Empirical Risk Minimization in the Interpolating Regime with Application to Neural Network Learning

Nicole Mücke
Institute for Mathematical Stochastics
Technical University of Braunschweig
nicole.muecke@tu-braunschweig.de

Ingo Steinwart
Institute for Stochastics and Applications
University of Stuttgart
ingo.steinwart@mathematik.uni-stuttgart.de

July 26, 2021

Abstract

A common strategy to train deep neural networks (DNNs) is to use very large architectures and to train them until they (almost) achieve zero training error. Empirically observed good generalization performance on test data, even in the presence of lots of label noise, corroborate such a procedure. On the other hand, in statistical learning theory it is known that over-fitting models may lead to poor generalization properties, occurring in e.g. empirical risk minimization (ERM) over too large hypotheses classes. Inspired by this contradictory behavior, so-called interpolation methods have recently received much attention, leading to consistent and optimally learning methods for some local averaging schemes with zero training error. However, there is no theoretical analysis of interpolating ERM-like methods so far. We take a step in this direction by showing that for certain, large hypotheses classes, some interpolating ERMs enjoy very good statistical guarantees while others fail in the worst sense. Moreover, we show that the same phenomenon occurs for DNNs with zero training error and sufficiently large architectures.

1 Introduction

During the last few decades statistical learning theory (SLT) has developed powerful techniques to analyze many variants of (regularized) empirical risk minimizers (ERMs), see e.g. [8, 23, 22, 10, 19, 21, 18]. The resulting learning guarantees, which include finite sample bounds, oracle inequalities, learning rates, adaptivity, and consistency, assume in most cases that the effective hypotheses space of the considered method is sufficiently small in terms of some notion of capacity such as VC-dimension, fat-shattering dimension, Rademacher complexities, covering numbers, or eigenvalues.

Most training algorithms for DNNs also optimize an (regularized) empirical error term over a hypotheses space, namely the class of functions that can be represented by the architecture of the considered DNN, see [9, Part II]. However, unlike for many classical ERMs, the hypotheses space is parametrized in a rather complicated manner. Consequently,
the optimization problem is, in general, harder to solve. A common way to address this is in practice is to use very large DNNs, since despite their size, training them is often easier, see e.g. [17, 13] and the references therein. Now, for sufficiently large DNNs it has been recently observed that common training algorithms can achieve zero training error on randomly, or arbitrarily labeled training sets, see [24]. Because of this ability, their effective hypotheses space can no longer have a sufficiently small capacity in the sense of classical SLT, so that the usual techniques for analyzing learning algorithms are no longer suitable, see e.g. the discussion on this in [24, 4, 15, 25]. In fact, SLT provides well known examples of large hypotheses spaces for which zero training error is possible but a simple ERM fails to learn. This phenomenon is known as over-fitting, and common wisdom suggests that successful learning algorithms need to avoid over-fitting, see e.g. [10, pp. 21-22]. The empirical evidence mentioned above thus stands in stark contrast to this credo of SLT.

This somewhat paradoxical behavior has recently sparked interests, leading to deeper theoretical investigations of the so called double/ multiple-descent phenomenon for different model settings. More specifically, [5] analyzed linear regression with random feature selection and investigated the random Fourier feature model. This model has also been analyzed by [14]. For linear regression, where model complexity is measured in terms of the number of parameters, the authors in [2, 20] show that over-parameterization is even essential for benign over-fitting. However, these results are highly distribution dependent and require a specific covariance structure and (sub-) Gaussian data. For more details we refer also to [4, 7, 12, 16, 1]. Another line of research [6] shows for classical learning methods, namely Nadaraya-Watson estimator with certain singular kernels, that interpolating the training data can achieve optimal rates for problems of nonparametric regression and prediction with square loss. Beyond empirical evidence there are therefore also theoretical results showing that interpolating the data and good learning performance is simultaneously possible. So far, however, the considered interpolating learning methods do not implement an empirical risk minimization (ERM) scheme nor do they closely resemble the learning mechanisms of DNNs. In this paper, we take a step towards closing this gap.

First, we explicitly construct, for data sets of size \( n \), large classes of hypotheses \( \mathcal{H}_n \) for which we show that some interpolating least squares ERM algorithms over \( \mathcal{H}_n \) enjoy very good statistical guarantees, while other interpolating least squares ERM algorithms over \( \mathcal{H}_n \) fail in a strong sense. To be more precise, we observe the following phenomena: There exists a universally consistent ERM and there exists an ERM whose predictors converge to the negative regression function for most distributions. In particular, the latter ERM is not consistent for most distributions, and even worse, the obtained risks are usually far off the best possible risk. We further construct modifications that enjoy minimax optimal rates of convergence up to some log factor under standard assumptions. In addition, there are also ERM algorithms that exhibit an intermediate behavior between these two extreme cases, with arbitrarily slow convergence. To put this in perspective, we note that classical SLT shows that for sufficiently small hypotheses classes, all versions of ERM enjoy good statistical guarantees. In contrast, our results demonstrate that this is no longer true for large hypotheses classes. For such hypotheses spaces, the description “ERM” is thus not sufficient to identify well-behaving learning algorithms. Instead, the class of algorithms described by “ERM” over such hypotheses spaces may encompass learning algorithms with extremely distinct learning behavior.

Second, we show that exactly the same phenomena occur for interpolating ReLU-DNNs of at least two hidden layers with widths growing linearly in both input dimension \( d \) and sample size \( n \). We present DNN training algorithms that produce interpolating predictors
and that enjoy consistency and optimal rates, at least up to some log factor. In addition, this training can be done in $O(d^2 \cdot n^2)$-time if the DNNs are implemented as fully connected networks. Since the constructed predictors have a particularly sparse structure, the training time can actually be reduced to $O(d \cdot n \cdot \log n)$ by implementing the DNNs as loosely connected networks. Moreover, we show that there are other efficient and feasible training algorithms for exactly the same architectures that fail in the worst possible sense, and like in the ERM case, there are also a variety of training algorithms performing in between these two extreme cases.

The rest of the paper is organized as follows: In Section 2 we firstly recall classical histograms as ERMs that we extend then to the class of inflated histograms. We provide specific examples of interpolating predictors from that class. In our main theorems we derive consistency results and learning rates. In the following Section 3 we explain how inflated histograms can be approximated by ReLU networks, having analogous learning properties. All our proofs are deferred to the Appendices A, B, C, and D. Finally, in the supplementary material E we derive general uniform bounds for histograms based on data-dependent partitions. This result is needed for proving our main results and is of independent interest.

2 The histogram rule revisited

In this section we reconsider the histogram rule in the framework of regression. In more detail, we recall the classical histogram rule and show how to change this appropriately in order to obtain a predictor that is able to interpolate given data. To this end, let us begin by introducing the necessary notations. Throughout this work, we consider $X := [-1,1]^d$ and $Y = [-1,1]$ if not specified otherwise. Moreover, $L : Y \times \mathbb{R} \to [0, \infty)$ denotes the least squares loss $L(y,t) = (y-t)^2$. Given a dataset $D := ((x_1,y_1),\ldots,(x_n,y_n)) \in (X \times Y)^n$ drawn i.i.d. from an unknown distribution $P$ on $X \times Y$, the aim of supervised learning is to build a function $f_D : X \to \mathbb{R}$ based on $D$ such that its risk

$$R_{L,P}(f_D) := \int_{X \times Y} L(y, f_D(x)) \, dP(x,y),$$

is close to the smallest possible risk

$$R^*_L = \inf_{f : X \to \mathbb{R}} R_{L,P}(f).$$

In the following, $R^*_{L,P}$ is called the Bayes risk and an $f^*_{L,P} : X \to \mathbb{R}$ satisfying $R_{L,P}(f^*_{L,P}) = R^*_{L,P}$ is called Bayes decision function. Recall, that for the least squares loss, $f^*_{L,P}$ equals the conditional mean function, i.e. $f^*_{L,P}(x) = \mathbb{E}_P(Y|x)$ for $P_X$-almost all $x \in X$, where $P_X$ denotes the marginal distribution of $P$ on $X$. In general, estimators $f_D$ having small excess risk

$$R_{L,P}(f_D) - R^*_{L,P} = \|f_D - f^*_{L,P}\|_{L^2(P_X)}^2,$$

where $\| \cdot \|_{L^2(P_X)}$ denotes the usual $L_2$-norm with respect to $P_X$, are considered as good in classical statistical learning theory.

Now, to describe the class of learning algorithms we are interested in, we need the empirical risk of an $f : X \to \mathbb{R}$, i.e.

$$R_{L,D}(f) := \frac{1}{n} \sum_{i=1}^n L(y_i, f(x_i)).$$
Recall, that an empirical risk minimizer (ERM) over some set $\mathcal{F}$ of functions $f : X \rightarrow \mathbb{R}$ chooses, for every data set $D$, an $f_D \in \mathcal{F}$ that satisfies
\[ R_{L,D}(f_D) = \inf_{f \in \mathcal{F}} R_{L,D}(f). \]

Note that the definition of ERMs implicitly requires that the infimum on the right hand side is attained, namely by $f_D$. In general, however, $f_D$ does not need to be unique. It is well-known that if we have a suitably increasing sequence of hypotheses classes $\mathcal{F}_n$ with controlled capacity, then every ERM $D \mapsto f_D$ that ensures $f_D \in \mathcal{F}_n$ for all data sets $D$ of length $n$ learns in the sense of e.g. universal consistency, and under additional assumptions it may also enjoy minmax optimal learning rates, see e.g. [8, 22, 10, 19].

### 2.1 Classical Histograms

Particular simple ERMs are histogram rules (HRs). To recall the latter, we fix a finite partition $A = (A_j)_{j \in J}$ of $X$ and for $x \in X$ we write $A(x)$ for the unique cell $A_j$ with $x \in A_j$. Moreover, we define
\[ \mathcal{H}_A := \left\{ \sum_{j \in J} c_j 1_{A_j} : c_j \in Y \right\}, \tag{4} \]

where $1_{A_j}$ denotes the indicator function of the cell $A_j$. Now, given a data set $D$ and a loss $L$ an $A$-histogram is an $h_{D,A} = \sum_{j=1}^m c_j^* 1_{A_j} \in \mathcal{H}_A$ that satisfies
\[ \sum_{i : x_i \in A_j} L(x_i, y_i, c_j^*) = \inf_{c \in Y} \sum_{i : x_i \in A_j} L(x_i, y_i, c) \tag{5} \]

for all, so-called non-empty cells $A_j$, that is, cells $A_j$ with $N_j := |\{i : x_i \in A_j\}| > 0$. Clearly, $D \mapsto h_{D,A}$ is an ERM. Moreover, note that in general $h_{D,A}$ is not uniquely determined, since $c_j^* \in Y$ can take arbitrary values for empty cells $A_j$. In particular, there are more than one ERM over $\mathcal{H}_A$ as soon as $m, n \geq 2$.

Before we proceed, let us consider the specific example of the least squares loss in more detail. Here, a simple calculation shows, see Lemma A.1, that for all non-empty cells $A_j$, the coefficient $c_j^*$ in (5) is uniquely determined by
\[ c_j^* := \frac{1}{N_j} \sum_{i : x_i \in A_j} y_i \tag{6} \]

provided that $Y$ is convex. In the following, we call every resulting $D \mapsto h_{D,A}$ with
\[ h_{D,A} := \sum_{j=1}^m c_j^* 1_{A_j} \in \mathcal{H}_A \]

an empirical HR for regression with respect to the least-squares loss $L$. For later use we also introduce an infinite sample version of a classical histogram
\[ h_{P,A} := \sum_{j \in J} c_j^* 1_{A_j}, \quad \text{ where } \quad c_j^* := \frac{1}{P_X(A_j)} \int_{A_j} f_{L,P}^*(x) dP_X(x) \tag{7} \]
for all cells $A_j$ with $P_X(A_j) > 0$. Similarly to empirical histograms one has

$$\mathcal{R}_{L,P}(h_{P,A}) = \inf_{h \in \mathcal{H}_A} \mathcal{R}_{L,P}(h).$$

We are mostly interested in HRs on $X = [-1, 1]^d$ whose underlying partition essentially consists of cubes with a fixed width. To rigorously deal with boundary effects, we first say that a partition $(B_j)_{j \geq 1}$ of $\mathbb{R}^d$ is a cubic partition of width $s > 0$, if each cell $B_j$ is a translated version of $[0, s]^d$, i.e. there is an $x^\dagger \in \mathbb{R}^d$ called offset such that for all $j \geq 1$ there exist $k_j := (k_1, \ldots, k_d) \in \mathbb{Z}^d$ with

$$B_j = x^\dagger + sk_j + [0, s)^d.$$ \hfill (8)

Now, a partition $\mathcal{A} = (A_j)_{j \in J}$ of $X = [-1, 1]^d$ is called a cubic partition of width $s > 0$, if there is a cubic partition $\mathcal{B} = (B_j)_{j \geq 1}$ of $\mathbb{R}^d$ with width $s > 0$ such that $J = \{ j \geq 1 : B_j \cap X \neq \emptyset \}$ and $A_j = B_j \cap X$ for all $j \in J$. If $s \in (0, 1]$, then, up to reordering, this $(B_j)_{j \geq 1}$ is uniquely determined by $\mathcal{A}$.

If the hypotheses space $[\mathcal{H}]$ is based on a cubic partition of $X = [-1, 1]^d$ with width $s > 0$, then the resulting HRs are well understood. For example, universal consistency and learning rates have been established, see e.g. [8, 10]. In general, these results only require a suitable choice for the widths $s_n$, for $n \to \infty$ but no specific choice of the cubic partition of width $s$. For this reason we write $\mathcal{H}_s := \bigcup \mathcal{H}_A$, where the union runs over all cubic partitions $\mathcal{A}$ of $X$ with fixed width $s \in (0, 1]$.

