boldsymbol{x}_{i}) - g_{*}(\boldsymbol{x}_{i}))^{2}} \qquad \text{for } \kappa \in [0, \infty), \Omega \in \mathcal{A}_{h}.$$
 (7)

This is a standard measure of how well the data generating function is learned. An interesting feature of the in-sample-prediction error is that it avoids any distributional assumptions on the data. Moreover, it also entails bounds on the generalization error (also called "out-of-sample-prediction error" or "prediction risk") for a new sample $(x, y) \in \mathbb{R}^d \times \mathbb{R}$

$$\operatorname{risk}(\kappa g_{\Omega}) := \mathbb{E}_{(\boldsymbol{x},y)} \Big[\left(\kappa g_{\Omega}(\boldsymbol{x}) - y \right)^2 \Big] \qquad \text{for } \kappa \in [0,\infty), \Omega \in \mathcal{A}_h \,,$$

which is more common in the deep-learning literature—see Lemma 5. We find the following guarantee:

Theorem 2 (Prediction guarantee) Assume that $\lambda \geq \lambda_{h,t}$ for a $t \in [0,1]$. Then,

$$\operatorname{err}^{2}(\hat{\kappa}_{h}g_{\widehat{\Omega}_{h}}) \leq \inf_{\substack{\kappa \in [0,\infty) \\ \Omega \in \mathcal{A}_{h}}} \left\{ \operatorname{err}^{2}(\kappa g_{\Omega}) + 2\lambda\kappa \right\}$$

with probability at least 1-t.

The bound is an analog of what has been called sparsity-bound in high-dimensional linear regression (Lederer et al., 2019). For neural networks, however, it is the first such bound. It states that the squared prediction error of the regularized estimator is governed by an approximation error or squared bias $\operatorname{err}^2(\kappa g_{\Omega})$ and an excess error or variance $2\lambda\kappa$. In other words, the estimator is guaranteed to have a small prediction error if (i) the quantile $\lambda_{h,t}$ is small and (ii) the data generating function can be represented well by a neural network with reasonably small κ . A typical example for (i) is provided in the following section; recent results on approximation theory support (ii) especially for wide and deep networks (Yarotsky, 2017).

Since z_h is a supremum over an empirical process, it allows us to connect our statistical theories with theories on empirical processes. Deviation inequalities that bound quantities such as $\lambda_{h,t}$ have been established even for noise u_i that has very heavy tails (Lederer and van de Geer, 2014). In Section 3, we derive an explicit bound for $\lambda_{h,t}$ for ℓ_1 -regularization and sub-Gaussian noise. Crucial in this derivation, and in controlling z_h in general, is that the index set of the empirical process is the constraint parameter space \mathcal{A}_h rather than the entire parameter space \mathcal{A} . This key feature of z_h is due to our novel way of regularizing.

The standard parametrization $\Theta \in \mathcal{A}$ of neural networks is ambiguous: there are typically uncountably many parameters $\Theta \in \mathcal{A}$ that yield the same network g_{Θ} . This ambiguity remains in our new framework with $(\kappa, \Omega) \in [0, \infty) \times \mathcal{A}_h$. But importantly, our guarantees hold for *every* solution $(\hat{\kappa}_h, \widehat{\Omega}_h)$.

3. An example: ℓ_1 -regularization

In view of its long-standing tradition in other parts of statistics and machine learning, sparsity-inducing regularization with ℓ_1 -terms has already sparked some theoretical research. This existing research has two components: first, general risk bounds in terms of the fat-shattering dimension or the Rademacher complexity such as Bartlett (1998, Theorem 2) and Bartlett and Mendelson (2002, Theorem 8), respectively; and second, bounds for the fat-shattering dimension and Rademacher complexity of classes of ℓ_1 -constraint neural networks such as Bartlett (1998, Section IV.B) and Golowich et al. (2018); Neyshabur et al. (2015), respectively. But these results have severe limitations: for example, they require bounded losses (which excludes the least-squares loss, for example); they consider constraints rather than regularization terms (which is the version used in practice); they do not provide insights into how the tuning parameters should scale with the dimensions of the problem, such as the sample size, the network size, and so forth (which can eventually lead to practical advise); and they have—except for Golowich et al. (2018)—a strong dependence on the network depth (which contradicts the current trend toward deep learning).

It turns out that our general theory applied to ℓ_1 -regularization can do away with these limitations. We define h as

$$h(\Omega) := \|\Omega\|_1 := \sum_{l=0}^L \sum_{k=1}^{p_{l+1}} \sum_{j=1}^{p_l} |U_{kj}^l|.$$

And to fix ideas, we impose two assumptions on the activation functions and the noise: First, we assume that the activation functions satisfy $\mathbf{f}^l(\mathbf{0}_{p_l}) = \mathbf{0}_{p_l}$ and are a_{Lip} -Lipschitz continuous for a constant $a_{\text{Lip}} \in [0, \infty)$ and with respect to the Euclidean norms on their input and output spaces:

$$\| \boldsymbol{f}^l(\boldsymbol{z}) - \boldsymbol{f}^l(\boldsymbol{z}') \|_2 \le a_{\text{Lip}} \| \boldsymbol{z} - \boldsymbol{z}' \|_2$$
 for all $\boldsymbol{z}, \boldsymbol{z}' \in \mathbb{R}^{p_l}$.

This assumption is satisfied by many popular activation functions: for example, the coordinates of the activation functions could be ReLU functions $x\mapsto 0 \vee x$ (Nair and Hinton, 2010), "leaky" versions of ReLU $x\mapsto (0\vee x)+(0\wedge cx)$ for $c\in (0,1)$, ELU functions $x\mapsto x\vee 0+c(e^{x\wedge 0}-1)$ for $c\in (0,1]$ (Clevert et al., 2015), hyperbolic tangent functions $x\mapsto (e^{2x}-1)/(e^{2x}+1)$, or SiL/Swish functions $x\mapsto x/(1+e^{-x})$ (Ramachandran et al., 2017; Elfwing et al., 2018) (throughout, we use the shorthands $r\vee s:=\max\{r,s\}$ and $r\wedge s:=\min\{r,s\}$ for $r,s\in\mathbb{R}$). Feasible Lipschitz constants for these examples are $a_{\rm Lip}=1.1$ for SiL/Swish and $a_{\rm Lip}=1$ for all other functions.

Second, we assume that the noise variables u_i are independent, centered, and uniformly sub-Gaussian for constants $K, \gamma \in (0, \infty)$ (van de Geer, 2000, Page 126; Vershynin, 2018, Section 2.5):

$$\max_{i \in \{1, \dots, n\}} K^2(\mathbb{E}e^{\frac{|u_i|^2}{K^2}} - 1) \le \gamma^2.$$

Using the shorthands $\mathcal{A}_1 := \{\Theta \in \mathcal{A} : \|\Theta\|_1 \le 1\}$ and $\|\boldsymbol{x}\|_n := \sqrt{\sum_{i=1}^n \|\boldsymbol{x}_i\|_2^2/n}$, we then find the following prediction guarantee for the estimator in (4):

Theorem 3 (Prediction guarantee for ℓ_1 -regularization) Assume that

$$\lambda \ge a \left(\frac{2a_{\text{Lip}}}{L}\right)^L \|\boldsymbol{x}\|_n \sqrt{L\log(2P)} \frac{\log(2n)}{\sqrt{n}},$$

where $a \in (0, \infty)$ is a constant that depends only on the sub-Gaussian parameters K and γ of the noise. Then, for n large enough,

$$\operatorname{err}^{2}(\hat{\kappa}_{h}g_{\widehat{\Omega}_{h}}) \leq \inf_{\substack{\kappa \in [0,\infty) \\ \Omega \in A_{1}}} \left\{ \operatorname{err}^{2}(\kappa g_{\Omega}) + 2\lambda\kappa \right\}$$

with probability at least 1 - 1/n.

The bound establishes essentially a $1/\sqrt{n}$ -decrease of the error in the sample size n, a mild logarithmic increase in the number of parameters P, and an almost exponential decrease in the number of hidden layers L if everything else is fixed (for example, the number of parameters P can depend on the number of hidden layers L). The dependencies on the sample size n and the number of parameters P match those of standard bounds in ℓ_1 -regularized

linear regression (Hebiri and Lederer, 2013). But one can argue that the logarithmic dependence on the number of parameters is even more crucial for neural networks: already a small network with L=10, $p_0=100$, and $p_1, \ldots, p_L=50$ involves $P=27\,550$ parameters, which highlights that neural networks typically involve very large P.

As an illustration, we can simplify Theorem 3 further in a parametric setting:

Corollary 4 (Parametric setting) Assume that

$$\lambda = a \left(\frac{2a_{\text{Lip}}}{L}\right)^{L} \|\boldsymbol{x}\|_{n} \sqrt{L \log(2P)} \frac{\log(2n)}{\sqrt{n}}$$

and that there exist parameters $(\kappa_*, \Omega_*) \in [0, \infty) \times \mathcal{A}_1$ such that $\kappa_* g_{\Omega_*}(\boldsymbol{x}_i) = g_*(\boldsymbol{x}_i)$ for all $i \in \{1, \ldots, n\}$. Then, for n large enough,

$$\operatorname{err}^{2}(\hat{\kappa}_{h}g_{\widehat{\Omega}_{h}}) \leq 2a\kappa_{*}\left(\frac{2a_{\operatorname{Lip}}}{L}\right)^{L} \|\boldsymbol{x}\|_{n} \sqrt{L\log(2P)} \frac{\log(2n)}{\sqrt{n}}$$

with probability at least 1 - 1/2n.

The above choice of h is not the only way to formulate ℓ_1 -constraints. Another way is, for example, $h(\Omega) := \max_{l \in \{0,\dots,L\}} \sum_{k=1}^{p_{l+1}} \sum_{j=1}^{p_l} |U^l_{kj}|$. The proofs and results remain virtually the same, and one may choose in practice whatever regularizer is more appropriate or easier to compute. And more broadly, our theories provide a general scheme for deriving prediction guarantees that could account for different regularizers (such as grouped versions of ℓ_1), activation functions (such as non-Lipschitz functions), and noise (such as heavy-tailed noise) through corresponding bounds for z_h .

The bounds in the in-sample-prediction error also entail bounds in the generalization error. We illustrate this here in the case of ℓ_1 -regularization. We assume that the input data are random and find:

Lemma 5 (Generalization guarantee for ℓ_1 -regularization) Assume that the conditions of Corollary 4 are satisfied and that the inputs x_1, \ldots, x_n are independent random vectors. Then, for n large enough,

$$\operatorname{risk}(\hat{\kappa}_h g_{\widehat{\Omega}_h}) \leq 1.01 \operatorname{risk}(\kappa_* g_{\Omega_*}) + a\kappa_* \left(\frac{2a_{\operatorname{Lip}}}{L}\right)^L \|\boldsymbol{x}\|_n \sqrt{L \log(2P)} \frac{\log(2n)}{\sqrt{n}} + a(\kappa_*)^2 \left(\frac{2a_{\operatorname{Lip}}}{L}\right)^{2L} \sqrt{L^2 \log(2P) \sum_{i=1}^n \|\boldsymbol{x}_i\|_2^4 \frac{\log(2n)}{n}}$$

with probability at least 1 - 1/n, where $a \in (0, \infty)$ is a constant that depends only on the sub-Gaussian parameters K and γ of the noise.

The result ensures that the estimator approaches the oracle risk at the above-discussed rate.

4. Further technical results

We now establish Lipschitz and complexity properties of neural networks. These results are used in our proofs but might also be of interest by themselves. To start, we define operator norms of the parameters and the weight matrices by

$$\|\Theta\|_2 := \sqrt{\sum_{l=0}^L \|W^l\|_2^2}$$
 and $\|W^l\|_2 := \sigma_{\max}(W^l)$,

respectively, where $\sigma_{\max}(W^l)$ is the largest singular value of W^l . We also define Frobenius norms of the parameter and weight matrices by

$$\|\!|\!|\!|\Theta \|\!|\!|_{\mathrm{F}} := \sqrt{\sum_{l=0}^L \|W^l\|_{\mathrm{F}}^2} \quad \text{ and } \quad \|W^l\|_{\mathrm{F}} := \sqrt{\sum_{k=1}^{p_{l+1}} \sum_{j=1}^{p_l} (W^l_{kj})^2}.$$

We then define the Euclidean norm of vectors by $\|\boldsymbol{v}\|_2 := \sqrt{\sum_{i=1}^d (v_i)^2}$ for $\boldsymbol{v} \in \mathbb{R}^d$. And finally, the prediction distance of any two networks g_{Θ} and g_{Γ} with $\Theta, \Gamma \in \mathcal{A}$ is

$$\|g_{\Theta} - g_{\Gamma}\|_n := \sqrt{\frac{1}{n} \sum_{i=1}^n (g_{\Theta}(\boldsymbol{x}_i) - g_{\Gamma}(\boldsymbol{x}_i))^2},$$

and similarly,

$$||g_{\Theta}||_n := \sqrt{\frac{1}{n} \sum_{i=1}^n (g_{\Theta}(x_i))^2}.$$

The Lipschitz property of neural networks is then as follows.