2.2 Interpolating Predictors and Inflated Histograms

In this section we construct particular interpolating ERMs. In a nutshell, the basic idea is to first consider classical histogram rules, and then to inflate their hypotheses space so that we can find interpolating ERMs in these inflated hypotheses spaces.

**Definition 2.1** (Interpolating Predictor). We say that an $f : X \to Y$ interpolates $D$, if

$$\mathcal{R}_{L,D}(f) = \mathcal{R}_{L,D}^* := \inf_{f : X \to \mathbb{R}} \mathcal{R}_{L,D}(\tilde{f}),$$

where we emphasize that the infimum is taken over all $\mathbb{R}$-valued functions, while $f$ is required to be $Y$-valued.

Clearly, an $f : X \to Y$ interpolates $D$ if and only if

$$\sum_{k : x_k = x_i^*} L(x_i, y_i, f(x_i^*)) = \inf_{c \in \mathbb{R}} \sum_{k : x_k = x_i^*} L(x_i, y_i, c), \quad i = 1, \ldots, m,$$ \hfill (9)

where $x_1^*, \ldots, x_m^*$ are the elements of $D_X := \{ x_i : i = 1, \ldots, n \}$.

It is easy to check that for the least squares loss $L$ and all data sets $D$ there exists an $f_D^*$ interpolating $D$. Moreover, we have $\mathcal{R}_{L,D}^* > 0$ if and only if $D$ contains contradicting samples, i.e. $x_i = x_k$ but $y_i \neq y_k$. Finally, if $\mathcal{R}_{L,D}^* = 0$, then any interpolating $f_D^*$ needs to satisfy $f_D^*(x_i) = y_i$ for all $i = 1, \ldots, n$.

**Definition 2.2** (Interpolatable Loss). We say that $L$ is interpolatable for $D$ if there exists an $f : X \to Y$ that interpolates $D$, i.e. $\mathcal{R}_{L,D}(f) = \mathcal{R}_{L,D}^*$. 

5
Note that (9) in particular ensures that the infimum over \( \mathbb{R} \) on the right is attained at some \( c^*_j \in Y \). Many common losses including the least squares, the hinge, and the classification loss interpolate all \( D \), and for the latter three losses we have \( \mathcal{R}^*_{L,D} > 0 \) if and only if \( D \) contains contradicting samples, i.e. \( x_i = x_k \) but \( y_i \neq y_k \). Moreover, for the least squares loss, \( c_i^* \) can be easily computed by averaging over all labels \( y_k \) that belong to some sample \( x_k \) with \( x_k = x_i \).

Let us now describe more precisely the inflated versions of \( \mathcal{H}_s \). For \( r, s > 0 \) and \( m \geq 0 \) we want to consider functions

\[
f = h + \sum_{i=1}^{m} b_i 1_{x_i^* + tB_{\infty}}
\]

with \( h \in \mathcal{H}_s, b_i \in 2Y, x_i^* \in X, \) and \( t \in [0, r] \), where \( B_{\infty} := [-1, 1]^d \). In other words, for \( m \geq 1 \), such an \( f \) changes a classical histogram \( h \in \mathcal{H}_s \) on at most \( m \) small neighborhoods of some arbitrary points \( x_1^*, \ldots, x_m^* \) in \( X \). Such changes are useful for finding interpolating predictors. In general, these small neighborhoods \( x_i^* + tB_{\infty} \) however may intersect and may be contained in more than one cell \( A_j \) of the considered partition \( \mathcal{A} \) with \( h \in \mathcal{H}_A \). To avoid undesired boundary effects we restrict the class of all admissible cubic partitions \( \mathcal{A} \) of \( X \) associated with \( h \). An additional technical difficulty arises in particular when constructing interpolating predictors since the set of points \( \{x_1^*, \ldots, x_m^*\} \subset X \) are naturally the random input variables. As a consequence, the admissible cubic partitions become data-dependent.

As a next step, we introduce the notion of a partitioning rule. To this end, we write

\[
\text{Pot}_m(X) := \{ A \subset X : |A| = m \}
\]

for the set of all subsets of \( X \) having cardinality \( m \). Moreover, we denote the set of all finite partitions of \( X \) by \( \mathcal{P}(X) \).

**Definition 2.3.** Given an integer \( m \geq 1 \), an \( m \)-sample partitioning rule for \( X \) is a map \( \pi_m : \text{Pot}_m(X) \to \mathcal{P}(X) \), i.e. a map that associates to every subset \( \{x_1^*, \ldots, x_m^*\} \subset X \) of cardinality \( m \) a finite partition \( \mathcal{A} \). Additionally, we will call an \( m \)-sample partitioning rule that assigns to any such \( \{x_1^*, \ldots, x_m^*\} \in \text{Pot}_m(X) \) a cubic partition with fixed width \( s \in (0, 1] \) an \( m \)-sample cubic partitioning rule and write \( \pi_{m,s} \).

Next we explain in more detail which particular partitions are considered as admissible.

**Definition 2.4 (Proper Alignment).** Let \( \mathcal{A} \) be a cubic partition of \( X \) with width \( s \in (0, 1] \), \( \mathcal{B} \) be the partition of \( \mathbb{R}^d \) that defines \( \mathcal{A} \), and \( r \in (0, s) \). We say that \( \mathcal{A} \) is properly aligned to the set of points \( \{x_1^*, \ldots, x_m^*\} \in \text{Pot}_m(X) \) with parameter \( r \), if for all \( i, k = 1, \ldots, m \) we have

\[
\begin{align*}
x_i^* + rB_{\infty} & \subset B(x_i^*), \\
x_i^* + rB_{\infty} \cap x_k^* + rB_{\infty} &= \emptyset \quad \text{whenever } i \neq k,
\end{align*}
\]

where \( B(x_i^*) \) is the unique cell\(^1\) of \( \mathcal{B} \) that contains \( x_i^* \).

\(^1\)Note that this gives \( A(x_i^*) = B(x_i^*) \cap X \).
cubic partition $\mathcal{A}$ of $X$ with width $s > 0$ is properly aligned with the parameter $r = 0$ for any set of points $\{x_j^*\}_{j=1}^m$ in $\text{Pot}_m(X)$.

In what follows, we establish the existence of cubic partitions $\mathcal{A}$ that are properly aligned to a given set of points with parameter $r > 0$ being sufficiently small. In other words, we construct a special $m$-sample cubic partitioning rule $\pi_{m,s}$. We call henceforth any such rule $\pi_{m,s}$ an $m$-sample properly aligned cubic partitioning rule. To this end, let $D_X := \{x_1^*,...,x_m^*\} \in \text{Pot}_m(X)$ be a set points and note that (12) holds for all $r > 0$ satisfying

$$r < \frac{1}{2} \min_{i,k: i \neq k} \|x_i^* - x_k^*\|_\infty.$$ 

Clearly, a brute-force algorithm finds such an $r$ in $\mathcal{O}(dm^2)$-time. However, a smarter approach is to first sort the first coordinates $x_{1,1}^*,...,x_{m,1}^*$ and to determine the smallest positive distance $r_1$ of two consecutive, non-identical ordered coordinates. This approach is then repeated for the remaining $d - 1$-coordinates, so at the end we have $r_1,\ldots,r_d > 0$. Then

$$r^* := r^*_{D_X} : = \frac{1}{3} \min\{r_1,\ldots,r_d\}$$

satisfies (12) and the used algorithm is $\mathcal{O}(d \cdot m \log m)$ in time. Our next result shows that we can also ensure (11) by jiggling the cubic partitions. Being rather technical, the proof is deferred to the Appendix [B]

**Theorem 2.5** (Existence of Properly Aligned Cubic Partitioning Rule). For all $d \geq 1$, $s \in (0,1]$, and $m \geq 1$ there exist an $m$-sample cubic partitioning rule $\pi_{m,s}$ with $|\text{Im}(\pi_{m,s})| \leq (m + 1)^d$ that assigns to each set of points $D_X := \{x_1^*,...,x_m^*\} \in \text{Pot}_m(X)$ a cubic partition $\mathcal{A}$ that is properly aligned to $\{x_1^*,...,x_m^*\}$ with parameter $r := r_{D_X} := \min\{r^*,\frac{s}{3m+3}\}$, where $r^* = r^*_{D_X}$ is defined in (13).

The construction of an $m$-sample cubic partitioning rule $\pi_{m,s}$ basically relies on the representation [8] of cubic partitions $\mathcal{B}$ of $\mathbb{R}^d$. In fact, the proof of Theorem 2.5 shows that there exists a finite set $x_{1,1}^*,...,x_{K}^* \in \mathbb{R}^d$ of candidate offsets, with $K = (m + 1)^d$. While at first glance this number seems to be prohibitively large for an efficient search, it turns out that the proof of Theorem 2.5 actually provides a simple algorithm that is $\mathcal{O}(d \cdot m)$ in time for identifying coordinate-wise the $x_k^*$ that leads to $\pi_{m,s}(\{x_1^*,...,x_m^*\})$.

Being now well prepared, we introduce the class of inflated histograms.

**Definition 2.6.** Let $s \in (0,1]$ and $m \geq 1$. Then a function $f : X \rightarrow Y$ is called an $m$-inflated histogram of width $s$, if there exist a subset $\{x_1^*,...,x_m^*\} \in \text{Pot}_m(X)$ and a cubic partition $\mathcal{A}$ of width $s$ that is properly aligned to $\{x_1^*,...,x_m^*\}$ with parameter $r \in [0,s)$ such that

$$f = h + \sum_{i=1}^{m} b_i 1_{x_i^*+tB_{\infty}},$$

where $h \in \mathcal{H}_A$, $t \in [0,r]$, and $b_i \in 2Y$ for all $i = 1,\ldots,m$. We denote the set of all $m$-inflated histograms of width $s$ by $\mathcal{F}_{s,m}$. Moreover, for $n \geq 1$ we write

$$\mathcal{F}_{s,n} := \mathcal{F}_{s,1} \cup \cdots \cup \mathcal{F}_{s,n}.$$
Figure 1: Left. Depiction of an inflated histogram for regression for a cubic partition \( \mathcal{A} = (A_j)_{j \in J} \) that is not properly aligned to the data (black crosses). The predictions \( c^*_i \) and \( c^*_j \) on the associated cells \( A_i \) and \( A_j \) are calculated according to (6), i.e. by a local average. Mispredicted samples are corrected according to (14) on a \( tB_\infty \)-neighborhood for some small \( t > 0 \). Note that one sample is too close to the cell boundary, i.e. (11) is violated. Right. An inflated histogram that is properly aligned to the same data set. Note that (11) ensures that boundary effects as for the left HR do not take place. For inflated histograms these effects seem to be a negligible technical nuisance. For their DNN counterparts considered in Section 3, however, such effects may significantly complicate the constructions of interpolating predictors, see Figure 2.

Note that the condition \( t \leq r < s \) ensures that the representation \( f = h + \sum_{i=1}^{m} b_i 1_{x^*_i + tB_\infty} \) of any \( f \in \mathcal{F}_{s,m} \) is unique. In addition, given an \( f \in \mathcal{F}_{s,n} \), the number \( m \) of inflation points \( \{x^*_1, \ldots, x^*_m\} \) is uniquely determined, too, and hence so is the representation of \( f \).

So far we have formalized the notion of interpolation and defined an appropriate inflated hypotheses class for modified histograms. In our next result we go a step further by providing a sufficient condition for the existence of interpolating predictors in \( \mathcal{F}_{s,m} \).

**Proposition 2.7.** Let \( L \) be a loss that is interpolatable for \( D = ((x_1, y_1), \ldots, (x_n, y_n)) \) and let \( x^*_1, \ldots, x^*_m \) be as in (9). Moreover, for \( s \in (0, 1] \) and \( r > 0 \) we fix an \( f^* \in \mathcal{F}_{s,m} \) with representation as given in Definition 2.6. For \( i = 1, \ldots, m \) let \( j_i \) be the index such that \( x^*_i \in A_{j_i} \). Then \( f^* \) interpolates \( D \), if for all \( i = 1, \ldots, m \) we have

\[
b_i = -c_{j_i} + \arg \min_{c \in \mathcal{Y}} \sum_{k : x_k = x^*_i} L(x_k, y_k, c).
\]
Proof of Proposition 2.7: By our assumptions we have
\[ c_i^*: = b_i + c_j \in \arg \min_{c \in Y} \sum_{k: x_k = x_i^*} L(x_k, y_k, c) = \arg \min_{c \in \mathbb{R}} \sum_{k: x_k = x_i^*} L(x_k, y_k, c), \]
where the last equality is a consequence of the fact that there is an \( f : X \rightarrow Y \) satisfying \( 9 \). Moreover, since \( 11 \) and \( 12 \) hold, we find \( f^*(x_i^*) = h(x_i^*) + b_i = c_j + b_i = c_i^* \), and therefore \( f^* \) interpolates \( D \) by \( 9 \).

Note that for all \( c_j \in Y \) the value \( b_i \) given by \( 14 \) satisfies \( b_i \in 2Y \) and we have \( b_i = 0 \) if \( c_j \) is contained in the \( \arg \min \) in \( 14 \). Consequently, defining \( b_i \) by \( 14 \) always gives an interpolating \( f^* \in \mathcal{F}_{s,m} \). Moreover, \( 14 \) shows that an interpolating \( f^* \in \mathcal{F}_{s,m} \) can have an arbitrary histogram part \( h \in \mathcal{H}_A \), that is, the behavior of \( f^* \) outside the small \( tB_{\infty} \)-neighborhoods around the samples of \( D \) can be arbitrary. In other words, as soon as we have found a properly aligned cubic partition \( A \) in the sense of \( \mathcal{F}_{s,m} \), we can pick an arbitrary histogram \( h \in \mathcal{H}_A \) and compute the \( b_i \)'s by \( 14 \). Intuitively, if the chosen \( tB_{\infty} \)-neighborhoods are small, then the prediction capabilities of the resulting interpolating predictor are (mostly) determined by the chosen histogram part \( h \in \mathcal{H}_A \).