Proposition 6 (Lipschitz property of neural networks) Assume that the activation functions $\mathbf{f}^l: \mathbb{R}^{p_l} \to \mathbb{R}^{p_l}$ are a_{Lip} -Lipschitz with respect to the Euclidean norms on their input and output spaces. Then, it holds for every $\mathbf{x} \in \mathbb{R}^d$ and $\Theta = (W^L, \dots, W^0), \Gamma = (V^L, \dots, V^0) \in \mathcal{A}$ that

$$|g_{\Theta}(\boldsymbol{x}) - g_{\Gamma}(\boldsymbol{x})| \le c_{\text{Lip}}(\boldsymbol{x}) \|\Theta - \Gamma\|_{\text{F}}$$

with $c_{\text{Lip}}(\boldsymbol{x}) := 2(a_{\text{Lip}})^L \sqrt{L} \|\boldsymbol{x}\|_2 \max_{l \in \{0,\dots,L\}} \prod_{j \in \{0,\dots,L\}, j \neq l} (\|W^j\|_2 \vee \|V^j\|_2)$.

And similarly, it holds that

$$\|g_{\Theta} - g_{\Gamma}\|_n \le \overline{c}_{\text{Lip}} \|\Theta - \Gamma\|_{\text{F}}$$

with
$$\overline{c}_{\text{Lip}} := 2(a_{\text{Lip}})^L \sqrt{L} \| \boldsymbol{x} \|_n \max_{l \in \{0, \dots, L\}} \prod_{j \in \{0, \dots, L\}, j \neq l} (\| W^j \|_2 \vee \| V^j \|_2).$$

This property is helpful in bounding the quantiles of the empirical processes. In particular, it can be used to show that the networks are Lipschitz and bounded over typical sets that originate from our regularization scheme. Such a result is given in the following lemma.

Lemma 7 (Lipschitz and boundedness on A_1) *Under the conditions of Proposition 6, it holds for every* $\Omega, \Gamma \in A_1$ *that*

$$||g_{\Omega} - g_{\Gamma}||_n \le c_{\text{Lip}1} |||\Omega - \Gamma|||_{\text{F}}$$

and that

$$||g_{\Omega}||_n \le c_{\text{Lip}1}$$

with
$$c_{\text{Lip1}} := 2(2a_{\text{Lip}}/L)^L \sqrt{L} \|\boldsymbol{x}\|_n$$
.

To derive the complexity properties, we denote covering numbers by $N(r, \mathcal{T}, \|\cdot\|)$ and entropy by $H(r, \mathcal{T}, \|\cdot\|) := \log N(r, \mathcal{T}, \|\cdot\|)$, where $r \in (0, \infty)$, \mathcal{T} is a set, and $\|\cdot\|$ is a (pseudo-)norm on an ambient space of \mathcal{T} (van der Vaart and Wellner, 1996, Page 98). We use these numbers to define a complexity measure for a collection of networks $\mathcal{G}_h := \{g_{\Omega} : \Omega \in \mathcal{A}_h\}$ by

$$J(\delta, \sigma, \mathcal{A}_h) := \int_{\delta/(8\sigma)}^{\infty} H^{1/2}(r, \mathcal{G}_h, \|\cdot\|_n) dr$$
 (8)

for $\delta, \sigma \in (0, \infty)$ (van de Geer, 2000, Section 3.3). Almost in line with standard terminology, we call this complexity measure the *Dudley integral* (Vershynin, 2018, Section 8.1). We can bound the complexity of the class of neural networks $\mathcal{G}_1 := \{g_{\Omega} : \Omega \in \mathcal{A}_1\}$ that have parameters in the constraint set \mathcal{A}_1 as follows:

Proposition 8 (Complexity properties of neural networks) Assume that the activation functions $\mathbf{f}^l: \mathbb{R}^{p_l} \to \mathbb{R}^{p_l}$ are a_{Lip} -Lipschitz continuous with respect to the Euclidean norms on their input and output spaces. Then, it holds for every $r \in (0, \infty)$ and $\delta, \sigma \in (0, \infty)$ that satisfy $\delta \leq 8\sigma c_{\text{Lip1}}$ that

$$H(r, \mathcal{G}_1, \|\cdot\|_n) \le \frac{6(c_{\text{Lip1}})^2}{r^2} \log\left(\frac{ePr^2}{(c_{\text{Lip1}})^2} \vee 2e\right)$$

and

$$J(\delta, \sigma, \mathcal{A}_1) \le \frac{5c_{\text{Lip1}}}{2} \sqrt{\log(eP \vee 2e)} \log\left(\frac{8\sigma c_{\text{Lip1}}}{\delta}\right),$$

where we recall that $c_{\text{Lip1}} = 2(2a_{\text{Lip}}/L)^L \sqrt{L} \|\boldsymbol{x}\|_n$.

5. Additional materials and proofs

We now state some auxiliary results and then prove our claims.

5.1 Additional materials

We first provide three auxiliary results that we use in our proofs. We start with a slightly adapted version of van de Geer (2000, Corollary 8.3):

Lemma 9 (Suprema over Gaussian processes) Consider a set $\mathcal{A}' \subset \mathcal{A}$ and a constant $R \in [0,\infty)$ such that $\sup_{\Theta \in \mathcal{A}'} \|g_{\Theta}\|_n \leq R$. Assume that the noise random variables u_1, \ldots, u_n are independent, centered, and uniformly sub-Gaussian as specified on

Page 7. Then, there is a constant $a_{\text{sub}} \in (0, \infty)$ that depends only on K and γ such that for all $\delta, \sigma \in (0, \infty)$ that satisfy $\delta < \sigma R$ and

$$\sqrt{n}\delta \geq a_{\text{sub}}(J(\delta, \sigma, \mathcal{A}') \vee R),$$

it holds that

$$\mathbb{P}\left(\left\{\sup_{\Theta\in\mathcal{A}'}\left|\frac{1}{n}\sum_{i=1}^{n}g_{\Theta}(\boldsymbol{x}_{i})u_{i}\right|\geq\delta\right\}\cap\left\{\frac{1}{n}\sum_{i=1}^{n}\left(u_{i}\right)^{2}\leq\sigma^{2}\right\}\right)\leq a_{\mathrm{sub}}e^{-\frac{n\delta^{2}}{(a_{\mathrm{sub}}R)^{2}}}.$$

This result is used to bound $\lambda_{\ell_1,t}$.

We then turn to a Lipschitz property of metric entropy:

Lemma 10 (Entropy transformation for Lipschitz functions) Consider sets $\mathcal{A}' \subset \mathcal{A}$ and $\mathcal{G}' := \{g_{\Theta} : \Theta \in \mathcal{A}'\}$ and a metric $\rho : \mathcal{A}' \times \mathcal{A}' \to \mathbb{R}$. Assume that $|g_{\Theta}(\mathbf{x}) - g_{\Gamma}(\mathbf{x})| \leq k_{\text{Lip}}(\mathbf{x})\rho(\Theta,\Gamma)$ for every $\Theta,\Gamma \in \mathcal{A}'$ and $\mathbf{x} \in \mathbb{R}^d$ and a fixed function $k_{\text{Lip}} : \mathbb{R}^d \to [0,\infty)$. Then,

$$H(r, \mathcal{G}', \|\cdot\|_n) \le H\left(\frac{r}{\|k_{\text{Lip}}\|_n}, \mathcal{A}', \rho\right) \quad \text{for all } r \in (0, \infty),$$

where $||k_{\text{Lip}}||_n := \sqrt{\sum_{i=1}^n (k_{\text{Lip}}(x_i))^2/n}$.

We use the convention $a/0 = \infty$ for $a \in (0, \infty)$. The result allows us to bound entropies on the parameter spaces instead of the network spaces. We prove the lemma in the following section.

We conclude with a deviation inequality for the noise.

Lemma 11 (Deviation of sub-Gaussian noise) Assume that the noise variables u_1, \ldots, u_n are independent, centered, and uniformly sub-Gaussian as stipulated on Page 7. Then,

$$\mathbb{P}\left(\frac{1}{n}\sum_{i=1}^{n} (u_i)^2 \ge v\right) \le e^{-\frac{nv}{12K^2}} \qquad \text{for all } v \in [2\gamma^2, \infty).$$

This deviation inequality is tailored to our needs in the proof of Theorem 3.

5.2 Proofs

We provide here the proofs of our claims.

5.2.1 Proof of Proposition 1

Proof We prove the two directions in order.

Direction 1: Fix a $\Theta = (W^L, \dots, W^0) \in \mathcal{A}$. Assume first that $W^l = \mathbf{0}_{p_{l+1} \times p_l}$ for an $l \in \{0, \dots, L\}$. In view of the definition of neural networks in (2) and the assumed nonnegative homogeneity of the activation functions, it then holds that

$$g_{\Theta}(\boldsymbol{x}) = W^{L} \boldsymbol{f}^{L}(\dots \boldsymbol{0}_{p_{l+1} \times p_{l}} \boldsymbol{f}^{l}(\dots W^{1} \boldsymbol{f}^{1}(W^{0} \boldsymbol{x})))$$
$$= W^{L} \boldsymbol{f}^{L}(\dots 0 \cdot \boldsymbol{0}_{p_{l+1} \times p_{l}} \boldsymbol{f}^{l}(\dots W^{1} \boldsymbol{f}^{1}(W^{0} \boldsymbol{x}))) = 0$$

for all $x \in \mathbb{R}^d$. Therefore, $\kappa := 0$ and all $\Omega \in \mathcal{A}_h$ satisfy $\kappa g_{\Omega} = g_{\Theta}$, as desired.

Assume now that $W^l \neq \mathbf{0}_{p_{l+1} \times p_l}$ for all $l \in \{0, \dots, L\}$. Define $\kappa := (h(\Theta))^{(L+1)/k}$ and $\Omega := \Theta/\kappa^{1/(L+1)} = (W^L/\kappa^{1/(L+1)}, \dots, W^0/\kappa^{1/(L+1)})$ if $\kappa^{1/(L+1)} \neq 0$. We need to show that $1. \kappa \in (0, \infty)$ and $\Omega \in \mathcal{A}_h$ and $2. g_{\Theta} = \kappa g_{\Omega}$.

Since h is assumed positive definite, it holds that $h(\Theta) \in (0, \infty)$ and, therefore, $\kappa \in (0, \infty)$. The fact that $\kappa > 0$ also ensures that the parameter Ω is well-defined, and we can invoke the assumed nonnegative homogeneity of degree k of h to derive

$$h(\Omega) = h(\Theta/\kappa^{1/(L+1)}) = (\kappa^{-1/(L+1)})^k h(\Theta) = ((h(\Theta))^{(L+1)/k})^{-k/(L+1)} h(\Theta) = 1.$$

This verifies 1.

We can then invoke the assumed nonnegative homogeneity of degree 1 of the activation functions to derive for all $x \in \mathbb{R}^d$ that

$$\kappa g_{\Omega}(\boldsymbol{x}) = \kappa \frac{W^L}{\kappa^{1/(L+1)}} \boldsymbol{f}^L \left(\dots \frac{W^1}{\kappa^{1/(L+1)}} \boldsymbol{f}^1 \left(\frac{W^0}{\kappa^{1/(L+1)}} \boldsymbol{x} \right) \right) \\
= \kappa \frac{W^L}{\kappa^{1/(L+1)}} \boldsymbol{f}^L \left(\dots \frac{W^1}{\left(\kappa^{1/(L+1)} \right)^2} \boldsymbol{f}^1 (W^0 \boldsymbol{x}) \right) \\
= \dots \\
= \frac{\kappa}{\left(\kappa^{1/(L+1)} \right)^{(L+1)}} W^L \boldsymbol{f}^L \left(\dots W^1 \boldsymbol{f}^1 (W^0 \boldsymbol{x}) \right) \\
= W^L \boldsymbol{f}^L \left(\dots W^1 \boldsymbol{f}^1 (W^0 \boldsymbol{x}) \right) \\
= g_{\Theta}(\boldsymbol{x}).$$

This verifies 2.

Direction 2: Fix a $\kappa \in [0, \infty)$ and a $\Omega = (U^L, \dots, U^0) \in \mathcal{A}_h$, and define $\Theta := \kappa^{1/(L+1)}\Omega = (\kappa^{1/(L+1)}U^L, \dots, \kappa^{1/(L+1)}U^0)$. We then invoke the assumed nonnegative homogeneity of degree 1 of the activation functions to derive for all $\boldsymbol{x} \in \mathbb{R}^d$ that

$$\begin{split} g_{\Theta}(\boldsymbol{x}) &= \kappa^{1/(L+1)} U^L \boldsymbol{f}^L \Big(\dots \kappa^{1/(L+1)} U^1 \boldsymbol{f}^1 \big(\kappa^{1/(L+1)} U^0 \boldsymbol{x} \big) \Big) \\ &= \kappa^{1/(L+1)} U^L \boldsymbol{f}^L \Big(\dots \big(\kappa^{1/(L+1)} \big)^2 U^1 \boldsymbol{f}^1 (U^0 \boldsymbol{x}) \Big) \\ &= \dots \\ &= \big(\kappa^{1/(L+1)} \big)^{(L+1)} U^L \boldsymbol{f}^L \big(\dots U^1 \boldsymbol{f}^1 (U^0 \boldsymbol{x}) \big) \\ &= \kappa U^L \boldsymbol{f}^L \big(\dots U^1 \boldsymbol{f}^1 (U^0 \boldsymbol{x}) \big) \\ &= \kappa g_{\Omega}(\boldsymbol{x}), \end{split}$$

as desired.

5.2.2 Proof of Theorem 2

Proof Since $(\hat{\kappa}_h, \widehat{\Omega}_h)$ is a minimizer of the objective function in (4), we find for every $\kappa \in [0, \infty)$ and $\Omega \in \mathcal{A}_h$ that

$$\frac{1}{n}\sum_{i=1}^{n} (y_i - \hat{\kappa}_h g_{\widehat{\Omega}_h}(\boldsymbol{x}_i))^2 + \lambda \hat{\kappa}_h \leq \frac{1}{n}\sum_{i=1}^{n} (y_i - \kappa g_{\Omega}(\boldsymbol{x}_i))^2 + \lambda \kappa.$$

Replacing the y_i 's via the model in (1) then yields

$$\frac{1}{n}\sum_{i=1}^{n} \left(g_*(\boldsymbol{x}_i) + u_i - \hat{\kappa}_h g_{\widehat{\Omega}_h}(\boldsymbol{x}_i)\right)^2 + \lambda \hat{\kappa}_h \leq \frac{1}{n}\sum_{i=1}^{n} \left(g_*(\boldsymbol{x}_i) + u_i - \kappa g_{\Omega}(\boldsymbol{x}_i)\right)^2 + \lambda \kappa.$$

Expanding the squared-terms and rearranging terms, we get

$$\frac{1}{n} \sum_{i=1}^{n} (\hat{\kappa}_h g_{\widehat{\Omega}_h}(\boldsymbol{x}_i) - g_*(\boldsymbol{x}_i))^2 \leq \frac{1}{n} \sum_{i=1}^{n} (\kappa g_{\Omega}(\boldsymbol{x}_i) - g_*(\boldsymbol{x}_i))^2 \\
+ \frac{2}{n} \sum_{i=1}^{n} \hat{\kappa}_h g_{\widehat{\Omega}_h}(\boldsymbol{x}_i) u_i - \frac{2}{n} \sum_{i=1}^{n} \kappa g_{\Omega}(\boldsymbol{x}_i) u_i + \lambda \kappa - \lambda \hat{\kappa}_h.$$

We can then bound the sums on the second line to obtain

$$\frac{1}{n} \sum_{i=1}^{n} (\hat{\kappa}_h g_{\widehat{\Omega}_h}(\boldsymbol{x}_i) - g_*(\boldsymbol{x}_i))^2 \leq \frac{1}{n} \sum_{i=1}^{n} (\kappa g_{\Omega}(\boldsymbol{x}_i) - g_*(\boldsymbol{x}_i))^2
+ \hat{\kappa}_h \sup_{\Omega \in \mathcal{A}_h} \left| \frac{2}{n} \sum_{i=1}^{n} g_{\Omega}(\boldsymbol{x}_i) u_i \right| + \kappa \sup_{\Omega \in \mathcal{A}_h} \left| \frac{2}{n} \sum_{i=1}^{n} g_{\Omega}(\boldsymbol{x}_i) u_i \right| + \lambda \kappa - \lambda \hat{\kappa}_h.$$

The second line can then be consolidated by virtue of the assumption on λ : with probability at least 1-t, it holds that

$$\frac{1}{n}\sum_{i=1}^{n}\left(\hat{\kappa}_{h}g_{\widehat{\Omega}_{h}}(\boldsymbol{x}_{i})-g_{*}(\boldsymbol{x}_{i})\right)^{2}\leq\frac{1}{n}\sum_{i=1}^{n}\left(\kappa g_{\Omega}(\boldsymbol{x}_{i})-g_{*}(\boldsymbol{x}_{i})\right)^{2}+2\lambda\kappa.$$

Taking the infimum over $\kappa \in [0, \infty)$ and $\Omega \in \mathcal{A}_h$ and invoking the definition of $\operatorname{err}^2(\cdot)$ on Page 5 gives the desired result.

5.2.3 Proof of Theorem 3

Proof The idea of the proof is to bound the effective noise and then apply Theorem 2. If $c_{\text{Lip1}} = 0$, then $g_{\Omega}(\boldsymbol{x}_i) = 0$ for all $\Omega \in \mathcal{A}_1$ and $i \in \{1, ..., n\}$ in view of Lemma 7. Hence,

$$\mathbb{P}\left(\sup_{\Omega\in\mathcal{A}_1}\left|\frac{2}{n}\sum_{i=1}^n g_{\Omega}(\boldsymbol{x}_i)u_i\right|\leq\delta\right)=\mathbb{P}(0\leq\delta)=1\quad\text{for all }\delta\in(0,\infty),$$

which makes a proof straightforward. We can thus assume $c_{\text{Lip1}} > 0$ in the following.

Our first step is to apply Lemma 9 about suprema of empirical processes with $\mathcal{A}' := \mathcal{A}_1$. For this, we need to find 1. a constant $R \in [0, \infty)$ that satisfies $\sup_{\Omega \in \mathcal{A}_1} \|g_{\Omega}\|_n \leq R$ and 2. suitable $\delta, \sigma \in (0, \infty)$ that satisfy $\delta < \sigma R$ and

$$\sqrt{n} \ge \frac{a_{\text{sub}}}{\delta} (J(\delta, \sigma, \mathcal{A}_1) \vee R).$$

Condition 1 is verified by $R := c_{\text{Lip1}}$ according to Lemma 7.

For Condition 2, we define $\delta \equiv \delta(n, P, a_{\text{sub}}, c_{\text{Lip1}}) := 10 a_{\text{sub}} c_{\text{Lip1}} \sqrt{\log(2P)/n} \log(2n) \in (0, \infty)$ and $\sigma := (2\delta/c_{\text{Lip1}}) \vee (\sqrt{2}\gamma)$. Then, $\delta < \sigma R$ by the definitions of δ, σ, R . Moreover, Proposition 8, the definitions of δ and R, and

$$\frac{8\sigma c_{\text{Lip1}}}{\delta} = 16 \lor \frac{8\sqrt{2}\gamma c_{\text{Lip1}}}{10a_{\text{sub}}c_{\text{Lip1}}\sqrt{\log(2P)/n}\log(2n)} \le 16 \lor \frac{2\gamma\sqrt{n}}{a_{\text{sub}}} \le 16\sqrt{n}$$

(we assume that $a_{\text{sub}} \geq \gamma/8$ without loss of generality and use that $\log(2) \geq 0.69$) yield

$$\frac{a_{\text{sub}}}{\delta} \left(J(\delta, \sigma, \mathcal{A}_{1}) \vee c_{\text{Lip1}} \right) \\
\leq \frac{a_{\text{sub}}}{\delta} \left(\frac{5c_{\text{Lip1}}}{2} \sqrt{\log(eP \vee 2e)} \log\left(\frac{8\sigma c_{\text{Lip1}}}{\delta}\right) \vee c_{\text{Lip1}} \right) \\
\leq \frac{\sqrt{n}a_{\text{sub}}}{10a_{\text{sub}}c_{\text{Lip1}} \sqrt{\log(2P)} \log(2n)} \left(\frac{5c_{\text{Lip1}}}{2} \sqrt{\log(eP \vee 2e)} \log(16\sqrt{n}) \vee c_{\text{Lip1}} \right) \\
\leq \frac{\sqrt{n}a_{\text{sub}}}{10a_{\text{sub}}c_{\text{Lip1}} \sqrt{\log(2P)} \log(2n)} \left(10c_{\text{Lip1}} \sqrt{\log(2P)} \log(2n) \vee c_{\text{Lip1}} \right) \\
= \sqrt{n},$$

which verifies Condition 2.

We can thus apply Lemma 9 with the above-specified parameters to obtain that

$$\mathbb{P}\left(\left\{\sup_{\Omega\in\mathcal{A}_1}\left|\frac{1}{n}\sum_{i=1}^n g_{\Omega}(\boldsymbol{x}_i)u_i\right|\geq\delta\right\}\cap\left\{\frac{1}{n}\sum_{i=1}^n (u_i)^2\leq\sigma^2\right\}\right)\leq a_{\mathrm{sub}}e^{-\frac{n\delta^2}{(a_{\mathrm{sub}}c_{\mathrm{Lip}1})^2}}.$$

We use that $\mathbb{P}(\mathcal{C} \cap \mathcal{D}) \leq \alpha$ implies $\mathbb{P}(\mathcal{C}^{\complement} \cup \mathcal{D}^{\complement}) \geq 1 - \alpha$ and that $\mathbb{P}(\mathcal{C}^{\complement}) \geq \mathbb{P}(\mathcal{C}^{\complement} \cup \mathcal{D}^{\complement}) - \mathbb{P}(\mathcal{D}^{\complement})$ to rewrite this inequality as

$$\mathbb{P}\left(\sup_{\Omega \in \mathcal{A}_{1}} \left| \frac{1}{n} \sum_{i=1}^{n} g_{\Omega}(\boldsymbol{x}_{i}) u_{i} \right| \leq \delta \right) \geq \mathbb{P}\left(\sup_{\Omega \in \mathcal{A}_{1}} \left| \frac{1}{n} \sum_{i=1}^{n} g_{\Omega}(\boldsymbol{x}_{i}) u_{i} \right| < \delta \right) \\
\geq 1 - a_{\text{sub}} e^{-\frac{n\delta^{2}}{(a_{\text{sub}} c_{\text{Lip1}})^{2}}} - \mathbb{P}\left(\frac{1}{n} \sum_{i=1}^{n} (u_{i})^{2} > \sigma^{2}\right).$$

Since $\sigma^2 \geq 2\gamma^2$ by the definition of σ , Lemma 11 with $v := \sigma^2$ allows us to bound the last term according to

$$\mathbb{P}\left(\frac{1}{n}\sum_{i=1}^{n}(u_{i})^{2} > \sigma^{2}\right) \leq \mathbb{P}\left(\frac{1}{n}\sum_{i=1}^{n}(u_{i})^{2} \geq \sigma^{2}\right) \leq e^{-\frac{n\sigma^{2}}{12K^{2}}}.$$

Combining this inequality with the previous one yields

$$\mathbb{P}\left(\sup_{\Omega\in\mathcal{A}_1}\left|\frac{1}{n}\sum_{i=1}^n g_{\Omega}(\boldsymbol{x}_i)u_i\right| \leq \delta\right) \geq 1 - a_{\text{sub}}e^{-\frac{n\delta^2}{(a_{\text{sub}}c_{\text{Lip1}})^2}} - e^{-\frac{n\sigma^2}{12K^2}}.$$

By the definitions of δ and σ , and assuming that n is large enough (depending on γ, K), we find that

$$a_{\text{sub}}e^{-\frac{n\delta^{2}}{(a_{\text{sub}}c_{\text{Lip1}})^{2}}} + e^{-\frac{n\sigma^{2}}{12K^{2}}}$$

$$\leq a_{\text{sub}}e^{-10^{2}\log(2P)(\log(2n))^{2}} + e^{-\frac{4\cdot10^{2}(a_{\text{sub}})^{2}\log(2P)(\log(2n))^{2}}{12K^{2}}} + e^{-\frac{n\gamma^{2}}{6K^{2}}}$$

$$\leq e^{-\log(4n)} + e^{-\log(4n)} + e^{-\frac{n\gamma^{2}}{6K^{2}}}$$

$$\leq \frac{1}{n},$$

that is.

$$\mathbb{P}\left(\sup_{\Omega \in \mathcal{A}_1} \left| \frac{1}{n} \sum_{i=1}^n g_{\Omega}(\boldsymbol{x}_i) u_i \right| \le \delta \right) \ge 1 - \frac{1}{n}.$$

In other words, $\lambda_{h,t} \leq 2\delta$ for t = 1/n.

The claim then follows directly from Theorem 2 with $\lambda \geq 2\delta = 20a_{\rm sub}c_{\rm Lip1}\sqrt{\log(2P)/n}$ $\log(2n), c_{\rm Lip1} = 2(2a_{\rm Lip}/L)^L\sqrt{L}\|\boldsymbol{x}\|_n$ (see Lemma 7), and $a := 40a_{\rm sub}$.

5.2.4 Proof of Lemma 5

Proof The idea of the proof is to disentangle the generalization error into the prediction error and additional terms. We then bound the prediction error by using Corollary 4 and the additional terms by using empirical-process theory.