Based on this observation, we can now construct different, interpolating \( f_D^+ \in \mathcal{F}_{s,m} \) that have particularly good and bad learning behaviors.

**Example 2.8** (Good interpolating histogram rule). Let \( L \) be the least squares loss, \( s \in (0,1] \) be a cell width, \( \rho \geq 0 \) be an inflation parameter, and \( D = ((x_1, y_1), \ldots, (x_n, y_n)) \) be a data set. By \( D_X = \{x_1^*, \ldots, x_m^*\} \) we denote the set of all covariates \( x_j \in X \) with \((x_j, y_j)\) belonging to the data set. For \( m = |D_X| \), Theorem 2.5 ensures the existence of a cubic partition \( A_D = \pi_{m,s}(D_X) \) with width \( s \in (0,1] \) being properly aligned to \( D_X \) with the data-dependent parameter \( r \). Based on this data-dependent cubic partition \( A_D \) we fix an empirical histogram for regression
\[ h_{D,A_D}^+ := \sum_{j \in J} c_j^+ \mathbf{1} A_j \in \mathcal{H}_s \]
with coefficients \( (c_j^+)_{j \in J} \) precisely given by \( 9 \). Applying now Proposition 2.7 gives us an \( f_{D,s,\rho}^+ \in \mathcal{F}_{s,m} \subset \mathcal{F}_{s,n} \), which interpolates \( D \) and has the representation
\[ f_{D,s,\rho}^+ := h_{D,A_D}^+ + \sum_{i=1}^m b_i^+ \mathbf{1}_{x_i^*} + tB_{\infty}, \]
where the \( b_1^+, \ldots, b_m^+ \) are calculated according to the rule \( 14 \), and \( t := \min\{r, \rho\} \) is again data-dependent. We call the map \( D \mapsto f_{D,s,\rho}^+ \) a good interpolating histogram rule.

**Example 2.9** (Bad interpolating histogram rule). Let \( L \) be the least squares loss, \( s \in (0,1] \) be a cell width, \( \rho \geq 0 \) be an inflation parameter, and \( D = ((x_1, y_1), \ldots, (x_n, y_n)) \) be a data set. Consider again a cubic partition \( A_D = \pi_{m,s}(D_X) \) with width \( s \in (0,1] \), that is properly aligned to \( D_X \) with parameter \( r \) and fix an empirical histogram \( h_{D,A_D}^- \in \mathcal{H}_s \) as in \( 15 \). Setting \( t := \min\{r, \rho\} \), we define a predictor \( f_{D,s,\rho}^- \in \mathcal{F}_{s,m} \) by
\[ f_{D,s,\rho}^- := h_{D,A_D}^- + \sum_{i=1}^m b_i^- \mathbf{1}_{x_i^*} + tB_{\infty}, \]
with \( \mathcal{H}_A \)-part \( h_{D,A_D}^- := -h_{D,A_D}^+ \). The \( b_1^-, \ldots, b_m^- \) are calculated according to \( 14 \) and satisfy
\[ b_i^- = b_i^+ + 2c_j^+ \]
for any \(i = 1, \ldots, m\) and where \(j_i\) denotes the index such that \(x_i^* \in A_{j_i}\). By writing

\[
D_X^{+t} := \bigcup_{i=1}^{m} (x_i^* + tB_{\infty})
\]

we easily see that the definition of \(f_{D,s,\rho}^\dagger\) gives \(f_{D,s,\rho}^\dagger \in \mathcal{F}_{s,m} \subset \mathcal{F}_{s,\infty}^\ast\) and

\[
f_{D,s,\rho}^\dagger(x) = \begin{cases} 
  f_{D,s,\rho}^\dagger(x) & \text{if } x \in D_X^{+t} \\
  -f_{D,s,\rho}^\dagger(x) & \text{if } x \notin D_X^{+t},
\end{cases}
\]

while Proposition \[2.7\] ensures that \(f_{D,s,\rho}^\dagger\) interpolates \(D\). We call the map \(D \mapsto f_{D,s,\rho}^\dagger\) a bad interpolating histogram rule and remark that it is, like for good interpolating histogram rules, data-dependent.

Our main results below show that the description good/ bad interpolating histogram rule from the above Examples \[2.8/2.9\] respectively, is indeed justified, provided the inflation parameter is chosen appropriately. Here we recall that good learning algorithms can be described by a small excess risk, or equivalently, a small distance to the Bayes decision function \(f_{L,P}^\ast\), see \([3]\). To describe bad learning behavior, we denote the point spectrum of \(P_X\) by

\[
\Delta := \{ x \in X : P_X(\{x\}) > 0 \},
\]

see \([1]\). One easily verifies that \(\Delta\) is at most countable, since \(P_X\) is finite. Moreover, for an arbitrary but fixed version \(f_{L,P}^\ast\) of the Bayes decision function, we write

\[
f_{L,P}^\dagger := 1_{\Delta} f_{L,P}^\ast - 1_{X \setminus \Delta} f_{L,P}^\ast \quad \text{and} \quad \mathcal{R}_{L,P}^\dagger := \mathcal{R}_{L,P}(f_{L,P}^\dagger),
\]

where we note that \(\mathcal{R}_{L,P}^\dagger\) does, of course, not depend on the choice of \(f_{L,P}^\ast\). Moreover, note that for \(x \notin \Delta\) the value \(f_{L,P}^\dagger(x)\) is also independent of the choice of \(f_{L,P}^\ast\) and it holds \(f_{L,P}^\dagger(x) = f_{L,P}^\ast(x)\). In contrast, for \(x \in X \setminus \Delta\) with \(f_{L,P}^\ast(x) \neq 0\) we have \(f_{L,P}^\dagger(x) \neq f_{L,P}^\ast(x)\). In fact, a quick calculation using \([3]\) shows

\[
\mathcal{R}_{L,P}^\dagger - \mathcal{R}_{L,P}^\ast = \|f_{L,P}^\dagger - f_{L,P}^\ast\|^2_{L_2(P_X)} = 4\|1_{X \setminus \Delta} f_{L,P}^\ast\|^2_{L_2(P_X)},
\]

and consequently we have \(\mathcal{R}_{L,P}^\dagger - \mathcal{R}_{L,P}^\ast > 0\) whenever \(P_X(\Delta) < 1\) and \(f_{L,P}^\dagger\) does not almost surely vanish on \(X \setminus \Delta\). It seems fair to say that the overwhelming majority of “interesting” \(P\) fall into this category. Finally, note that in general we do not have an equality of the form \([3]\), when we replace \(\mathcal{R}_{L,P}^\ast\) and \(f_{L,P}^\dagger\) by \(\mathcal{R}_{L,P}^\dagger\) and \(f_{L,P}^\dagger\). However, for \(y,t,t' \in Y = [-1,1]\) we have \(|L(y,t) - L(y,t')| \leq 4|t - t'|\), and consequently we find

\[
|\mathcal{R}_{L,P}(f) - \mathcal{R}_{L,P}^\dagger| \leq 4 \|f - f_{L,P}^\dagger\|_{L_2(P_X)}
\]

for all \(f : X \to Y\). For this reason, we will investigate the bad interpolating histogram rule only with respect to its \(L_2\)-distance to \(f_{L,P}^\dagger\).

Before the state our main result of this section we need to introduce one more assumption that will be required for parts of our results.

**Assumption 2.10.** There exists a non-decreasing continuous map \(\varphi : \mathbb{R}_+ \to \mathbb{R}_+\) with \(\varphi(0) = 0\) such that for any \(t \geq 0\) and \(x \in X\) one has \(P_X(x + tB_{\infty}) \leq \varphi(t)\).
Note that this assumption implies $P_X(\{x\}) = 0$ for any $x \in X$. Moreover, it is satisfied for the uniform distribution $P_X$, if we consider $\phi(t) := 2^{d\beta}$, and a simple argument shows that modulo the constant appearing in $\phi$ the same is true if $P_X$ only has a bounded Lebesgue density. The latter is, however, not necessary. Indeed, for $X = [-1, 1]$ and $0 < \beta < 1$ it is easy to construct unbounded Lebesgue densities that satisfy Assumption $2.10$ for $\phi$ of the form $\phi(t) = ct^\beta$, and higher dimensional analogs are also easy to construct. Moreover, in higher dimensions Assumption $2.10$ also applies to various distributions living on sufficiently smooth low-dimensional manifolds.

With these preparations we can now establish the following theorem that shows that for $\rho = 0$ the good interpolating histogram rule is universally consistent while the bad interpolating histogram rule fails to be consistent in a stark sense. It further shows consistency, respectively non-consistency for $\rho = \rho_n > 0$ with $\rho_n \to 0$.

**Theorem 2.11.** Let $L$ be the least-squares loss and let $D \in (X \times Y)^n$ be an i.i.d. sample of size $n \geq 1$. Let $D \mapsto f^+_{D,s,\rho}$ denote the good interpolating histogram rule from Example $2.8$. Similarly, let $D \mapsto f^-_{D,s,\rho}$ denote the bad interpolating histogram rule from Example $2.9$. Assume that $(s_n)_{n \in \mathbb{N}}$ is a sequence with $s_n \to 0$ as well as $\frac{\ln(n)}{ns_n} \to 0$ as $n \to \infty$.

i) (Non)-consistency for $\rho_n = 0$. We have in probability for $|D| \to \infty$

\[
\|f^+_{D,s_n,0} - f^*_{L,P}\|_{L_2(P_X)} \to 0, \tag{21}
\]

\[
\|f^-_{D,s_n,0} - f^*_{L,P}\|_{L_2(P_X)} \to 0. \tag{22}
\]

ii) (Non)-consistency for $\rho_n > 0$. Let $(\rho_n)_{n \in \mathbb{N}}$ be a non-negative sequence with $\rho_n \to 0$ as $n \to \infty$. Then for all distributions $P$ that satisfy Assumption $2.10$ for a function $\varphi$ with $n\varphi(\rho_n) \to 0$ for $n \to \infty$, we have

\[
\|f^+_{D,s_n,\rho_n} - f^*_{L,P}\|_{L_2(P_X)} \to 0, \tag{23}
\]

\[
\|f^-_{D,s_n,\rho_n} - f^*_{L,P}\|_{L_2(P_X)} \to 0. \tag{24}
\]

in probability for $|D| \to \infty$.

The proof of Theorem $2.11$ is provided in Appendix $C.2$. Our second main result, whose proof is provided in Appendix $C.3$, refines the above theorem and establishes learning rates for the good and bad interpolating histogram rules, provided the width $s_n$ and the inflation parameter $\rho_n$ decrease sufficiently fast as $n \to \infty$.

**Theorem 2.12** (Learning Rates). Let $L$ be the least-squares loss and let $D \in (X \times Y)^n$ be an i.i.d. sample of size $n \geq 1$. Let $D \mapsto f^+_{D,s,\rho}$ denote the good interpolating histogram rule from Example $2.8$. Similarly, let $D \mapsto f^-_{D,s,\rho}$ denote the bad interpolating histogram rule from Example $2.9$. Suppose that $f^*_{L,P}$ is $\alpha$-Hölder continuous with $\alpha \in (0, 1]$ and that $P$ satisfies Assumption $2.10$ for some function $\varphi$. Assume further that $(s_n)_{n \in \mathbb{N}}$ is a sequence with

\[
s_n = n^{-\gamma}, \quad \gamma = \frac{1}{2\alpha + d}
\]

and that $(\rho_n)_{n \geq 1}$ is a non-negative sequence with $n\varphi(\rho_n) \leq \ln(n)n^{-2/3}$ for all $n \geq 1$. Then there exists a constant $c_{d,\alpha} > 0$ only depending on $d$, $\alpha$, and $f^*_{L,P}|_{\alpha}$, such that for all $n \geq 1$ the good interpolating histogram rule satisfies

\[
\|f^+_{D,s_n,\rho_n} - f^*_{L,P}\|_{L_2(P_X)} \leq c_{d,\alpha} \sqrt{\frac{\ln(n)}{n}} \left(\frac{1}{n}\right)^{\alpha \gamma}, \tag{25}
\]
with probability $P_n$ not less than $1 - 2^d n^{1+d} e^{-nd^\gamma}$. Furthermore, for all $n \geq 1$, the bad interpolating histogram rule satisfies

$$\|f_{D, s_n, \rho_n} - f_{l_P}^\dagger\|_{L_2(P_X)} \leq c_{\alpha, d} \sqrt{\ln(n)} \left( \frac{1}{n} \right)^{\alpha \gamma}.$$  \hspace{1cm} (26)$$

with probability $P_n$ not less than $1 - 2^d n^{1+d} e^{-nd^\gamma}$.

To set the results above in context, let us first recall that even for a fixed hypotheses class, ERM is, in general, not a single algorithm, but a collection of algorithms. In fact, this ambiguity appears, as soon as the ERM-optimization problem has not a unique solution for certain data sets, and as Lemma A.1 shows, this non-uniqueness may even occur for strictly convex loss functions such as the least squares loss. Now, the standard techniques of statistical learning theory are capable of showing that for sufficiently small hypotheses classes, all versions of ERM enjoy good statistical guarantees. In other words, the non-uniqueness of ERM does not affect its learning capabilities as long as the hypotheses class is sufficiently small. In addition, it is folklore that in some large hypotheses classes, there may be heavily overfitting ERM solutions, leading to the usual conclusion that such hypotheses classes should be avoided.

In contrast to this common wisdom, however, Theorem 2.11 demonstrates that for large hypotheses classes, the situation may be substantially more complicated: First, it shows that there exist ERMs, whose predictors converge to a function $f_{l_P}^\dagger$, see (22), that in almost all interesting cases is far off the target regression function, see (19), confirming that the overfitting issue is indeed present for the chosen hypotheses classes. Moreover, this strong overfitting may actually take place with fast convergence, see (26). Despite this negative result, however, we can also find ERMs that enjoy a good learning behavior in terms of consistency (21) and almost optimal learning rates (25). In other words, both the expected overfitting and standard learning guarantees may be realized by suitable versions of ERM over these hypotheses classes. In fact, these two different behaviors are just extreme examples, and a variety of intermediate behaviors are possible, too: Indeed, as the training error can be solely controlled by the corrections on the inflating parts, the behaviour of the histogram part $h$ can be arbitrarily chosen. For our theorems above, we have chosen a particular good and bad $h$-part, respectively, but of course, a variety of other choices leading to intermediate behavior are also possible. As a consequence, the ERM property of an algorithm working with a large hypotheses class is, in general, no longer a sufficient notion for describing its learning behavior. Instead, additional assumptions are required to determine its learning behavior. In this respect we also note that for our inflated hypotheses classes, other learning algorithms that do not (approximately) minimize the empirical risk may also enjoy good learning properties. Indeed, by setting the inflating parts to zero, we recover standard histograms, which in general do not have close-to-zero training error, but for which the guarantees of our good interpolating predictors also hold true.

Of course, the chosen hypotheses classes may, to some extent, appear artificial. Nonetheless, in the following section they will be key for showing that for sufficiently large DNN architectures exactly the same phenomena occur for some of their global minima.

3 Approximation of histograms with ReLU networks

The goal of this section is to build neural networks of suitable depth and width that mimic the learning properties of inflated histogram rules. To be more precise, we aim to construct
a particular class of inflated networks that contains good and bad interpolating predictors, similar to the good and bad interpolating histogram rules from Example 2.8 and Example 2.9, respectively.

We begin with describing in more detail the specific networks that we will consider. Given an activation function $\sigma : \mathbb{R} \to \mathbb{R}$ and $b \in \mathbb{R}^p$ we define the shifted activation function $\sigma_b : \mathbb{R}^p \to \mathbb{R}^p$ as

$$\sigma_b(y) := (\sigma(y_1 + b_1), \ldots, \sigma(y_p + b_p))^T.$$

A hidden layer with activation $\sigma$, of width $p \in \mathbb{N}$ and with input dimension $q \in \mathbb{N}$ is a function $H_\sigma : \mathbb{R}^q \to \mathbb{R}^p$ of the form

$$H_\sigma(x) := (\sigma \circ A)(x), \quad x \in \mathbb{R}^q,$$

where $A$ is a $p \times q$ weight matrix and $b \in \mathbb{R}^p$ is a shift vector or bias. Clearly, each pair $(A,b)$ describes a layer, but in general, a layer, if viewed as a function, can be described by more than one such pair. The class of networks we consider is given in the following definition.

**Definition 3.1.** Given an activation function $\sigma : \mathbb{R} \to \mathbb{R}$ and an integer $L \geq 1$, a neural network with architecture $p \in \mathbb{N}_L^{L+1}$ is a function $f : \mathbb{R}^{p_0} \to \mathbb{R}^{p_L}$, having a representation of the form

$$f(x) = H_{id,L} \circ H_{\sigma_{L-1}} \circ \cdots \circ H_{\sigma_1}(x), \quad x \in \mathbb{R}^{p_0},$$

where $H_{\sigma_l} : \mathbb{R}^{p_{l-1}} \to \mathbb{R}^{p_l}$ is a hidden layer of width $p_l \in \mathbb{N}$ and input dimension $p_{l-1} \in \mathbb{N}$, $l = 1, \ldots, L - 1$. Here, the last layer $H_{id,L} : \mathbb{R}^{p_{L-1}} \to \mathbb{R}^{p_L}$ is associated to the identity id : $\mathbb{R} \to \mathbb{R}$.

A network architecture is therefore described by an activation function $\sigma$ and a width vector $p = (p_0, \ldots, p_L) \in \mathbb{N}_L^{L+1}$. The positive integer $L$ is the number of layers, $L - 1$ is the number of hidden layers or the depth. Here, $p_0$ is the input dimension and $p_L$ is the output dimension. In the sequel, we confine ourselves to the ReLU-activation function $| \cdot |_+ : \mathbb{R} \to [0, \infty)$ defined by

$$|t|_+ := \max\{0, t\}, \quad t \in \mathbb{R}.$$ 

Moreover, we consider networks with fixed input dimension $p_0 = d$ and output dimension $p_L = 1$, that is,

$$H_{id,L}(x) = \langle a, x \rangle + b, \quad x \in \mathbb{R}^{p_{L-1}}.$$ 

Thus, we may parameterize the (inner) architecture by the width vector $(p_1, \ldots, p_{L-1}) \in \mathbb{N}^{L-1}$ of the hidden layers only. In the following, we denote the set of all such neural networks by $\mathcal{A}_{p_1, \ldots, p_{L-1}}$.

### 3.1 \(\varepsilon\)-Approximate Inflated Histograms

Motivated by the representation \([1]\) for histograms, the first step of our construction approximates the indicator function of an multi-dimensional interval by a small part of a possibly large DNN. This will be our main building block. We emphasize that the ReLU activation function is particularly suited for this approximation and it thus plays a key role in our entire construction.

For the formulation of the corresponding result we fix some notation. For $z_1, z_2 \in \mathbb{R}^d$ we write $z_1 \leq z_2$ if each coordinate satisfies $z_{1,i} \leq z_{2,i}, \ i = 1, \ldots, d$. We define $z_1 < z_2$
Figure 2: Left. Approximation $1_A^{(ε)}$ (orange) of the indicator function $1_A$ for $A = [0.05, 0.45]$ (blue) according to Lemma 3.3 for $ε = 0.1$ on $X = [0, 1]$. The construction of $1_A^{(ε)}$ ensures that $1_A^{(ε)}$ coincides with $1_A$ modulo a small set that is controlled by $ε > 0$. Right. A DNN (orange) for regression that approximates the histogram $1_{[0,0.5]} + 0.8 \cdot 1_{[0.5,1]}$ and a DNN (green) that additionally tries to interpolate two samples $x_1 = 0.15$ and $x_2 = 0.975$ (located at the two vertical dotted lines) with $y_i = -0.5$. The label $y_1$ is correctly interpolated since the alignment condition (11) is satisfied for $x_1$ with $t = 0.15$ and $ε = δ = t/3 = 0.05$ as in Example 3.6. In contrast, $y_2$ is not correctly interpolated since condition (11) is violated for this $t$ and hence $ε$ and $δ$ are too large.

analogously. In addition, if $z_1 \leq z_2$, then the multi-dimensional interval is $[z_1, z_2] := \{z \in \mathbb{R}^d : z_1 \leq z \leq z_2\}$, and we similarly define $(z_1, z_2)$ if $z_1 < z_2$. Finally, for $s \in \mathbb{R}$, we let $z_1 + s := (z_{1,1} + s, \ldots, z_{1,d} + s)$.

**Definition 3.2** ($ε$-Approximation). Let $A \subset X$, $z_1, z_2 \in \mathbb{R}^d$ with $z_1 < z_2$ and $ε > 0$ with $ε < \min\{z_{2,i} - z_{1,i} : i = 1, \ldots, d\}$. Then a network $1_A^{(ε)} \in \mathcal{A}_{2d,1}$ is called an $ε$-Approximation of the indicator function $1_A : X \to [0, 1]$ if

$$\{1_A^{(ε)} = 1_A\} = [z_1 + ε, z_2 - ε] \cup (X \setminus A),$$

and if

$$\{1_A^{(ε)} > 1\} = \emptyset, \quad \{1_A^{(ε)} < 0\} = \emptyset.$$

The next lemma ensures the existence of such approximations. The full construction is elementary calculus and is provided in Appendix D.2 in particular in Lemma D.3. Lemma D.5 provides then the desired properties.

**Lemma 3.3** (Existence of $ε$-Approximations). Let $z_1, z_2 \in \mathbb{R}^d$ and $ε > 0$ as in Definition 3.2. Then for all $A \subset X$ with $[z_1 + ε, z_2 - ε] \subset A \subset [z_1, z_2]$ there exists an $ε$-Approximation $1_A^{(ε)}$ of $1_A$.

Figure 2 illustrates $1_A^{(ε)}$ for $d = 1$. Moreover, the proof of Lemma D.3 shows that out of the $2d^2$ weight parameters of the first layer, only $2d$ are non-zero. In addition, the $2d$ weight parameters of the neuron in the second layer are all identical. In order to approximate inflated histograms we need to know how to combine several functions of the form provided by Lemma 3.3 into a single neural network. An appealing feature of our DNNs is that the concatenation of layer structures is very easy.
Lemma 3.4. If $c \in \mathbb{R}$, $(p_1, p_2) \in \mathbb{N}^2$, and $g \in \mathcal{A}_p$, $g' \in \mathcal{A}_{p'}$, then $cg \in \mathcal{A}_p$ and $g + g' \in \mathcal{A}_{p+p'}$.

For an extended version of this result, see Lemma 4.2. In particular, our constructed DNNs have a particularly sparse structure and the number of required neurons behaves in a very controlled and natural fashion.

With these insights, we are now able to find a representation similar to (4). To this end, we choose a cubic partition $\mathcal{A} = (A_j)_{j \in J}$ of $X$ with width $s > 0$ and define for $\varepsilon \in (0, \frac{2}{3}]$

$$
\mathcal{H}_\varepsilon^{(e)} := \left\{ \sum_{j \in J} c_j 1_{A_j}^{(e)} : c_j \in Y \right\},
$$

where $1_{A_j}^{(e)} := (1_{B_j})_{|A_j}$ is the restriction of $1_{B_j}^{(e)}$ to $A_j$ and $1_{B_j}^{(e)}$ is an $\varepsilon$-approximation of $1_{B_j}$ of Lemma 3.3. Here, $B_j$ is the cell with $A_j = B_j \cap X$, see the text around (8). We call any function in $\mathcal{H}_\varepsilon^{(e)}$ an $\varepsilon$-approximate histogram.

Our considerations above show that we have $\mathcal{H}_\varepsilon^{(e)} \subset \mathcal{A}_{p_1,p_2}$ with $p_1 = 2d|J|$ and $m_2 = |J|$. Thus, any $\varepsilon$-approximate histogram can be represented by a neural network with 2 hidden layers. Inflated versions are now straightforward.

Definition 3.5. Let $s \in (0, 1]$, $m \geq 1$, and $\varepsilon \in (0, s/3]$. Then a function $f : X \to Y$ is called an $\varepsilon$-approximated $m$-inflated histogram of width $s$ if there exist a subset $\{x_1^*, ..., x_m^*\} \in \text{Pot}_m(X)$ and a cubic partition $\mathcal{A}$ of width $s$ that is properly aligned to $\{x_1^*, ..., x_m^*\}$ with parameter $r \in [0, s)$ such that

$$
f^{(e)} = h^{(e)} + \sum_{i=1}^{m} b_i 1_{x_i^*+tB_\infty}^{(s)},
$$

where $h^{(e)} \in \mathcal{H}_\varepsilon^{(e)}$, $t \in (0, r]$, $\delta \in (0, t/3]$, $b_i \in 2Y$ and where $1_{x_i^*+tB_\infty}^{(s)}$ is a $\delta$-approximation of $1_{x_i^*+tB_\infty}$ for all $i = 1, ..., m$. We denote the set of all $\varepsilon$-approximated $m$-inflated histograms of width $s$ by $\mathcal{F}_{s,m}^{(e)}$.

A short calculation shows that $\mathcal{F}_{s,m}^{(e)} \subset \mathcal{A}_{p_1,p_2}$ with $p_1 = 2d(m + |J|)$, $p_2 = m + |J|$ and $|J| \leq (2/s)^d$. With these preparations, we can now introduce good and bad interpolating DNNs.

Example 3.6 (Good and bad interpolating DNN). Let $L$ be the least squares loss, $s \in (0, 1]$ be a cell width and let $\rho > 0$ be an inflation parameter. For a data set $D = ((x_1, y_1), ..., (x_n, y_n))$ we consider again a cubic partition $\mathcal{A}_D = \pi_{m,s}(D_X)$, with $m = |D_X|$, being properly aligned to $D_X$ with parameter $r$. Set $t := \min\{r, \rho\}$. According to Example 2.8, a good interpolating HR is given by

$$
f_{D,s,\rho}^+ := \sum_{j \in J} c_j^+ 1_{A_j}^+ + \sum_{i=1}^{m} b_i^+ 1_{x_i^*+tB_\infty},
$$

where the $(c_j^+)_{j \in J}$ are given in (6) and $b_1^+, ..., b_m^+$ are from (14). For $\varepsilon := \delta := t/3$ we then define the good interpolating DNN by

$$
g_{D,s,\rho}^+ = \sum_{j \in J} c_j^+ 1_{A_j}^{(e)} + \sum_{i=1}^{m} b_i^+ 1_{x_i^*+tB_\infty}^{(s)}.\]
Clearly, we have \( g_{D,s,\rho}^\dagger \in \mathcal{F}^{(\xi)}_{s,m} \). We call the map \( D \mapsto g_{D,s,\rho}^\dagger \) a good interpolating DNN and it is easy to see that this network indeed interpolates \( D \). Finally, the bad interpolating DNN \( g_{D,s,\rho}^\ominus \) is defined analogously using the bad interpolating HR from Example 2.9 instead.

Similarly to our inflated histograms from the previous section, the next theorem shows that the good interpolating DNN is consistent while the bad interpolating DNN fails to be. The proof of this result is given in Appendix D.3.