We 1. replace the output y by using the model in (1), 2. use monotone convergence together with the fact that $(r+s)^2 \leq br^2 + 1.01s^2$ for a numerical constant $b \in (0, \infty)$, 3. use the linearity of expectations, 4. add a zero-valued term, and 5. take an absolute value to get

$$\mathbb{E}_{(\boldsymbol{x},y)} \Big[\big(\hat{\kappa}_h g_{\widehat{\Omega}_h}(\boldsymbol{x}) - y \big)^2 \Big] \\
= \mathbb{E}_{(\boldsymbol{x},y)} \Big[\big(\hat{\kappa}_h g_{\widehat{\Omega}_h}(\boldsymbol{x}) - g_*(\boldsymbol{x}) - u \big)^2 \Big] \\
\leq \mathbb{E}_{(\boldsymbol{x},y)} \Big[b \big(\hat{\kappa}_h g_{\widehat{\Omega}_h}(\boldsymbol{x}) - g_*(\boldsymbol{x}) \big)^2 + 1.01 u^2 \Big] \\
= b \mathbb{E}_{(\boldsymbol{x},y)} \Big[\big(\hat{\kappa}_h g_{\widehat{\Omega}_h}(\boldsymbol{x}) - g_*(\boldsymbol{x}) \big)^2 \Big] + 1.01 \mathbb{E}_{(\boldsymbol{x},y)} [u^2] \\
= \frac{b}{n} \sum_{i=1}^{n} \big(\hat{\kappa}_h g_{\widehat{\Omega}_h}(\boldsymbol{x}_i) - g_*(\boldsymbol{x}_i) \big)^2 + 1.01 \mathbb{E}_{(\boldsymbol{x},y)} [u^2] \\
- \frac{b}{n} \sum_{i=1}^{n} \big(\hat{\kappa}_h g_{\widehat{\Omega}_h}(\boldsymbol{x}_i) - g_*(\boldsymbol{x}_i) \big)^2 + b \mathbb{E}_{(\boldsymbol{x},y)} \Big[\big(\hat{\kappa}_h g_{\widehat{\Omega}_h}(\boldsymbol{x}) - g_*(\boldsymbol{x}) \big)^2 \Big]$$

$$\leq \frac{b}{n} \sum_{i=1}^{n} (\hat{\kappa}_h g_{\widehat{\Omega}_h}(\boldsymbol{x}_i) - g_*(\boldsymbol{x}_i))^2 + 1.01 \mathbb{E}_{(\boldsymbol{x},y)}[u^2] \\
+ \left| \frac{b}{n} \sum_{i=1}^{n} (\hat{\kappa}_h g_{\widehat{\Omega}_h}(\boldsymbol{x}_i) - g_*(\boldsymbol{x}_i))^2 - b \mathbb{E}_{(\boldsymbol{x},y)} \left[(\hat{\kappa}_h g_{\widehat{\Omega}_h}(\boldsymbol{x}) - g_*(\boldsymbol{x}))^2 \right] \right|.$$

The remaining challenge is now to bound the last term of this display. We devise an approach based on symmetrization for probabilities (van de Geer, 2016, Lemma 16.1). We first use 1. the fact that $\widehat{\Omega}_h \in \mathcal{A}_1$ and 2. the independence assumption on the data to get

$$\left| \frac{b}{n} \sum_{i=1}^{n} \left(\hat{\kappa}_{h} g_{\widehat{\Omega}_{h}}(\boldsymbol{x}_{i}) - g_{*}(\boldsymbol{x}_{i}) \right)^{2} - b \mathbb{E}_{(\boldsymbol{x},y)} \left[\left(\hat{\kappa}_{h} g_{\widehat{\Omega}_{h}}(\boldsymbol{x}) - g_{*}(\boldsymbol{x}) \right)^{2} \right] \right| \\
\leq \sup_{\Omega \in \mathcal{A}_{1}} \left| \frac{b}{n} \sum_{i=1}^{n} \left(\hat{\kappa}_{h} g_{\Omega}(\boldsymbol{x}_{i}) - g_{*}(\boldsymbol{x}_{i}) \right)^{2} - b \mathbb{E}_{(\boldsymbol{x},y)} \left[\left(\hat{\kappa}_{h} g_{\Omega}(\boldsymbol{x}) - g_{*}(\boldsymbol{x}) \right)^{2} \right] \right| \\
= \sup_{\Omega \in \mathcal{A}_{1}} \left| \frac{b}{n} \sum_{i=1}^{n} \left(\left(\hat{\kappa}_{h} g_{\Omega}(\boldsymbol{x}_{i}) - g_{*}(\boldsymbol{x}_{i}) \right)^{2} - \mathbb{E}_{(\boldsymbol{x}_{1},y_{1}),\dots,(\boldsymbol{x}_{n},y_{n})} \left[\left(\hat{\kappa}_{h} g_{\Omega}(\boldsymbol{x}_{i}) - g_{*}(\boldsymbol{x}_{i}) \right)^{2} \right] \right) \right|.$$

We now prepare the application of van de Geer (2016, Lemma 16.1). We use 1. the definition of $(R_A)^2$, which is called " R^2 " in van de Geer (2016, Lemma 16.1), 2. the fact that $(r+s)^4 \leq 8r^4 + 8s^4$ and dominated convergence, 3. the fact that $\kappa_* g_{\Omega_*}(\boldsymbol{x}_i) = g_*(\boldsymbol{x}_i)$ by assumption and the linearity of finite sums and expectations, 4. again the linearity of finite sums and expectations, the fact that $\Omega_* \in \mathcal{A}_1$, and dominated convergence, 5. the fact that $\sum_{i=1}^n (g_{\Omega}(\boldsymbol{x}_i))^4/n \leq 16(2a_{\text{Lip}}/L)^{4L}L^2\sum_{i=1}^n \|\boldsymbol{x}_i\|_2^4/n$ and analogs of Proposition 6 and Lemma 7, 6. $\hat{\kappa}_h \leq 3\kappa_*$, which can be proved easily along the lines of the proof of Theorem 2 (just double the tuning parameter), and once more the linearity of integrals, and 7. a simplification with a numerical constant $\tilde{a} \in (0, \infty)$, which may change from line to line in the proof, to obtain

$$(R_{\mathcal{A}})^{2} = \sup_{\Omega \in \mathcal{A}_{1}} \frac{1}{n} \sum_{i=1}^{n} \mathbb{E}_{(\boldsymbol{x}_{i}, y_{i})} \left[\left(\hat{\kappa}_{h} g_{\Omega}(\boldsymbol{x}_{i}) - g_{*}(\boldsymbol{x}_{i}) \right)^{4} \right]$$

$$\leq \sup_{\Omega \in \mathcal{A}_{1}} \frac{1}{n} \sum_{i=1}^{n} \mathbb{E}_{(\boldsymbol{x}_{i}, y_{i})} \left[8 \left(\hat{\kappa}_{h} g_{\Omega}(\boldsymbol{x}_{i}) \right)^{4} + 8 \left(g_{*}(\boldsymbol{x}_{i}) \right)^{4} \right]$$

$$= 8 \left(\hat{\kappa}_{h} \right)^{4} \sup_{\Omega \in \mathcal{A}_{1}} \frac{1}{n} \sum_{i=1}^{n} \mathbb{E}_{(\boldsymbol{x}_{i}, y_{i})} \left[\left(g_{\Omega}(\boldsymbol{x}_{i}) \right)^{4} \right] + \frac{8 \left(\kappa_{*} \right)^{4}}{n} \sum_{i=1}^{n} \mathbb{E}_{(\boldsymbol{x}_{i}, y_{i})} \left[\left(g_{\Omega_{*}}(\boldsymbol{x}_{i}) \right)^{4} \right]$$

$$\leq 8 \left(\left(\hat{\kappa}_{h} \right)^{4} + \left(\kappa_{*} \right)^{4} \right) \mathbb{E}_{(\boldsymbol{x}_{1}, y_{1}), \dots, (\boldsymbol{x}_{n}, y_{n})} \left[\sup_{\Omega \in \mathcal{A}_{1}} \frac{1}{n} \sum_{i=1}^{n} \left(g_{\Omega}(\boldsymbol{x}_{i}) \right)^{4} \right]$$

$$\leq 8 \left(\left(\hat{\kappa}_{h} \right)^{4} + \left(\kappa_{*} \right)^{4} \right) \mathbb{E}_{(\boldsymbol{x}_{1}, y_{1}), \dots, (\boldsymbol{x}_{n}, y_{n})} \left[16 \left(\frac{2a_{\text{Lip}}}{L} \right)^{4L} \frac{L^{2}}{n} \sum_{i=1}^{n} \|\boldsymbol{x}_{i}\|_{2}^{4} \right]$$

$$\leq 128 \left(\left(3\kappa_{*} \right)^{4} + \left(\kappa_{*} \right)^{4} \right) \left(\frac{2a_{\text{Lip}}}{L} \right)^{4L} L^{2} \mathbb{E}_{(\boldsymbol{x}_{1}, y_{1}), \dots, (\boldsymbol{x}_{n}, y_{n})} \left[\frac{1}{n} \sum_{i=1}^{n} \|\boldsymbol{x}_{i}\|_{2}^{4} \right]$$

$$= \tilde{a}(\kappa_*)^4 \left(\frac{2a_{\text{Lip}}}{L}\right)^{4L} L^2 \mathbb{E}_{(\boldsymbol{x}_1, y_1), \dots, (\boldsymbol{x}_n, y_n)} \left[\frac{1}{n} \sum_{i=1}^n \|\boldsymbol{x}_i\|_2^4\right].$$

Then, we use 1. the penultimate inequality and a rearrangement, 2. the symmetrization bound of van de Geer (2016, Lemma 16.1) with an i.i.d. Rademacher variables $\zeta_1, \ldots, \zeta_n \in \{\pm 1\}$ that are independent of the data, 3. multiplying by a one-valued factor, 4 the contraction principle (Ledoux and Talagrand, 1991, Theorem 4.4) with $\alpha_i = (\hat{\kappa}_h g_{\Omega}(\boldsymbol{x}_i) - g_*(\boldsymbol{x}_i))^2/(2(\hat{\kappa}_h g_{\Omega}(\boldsymbol{x}_i))^2 + 2(g_*(\boldsymbol{x}_i))^2) \in [0,1]$, 5. the fact that $\mathbb{P}(r+s>w) \leq \mathbb{P}(r>w/2) + \mathbb{P}(s>w/2)$, 6. the linearity of finite sums, $\kappa_* g_{\Omega_*}(\boldsymbol{x}_i) = g_*(\boldsymbol{x}_i)$, and the fact that $\Omega_* \in \mathcal{A}_1$, and 7. $\hat{\kappa}_h \leq 3\kappa_*$ to get for all $t \in [4,\infty)$

$$\begin{split} & \mathbb{P}\left(\left|\frac{b}{n}\sum_{i=1}^{n}\left(\hat{\kappa}_{h}g_{\widehat{\Omega}_{h}}(\boldsymbol{x}_{i})-g_{*}(\boldsymbol{x}_{i})\right)^{2}-b\mathbb{E}_{(\boldsymbol{x},y)}\left[\left(\hat{\kappa}_{h}g_{\widehat{\Omega}_{h}}(\boldsymbol{x})-g_{*}(\boldsymbol{x})\right)^{2}\right]\right|>4bR_{\mathcal{A}}\sqrt{\frac{2t}{n}}\right) \\ & \leq \mathbb{P}\left(\sup_{\Omega\in\mathcal{A}_{1}}\left|\frac{1}{n}\sum_{i=1}^{n}\left(\left(\hat{\kappa}_{h}g_{\Omega}(\boldsymbol{x}_{i})-g_{*}(\boldsymbol{x}_{i})\right)^{2}-\mathbb{E}_{(\boldsymbol{x}_{1},y_{1}),\dots,(\boldsymbol{x}_{n},y_{n})}\left[\left(\hat{\kappa}_{h}g_{\Omega}(\boldsymbol{x}_{i})-g_{*}(\boldsymbol{x}_{i})\right)^{2}\right]\right)\right|>4R_{\mathcal{A}}\sqrt{\frac{2t}{n}}\right) \\ & \leq 4\mathbb{P}\left(\sup_{\Omega\in\mathcal{A}_{1}}\left|\frac{1}{n}\sum_{i=1}^{n}\zeta_{i}\left(\hat{\kappa}_{h}g_{\Omega}(\boldsymbol{x}_{i})-g_{*}(\boldsymbol{x}_{i})\right)^{2}\right|>R_{\mathcal{A}}\sqrt{\frac{2t}{n}}\right) \\ & = 4\mathbb{P}\left(\sup_{\Omega\in\mathcal{A}_{1}}\left|\frac{1}{n}\sum_{i=1}^{n}\zeta_{i}\left(2\left(\hat{\kappa}_{h}g_{\Omega}(\boldsymbol{x}_{i})\right)^{2}+2\left(g_{*}(\boldsymbol{x}_{i})\right)^{2}\right)\frac{\left(\hat{\kappa}_{h}g_{\Omega}(\boldsymbol{x}_{i})-g_{*}(\boldsymbol{x}_{i})\right)^{2}}{2\left(\hat{\kappa}_{h}g_{\Omega}(\boldsymbol{x}_{i})\right)^{2}+2\left(g_{*}(\boldsymbol{x}_{i})\right)^{2}}\right|>R_{\mathcal{A}}\sqrt{\frac{2t}{n}}\right) \\ & \leq 8\mathbb{P}\left(\sup_{\Omega\in\mathcal{A}_{1}}\left|\frac{1}{n}\sum_{i=1}^{n}\zeta_{i}\left(2\left(\hat{\kappa}_{h}g_{\Omega}(\boldsymbol{x}_{i})\right)^{2}+2\left(g_{*}(\boldsymbol{x}_{i})\right)^{2}\right)\right|>R_{\mathcal{A}}\sqrt{\frac{2t}{n}}\right) \\ & \leq 8\mathbb{P}\left(\sup_{\Omega\in\mathcal{A}_{1}}\left|\frac{1}{n}\sum_{i=1}^{n}\zeta_{i}\left(2\left(\hat{\kappa}_{h}g_{\Omega}(\boldsymbol{x}_{i})\right)^{2}\right|>\frac{R_{\mathcal{A}}}{2}\sqrt{\frac{2t}{n}}\right)+8\mathbb{P}\left(\left|\frac{1}{n}\sum_{i=1}^{n}2\zeta_{i}\left(g_{*}(\boldsymbol{x}_{i})\right)^{2}\right|>\frac{R_{\mathcal{A}}}{2}\sqrt{\frac{2t}{n}}\right) \\ & = 8\mathbb{P}\left(\sup_{\Omega\in\mathcal{A}_{1}}\left|\frac{2\left(\hat{\kappa}_{h}\right)^{2}}{n}\sum_{i=1}^{n}\zeta_{i}\left(g_{\Omega}(\boldsymbol{x}_{i})\right)^{2}\right|>\frac{R_{\mathcal{A}}}{2}\sqrt{\frac{2t}{n}}\right)+8\mathbb{P}\left(\sup_{\Omega\in\mathcal{A}_{1}}\left|\frac{2\left(\kappa_{*}\right)^{2}}{n}\sum_{i=1}^{n}\zeta_{i}\left(g_{\Omega}(\boldsymbol{x}_{i})\right)^{2}\right|>\frac{R_{\mathcal{A}}}{2}\sqrt{\frac{2t}{n}}\right) \\ & \leq 16\mathbb{P}\left(\sup_{\Omega\in\mathcal{A}_{1}}\left|\frac{18\left(\kappa_{*}\right)^{2}}{n}\sum_{i=1}^{n}\zeta_{i}\left(g_{\Omega}(\boldsymbol{x}_{i})\right)^{2}\right|>\frac{R_{\mathcal{A}}}{2}\sqrt{\frac{2t}{n}}\right). \end{split}$$