**Theorem 3.7** ((Non)-consistency). Let \( L \) be the least-squares loss and let \( D \in (X \times Y)^n \) be an i.i.d. sample of size \( n \geq 1 \). Let \( D \mapsto g_{D,s,\rho}^\dagger \) denote the good interpolating DNN from Example 3.6. Similarly, let \( D \mapsto g_{D,s,\rho}^\ominus \) denote the bad interpolating DNN from Example 3.6. Assume that \((s_n)_{n \in \mathbb{N}}\) is a sequence with \( s_n \to 0 \), \( \frac{\ln(n)s_n^d}{n} \to 0 \) as \( n \to \infty \) as well as \( s_n > 2n^{-1/d} \). Additionally, let \((\rho_n)_{n \in \mathbb{N}}\) be a non-negative sequence with \( \rho_n \leq 2n^{-1/d} \). Then \( g_{D,s_n,\rho_n}^\dagger \in \mathcal{A}_{dn,2n} \). Moreover, for all distributions \( P \) that satisfy Assumption 2.18 for a function \( \varphi \) with \( \rho_n^{-d}\varphi(\rho_n) \to 0 \) for \( n \to \infty \), we have

\[
\|g_{D,s_n,\rho_n}^\dagger - f_{L,P}^*\|_{L_2(P_X)} \to 0, \\
\|g_{D,s_n,\rho_n}^\ominus - f_{L,P}^*\|_{L_2(P_X)} \to 0,
\]

in probability for \(|D| \to \infty \).

The above result can further be refined to establishing rates of convergence if the width \( s_n \) and the inflation parameter \( \rho_n \) converge to zero sufficiently fast as \( n \to \infty \). The proof is provided in Appendix D.4.

**Theorem 3.8** (Learning Rates). Let \( L \) be the least-squares loss and let \( D \in (X \times Y)^n \) be an i.i.d. sample of size \( n \geq 1 \). Let \( D \mapsto g_{D,s,\rho}^\dagger \) denote the good interpolating DNN from Example 3.6. Similarly, let \( D \mapsto g_{D,s,\rho}^\ominus \) denote the bad interpolating DNN from Example 3.6. Suppose that \( f_{L,P}^* \) is \( \alpha \)-Hölder continuous with \( \alpha \in (0,1] \) and that \( P \) satisfies Assumption 2.18 for some function \( \varphi \). Assume further that \((s_n)_{n \in \mathbb{N}}\) is a sequence with

\[
s_n = n^{-\gamma}, \quad \gamma = \frac{1}{2\alpha + d}
\]

and that \((\rho_n)_{n \geq 1}\) is a non-negative sequence with \( \rho_n \leq 2n^{-1/d} \) and \( \rho_n^{-d}\varphi(\rho_n) \leq \ln(n)n^{-2/3} \) for all \( n \geq 1 \). Then there exists a constant \( c_{d,\alpha} > 0 \) only depending on \( d \), \( \alpha \), and \( |f_{L,P}^*|_\alpha \), such that for all \( n \geq 2 \) the good interpolating histogram rule satisfies

\[
\|g_{D,s_n,\rho_n}^\dagger - f_{L,P}^*\|_{L_2(P_X)} \leq c_{d,\alpha}\sqrt{\ln(n)}\left(\frac{1}{n}\right)^{\alpha\gamma},
\]

with probability \( P^n \) not less than \( 1 - 2^{d}n^{1+d}e^{-n^{d\gamma}} \). Furthermore, for all \( n \geq 2 \), the bad interpolating histogram rule satisfies

\[
\|g_{D,s_n,\rho_n}^\ominus - f_{L,P}^*\|_{L_2(P_X)} \leq c_{d,\alpha}\sqrt{\ln(n)}\left(\frac{1}{n}\right)^{\alpha\gamma}.
\]

with probability \( P^n \) not less than \( 1 - 2^{d}n^{1+d}e^{-n^{d\gamma}} \). Finally, there exists a natural number \( n_{d,\alpha} > 0 \) such that for any \( n \geq n_{d,\alpha} \) we have \( g_{D,s_n,\rho_n}^\ominus \in \mathcal{A}_{4dn,2n} \).
Note that the rates of convergence in (32) and (33) remain true if we consider a sequence $s_n$ with $e^{-1}n^{-\gamma} \leq s_n \leq cn^{-\gamma}$ for some constant $c$ independent of $n$. In fact, the only reason why we have formulated Theorem 3.8 with $s_n = n^{-\gamma}$ is to avoid another constant appearing in the statements. Moreover, if we choose $s_n := 2a(n^{-\gamma})^{-1}$ with $a := 3^{1/d}/(3^{1/d} - 2)$, then we have $|J| \leq (2s_n^{-1} + 2)^d \leq (a^{-1}n^{1/d} + 2)^d \leq n$ for all $n \geq 3$. Consequently, for $m := n$, we can choose $n_{d,\alpha} := 3$, and hence we have $g_{D,s_n,\rho_n}^g \in A_{4dn,2n}$ for all $n \geq 3$ while (32) and (33) hold true modulo a change in the constant $c_{\alpha,d}$.

**Discussion of results.** To fully appreciate Theorems 3.7 and 3.8 as well as their underlying construction let us discuss its various consequences:

First, the good interpolating DNN predictors $g_{D,s_n,\rho_n}^g$ show that its is actually possible to train sufficiently large, over-parameterized DNNs such that they become consistent and enjoy optimal learning rates up to a logarithmic factor without adapting the network size to the particular smoothness of the target function. In fact, it suffices to consider DNNs with two hidden layers and $4dn$, respectively $2n$ neurons in the first, respectively second, hidden layer. In other words, Theorems 3.7 and 3.8 already apply to moderately over-parameterized DNNs, and by the particular properties of the ReLU-activation function, also for all larger network architectures. In addition, when using architectures of minimal size, training, that is constructing $g_{D,s_n,\rho_n}^g$, can be done in $O(d^2 \cdot n^2)$-time if the DNNs are implemented as fully connected networks. Moreover, the constructed DNNs have a particularly sparse structure and exploiting this can actually reduce the training time to $O(d \cdot n \cdot \log n)$. While we believe that this is one of the very first statistically sound end-to-end proofs of consistency and optimal rates for DNNs, we also need to admit that our training algorithm is mostly interesting from a theoretical point of view, but useless for practical purposes.

Second, Theorems 3.7 and 3.8 also have its consequences for DNNs trained by variants of stochastic gradient descent (SGD) if the resulting predictor is interpolating. Indeed, these theorems show that ending in a global minimum may result in either a very good learning behavior or an extremely overfitting, bad behavior. In fact, all the observations made for histograms at the end of Section 2 apply to DNNs, too. In particular, since for $n \geq n_{d,\alpha}$ the $A_{4dn,2n}$-networks can $\varepsilon$-approximate all functions in $F_{d,n}^\varepsilon$ for all $\varepsilon \geq 0$ and all $s \in \{n^{-1/d}, 1\}$, we can, for example, find, for each polynomial learning rate slower than $n^{-\alpha \gamma}$, an interpolating learning method $D \mapsto f_D$ with $f_D \in A_{4dn,2n}$ that learns with this rate. Similarly, we can find interpolating $f_D \in A_{4dn,2n}$ with various degrees of bad learning behavior. In summary, the optimization landscape induced by $A_{4dn,2n}$ contains a wide variety of global minima whose learning properties range somewhat continuously from essentially optimal to extremely poor. Consequently, an optimization guarantee for (S)GD, that is, a guarantee that (S)GD finds a global minimum in the optimization landscape, is useless for learning guarantees unless more information about the particular nature of the minimum found is provided. Moreover, it becomes clear that considering (S)GD without the initialization of the weights and biases is a meaningless endeavor: For example, constructing $g_{D,s_n,\rho_n}^g$ can be viewed as a very particular form of initialization for which (S)GD won’t change the parameters anymore. More generally, when initializing the parameters randomly in the attraction basin of $g_{D,s_n,\rho_n}^g \pm$ then GD will converge to $g_{D,s_n,\rho_n}^g$ and therefore the behavior of GD is completely determined by the initialization. In this respect note that so far there is no statistically sound way to distinguish between good and bad interpolating DNNs on the basis of the training set alone, and hence the only way to identify good interpolating

\footnote{By “end-to-end” we mean the explicit construction of an efficient, feasible, and implementable training algorithm and the rigorous statistical analysis of this very particular algorithm under minimal assumptions.}
DNNs obtained by SGD is to use a validation set. Now, for the good interpolating DNNs of Theorem 3.7 it is actually possible to construct a finite set of candidates such that the one with the best validation error achieves the optimal learning rates without knowing $\alpha$. For DNNs trained by SGD, however, we do not have this luxury anymore. Indeed, while we can still identify the best predicting DNN from a finite set of SGD-learned interpolating DNNs we no longer have any theoretical understanding of whether there is any useful candidate among them, or whether they all behave like a $g_{D,s,D,n}$. 

Third, for both consistency and learning with essentially optimal rates it is by no means necessary to find a global minimum, or at least a local minimum, in the optimization landscape. For example, the positive learning rates (25) also hold for ordinary cubic histograms with widths $s_n := n^{-\gamma}$, and the latter can, of course, also be approximated by $A_{4dn,2n}$. Repeating the proof of Theorem 3.8 it is easy to verify that these approximations also enjoy the good learning rates (32). Moreover, these approximations $f_D$ are almost never global minima, or more precisely, $f_D$ is not a global minimum as soon as there exist a cubic cell $A$ containing two samples $x_i$ and $x_j$ with different labels, i.e. $y_i \neq y_j$. In fact, in this case, $f_D$ is not even a local minimum. To see this, assume without loss of generality that $x_i$ is one of the samples in $A$ with $y_i \neq f_D(x_i)$. Considering $f_{D,\lambda} := f_D + \lambda h^\top \mathbf{1}_{x_i+\mathbb{B}_\infty}$ for all $\lambda \in [0,1]$ and $t := \min\{r, \rho\}$ we then see that there is a continuous path in the parameter space of $A_{4dn,2n}$ that corresponds to the $\|\cdot\|_\infty$-continuous path $\lambda \mapsto f_{D,\lambda}$ in the set of functions $A_{4dn,2n}$ for which we have $R_{L,D}(f_{D,\lambda}) < R_{L,D}(f_D)$ for all $\lambda \in (0,1)$. In other words, $f_D$ is not a local minimum. In this respect we note that this phenomenon also occurs to some extend in under-parameterized DNNs, at least for $d = 1$. Indeed, if we consider $m := 1$ and $s_n := n^\gamma$, then $f_D, f_{D,\lambda} \in A_{4dn^{-\gamma}d,2n^{-\gamma}d}$ for all sufficiently large $n$. Now, the functions in $A_{4dn^{-\gamma}d,2n^{-\gamma}d}$ have $O(d^2n^{2\gamma d})$ many parameters and for $2\gamma d = \frac{2d}{2a+d} < 1$, that is $\alpha > d/2 = 1/2$, we then see that we have strictly less than $O(\sqrt{n})$ neurons with $O(n)$ parameters, while all the observations made so far still hold.

References

[1] Zeyuan Allen-Zhu, Yuanzhi Li, and Yingyu Liang. Learning and generalization in overparameterized neural networks, going beyond two layers. In Proceedings of the 33rd International Conference on Neural Information Processing Systems, pages 6158–6169, 2019.

[2] Peter L Bartlett, Philip M Long, Gábor Lugosi, and Alexander Tsigler. Benign overfitting in linear regression. Proceedings of the National Academy of Sciences, 117(48):30063–30070, 2020.

[3] H. Bauer. Measure and Integration Theory. De Gruyter, Berlin, 2001.

[4] M. Belkin, D. J. Hsu, and P. Mitra. Overfitting or perfect fitting? Risk bounds for classification and regression rules that interpolate. In S. Bengio, H. Wallach, H. Larochelle, K. Grauman, N. Cesa-Bianchi, and R. Garnett, editors, Advances in Neural Information Processing Systems 31, pages 2300–2311. Curran Associates, Inc., 2018.

[5] Mikhail Belkin, Daniel Hsu, and Ji Xu. Two models of double descent for weak features. SIAM Journal on Mathematics of Data Science, 2(4):1167–1180, 2020.
[6] Mikhail Belkin, Alexander Rakhlin, and Alexandre B Tsybakov. Does data interpolation contradict statistical optimality? In The 22nd International Conference on Artificial Intelligence and Statistics, pages 1611–1619. PMLR, 2019.

[7] Lin Chen, Yifei Min, Mikhail Belkin, and Amin Karbasi. Multiple descent: Design your own generalization curve. arXiv preprint arXiv:2008.01036, 2020.

[8] L. Devroye, L. Györfi, and G. Lugosi. A Probabilistic Theory of Pattern Recognition. Springer, New York, 1996.

[9] I. Goodfellow, Y. Bengio, and A. Courville. Deep Learning. MIT Press, Cambridge, MA, 2016.

[10] L. Györfi, M. Kohler, A. Krzyżak, and H. Walk. A Distribution-Free Theory of Nonparametric Regression. Springer-Verlag, New York, 2002.

[11] J Hoffman-Jorgensen. Probability With a View Towards Statistics, Volume I. Routledge, 2017.

[12] Tengyuan Liang, Alexander Rakhlin, and Xiyu Zhai. On the multiple descent of minimum-norm interpolants and restricted lower isometry of kernels. In Conference on Learning Theory, pages 2683–2711. PMLR, 2020.

[13] S. Ma, R. Bassily, and M. Belkin. The power of interpolation: Understanding the effectiveness of SGD in modern over-parametrized learning. In J. Dy and A. Krause, editors, Proceedings of the 35th International Conference on Machine Learning, volume 80 of Proceedings of Machine Learning Research, pages 3325–3334, 2018.

[14] Song Mei and Andrea Montanari. The generalization error of random features regression: Precise asymptotics and the double descent curve. Communications on Pure and Applied Mathematics, 2019.

[15] Vaishnavh Nagarajan and J Zico Kolter. Uniform convergence may be unable to explain generalization in deep learning. arXiv preprint arXiv:1902.04742, 2019.

[16] Behnam Neyshabur, Zhiyuan Li, Srinadh Bhojanapalli, Yann LeCun, and Nathan Srebro. Towards understanding the role of over-parametrization in generalization of neural networks. In International Conference on Learning Representations (ICLR), 2019.