In the case $\kappa_* = 0$, the probability equals zero (notice that $R_{\mathcal{A}} \in [0, \infty)$, $t \in [4, \infty)$, and $n \in [1, \infty)$), which is commensurate with the bound in Lemma 5. So, for the rest of the proof we can assume without loss of generality that $\kappa_* > 0$. Rearranging the above display then gives

$$\mathbb{P}\left(\left|\frac{b}{n}\sum_{i=1}^{n}\left(\hat{\kappa}_{h}g_{\widehat{\Omega}_{h}}(\boldsymbol{x}_{i})-g_{*}(\boldsymbol{x}_{i})\right)^{2}-b\mathbb{E}_{(\boldsymbol{x},y)}\left[\left(\hat{\kappa}_{h}g_{\widehat{\Omega}_{h}}(\boldsymbol{x})-g_{*}(\boldsymbol{x})\right)^{2}\right]\right|>4bR_{\mathcal{A}}\sqrt{\frac{2t}{n}}\right)$$

$$\leq 16\mathbb{P}\left(\sup_{\Omega\in\mathcal{A}_{1}}\left|\frac{1}{n}\sum_{i=1}^{n}\zeta_{i}\left(g_{\Omega}(\boldsymbol{x}_{i})\right)^{2}\right|>\frac{R_{\mathcal{A}}}{36(\kappa_{*})^{2}}\sqrt{\frac{2t}{n}}\right).$$

Following the same approach as in the proof of Theorem 3 (with $\delta = 1280 a_{\text{sub}} (2a_{\text{Lip}}/L)^{2L} \sqrt{L^2 \log(2P) \sum_{i=1}^n \|\boldsymbol{x}_i\|_2^4/n^2 \log(2n)}$), we get

$$\left\| \left(\sup_{\Omega \in \mathcal{A}_1} \left| \frac{1}{n} \sum_{i=1}^n \zeta_i (g_{\Omega}(\boldsymbol{x}_i))^2 \right| \le \frac{R_{\mathcal{A}}}{36(\kappa_*)^2} \sqrt{\frac{2t}{n}} \right) \ge 1 - \frac{1}{32n} \right\|$$

for $t:=(\tilde{a}a_{\mathrm{sub}}(\kappa_*)^2(2a_{\mathrm{Lip}}/L)^{2L}\sqrt{L^2\log(2P)\sum_{i=1}^n\|\boldsymbol{x}_i\|_2^4/n}\log(2n)/R_{\mathcal{A}})^2/2$. (note that $t\in[4,\infty)$ as long as n is large enough such that $\tilde{a}(a_{\mathrm{sub}})^2\log(2P)(\log(2n))^2\geq 4$; and also let remind our assumption in Theorem 3 that $a_{\mathrm{sub}}\geq\gamma/8$). Hence, we obtain

$$\mathbb{P}\left(\sup_{\Omega\in\mathcal{A}_1}\left|\frac{1}{n}\sum_{i=1}^n\zeta_i(g_{\Omega}(\boldsymbol{x}_i))^2\right|>\frac{R_{\mathcal{A}}}{36(\kappa_*)^2}\sqrt{\frac{2t}{n}}\right)<\frac{1}{32n}.$$

Now, we combine the above inequality with the previous result and using some rearrangements to obtain

$$\mathbb{P}\left(\left|\frac{b}{n}\sum_{i=1}^{n}\left(\left(\hat{\kappa}_{h}g_{\widehat{\Omega}_{h}}(\boldsymbol{x}_{i})-g_{*}(\boldsymbol{x}_{i})\right)^{2}\right)-b\mathbb{E}_{(\boldsymbol{x},y)}\left[\left(\hat{\kappa}_{h}g_{\widehat{\Omega}_{h}}(\boldsymbol{x})-g_{*}(\boldsymbol{x})\right)^{2}\right]\right|>4bR_{\mathcal{A}}\sqrt{\frac{2t}{n}}\right)<\frac{1}{2n}.$$

Collecting all pieces of the proof, we obtain

$$\mathbb{E}_{(\boldsymbol{x},y)} \left[\left(\hat{\kappa}_h g_{\widehat{\Omega}_h}(\boldsymbol{x}) - y \right)^2 \right] \\
\leq \frac{b}{n} \sum_{i=1}^n \left(\hat{\kappa}_h g_{\widehat{\Omega}_h}(\boldsymbol{x}_i) - g_*(\boldsymbol{x}_i) \right)^2 + 1.01 \mathbb{E}_{(\boldsymbol{x},y)} [u^2] \\
+ \left| \frac{b}{n} \sum_{i=1}^n \left(\hat{\kappa}_h g_{\widehat{\Omega}_h}(\boldsymbol{x}_i) - g_*(\boldsymbol{x}_i) \right)^2 - b \mathbb{E}_{(\boldsymbol{x},y)} \left[\left(\hat{\kappa}_h g_{\widehat{\Omega}_h}(\boldsymbol{x}) - g_*(\boldsymbol{x}) \right)^2 \right] \right| \\
\leq \frac{b}{n} \sum_{i=1}^n \left(\hat{\kappa}_h g_{\widehat{\Omega}_h}(\boldsymbol{x}_i) - g_*(\boldsymbol{x}_i) \right)^2 + 1.01 \mathbb{E}_{(\boldsymbol{x},y)} [u^2] \\
+ \tilde{a} b a_{\text{sub}}(\kappa_*)^2 \left(\frac{2a_{\text{Lip}}}{L} \right)^{2L} \sqrt{\frac{L^2 \log(2P) \sum_{i=1}^n \|\boldsymbol{x}_i\|_2^4}{n^2} \log(2n)}$$

with probability at least 1 - 1/2n.

We finally 1. invoke the inequality of Corollary 4 to bound the in-sample-prediction error in the above display with probability at least 1 - 1/2n, 2. define $a := \tilde{a}ba_{\text{sub}}$ and 3. use the fact that $\text{risk}(\kappa_*g_{\Omega_*}) = \mathbb{E}_{(x,y)}[u^2]$ to get the desired bound with probability at least 1 - 1/n.

5.2.5 Proof of Proposition 6

Proof The proof peels the networks into inner and outer subnetworks. The inner subnetworks of a network $g_{\Theta} \in \mathcal{G} := \{g_{\Theta} : \Theta \in \mathcal{A}\}$ are vector-valued functions defined by

$$S_0 g_{\Theta} : \mathbb{R}^d o \mathbb{R}^d \ oldsymbol{x} \mapsto S_0 g_{\Theta}(oldsymbol{x}) := oldsymbol{x}$$

and

$$S_{l}g_{\Theta} : \mathbb{R}^{d} \to \mathbb{R}^{p_{l}}$$

$$\boldsymbol{x} \mapsto S_{l}g_{\Theta}(\boldsymbol{x}) := \boldsymbol{f}^{l} \Big(W^{l-1} \boldsymbol{f}^{l-1} \big(\dots W^{1} \boldsymbol{f}^{1} (W^{0} \boldsymbol{x}) \big) \Big)$$

for $l \in \{1, ..., L\}$. Similarly, the outer subnetworks of g_{Θ} are real-valued functions defined by

$$S^l g_{\Theta} : \mathbb{R}^{p_{l-1}} \to \mathbb{R}$$

 $oldsymbol{z} \mapsto S^l g_{\Theta}(oldsymbol{z}) := W^L oldsymbol{f}^L (\dots W^l oldsymbol{f}^l (W^{l-1} oldsymbol{z}))$

for $l \in \{1, \dots, L\}$ and

$$S^{L+1}g_{\Theta}: \mathbb{R}^{L} \to \mathbb{R}$$

 $\mathbf{z} \mapsto S^{L+1}g_{\Theta}(\mathbf{z}) := W^{L}\mathbf{z}.$

The initial network can be split into an inner and an outer network along every layer $l \in \{1, \ldots, L+1\}$:

$$g_{\Theta}(\boldsymbol{x}) = S^l g_{\Theta}(S_{l-1} g_{\Theta}(\boldsymbol{x})).$$

This observation is the basis for the following derivations.

We now show a contraction property for the inner subnetworks and a Lipschitz property for the outer subnetworks. Using the assumption that $\mathbf{z} \mapsto \mathbf{f}^{l-1}(\mathbf{z})$ is a_{Lip} -Lipschitz, we get for every $\Theta = (W^L, \dots, W^0)$ and $\mathbf{x} \in \mathbb{R}^d$ that

$$||S_{l-1}g_{\Theta}(\boldsymbol{x})||_{2} = ||\boldsymbol{f}^{l-1}(W^{l-2}S_{l-2}g_{\Theta}(\boldsymbol{x}))||_{2}$$

$$\leq a_{\text{Lip}}||W^{l-2}S_{l-2}g_{\Theta}(\boldsymbol{x})||_{2}$$

$$\leq a_{\text{Lip}}||W^{l-2}||_{2}||S_{l-2}g_{\Theta}(\boldsymbol{x})||_{2}$$

$$\leq \dots$$

$$\leq (a_{\text{Lip}})^{l-1}||\boldsymbol{x}||_{2}\prod_{j=0}^{l-2}||W^{j}||_{2}$$

for all $l \in \{2, ..., L+1\}$; and one can verify readily that $||S_0 g_{\Theta}(\boldsymbol{x})||_2 = ||\boldsymbol{x}||_2$. In other words, $\boldsymbol{x} \mapsto S_{l-1} g_{\Theta}(\boldsymbol{x})$ and $\boldsymbol{x} \mapsto S_0 g_{\Theta}(\boldsymbol{x})$ are "contractions" with constants $(a_{\text{Lip}})^{l-1} \prod_{j=0}^{l-2} ||W^j||_2$ and 1, respectively, with respect to the Euclidean norms on the input space \mathbb{R}^d and output spaces $\mathbb{R}^{p_{l-1}}$ and \mathbb{R}^d , respectively.