[17] R. Salakhutdinov. Deep learning tutorial at the Simons Institute, 2017. https://simons.berkeley.edu/talks/ruslan-salakhutdinov-01-26-2017-1

[18] S. Shalev-Shwartz and S. Ben-David. Understanding Machine Learning: From Theory to Algorithms. Cambridge University Press, Cambridge, 2014.

[19] I. Steinwart and A. Christmann. Support Vector Machines. Springer, New York, 2008.

[20] Alexander Tsigler and Peter L Bartlett. Benign overfitting in ridge regression. arXiv preprint arXiv:2009.14286, 2020.

[21] A. B. Tsybakov. Introduction to Nonparametric Estimation. Springer-Verlag, New York, 2009.
A Characterization of empirical risk minimizers

In this section we briefly provide a full characterization of empirical risk minimizers that we use several times for proving our main results.

**Lemma A.1** (Characterization of ERMs). Let $Y$ be convex, $A \subseteq X$ be non-empty, $A = (A_j)_{j \in J}$ be a finite partition of $A$, and

$$\mathcal{H}_A := \left\{ \sum_{j \in J} c_j 1_{A_j} : c_j \in Y \right\}.$$ 

Moreover, let $D = ((x_1,y_1),\ldots,(x_n,y_n)) \in (X \times Y)^n$ be a data set and let $L_A(x,y,t) = 1_A(x)L(y,t)$, with $L$ being the least squares loss. Furthermore, denote the number of samples whose covariates fall into cell $A_j$ by $N_j$, that is $N_j := |\{i : x_i \in A_j\}|$. Then, for every $f^* \in \mathcal{H}_A$ with representation $f^* = \sum_{j \in J} c_j 1_{A_j}$, the following statements are equivalent:

i) The function $f^*$ is an empirical risk minimizer, that is

$$R_{L,A,D}(f^*) = \min_{f \in \mathcal{H}_A} R_{L,A,D}(f).$$

ii) For all $j \in J$ satisfying $N_j \neq 0$ we have

$$c_j = \frac{1}{N_j} \sum_{i : x_i \in A_j} y_i.$$

**Proof of Lemma A.1** We first note that for an $f^* \in \mathcal{H}_A$ with representation $f^* = \sum_{j \in J} c_j 1_{A_j}$ we have

$$R_{L,A,D}(f^*) = \frac{1}{n} \sum_{i=1}^n 1_A(x_i)L(y_i,f^*(x_i)) = \frac{1}{n} \sum_{j \in J \atop i : x_i \in A_j} \sum_{i : x_i \in A_j} L(y_i,c_j).$$

Consequently, $f^*$ is an empirical risk minimizer, if and only if $c_j$ minimizes $\sum_{i : x_i \in A_j} L(y_i,\cdot)$ for all $j \in J$. Now, if $N_j = 0$, the sum is empty, and hence there is nothing to consider. For $j \in J$ with $N_j$ we observe that

$$\sum_{i : x_i \in A_j} L(y_i,c_j) = N_j c_j^2 - 2c_j \left( \sum_{i : x_i \in A_j} y_i \right) + \sum_{i : x_i \in A_j} y_i^2,$$

which is minimized for $c_j$ given by (34).
B Existence of properly aligned cubic partitioning rule

In this section we prove the existence of a properly aligned cubic partitioning rule.

Proof of Theorem 2.5: Recall that cubic partitions $\mathcal{B}$ of $\mathbb{R}^d$ have a representation of the form $[s]$. Now, to construct $\pi_{m,s}$ we will consider a finite set of candidate offsets $x_1, \ldots, x_K \in \mathbb{R}^d$. For the construction of these offsets we write $\delta := s/(m+1)$ and for $j \in \{0, \ldots, m\}$ we further define
$$z_j := \left(j + \frac{1}{2}\right) \delta.$$ 

Now, our candidate offsets $x_1, \ldots, x_K \in \mathbb{R}^d$ are exactly those vectors whose coordinates are taken from $z_0, \ldots, z_m$. Clearly, this gives $K = (m + 1)^d$. Now let $\{x_1, \ldots, x_m\} \in \text{Pot}_m([-1,1]^d)$. In the following, we will identify the offset $x_j$ that leads to $\pi_{m,s}(\{x_1, \ldots, x_m\})$ coordinate-wise. We begin by determining its first coordinate $x_{\ell,1}$. To this end, we define
$$I_j := \bigcup_{k \in \mathbb{Z}} [ks + j \delta, ks + (j + 1) \delta).$$

Our first goal is to show that $I_0, \ldots, I_m$ are a partition of $\mathbb{R}$. To this end, we fix an $x \in \mathbb{R}$. Then there exists a unique $k \in \mathbb{Z}$ with $ks \leq x < (k + 1)s$. Moreover, for $y := x - ks \in [0,s)$, there exists a unique $j \in \{0, \ldots, m\}$ with $j \delta \leq y < (j + 1)\delta$. Consequently, we have found $x \in [ks + j \delta, ks + (j + 1)\delta)$. This shows $\mathbb{R} \subset I_0 \cup \cdots \cup I_m$, and the converse inclusion is trivial. Let us now fix some $j, j' \in \{0, \ldots, m\}$ and assume that there is an $x \in I_j \cap I_{j'}$. Then there exist $k, k' \in \mathbb{Z}$ such that
$$x \in [ks + j \delta, ks + (j + 1)\delta) \cap [ks + j' \delta, k's + (j' + 1)\delta).$$

Since $(j + 1)\delta \leq s$ and $(j' + 1)\delta \leq s$, we conclude that $ks \leq x < (k + 1)s$ and $k's \leq x < (k' + 1)s$. As observed above this implies $k = k'$. Now consider $y := x - ks \in [0,s)$. Then
$$y \in [j \delta, (j + 1)\delta) \cap [j' \delta, (j' + 1)\delta),$$
and again we have seen above that this implies $j = j'$. This shows $I_j \cap I_{j'} = \emptyset$ for all $j \neq j'$.

Let us now denote the first coordinate of $x_i$ by $x_{i,1}$. Then $D_{X,1} := \{x_{i,1} : i = 1, \ldots, m\}$ satisfies $|D_{X,1}| \leq m$ and since we have $m + 1$ cells $I_j$, we conclude that there exists a $j \in \{0, \ldots, m\}$ with $D_{X,1} \cap I_{j^*} = \emptyset$. We define
$$x_{\ell,1} := x_{j^*,1} = \left(j^* + \frac{1}{2}\right) \delta.$$ 

Next we repeat this construction for the remaining $d - 1$ coordinates, so that we finally obtain $x_k := (z_{j^*,1}, \ldots, z_{j^*_d}) \in \mathbb{R}^d$ for indices $j^*_1, \ldots, j^*_d \in \{0, \ldots, m\}$ found by the above reasoning.

It remains to show that $[8]$ holds the cubic partition $[s]$ with offset $x_1^*$ and all $t > 0$ with $t \leq \frac{\delta}{3m+3} = \delta/3$. To this end, we fix an $x_1^*$. Then its cell $B(x_1^*)$ is described by a unique $k := (k_1, \ldots, k_d) \in \mathbb{Z}^d$, namely
$$B(x_1^*) = [x_{\ell,1}^* + k_1 s, x_{\ell,1}^* + (k_1 + 1) s) \times \cdots \times [x_{\ell,d}^* + k_d s, x_{\ell,d}^* + (k_d + 1) s).$$

Let us now consider the first coordinate $x_{\ell,1}^*$. By construction we know that $x_{i,1}^* \notin I_{j^*}$ and
$$\left(j^*_1 + \frac{1}{2}\right) \delta + k_1 s \leq x_{i,1}^* < \left(j^*_1 + \frac{1}{2}\right) \delta + (k_1 + 1) s. \quad (36)$$
Now, \( x_{i,1}^* \not\in I_{j_1^*} \) implies
\[
x_{i,1}^* \not\in [(k_1 + 1)s + j_1^* \delta, (k_1 + 1)s + (j_1^* + 1)\delta)
\]
Since the right hand side of (36) excludes the case \( x_{i,1}^* \geq (k_1 + 1)s + (j_1^* + 1)\delta \), we hence find
\[
x_{i,1}^* < (k_1 + 1)s + j_1^* \delta = x_{j_1^*} + (k_1 + 1)s - \delta/2.
\]
This shows \( x_{i,1}^* + r < x_{j_1^*} + (k_1 + 1)s \) for all \( r \in [-t, t] \). To show that \( x_{i,1}^* + r > x_{j_1^*} + k_1s \) holds for all \( r \in [-t, t] \) we first observe that \( x_{i,1}^* \not\in I_{j_1} \) also implies
\[
x_{i,1}^* \not\in [k_1s + j_1^* \delta, k_1s + (j_1^* + 1)\delta).
\]
Now, the left hand side of (36) excludes the case \( x_{i,1}^* < k_1s + j_1^* \delta \). Consequently, we have
\[
x_{i,1}^* \geq k_1s + (j_1^* + 1)\delta = x_{j_1^*} + k_1s + \delta/2
\]
and this yields \( x_{i,1}^* + r > x_{j_1^*} + k_1s \) for all \( r \in [-t, t] \). Finally, by repeating these considerations for the remaining \( d - 1 \) coordinates, we conclude that \( x_i^* + tB_\infty \subset B(x_1^*) \). \( \square \)

### C Learning properties of inflated histograms

In this section we provide the proofs of the results for the good and bad interpolating histogram rules from Section 2.2. To this end let us introduce some more notation. For a measurable set \( A \) and a loss \( L : Y \times \mathbb{R} \to [0, \infty) \) we therefore introduce the loss \( L_A : X \times Y \times \mathbb{R} \to [0, \infty) \) by
\[
L_A(x, y, t) = 1_A(x)L(y, t).
\]
Obviously, for any measurable function \( f : X \to \mathbb{R} \) it holds
\[
\mathcal{R}_{L_A, P}(f) = \mathcal{R}_{L_A, P}(1_A f).
\]
Moreover, by linearity, for every measurable sets \( B \subset A \), the risk then decomposes as
\[
\mathcal{R}_{L_A, P}(f) = \mathcal{R}_{L_A, B, P}(f) + \mathcal{R}_{L_B, P}(f).
\]
The next result shows that also the Bayes risk enjoys a similar decomposition.

**Lemma C.1.** Let \( A, B \subset X \) be non-empty, disjoint, and measurable with \( A \cup B = X \). Then we have
\[
\mathcal{R}_{L_A, P}^* = \mathcal{R}_{L_A, A, P}^* + \mathcal{R}_{L_B, P}^*.
\]

**Proof of Lemma C.1** Basically, this is a consequence of the presence of the indicator functions \( 1_A, 1_B \) in the definition of \( L_A, L_B \), see (37). More precisely, there is a sequence of functions \( f_n^A \) with \( \{f_n^A \neq 0\} \subset A \) such that
\[
\mathcal{R}_{L_A, P}(f_n^A) \to \mathcal{R}_{L_A, A, P}^*,
\]
as \( n \to \infty \), and similarly for \( A \) replaced by \( B \). Thus, for \( f_n := f_n^A + f_n^B \), one has
\[
\mathcal{R}_{L, P} \leq \lim_{n \to \infty} \mathcal{R}_{L, P}(f_n) = \lim_{n \to \infty} \mathcal{R}_{L_A, P}(f_n^A) + \lim_{n \to \infty} \mathcal{R}_{L_B, P}(f_n^B) = \mathcal{R}_{L_A, P}^* + \mathcal{R}_{L_B, P}^*.
\]
Since the converse inequality is trivial, this proves the lemma. \( \square \)
C.1 Preparatory Lemmata

The next lemma provides a bound on the difference of the risks of two measurable functions.

**Lemma C.2.** Let $Y = [-1, 1]$ and let $f_1, f_2 : X \to Y$ be measurable functions. For $A \subset X$ measurable and non-empty we define $L_A(x, y, t) = 1_A(x)L(y, t)$ with $L$ being the least square loss. Then the following two inequalities hold:

$$
|\mathcal{R}_{L_A,P}(f_1) - \mathcal{R}_{L_A,P}(f_2)| \leq 4 P_X(A \cap \{f_1 \neq f_2\}) ,

||1_A(f_1 - f_2)||^2_{L_2(P_X)} \leq 4 P_X(A \cap \{f_1 \neq f_2\}) .
$$

**Proof of Lemma C.2** We begin by proving the first inequality. To this end, we note that

$$
\mathcal{R}_{L,P}(f_1) - \mathcal{R}_{L,P}(f_2) = \int_A \int_Y (y - f_1(x))^2 - (y - f_2(x))^2 P(dy|x)dP_X(x)
$$

$$
= \int_{A \cap \{f_1 \neq f_2\}} \int_Y (y - f_1(x))^2 - (y - f_2(x))^2 P(dy|x)dP_X(x) .
$$

Now observe that $y, f_i(x) \in [-1, 1]$ implies $(y - f_i(x))^2 \leq 4$. Moreover, we also have $(y - f_i(x))^2 \geq 0$, and hence we conclude that

$$
|(y - f_1(x))^2 - (y - f_2(x))^2| \leq 4 .
$$

Combining these considerations we find

$$
|\mathcal{R}_{L,P}(f_1) - \mathcal{R}_{L,P}(f_2)| \leq \int_{A \cap \{f_1 \neq f_2\}} \int_Y |(y - f_1(x))^2 - (y - f_2(x))^2| P(dy|x)dP_X(x)
$$

$$
\leq 4 P_X(A \cap \{f_1 \neq f_2\}) .
$$

The second inequality can be show similarly. Namely, we have

$$
||1_A(f_1 - f_2)||^2_{L_2(P_X)} = \int_A (f_1(x) - f_2(x))^2 dP_X(x)
$$

$$
= \int_{A \cap \{f_1 \neq f_2\}} (f_1(x) - f_2(x))^2 dP_X(x)
$$

$$
\leq 4 P_X(A \cap \{f_1 \neq f_2\}) ,
$$

where we again used $f_i(x) \in [-1, 1]$.