By similar arguments, we get for every $z_1, z_2 \in \mathbb{R}^{p_l}$ that

$$\begin{split} &|S^{l+1}g_{\Theta}(\boldsymbol{z}_{1}) - S^{l+1}g_{\Theta}(\boldsymbol{z}_{2})| \\ &= \left| W^{L}\boldsymbol{f}^{L}\big(\dots W^{l+1}\boldsymbol{f}^{l+1}(W^{l}\boldsymbol{z}_{1}) \big) - W^{L}\boldsymbol{f}^{L}\big(\dots W^{l+1}\boldsymbol{f}^{l+1}(W^{l}\boldsymbol{z}_{2}) \big) \right| \\ &\leq \|W^{L}\|_{2}\|\boldsymbol{f}^{L}\big(\dots W^{l+1}\boldsymbol{f}^{l+1}(W^{l}\boldsymbol{z}_{1}) \big) - \boldsymbol{f}^{L}\big(\dots W^{l+1}\boldsymbol{f}^{l+1}(W^{l}\boldsymbol{z}_{2}) \big) \|_{2} \\ &\leq a_{\operatorname{Lip}}\|W^{L}\|_{2}\|W^{L-1}\boldsymbol{f}^{L-1}\big(\dots W^{l+1}\boldsymbol{f}^{l+1}(W^{l}\boldsymbol{z}_{1}) \big) - W^{L-1}\boldsymbol{f}^{L-1}\big(\dots W^{l+1}\boldsymbol{f}^{l+1}(W^{l}\boldsymbol{z}_{2}) \big) \|_{2} \\ &< \dots \end{split}$$

$$\leq (a_{\operatorname{Lip}})^{L-l} \|oldsymbol{z}_1 - oldsymbol{z}_2\|_2 \prod_{j=l}^L \|W^j\|_2$$

for $l \in \{0, \dots, L\}$. In other words, $\boldsymbol{z} \mapsto S^{l+1} g_{\Theta}(\boldsymbol{z})$ is Lipschitz with constant $(a_{\text{Lip}})^{L-l} \prod_{j=l}^{L} \|W^{j}\|_{2}$ with respect to the Euclidean norms on the input space $\mathbb{R}^{p_{l}}$ and output space \mathbb{R} .

We now use these contraction and Lipschitz properties for the subnetworks to derive a Lipschitz property for the entire network. We consider two networks g_{Θ} and g_{Γ} with parameters $\Theta = (W^L, \dots, W^0) \in \mathcal{A}$ and $\Gamma = (V^L, \dots, V^0) \in \mathcal{A}$, respectively. Our above splitting of the networks applied to l = 1 and l = L + 1 and the fact that $S_0 g_{\Theta}(\mathbf{x}) = S_0 g_{\Gamma}(\mathbf{x}) = \mathbf{x}$ yield

$$|g_{\Theta}(\boldsymbol{x}) - g_{\Gamma}(\boldsymbol{x})| = |S^{1}g_{\Theta}(S_{0}g_{\Theta}(\boldsymbol{x})) - S^{L+1}g_{\Gamma}(S_{L}g_{\Gamma}(\boldsymbol{x}))|$$

= $|S^{1}g_{\Theta}(S_{0}g_{\Gamma}(\boldsymbol{x})) - S^{L+1}g_{\Gamma}(S_{L}g_{\Gamma}(\boldsymbol{x}))|.$

Elementary algebra and the fact that $S^{l+1}g_{\Theta}(S_lg_{\Gamma}(\boldsymbol{x})) = S^{l+1}g_{\Theta}(\boldsymbol{f}^l(V^{l-1}S_{l-1}g_{\Gamma}(\boldsymbol{x}))) = S^{l+2}g_{\Theta}(\boldsymbol{f}^{l+1}(W^lS_lg_{\Gamma}(\boldsymbol{x})))$ then allow us to derive

$$\begin{split} &|g_{\Theta}(\boldsymbol{x}) - g_{\Gamma}(\boldsymbol{x})| \\ &= \left| S^{1}g_{\Theta}(S_{0}g_{\Gamma}(\boldsymbol{x})) - \sum_{l=1}^{L-1} \left(S^{l+1}g_{\Theta}(S_{l}g_{\Gamma}(\boldsymbol{x})) - S^{l+1}g_{\Theta}(S_{l}g_{\Gamma}(\boldsymbol{x})) \right) \right. \\ &- \left(S^{L+1}g_{\Theta}(S_{L}g_{\Gamma}(\boldsymbol{x})) - S^{L+1}g_{\Theta}(S_{L}g_{\Gamma}(\boldsymbol{x})) \right) - S^{L+1}g_{\Gamma}(S_{L}g_{\Gamma}(\boldsymbol{x})) \right| \\ &= \left| S^{2}g_{\Theta}\left(\boldsymbol{f}^{1}(W^{0}S_{0}g_{\Gamma}(\boldsymbol{x})) \right) - S^{L+1}g_{\Theta}(S_{L}g_{\Gamma}(\boldsymbol{x})) \right| \\ &- \sum_{l=1}^{L-1} \left(S^{l+1}g_{\Theta}\left(\boldsymbol{f}^{l}(V^{l-1}S_{l-1}g_{\Gamma}(\boldsymbol{x})) \right) - S^{l+2}g_{\Theta}\left(\boldsymbol{f}^{l+1}(W^{l}S_{l}g_{\Gamma}(\boldsymbol{x})) \right) \right) \\ &- S^{L+1}g_{\Theta}\left(\boldsymbol{f}^{L}(V^{L-1}S_{L-1}g_{\Gamma}(\boldsymbol{x})) \right) + S^{L+1}g_{\Theta}\left(S_{L}g_{\Gamma}(\boldsymbol{x}) \right) - S^{L+1}g_{\Gamma}\left(S_{L}g_{\Gamma}(\boldsymbol{x}) \right) \right) \\ &= \left| \sum_{l=1}^{L} \left(S^{l+1}g_{\Theta}\left(\boldsymbol{f}^{l}(W^{l-1}S_{l-1}g_{\Gamma}(\boldsymbol{x})) \right) - S^{l+1}g_{\Theta}\left(\boldsymbol{f}^{l}(V^{l-1}S_{l-1}g_{\Gamma}(\boldsymbol{x})) \right) \right) \right. \\ &+ S^{L+1}g_{\Theta}\left(S_{L}g_{\Gamma}(\boldsymbol{x}) \right) - S^{L+1}g_{\Gamma}\left(S_{L}g_{\Gamma}(\boldsymbol{x}) \right) \right| \\ &= \left| \sum_{l=1}^{L} \left(S^{l+1}g_{\Theta}\left(\boldsymbol{f}^{l}(W^{l-1}S_{l-1}g_{\Gamma}(\boldsymbol{x})) \right) - S^{l+1}g_{\Theta}\left(\boldsymbol{f}^{l}(V^{l-1}S_{l-1}g_{\Gamma}(\boldsymbol{x})) \right) \right) \right. \\ &+ W^{L}S_{L}g_{\Gamma}(\boldsymbol{x}) - V^{L}S_{L}g_{\Gamma}(\boldsymbol{x}) \right| \\ &\leq \sum_{l=1}^{L} \left| S^{l+1}g_{\Theta}\left(\boldsymbol{f}^{l}(W^{l-1}S_{l-1}g_{\Gamma}(\boldsymbol{x})) \right) - S^{l+1}g_{\Theta}\left(\boldsymbol{f}^{l}(V^{l-1}S_{l-1}g_{\Gamma}(\boldsymbol{x})) \right) \right| \\ &+ |(W^{L} - V^{L})S_{L}g_{\Gamma}(\boldsymbol{x})|. \end{split}$$

We bound this further by using 1. the above-derived Lipschitz property of $S^{l+1}g_{\Theta}$, 2. the assumption that the \mathbf{f}^l are a_{Lip} -Lipschitz, 3. the properties of the ℓ_2 -norm, and 4. the above-derived contraction property of $S_{l-1}g_{\Gamma}$:

$$\begin{split} &|g_{\Theta}(\boldsymbol{x}) - g_{\Gamma}(\boldsymbol{x})| \\ &\leq \sum_{l=1}^{L} \left[(a_{\text{Lip}})^{L-l} \prod_{j=l}^{L} \|W^{j}\|_{2} \right] \|\boldsymbol{f}^{l}(W^{l-1}S_{l-1}g_{\Gamma}(\boldsymbol{x})) - \boldsymbol{f}^{l}(V^{l-1}S_{l-1}g_{\Gamma}(\boldsymbol{x})) \|_{2} \\ &+ \left| (W^{L} - V^{L})S_{L}g_{\Gamma}(\boldsymbol{x}) \right| \\ &\leq \sum_{l=1}^{L} \left[(a_{\text{Lip}})^{L-l+1} \prod_{j=l}^{L} \|W^{j}\|_{2} \right] \|W^{l-1}S_{l-1}g_{\Gamma}(\boldsymbol{x}) - V^{l-1}S_{l-1}g_{\Gamma}(\boldsymbol{x}) \|_{2} + \left| (W^{L} - V^{L})S_{L}g_{\Gamma}(\boldsymbol{x}) \right| \\ &\leq \sum_{l=1}^{L} \left[(a_{\text{Lip}})^{L-l+1} \prod_{j=l}^{L} \|W^{j}\|_{2} \right] \|W^{l-1} - V^{l-1}\|_{2} \|S_{l-1}g_{\Gamma}(\boldsymbol{x})\|_{2} + \|W^{L} - V^{L}\|_{2} \|S_{L}g_{\Gamma}(\boldsymbol{x})\|_{2} \\ &\leq \sum_{l=1}^{L} \left[(a_{\text{Lip}})^{L-l+1} \prod_{j=l}^{L} \|W^{j}\|_{2} \right] \|W^{l-1} - V^{l-1}\|_{2} \left[(a_{\text{Lip}})^{l-1} \prod_{j=0}^{l-2} \|V^{j}\|_{2} \right] \|\boldsymbol{x}\|_{2} \\ &+ \|W^{L} - V^{L}\|_{2} \left[(a_{\text{Lip}})^{L} \prod_{j=0}^{L-1} \|V^{j}\|_{2} \right] \|\boldsymbol{x}\|_{2}, \end{split}$$

where we set $\prod_{j=0}^{-1} \|V^j\|_2 := 1$. Consolidating and rearranging then yields

$$\begin{split} &|g_{\Theta}(\boldsymbol{x}) - g_{\Gamma}(\boldsymbol{x})| \\ &\leq (a_{\operatorname{Lip}})^{L} \Biggl(\sum_{l=1}^{L} \Biggl[\prod_{\substack{j \in \{0, \dots, L\} \\ j \neq l-1}} \left(\|W^{j}\|_{2} \vee \|V^{j}\|_{2} \right) \Biggr] \|W^{l-1} - V^{l-1}\|_{2} \|\boldsymbol{x}\|_{2} \\ &+ \Biggl[\prod_{j=0}^{L-1} \left(\|W^{j}\|_{2} \vee \|V^{j}\|_{2} \right) \Biggr] \|W^{L} - V^{L}\|_{2} \|\boldsymbol{x}\|_{2} \Biggr) \\ &= (a_{\operatorname{Lip}})^{L} \sum_{l=1}^{L+1} \Biggl[\prod_{\substack{j \in \{0, \dots, L\} \\ j \neq l-1}} \left(\|W^{j}\|_{2} \vee \|V^{j}\|_{2} \right) \Biggr] \|W^{l-1} - V^{l-1}\|_{2} \|\boldsymbol{x}\|_{2} \\ &\leq (a_{\operatorname{Lip}})^{L} \|\boldsymbol{x}\|_{2} \max_{l \in \{1, \dots, L+1\}} \Biggl\{ \prod_{\substack{j \in \{0, \dots, L\} \\ j \neq l-1}} \left(\|W^{j}\|_{2} \vee \|V^{j}\|_{2} \right) \Biggr\} \sum_{m=1}^{L+1} \|W^{m-1} - V^{m-1}\|_{2} \\ &= (a_{\operatorname{Lip}})^{L} \|\boldsymbol{x}\|_{2} \max_{l \in \{0, \dots, L\}} \Biggl\{ \prod_{\substack{j \in \{0, \dots, L\} \\ j \neq l}} \left(\|W^{j}\|_{2} \vee \|V^{j}\|_{2} \right) \Biggr\} \sum_{m=0}^{L} \|W^{m} - V^{m}\|_{2}. \end{split}$$

We now study the last sum in that bound: First, we observe that

$$\begin{split} \sum_{m=0}^{L} \|W^m - V^m\|_2 &= \sqrt{\left(\sum_{m=0}^{L} \|W^m - V^m\|_2\right)^2} \\ &\leq \sqrt{(L+1)\sum_{m=0}^{L} \|W^m - V^m\|_2^2} \\ &= \sqrt{L+1} \sqrt{\sum_{m=0}^{L} \|W^m - V^m\|_2^2}, \end{split}$$

where we use $\left(\sum_{m=0}^{L} a_m\right)^2 \leq (L+1) \sum_{m=0}^{L} (a_m)^2$ with $a_m := \|W^m - V^m\|_2$. We then bound the last line further to obtain

$$\begin{split} \sum_{m=0}^{L} \|W^m - V^m\|_2 &\leq \sqrt{L+1} \|\Theta - \Gamma\|_2 \\ &\leq 2\sqrt{L} \|\Theta - \Gamma\|_2 \\ &\leq 2\sqrt{L} \|\Theta - \Gamma\|_F, \end{split}$$

where we use 1. the definition of the operator norm on Page 9, 2. $\sqrt{1+L} \leq 2\sqrt{L}$, and 3. $\|\Theta - \Gamma\|_2 \leq \|\Theta - \Gamma\|_F$. Combining this result with the previous display yields

$$\begin{split} |g_{\Theta}(\boldsymbol{x}) - g_{\Gamma}(\boldsymbol{x})| &\leq 2(a_{\text{Lip}})^{L} \sqrt{L} \|\boldsymbol{x}\|_{2} \max_{l \in \{0, \dots, L\}} \bigg\{ \prod_{j \in \{0, \dots, L\}} \big(\|W^{j}\|_{2} \vee \|V^{j}\|_{2} \big) \bigg\} \|\Theta - \Gamma\|_{\text{F}} \\ &= c_{\text{Lip}}(\boldsymbol{x}) \|\Theta - \Gamma\|_{\text{F}}, \end{split}$$

as desired.

The second claim then follows readily:

$$\begin{split} \|g_{\Theta} - g_{\Gamma}\|_{n} &= \sqrt{\frac{1}{n} \sum_{i=1}^{n} \left(g_{\Theta}(\boldsymbol{x}_{i}) - g_{\Gamma}(\boldsymbol{x}_{i})\right)^{2}} \\ &\leq \sqrt{\frac{1}{n} \sum_{i=1}^{n} \left(c_{\text{Lip}}(\boldsymbol{x}_{i}) \|\Theta - \Gamma\|_{\text{F}}\right)^{2}} \\ &= \sqrt{\frac{1}{n} \sum_{i=0}^{n} \left(2(a_{\text{Lip}})^{L} \sqrt{L} \|\boldsymbol{x}_{i}\|_{2} \max_{l \in \{0, \dots, L\}} \left\{ \prod_{j \in \{0, \dots, L\}} (\|W^{j}\|_{2} \vee \|V^{j}\|_{2}) \right\} \|\Theta - \Gamma\|_{\text{F}}\right)^{2}} \\ &= 2(a_{\text{Lip}})^{L} \sqrt{L} \sqrt{\frac{1}{n} \sum_{i=0}^{n} \|\boldsymbol{x}_{i}\|_{2}^{2} \max_{l \in \{0, \dots, L\}} \left\{ \prod_{j \in \{0, \dots, L\}} (\|W^{j}\|_{2} \vee \|V^{j}\|_{2}) \right\} \|\Theta - \Gamma\|_{\text{F}}} \\ &= \overline{c}_{\text{Lip}} \|\Theta - \Gamma\|_{\text{F}}, \end{split}$$

as desired.

5.2.6 Proof of Lemma 7

Proof The proof follows from Proposition 6 and restricting the parameter space to A_1 . Since $\Omega, \Gamma \in A_1$, we can get

$$\begin{split} \sum_{j=0}^{L} \left(\|W^{j}\|_{2} \vee \|V^{j}\|_{2} \right) &\leq \sum_{j=0}^{L} \left(\|W^{j}\|_{2} + \|V^{j}\|_{2} \right) \\ &\leq \sum_{j=0}^{L} \left(\|W^{j}\|_{1} + \|V^{j}\|_{1} \right) \\ &= \|\Omega\|_{1} + \|\Gamma\|_{1} \\ &\leq 2. \end{split}$$

Using 1. the inequality of arithmetic and geometric means, 2. the nonnegativity of norms $(\|\cdot\|_2 \ge 0)$, and 3. the above display, we obtain

$$\begin{aligned} \max_{l \in \{0, \dots, L\}} \prod_{j \in \{0, \dots, L\}} \left(\|W^j\|_2 \vee \|V^j\|_2 \right) &\leq \max_{l \in \{0, \dots, L\}} \left(\frac{1}{L} \sum_{j=0, j \neq l}^{L} \left(\|W^j\|_2 \vee \|V^j\|_2 \right) \right)^L \\ &\leq \left(\frac{1}{L} \sum_{j=0}^{L} \left(\|W^j\|_2 \vee \|V^j\|_2 \right) \right)^L \\ &\leq \left(\frac{2}{L} \right)^L. \end{aligned}$$

We can plug this inequality into the definition of $\overline{c}_{\mathrm{Lip}}$ in Proposition 6 to get

$$c_{\text{Lip1}} = 2(a_{\text{Lip}})^L \sqrt{L} \|\boldsymbol{x}\|_n \left(\frac{2}{L}\right)^L,$$

as desired in the first claim. The second claim then follows by setting Γ equal to the all-zeros parameter in the first claim.

5.2.7 Proof of Proposition 8

Proof We prove the two claims in order.

Claim 1: entropy bound

Our strategy is to move from $H(r, \mathcal{G}_1, \|\cdot\|_n)$ to $H(r/c_{\text{Lip1}}, \mathcal{A}_1, \|\cdot\|_F)$ via Proposition 6 and Lemma 10 and then bound the latter covering number using a bound on the entropy of ℓ_1 -balls.

Lemma 7 ensures that the function $\Omega \mapsto g_{\Omega}$ restricted to the parameter space \mathcal{A}_1 is c_{Lip1} -Lipschitz with respect to the prediction distance $\|\cdot\|_n$ on the network space and

Frobenius norm $\|\cdot\|_{\mathrm{F}}$ on the parameter space with $c_{\mathrm{Lip1}} = 2(2a_{\mathrm{Lip}}/L)^L\sqrt{L}\|\boldsymbol{x}\|_n$. If $c_{\mathrm{Lip1}} = 0$, then $N(r, \mathcal{G}_1, \|\cdot\|_n) = 1$ for all $r \in (0, \infty)$ and, therefore, $H(r, \mathcal{G}_1, \|\cdot\|_n) = 0$ for all $r \in (0, \infty)$, which is commensurate with the alleged bound. We can thus assume $c_{\mathrm{Lip1}} > 0$ in the following.

Since $\|g_{\Gamma} - g_{\mathbf{0}_{\mathcal{A}}}\|_n = \|g_{\Gamma}\|_n \leq \sup_{\Omega \in \mathcal{A}_1} \|g_{\Omega}\|_n =: R \text{ for all } \Gamma \in \mathcal{A}_1 \text{ and } \mathbf{0}_{\mathcal{A}} := (\mathbf{0}_{p_{L+1} \times p_L}, \dots, \mathbf{0}_{p_1 \times p_0}),$ it holds that $N(r, \mathcal{G}_1, \|\cdot\|_n) = 1$ for all r > R and, consequently, $H(r, \mathcal{G}_1, \|\cdot\|_n) = 0$ for all r > R, which is commensurate with the alleged bound. We can thus assume $r \leq R$ in the following.

We then apply Lemma 10 with $\mathcal{A}' := \mathcal{A}_1$, $\mathcal{G}' := \mathcal{G}_1$, $||k_{\text{Lip}}||_n := c_{\text{Lip}1}$, and $\rho := ||| \cdot |||_{\text{F}}$ to obtain

 $H(r,\mathcal{G}_1,\|\cdot\|_n) \leq H\left(\frac{r}{c_{\text{Lip1}}},\mathcal{A}_1,\|\cdot\|_{\text{F}}\right).$

We now think of \mathcal{A}_1 as a set in \mathbb{R}^P . Defining $\mathcal{A}'' := \{ \boldsymbol{\omega} = (\omega_1, \dots, \omega_P)^\top \in \mathbb{R}^P : \sum_{j=1}^P |\omega_j| \leq 1 \}$, we find for every $r \leq R$ and $\epsilon := r/(\sqrt{2}c_{\text{Lip}1}) \in (0,1)$, where $\epsilon \in (0,1)$ comes by the definition of ϵ together with $r \leq R$ and $R \leq c_{\text{Lip}1}$ (by Lemma 7),

$$H\left(\frac{r}{c_{\text{Lip1}}}, \mathcal{A}_1, \|\cdot\|_{\text{F}}\right) = H\left(\sqrt{2}\epsilon, \mathcal{A}'', \|\cdot\|_2\right).$$

We then bound the right-hand side of this equality using 1. the definition of the entropy, 2. the entropy bound of Lederer (2010, Page 9) (with $k = \lceil 2nA^2M^2/\epsilon^2 \rceil$, M = 1, and $A = 1/\sqrt{n}$), and 3. a simplification (by $\epsilon \in (0,1)$) to get

$$H(\sqrt{2\epsilon}, \mathcal{A}'', \|\cdot\|_2) = \log N(\sqrt{2\epsilon}, \mathcal{A}'', \|\cdot\|_2)$$

$$\leq \left(\frac{2}{\epsilon^2} + 1\right) \log(e(1 + P\epsilon^2))$$

$$\leq \frac{3}{\epsilon^2} \log(2eP\epsilon^2 \vee 2e).$$

Collecting the pieces and recalling that $\epsilon = r/(\sqrt{2}c_{\text{Lip1}})$ then yields

$$H(r, \mathcal{G}_1, \|\cdot\|_n) \le H(\sqrt{2}\epsilon, \mathcal{A}'', \|\cdot\|_2)$$

$$\le \frac{6(c_{\text{Lip1}})^2}{r^2} \log\left(\frac{ePr^2}{(c_{\text{Lip1}})^2} \vee 2e\right),$$

as desired.

Claim 2: Dudley bound

Our strategy is to use Claim 1 to prove that

$$J(\delta, \sigma, A_1) \le \frac{5c_{\text{Lip1}}}{2} \sqrt{\log(eP \vee 2e)} \log\left(\frac{8\sigma R}{\delta}\right)$$

and then to use Lemma 7 to formulate the bound in the desired way.

We first split the Dudley integral into two parts according to

$$J(\delta, \sigma, \mathcal{A}_1) = \int_{\delta/(8\sigma)}^R H^{1/2}(r, \mathcal{G}_1, \|\cdot\|_n) dr + \int_{r>R} H^{1/2}(r, \mathcal{G}_1, \|\cdot\|_n) dr.$$

Recalling $H(r, \mathcal{G}_1, \|\cdot\|_n) = 0$ for all r > R, the Dudley integral simplifies to

$$J(\delta, \sigma, \mathcal{A}_1) = \int_{\delta/(8\sigma)}^R H^{1/2}(r, \mathcal{G}_1, \|\cdot\|_n) dr.$$

Using this equality together with the bound from Claim 1, we obtain that

$$J(\delta, \sigma, \mathcal{A}_{1}) = \int_{\delta/(8\sigma)}^{R} H^{1/2}(r, \mathcal{G}_{1}, \|\cdot\|_{n}) dr$$

$$\leq \int_{\delta/(8\sigma)}^{R} \left(\frac{6(c_{\text{Lip1}})^{2}}{r^{2}} \log\left(\frac{ePr^{2}}{(c_{\text{Lip1}})^{2}} \vee 2e\right)\right)^{1/2} dr$$

$$\leq \frac{5c_{\text{Lip1}}}{2} \sqrt{\log\left(\frac{ePR^{2}}{(c_{\text{Lip1}})^{2}} \vee 2e\right)} \int_{\delta/(8\sigma)}^{R} \frac{1}{r} dr$$

$$= \frac{5c_{\text{Lip1}}}{2} \sqrt{\log\left(\frac{ePR^{2}}{(c_{\text{Lip1}})^{2}} \vee 2e\right)} \log\left(\frac{8\sigma R}{\delta}\right).$$

Since $R \leq c_{\text{Lip1}}$ by Lemma 7, we can get

$$J(\delta, \sigma, \mathcal{A}_1) \le \frac{5c_{\text{Lip1}}}{2} \sqrt{\log(eP \vee 2e)} \log\left(\frac{8\sigma c_{\text{Lip1}}}{\delta}\right),$$

as desired.

5.2.8 Proof of Lemma 10

Proof The case $||k_{\text{Lip}}||_n = 0$ follows directly from our convention $a/0 = \infty$ for $a \in (0, \infty)$ on Page 11 and the definition of the entropy on Page 10. We thus assume $||k_{\text{Lip}}||_n > 0$ in the following.

Using the definition of the prediction distance on Page 9 and the Lipschitz property stipulated in the lemma, we find that

$$\|g_{\Theta} - g_{\Gamma}\|_{n} = \sqrt{\frac{1}{n} \sum_{i=1}^{n} (g_{\Theta}(\boldsymbol{x}_{i}) - g_{\Gamma}(\boldsymbol{x}_{i}))^{2}}$$

$$\leq \sqrt{\frac{1}{n} \sum_{i=1}^{n} (k_{\text{Lip}}(\boldsymbol{x}_{i}))^{2} (\rho(\Theta, \Gamma))^{2}}$$

$$= \|k_{\text{Lip}}\|_{n} \rho(\Theta, \Gamma).$$

Now, let \mathcal{A}'_r be an $r/\|k_{\text{Lip}}\|_n$ -covering of \mathcal{A}' with respect to the metric ρ . This means that for every $\Theta \in \mathcal{A}'$, there is a $\Theta_r \in \mathcal{A}'_r$ such that $\rho(\Theta, \Theta_r) \leq r/\|k_{\text{Lip}}\|_n$. This insight together with the first display applied to $\Gamma = \Theta_r$ yield that for every function $g_{\Theta} \in \mathcal{G}'$, there

is a $g_{\Theta_r} \in \{g_{\Theta_r} : \Theta_r \in \mathcal{A}'_r\}$ such that

$$||g_{\Theta} - g_{\Theta_r}||_n \le ||k_{\text{Lip}}||_n \rho(\Theta, \Theta_r)$$

$$\le ||k_{\text{Lip}}||_n \cdot \frac{r}{||k_{\text{Lip}}||_n}$$

$$= r.$$

Hence, $\{g_{\Theta_r} : \Theta_r \in \mathcal{A}'_r\}$ is an r-covering of \mathcal{G}' with respect to $\|\cdot\|_n$. The proof then follows directly from the definition of the entropy on Page 10 as the logarithm of the covering number.