**Lemma C.3.** Let $h : X \to \mathbb{R}$ be measurable, $A \subset X$, and $L$ be the least-squares loss. Then we have the identity

$$
\mathcal{R}_{L_A,P}(-h) - \mathcal{R}_{L_A,P}(-f_{L,P}^*) = \mathcal{R}_{L_A,P}(h) - \mathcal{R}_{L_A,P}^* + 4 (1_A f_{L,P}^* , h - f_{L,P}^*)_2 .
$$

**Proof of Lemma C.3** Given $x \in X$ and using

$$
(a + b)^2 - (a - b)^2 = 4ab ,
$$

23
we obtain for the difference of inner risks
\[
\int_Y (y + h(x))^2 P(\text{d}y|x) - \int_Y (y + f^*_{L,P}(x))^2 P(\text{d}y|x)
= \int_Y (y + h(x))^2 - (y + h(x))^2 + (y - h(x))^2 \\
- (y + f^*_{L,P}(x))^2 + (y - f^*_{L,P}(x))^2 - (y - f^*_{L,P}(x))^2 P(\text{d}y|x)
= \int_Y (y - h(x))^2 - (y - f^*_{L,P}(x))^2 + 4yh(x) - 4yf^*_{L,P}(x) P(\text{d}y|x).
\]
Thus, since
\[
f^*_{L,P}(x) = \int_Y y P(\text{d}y|x),
\]
we arrive at
\[
\mathcal{R}_{L,A,P}(-h) - \mathcal{R}_{L,A,P}(-f^*_{L,P})
= \mathcal{R}_{L,A,P}(h) - \mathcal{R}^*_{L,A,P} + 4 \int_A \int_Y yh(x) - yf^*_{L,P}(x) P(\text{d}y|x)P_X(\text{d}x)
= \mathcal{R}_{L,A,P}(h) - \mathcal{R}^*_{L,A,P} + 4(1_A f^*_{L,P} , h - f^*_{L,P})_2,
\]
i.e., we have shown the assertion.

With these preparations we can now present the following key lemma that shows that it suffices to understand the behavior of the good and bad interpolating histogram rules on \(\Delta\) and the behavior of \(h^+_{D_A D_B}\).

**Lemma C.4.** Let \(L\) be the least squares loss, \(P\) be a distribution on \(X \times Y\) with point spectrum \(\Delta\), see (18), and \(D \in (X \times Y)^n\) be a data set. Then for all \(s \in (0,1]\) and all \(\rho \geq 0\) the good interpolating histogram rule satisfies
\[
\mathcal{R}_{L,P}(f^+_{D,s,\rho}) - \mathcal{R}^*_{L,P} \leq \mathcal{R}_{L,\Delta,P}(f^+_{D,s,\rho}) - \mathcal{R}^*_{L,\Delta,P} + 4P_X(D^+_{X} \setminus \Delta)
+ \mathcal{R}_{L,P}(h^+_{D_A D_B}) - \mathcal{R}^*_{L,P}.
\]
where \(D^+_{X}\) is defined by (16). Moreover, for all \(s \in (0,1]\) and all \(\rho \geq 0\) the bad interpolating histogram rule satisfies
\[
\|f^-_{D,s,\rho} - f^+_{L,P}\|^2_{L2(P_X)} \leq \mathcal{R}_{L,\Delta,P}(f^-_{D,s,\rho}) - \mathcal{R}^*_{L,\Delta,P} + 4P_X(D^+_{X} \setminus \Delta)
+ \mathcal{R}_{L,P}(h^+_{D_A D_B}) - \mathcal{R}^*_{L,P}.
\]

**Proof of Lemma [C.4].** To simplify notation, we write \(A := D^+_{X} \setminus \Delta\) and \(B := X \setminus (D^+_{X} \cup \Delta)\). Note that this yields the partition \(X = \Delta \cup A \cup B\). In addition, we have \(f^+_{D,s,\rho}(x) = h^+_{D_A D_B}(x)\) for all \(x \in X \setminus D^+_{X}\). Using this in combination with \(B \subset X \setminus D^+_{X}\) as well as the risk decomposition formula (39) and Lemma C.1 we then find
\[
\mathcal{R}_{L,P}(f^+_{D,s,\rho}) - \mathcal{R}^*_{L,P} = \mathcal{R}_{L,\Delta,P}(f^+_{D,s,\rho}) - \mathcal{R}^*_{L,\Delta,P} \\
+ \mathcal{R}_{L,A,P}(f^+_{D,s,\rho}) - \mathcal{R}^*_{L,A,P} \\
+ \mathcal{R}_{L,B,P}(h^+_{D_A D_B}) - \mathcal{R}^*_{L,B,P}.
\]

Moreover, Lemma [C.2] applied to \( f_1 := f_{D,s,\rho}^+ \) and \( f_2 := f_{L,P}^+ \) implies
\[
\mathcal{R}_{L,A,P}(f_{D,s,\rho}^+) - \mathcal{R}_{L,A,P}^* \leq 4P_X(\{ f_{D,s,\rho}^+ \neq f_{L,P}^+ \}) \leq 4P_X(A).
\]
In addition, we have
\[
\mathcal{R}_{L,B,P}(h_{D,\rho}^{+}) - \mathcal{R}_{L,B,P}^* \leq \mathcal{R}_{L,B,P}(h_{D,\rho}^{+}) - \mathcal{R}_{L,B,P}^* + \mathcal{R}_{L,B,P}(h_{D,\rho}^{+}) - \mathcal{R}_{L,B,P}^*
= \mathcal{R}_{L,P}(h_{D,\rho}^{+}) - \mathcal{R}_{L,P}^*,
\]
where again we used [39] and Lemma [C.1]. Combining these estimates we then obtain the assertion for the good interpolating ERM.

To prove the inequality for the bad interpolating histogram rule, we consider the decomposition
\[
\|f_{D,s,\rho} - f_{L,P}^+\|_{L_2(P_X)}^2 = \int_\Delta (f_{D,s,\rho} - f_{L,P}^+)^2 \, dP_X
+ \int_A (f_{D,s,\rho} - f_{L,P}^+)^2 \, dP_X
+ \int_B (f_{D,s,\rho} - f_{L,P}^+)^2 \, dP_X,
\]
where in the first integral we used \( f_{L,P}^+(x) = f_{L,P}^-(x) \) for all \( x \in \Delta \). Now, \( f_{D,s,\rho}^-(x) \in [-1,1] \) and \( f_{L,P}^+(x) \in [-1,1] \) for all \( x \in X \) gives
\[
\int_A (f_{D,s,\rho} - f_{L,P}^+)^2 \, dP_X \leq 4P_X(A).
\]
Moreover, by [17] we find \( f_{D,s,\rho}^-(x) = -f_{D,s,\rho}^+(x) = -h_{D,\rho}^{+}(x) \) for all \( x \in X \setminus D_{X}^{+} \) and thus also for all \( x \in B \). In addition, \( B \subset X \setminus \Delta \) shows \( f_{L,P}^+(x) = -f_{L,P}^-(x) \) for all \( x \in B \). Together, these considerations give \( f_{D,s,\rho}^-(x) - f_{L,P}^+(x) = -h_{D,\rho}^{+}(x) + f_{L,P}^-(x) \) for all \( x \in B \), and consequently we obtain
\[
\int_B (f_{D,s,\rho} - f_{L,P}^+)^2 \, dP_X \leq \int_B (h_{D,\rho}^{+} - f_{L,P}^+)^2 \, dP_X = \mathcal{R}_{L,P}(h_{D,\rho}^{+}) - \mathcal{R}_{L,P}^*.
\]
Combining these considerations finishes the proof.

### C.2 Proof of Theorem [2.11]

Throughout this section we assume that the general assumptions of Theorem [2.11] are satisfied. In particular, \( D \in (X \times Y)^n \) is an i.i.d. sample of size \( n \geq 1 \) and \( D_X := \{ x_1^*, ..., x_m^* \} \in \text{Pot}_m(X) \) is the set of input observations. Moreover, \( (s_n)_{n \in \mathbb{N}} \) is a sequence with \( s_n \to 0 \) as well as \( \frac{\ln(n s_n^2)}{n s_n^2} \to 0 \) as \( n \to \infty \).

#### C.2.1 The good interpolating histogram rule

We begin by introducing the basic strategy of our proof. To this end, consider the good interpolating histogram rule from Example [2.8] with representation
\[
f_{D,s,\rho}^+ = h_{D,\rho}^+ + \sum_{i=1}^m b_i \mathbb{1}_{\{x_i^* + tB_{\infty}\}} \in \mathcal{F}_{s,m}.
\]
In view of (3) it suffices to consider the excess risk of \( f_{D,s,ρ}^+ \). Now observe that in the case \( i) \), i.e. for \( ρ = 0 \), we have \( t = 0 \) and thus \( D_{X}^+ = D_{X} \). Since \( P_{X}(D_{X} \setminus Δ) = 0 \) by the definition of \( Δ \), we then find by Lemma [C.4] that

\[
\mathcal{R}_{L,P}(f_{D,s,0}^+) - \mathcal{R}_{L,P}^* \leq \mathcal{R}_1(h_{D,A_D}^+) + \mathcal{R}_2(f_{D,s,0}^+) ,
\]

where

\[
\begin{align*}
\mathcal{R}_1(h_{D,A_D}^+) & := \mathcal{R}_{L,P}(h_{D,A_D}^+) - \mathcal{R}_{L,P}^* , \\
\mathcal{R}_2(f_{D,s,0}^+) & := \mathcal{R}_{L,P}(f_{D,s,0}^+) - \mathcal{R}_{L,P}^* .
\end{align*}
\]

Moreover, in the case \( ii) \), i.e. for \( ρ = ρ_n > 0 \) the distribution \( P \) satisfies Assumption [2.10] which ensures \( Δ = 0 \). The latter implies \( \mathcal{R}_2(f_{D,s,0}^+) = 0 \), and therefore we find by Lemma [C.4] that

\[
\mathcal{R}_{L,P}(f_{D,s,ρ}^+) - \mathcal{R}_{L,P}^* \leq 4P_X(D_{X}^+ \setminus Δ) + \mathcal{R}_1(h_{D,A_D}^+) .
\]

Moreover, by Assumption [2.10] and \( t \leq ρ = ρ_n \) we obtain

\[
P_X(D_{X}^+ \setminus Δ) \leq P_X(D_{X}^{+n}) \leq \sum_{i=1}^{n} P_X(x_i + ρ_n B_∞) \leq n ϕ(ρ_n) \rightarrow 0 , \tag{41}
\]

and consequently, it suffices to bound \( \mathcal{R}_1(h_{D,A_D}^+) \). Therefore, the rest of this subsection is devoted to bounding \( \mathcal{R}_1(h_{D,A_D}^+) \) and \( \mathcal{R}_2(f_{D,s,0}^+) \) individually.

**Bounding \( \mathcal{R}_1(h_{D,A_D}^+) \).** Thanks to Proposition [E.5] we already know that

\[
\mathcal{R}_1(h_{D,A_D}^+) = \mathcal{R}_{L,P}(h_{D,A_D}^+) - \mathcal{R}_{L,P}^* \rightarrow 0
\]

in probability for \( n \to ∞ \).

**Bounding \( \mathcal{R}_2(f_{D,s,0}^+) \).** If \( Δ = 0 \) we obviously have \( \mathcal{R}_2(f_{D,s,0}^+) = 0 \), and hence we assume \( Δ \neq 0 \) in the following. In this case, \( Δ \) can be at most countable, and therefore we fix an at most countable enumeration \( (\tilde{x}_j)_{j \in J} \) of \( Δ \), i.e.

\[
Δ = \bigcup_{j \in J} \{ \tilde{x}_j \} .
\]

Let us further fix an \( ϵ > 0 \) and a finite subset \( Δ_0 \subset Δ \) such that \( P_X(Δ \setminus Δ_0) \leq ϵ \). With the help of (39) and Lemma [C.1] we then observe that

\[
\mathcal{R}_{L,A,D}(f_{D,s,0}^+) - \mathcal{R}_{L,A,D}^* = \mathcal{R}_{L,A_0}(f_{D,s,0}^+) - \mathcal{R}_{L,A_0}^* + \mathcal{R}_{L,A_0}(f_{D,s,0}^+) - \mathcal{R}_{L,A_0}^* . \tag{42}
\]

Since \( Y = [-1,1] \) is bounded the second difference can be bounded by

\[
|\mathcal{R}_{L,A_0}(f_{D,s,0}^+) - \mathcal{R}_{L,A_0}^*| = \int_{X \times Y} 1_{Δ \setminus Δ_0}(x) (f_{D,s,0}^+(x) - f^*_P(x))^2 \, dP(x,y) \\
\leq 4 P_X(Δ \setminus Δ_0) \leq 4 ϵ . \tag{43}
\]

26
Our next step is to bound the first difference in (42). To this end, we write
\[ J_0 := \{ j \in J : \tilde{x}_j \in \Delta_0 \} , \]
\[ C_j := \{ \tilde{x}_j \} \text{ for } j \in J_0 , \text{ and } C := (C_j)_{j \in J_0} . \]
Then \( C \) is a finite partition of \( \Delta_0 \), and we set
\[ \mathcal{F}_C := \left\{ \sum_{j \in J_0} c_j \mathbf{1}_{C_j} : c_j \in Y \right\} . \tag{44} \]
Since all \( C_j \) are singletons, every measurable function \( f : X \to Y \) satisfies \( 1_{\Delta_0} f \in \mathcal{F}_C \). We thus conclude that \( f_D := 1_{\Delta_0} f_{D,s_n,0}^+ \in \mathcal{F}_C \), too. Moreover, by (38) we know
\[ \mathcal{R}_{L_{\Delta_0},P}(f_D) = \mathcal{R}_{L_{\Delta_0},P}(f_{D,s_n,0}^+) . \tag{45} \]

Our next goal is to show that \( f_D \) minimizes the empirical risk over \( \mathcal{F}_C \) with respect to \( L_{\Delta_0} \). To this end, we fix a \( j \in J_0 \) for which we have \( N_j := |\{ i : x_i \in C_j \}| > 0 \). Since \( f_{D,s_n,0}^+ \) interpolates \( D \) by construction, Proposition 2.7 then gives
\[ f_D(\tilde{x}_j) = 1_{\Delta_0}(x) f_{D,s_n,0}^+(\tilde{x}_j) = f_{D,s_n,0}^+(\tilde{x}_j) = \frac{1}{N_j} \sum_{i : x_i \in C_j} y_i . \tag{46} \]
Thus, Lemma A.1 shows that \( f_D \) is indeed an empirical risk minimizer with respect to \( L_{\Delta_0} \) and \( \mathcal{F}_C \).