5.2.9 Proof of Lemma 11

Proof There are several ways to derive such a deviation inequality. We choose an approach based on a version of Bernstein's inequality.

A Taylor expansion of the sub-Gaussian assumption on Page 7 gives

$$\max_{i \in \{1,\dots,n\}} K^2 \Big(\mathbb{E} \big[|u_i|^2 / K^2 + \big(|u_i|^2 / K^2 \big)^2 / 2! + \big(|u_i|^2 / K^2 \big)^3 / 3! + \dots \big] \Big) \le \gamma^2.$$

Hence, the individual terms of the expansion satisfy the moment inequality

$$\max_{i \in \{1, ..., n\}} K^2 \mathbb{E} \Big[(|u_i|^2 / K^2)^m / m! \Big] \le \gamma^2 \qquad \text{for all } m \in \{1, 2, ... \}.$$

By exchanging the maximum for an average, we then find

$$\frac{1}{n} \sum_{i=1}^{n} K^2 \mathbb{E}\left[\left(|u_i|^2/K^2\right)^m/m!\right] \le \gamma^2 \qquad \text{for all } m \in \{1, 2, \dots\},$$

which can be reformulated as

$$\sum_{i=1}^{n} \mathbb{E}\left[\left(|u_i|^2\right)^m\right] \le \frac{m!}{2} (2n\gamma^2 K^2) (K^2)^{m-2} \qquad \text{for all } m \in \{1, 2, \dots\}.$$

This means that the squared noise random variables satisfy a "Bernstein condition" (van de Geer and Lederer, 2013).

We can thus apply a Bernstein-type deviation inequality such as Boucheron et al. (2013, Corollary 2.11) to derive

$$\mathbb{P}\left(\sum_{i=1}^{n} \left((u_i)^2 - \mathbb{E}\left[(u_i)^2 \right] \right) \ge \frac{nv}{2} \right) \le e^{-\frac{n^2 v^2/4}{2(2n\gamma^2 K^2 + K^2 nv/2)}},$$

which can be reformulated as

$$\mathbb{P}\left(\frac{1}{n}\sum_{i=1}^{n} \left((u_i)^2 - \mathbb{E}\left[(u_i)^2 \right] \right) \ge \frac{v}{2} \right) \le e^{-\frac{nv^2}{16\gamma^2 K^2 + 4vK^2}}.$$

Using that $v \geq 2\gamma^2$ by assumption, we then find further

$$\mathbb{P}\left(\frac{1}{n}\sum_{i=1}^{n} \left((u_i)^2 - \mathbb{E}\left[(u_i)^2 \right] \right) \ge \frac{v}{2} \right) \le e^{-\frac{nv^2}{8vK^2 + 4vK^2}} = e^{-\frac{nv}{12K^2}}.$$

By 1. adding a zero-valued term, 2. invoking the above-derived property on the $(u_i)^2$ (set m=1), 3. using again that $v \geq 2\gamma^2$, and 4. invoking the above display, we conclude that

$$\mathbb{P}\left(\frac{1}{n}\sum_{i=1}^{n}(u_{i})^{2} \geq v\right) = \mathbb{P}\left(\frac{1}{n}\sum_{i=1}^{n}\left((u_{i})^{2} - \mathbb{E}\left[(u_{i})^{2}\right]\right) \geq v - \frac{1}{n}\sum_{i=1}^{n}\mathbb{E}\left[(u_{i})^{2}\right]\right) \\
\leq \mathbb{P}\left(\frac{1}{n}\sum_{i=1}^{n}\left((u_{i})^{2} - \mathbb{E}\left[(u_{i})^{2}\right]\right) \geq v - \gamma^{2}\right) \\
\leq \mathbb{P}\left(\frac{1}{n}\sum_{i=1}^{n}\left((u_{i})^{2} - \mathbb{E}\left[(u_{i})^{2}\right]\right) \geq \frac{v}{2}\right) \\
\leq e^{-\frac{nv}{12K^{2}}},$$

as desired.

6. Discussion

Our theories in Section 3 show that ℓ_1 -regularization can guarantee accurate prediction even when the neural networks are very wide (see the logarithmic increase of the error in the number of parameters) and deep (see the decrease of the error in the number of layers). More generally, our theories in Section 2 facilitate the derivation of concrete guarantees by connecting regularization with the rich literature on suprema of empirical processes.

Another related contribution is Schmidt-Hieber (2017), which uses ideas from nonparameteric statistics to derive bounds for empirical-risk minimization over classes of sparse networks. Direct sparsity constraints, in contrast to ℓ_1 -regularization, are not feasible in practice. But Schmidt-Hieber (2017) provides a number of new insights, two of which are also important here: first, it highlights the statistical benefits of sparsity and, therefore, supports our results in Section 3; and second, it indicates that—arguably under strict assumptions—one can achieve the rate 1/n rather than $1/\sqrt{n}$. However, again, we believe that the $1/\sqrt{n}$ -rate cannot be improved in general: while a formal proof still needs to be established, a corresponding statement has already been proved for ℓ_1 -regularized linear regression (Dalalyan et al., 2017, Proposition 4). In this sense, we might claim some optimality of our results.

Our theory considers only global minima of the estimators' objective functions, while the objective functions might also have saddle points or suboptimal local minima. However, current research suggests that at least for wide networks, global optimization is feasible—see Lederer (2020) and references therein.

In summary, our paper highlights the effectiveness of regularisation in deep learning, and it furthers the mathematical understanding of neural networks more broadly. As practical

advice, our results suggest the use of wide networks (to minimize approximation errors and to facilitate optimizations) with many layers (to improve statistical accuracy) together with regularization (to avoid overfitting).

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References

- M. Anthony and P. Bartlett. *Neural network learning: Theoretical foundations*. Cambridge Univ. Press, 2009.
- V. Badrinarayanan, A. Kendall, and R. Cipolla. SegNet: A deep convolutional encoder-decoder architecture for image segmentation. *IEEE Trans. Pattern Anal. Mach. Intell.*, 39(12):2481–2495, 2017.
- A. Barron and J. Klusowski. Approximation and estimation for high-dimensional deep learning networks. arXiv:1809.03090, 2018.
- A. Barron and J. Klusowski. Complexity, statistical risk, and metric entropy of deep nets using total path variation. arXiv:1902.00800, 2019.
- P. Bartlett. The sample complexity of pattern classification with neural networks: The size of the weights is more important than the size of the network. *IEEE Trans. Inform. Theory*, 44(2): 525–536, 1998.
- P. Bartlett and S. Mendelson. Rademacher and Gaussian complexities: risk bounds and structural results. J. Mach. Learn. Res., 3:463–482, 2002.
- S. Boucheron, G. Lugosi, and P. Massart. Concentration inequalities: A nonasymptotic theory of independence. Oxford Univ. Press, 2013.
- E. Candès, J. Romberg, and T. Tao. Stable signal recovery from incomplete and inaccurate measurements. *Commun. Pure Appl. Math.*, 59(8):1207–1223, 2006.
- J. Chorowski, D. Bahdanau, D. Serdyuk, K. Cho, and Y. Bengio. Attention-based models for speech recognition. In *NIPS*, pages 577–585, 2015.
- D. Clevert, T. Unterthiner, and S. Hochreiter. Fast and accurate deep network learning by exponential linear units (ELUs). arXiv:1511.07289, 2015.
- A. Dalalyan, M. Hebiri, and J. Lederer. On the prediction performance of the lasso. *Bernoulli*, 23 (1):552–581, 2017.
- D. Donoho. Compressed sensing. IEEE Trans. Inform. Theory, 52(4):1289–1306, 2006.
- S. Du, W. Hu, and J. Lee. Algorithmic regularization in learning deep homogeneous models: layers are automatically balanced. In *NIPS*, pages 384–395, 2018.
- S. Elfwing, E. Uchibe, and K. Doya. Sigmoid-weighted linear units for neural network function approximation in reinforcement learning. *Neural Networks*, 107:3–11, 2018.

- R. Girshick, J. Donahue, T. Darrell, and J. Malik. Rich feature hierarchies for accurate object detection and semantic segmentation. In *CVPR*, pages 580–587, 2014.
- X. Glorot, A. Bordes, and Y. Bengio. Deep sparse rectifier neural networks. In *AISTATS*, pages 315–323, 2011.
- N. Golowich, A. Rakhlin, and O. Shamir. Size-independent sample complexity of neural networks. In *COLT*, volume 75, pages 297–299, 2018.
- A. Graves, A. Mohamed, and G. Hinton. Speech recognition with deep recurrent neural networks. In ICASSP, pages 6645–6649, 2013.
- M. Hebiri and J. Lederer. How correlations influence lasso prediction. *IEEE Trans. Inform. Theory*, 59(3):1846–1854, 2013.
- M. Hebiri and J. Lederer. Layer sparsity in neural networks. arXiv:2006.15604, 2020.
- G. Hinton, L. Deng, D. Yu, G. Dahl, A. Mohamed, N. Jaitly, A. Senior, V. Vanhoucke, P. Nguyen, T. Sainath, and B. Kingsbury. Deep neural networks for acoustic modeling in speech recognition: The shared views of four research groups. *IEEE Signal Process. Mag.*, 29(6):82–97, 2012.
- R. Jozefowicz, O. Vinyals, M. Schuster, N. Shazeer, and Y. Wu. Exploring the limits of language modeling. arXiv:1602.02410, 2016.
- J. Lederer. Bounds for Rademacher processes via chaining. arXiv:1010.5626, 2010.
- J. Lederer. No spurious local minima: on the optimization landscapes of wide and deep neural networks. arXiv:2010.00885, 2020.
- J. Lederer and S. van de Geer. New concentration inequalities for suprema of empirical processes. Bernoulli, 20(4):2020–2038, 2014.
- J. Lederer and M. Vogt. Estimating the lasso's effective noise. arXiv:2004.11554, 2020.
- J. Lederer, L. Yu, and I. Gaynanova. Oracle inequalities for high-dimensional prediction. *Bernoulli*, 25(2):1225–1255, 2019.
- M. Ledoux and M. Talagrand. *Probability in Banach spaces: Isoperimetry and processes*. Springer-Verlag Berlin, 1991.
- H. Liu and Y. Ye. High-dimensional learning under approximate sparsity: A unifying framework for nonsmooth learning and regularized neural networks. *arXiv:1903.00616*, 2019.
- J. Long, E. Shelhamer, and T. Darrell. Fully convolutional networks for semantic segmentation. In CVPR, pages 3431–3440, 2015.
- V. Nair and G. Hinton. Rectified linear units improve restricted Boltzmann machines. In ICLM, pages 807–814, 2010.
- B. Neyshabur, R. Tomioka, and N. Srebro. In search of the real inductive bias: on the role of implicit regularization in deep learning. arXiv:1412.6614, 2014.
- B. Neyshabur, R. Tomioka, and N. Srebro. Norm-based capacity control in neural networks. In *COLT*, pages 1376–1401, 2015.
- P. Ramachandran, B. Zoph, and Q. Le. Swish: A self-gated activation function. arXiv:1710.05941, 2017.

- S. Scardapane, D. Comminiello, A. Hussain, and A. Uncini. Group sparse regularization for deep neural networks. *Neurocomputing*, 241:81–89, 2017.
- J. Schmidt-Hieber. Nonparametric regression using deep neural networks with ReLU activation function. arXiv:1708.06633, 2017.
- C. Szegedy, W. Liu, Y. Jia, P. Sermanet, S. Reed, D. Anguelov, D. Erhan, V. Vanhoucke, and A. Rabinovich. Going deeper with convolutions. In CVPR, pages 1–9, 2015.
- R. Tibshirani. Regression shrinkage and selection via the lasso. J. R. Stat. Soc. Ser. B. Stat. Methodol., 58(1):267–288, 1996.
- S. van de Geer. Empirical processes in M-estimation. Cambridge Univ. Press, 2000.
- S. van de Geer. Estimation and testing under sparsity. Springer, 2016.
- S. van de Geer and J. Lederer. The Bernstein-Orlicz norm and deviation inequalities. *Probab. Theory Related Fields*, 157:225–250., 2013.
- A. van der Vaart and J. Wellner. Weak convergence and empirical processes. Springer, 1996.
- R. Vershynin. *High-dimensional probability: An introduction with applications in data science*. Cambridge Univ. Press, 2018.
- D. Yarotsky. Error bounds for approximations with deep ReLU networks. *Neural Networks*, 94: 103–114, 2017.
- Y. Zhang, J. Lee, and M. Jordan. ℓ_1 -regularized neural networks are improperly learnable in polynomial time. In ICML, pages 993–1001, 2016.