Our next goal is to apply Theorem E.2, which holds for all ERM with respect to \( L_{\Delta_0} \) and \( \mathcal{F}_C \), to our specific ERM \( f_D \). To this end, we first observe, as in the proof of Corollary E.3 that since \( L \) is the least squares loss, the assumptions (72) and (73) of Theorem E.2 are satisfied for \( L_{\Delta_0} \) with \( d = 1, B = 4 \), and \( V = 16 \). Moreover, our assumption \( Y = [-1,1] \) ensures that \( L_{\Delta_0} \) is locally Lipschitz continuous with \( |L_{\Delta_0}|_{1,1} \leq 4 \). In addition, we have
\[ \mathcal{N}(\mathcal{F}_C, ||| . |||_{\infty}, \varepsilon) \leq (2/\varepsilon)^{|\Delta_0|} . \]
Applying Theorem E.2 and optimizing the resulting oracle inequality with respect to \( \varepsilon \) like at the end of the proof of Corollary E.3, we then see that, for all \( n \geq 1 \) and \( \tau > 0 \),
\[ \mathcal{R}_{L_{\Delta_0},P}(f_D) - \mathcal{R}_{L_{\Delta_0},P}(f_D) \leq 4 (\mathcal{R}_{L_{\Delta_0},P,\mathcal{F}_C} - \mathcal{R}_{L_{\Delta_0},P}^*) + 1024 \frac{\tau}{n} + 512 \frac{|\Delta_0|}{n} \left( 1 + \ln \left( \frac{n}{|\Delta_0|} \right) \right) \]
holds with probability \( P^n \) not less than \( 1 - e^{-\tau} \). Now, to bound the approximation error term, we note that
\[ \mathcal{F}_C = \left\{ f : X \to Y \mid f \text{ measurable and } f(x) = 0 \text{ for all } x \notin \Delta_0 \right\} , \]
and hence we easily find
\[ \mathcal{R}_{L_{\Delta_0},P}(f_D) = \inf_{f:X \to Y} \mathcal{R}_{L_{\Delta_0},P}(f) = \inf_{f:X \to Y} \mathcal{R}_{L_{\Delta_0},P}(1_{\Delta_0} f) = \mathcal{R}_{L_{\Delta_0},P,\mathcal{F}_C}^* . \]
Setting \( \tau := \ln(n) \) we conclude that
\[ \mathcal{R}_{L_{\Delta_0},P}(f_D) - \mathcal{R}_{L_{\Delta_0},P}^* \leq 1024 \frac{\tau}{n} + 512 \frac{|\Delta_0|}{n} \left( 1 + \ln \left( \frac{n}{|\Delta_0|} \right) \right) \tag{47} \]
holds with probability \( P^n \) not less than \( 1 - 1/n \). For later use note that this oracle inequality actually holds for all ERM respect to \( L_{\Delta_0} \) and \( \mathcal{F}_C \), since so does Theorem E.2 and we have not used any property of our specific ERM \( f_D \) to derive (47). Finally, combining this with (42), (43), (45), and the obvious \( \mathcal{R}_{L_{\Delta_0},P}(f_{D,s_n,0}^+) - \mathcal{R}_{L_{\Delta_0},P}^* \geq 0 \), we conclude that
\[ \mathcal{R}_{\Delta}(f_{D,s_n,0}^+) = \mathcal{R}_{L_{\Delta},P}(f_{D,s_n,0}^+) - \mathcal{R}_{L_{\Delta},P}^* \to 0 \]
in probability for \( n \to \infty \).
In this subsection we consider the bad interpolating histogram rule from Example 2.9 with representation
\[
f_{D,s,\rho} = h_{D,A_D} - \sum_{i=1}^{m} b_i \mathbb{1}_{x_t^*_i + tB_\infty} \in F_{s,m}.
\]
Now observe that in the case \(i)\) of Theorem 2.11, i.e. for \(\rho = 0\), we have \(t = 0\) and thus \(D_X^{+t} = D_X\). Since \(P_X(D_X \setminus \Delta) = 0\) by the definition of \(\Delta\), we then see by Lemma C.4 and Proposition E.5 that it suffices to show that
\[
\mathcal{R}_{L,\rho}(f_{D,s,0}) - \mathcal{R}^*_{L,\rho} \to 0
\]
in probability for \(n \to \infty\). To this end, we fix an \(\epsilon > 0\) and a finite \(\Delta_0 \subseteq \Delta\) with \(P_X(\Delta \setminus \Delta_0) \leq \epsilon\). Then we note that the decomposition (42) and the estimate (43) for \(f_{D,s,0}^+\) also holds for \(f_{D,s,0}^+\). Consequently, it suffices to bound the term
\[
\mathcal{R}_{L,\Delta_0}(f_{D,s,0}) - \mathcal{R}^*_{L,\Delta_0}\cdot
\]
To this end, recall that \(f_{D,s,0}^+\) and \(f_{D,s,0}^-\) are both interpolating predictors, and hence we have
\[
f_{D,s,0}(x_i) = f_{D,s,0}^+(x_i)
\](49)
for all samples \((x_i, y_i)\) of \(D\), and thus in particular for all samples \((x_i, y_i)\) of \(D_0\) with \(x_i \in \Delta\). Let us define \(f_D := \mathbb{1}_{\Delta_0}f_{D,s,0}^+.\) Combining (49) with (46) we see that \(f_D\) is an empirical risk minimizer over the hypotheses set \(F_C\) defined (44) with respect to \(L_{\Delta_0}\). Since (47) has been shown for all ERM respect to \(L_{\Delta_0}\) and \(F_C\) we thus find
\[
\mathcal{R}_{L,\Delta_0}(f_{D,s,0}^-) - \mathcal{R}^*_{L,\Delta_0} \to 0
\]
in probability for \(n \to \infty\). This finishes the proof in the case \(i)\) of Theorem 2.11. Moreover, in the case \(ii)\), i.e. for \(\rho = \rho_n > 0\) the distribution \(P\) satisfies Assumption 2.10 which ensures \(\Delta = \emptyset\). In combination with Lemma C.4 the latter implies
\[
\|f_{D,s,\rho}^+ - f_{L,P}^+\|^2_{L_2(P_X)} \leq 4P_X(D_X^{+t} \setminus \Delta) + \mathcal{R}_{L,P}(h_{D,A_D}^+) - \mathcal{R}^*_{L,P}.
\]
Now, the first term has already been bounded in (41) and the excess risk of \(h_{D,A_D}^+\) can again be bounded by Proposition E.5.

**C.3 Proof of Theorem 2.12 (Learning Rates)**

In the following we suppose that all assumption of Theorem 2.12 are satisfied.

Let us first prove the assertions for the good interpolating histogram rule. To this end, we first recall that Assumption 2.10 implies \(\Delta = \emptyset\). By (3) and Lemma C.4 we then obtain
\[
\|f_{D,s,\rho}^+ - f_{L,P}^+\|^2_{L_2(P_X)} = \mathcal{R}_{L,P}(f_{D,s,\rho}^+) - \mathcal{R}^*_{L,P} \leq 4P_X(D_X^{+t} \setminus \Delta) + \mathcal{R}_{L,P}(h_{D,A_D}^+) - \mathcal{R}^*_{L,P}.
\]
Now, (41) shows
\[
P_X(D_X^{+t} \setminus \Delta) \leq n\varphi(\rho_n) \leq \ln(n) n^{-2/3} \leq \ln(n) n^{-2\alpha\gamma}.
\]
(50)
Moreover, by Theorem 2.5 we know that $|\text{Im}(\pi_{m,a})| \leq (m + 1)^d \leq 2^d n^d$ for all $m \leq n$. Consequently, applying Proposition E.6 with $c = 2^d$ and $\beta := d$ we find

$$R_{L,P}(h^+_{D,A_D}) - R^*_{L,P} \leq c_{d,\alpha} \ln(n) n^{-2\alpha\gamma}$$

(51)

with probability $P^n$ at least $1 - 2^{d_N} n^{d^*} e^{-n^{d^{*\gamma}}}$, where $c_{d,\alpha} > 0$ is a constant only depending on $d, \alpha$, and $|f^*_{L,P}|_{\alpha}$. Combining this with (50) we then obtain (25).

Finally, inequality (25) for the bad interpolating histogram rule follows analogously; since in this case Lemma C.4 shows

$$||f^-_{D,s_n,p_n} - f^1_{L,P}||^2_{L_2(P_X)} \leq 4P_X(D^-_{X} \setminus \Delta) + R_{L,P}(h^+_{D,A_D}) - R^*_{L,P}.$$  

**D Learning properties of approximating neural networks**

**D.1 Auxiliary Results on Functions that can be represented by DNNs**

In this section we present some results on algebraic properties of the set of functions that can be represented by DNNs. We particularly focus on the network sizes required to perform algebraic transformations of such functions.

To this end, recall that throughout this work we solely consider the ReLU-activation function $\sigma := |\cdot|_+$ and its shifted extensions [27]. Given an input dimension $d$, a depth $L \geq 2$, and a width vector $(p_1, \ldots, p_{L-1}) \in \mathbb{N}^{L-1}$, a function $f \in \mathcal{A}_{p_1, \ldots, p_{L-1}}$ is then of the form [29], i.e.

$$f(x) = H_L \circ H_{L-1} \circ \cdots \circ H_1(x), \quad x \in \mathbb{R}^{p_0},$$

where each layer $H_l$, $l = 1, \ldots, L$, is of the form [28], where we drop the index for the activation to ease notation. Specifically, each layer can be represented by a $p_l \times p_{l-1}$ weight matrix $A^{(l)}$ with $p_0 := d$ and $p_L := 1$ and a shift vector $b^{(l)} \in \mathbb{R}^{p_l}$, and the last layer $H_L$ has the identity as an activation function. In the following, we thus say that the network $f$ is represented by $(\mathfrak{A}, \mathfrak{B})$, where $\mathfrak{A} := (A^{(1)}, \ldots, A^{(L)})$ and $\mathfrak{B} := (b^{(1)}, \ldots, b^{(L)})$. For later use we emphasize that $p_L = 1$ implies $b^{(L)} \in \mathbb{R}$. Moreover note that each pair $(\mathfrak{A}, \mathfrak{B})$ determines a neural network, but in general, a neural network, if viewed as a function, can be described by more than one such pair.

Now, our first lemma describes the changes in the representation when manipulating a single neural network.

**Lemma D.1.** Let $d \geq 1$, $L \geq 2$, and $p := (p_1, \ldots, p_{L-1}) \in \mathbb{N}^{L-1}$. Moreover, let $f \in \mathcal{A}_p$ be a neural network with representation $\mathfrak{A} := (A^{(1)}, \ldots, A^{(L)})$ and $\mathfrak{B} := (b^{(1)}, \ldots, b^{(L)})$. Then the following statements hold true:

i) For all $\alpha \in \mathbb{R}$ and $c \in \mathbb{R}$ we have $\alpha f + c \in \mathcal{A}_p$ with representation

$$(A^{(1)}, \ldots, A^{(L-1)}, \alpha A^{(L)}) \quad \text{and} \quad (b^{(1)}, \ldots, b^{(L-1)}, \alpha b^{(L)} + c).$$

ii) We have $|f|_+ \in \mathcal{A}_{p,1}$ with representation

$$(A^{(1)}, \ldots, A^{(L)}, 1) \quad \text{and} \quad (b^{(1)}, \ldots, b^{(L)}, 0).$$
Proof of Lemma D.1. This immediately follows from the representation (29) and the fact that $H_l$ does not have an activation function.

ii). Let $\tilde{H}_1, \ldots, \tilde{H}_{L+1}$ be the layers of the neural network $\tilde{f}$ given by the new representation. Then we have $H_l = \tilde{H}_l$ for all $l = 1, \ldots, L-1$ as well as $\tilde{H}_L = |H_L|_+$ and $\tilde{H}_{L+1} = \text{id}_{\mathbb{R}}$. Applying the representation (29) for $f$ and $\tilde{f}$ then gives the assertion.

Our next lemma describes a possible representation of the sum of two nets with the same depth $L$.

Lemma D.2. Let $d \geq 1$, $L \geq 2$, and $\tilde{p} := (\tilde{p}_1, \ldots, \tilde{p}_{L-1}) \in \mathbb{N}^{L-1}$ and $\bar{p} := (\bar{p}_1, \ldots, \bar{p}_{L-1}) \in \mathbb{N}^{L-1}$ be two width vectors. Then for all $\tilde{f} \in \mathcal{A}_{\tilde{p}}$ and $\bar{f} \in \mathcal{A}_{\bar{p}}$ we have

$$\tilde{f} + \bar{f} \in \mathcal{A}_{\tilde{p} + \bar{p}}.$$

In addition, if $(\mathfrak{A}, \mathfrak{B})$ and $(\mathfrak{\bar{A}}, \mathfrak{\bar{B}})$ are representations of $\tilde{f}$ and $\bar{f}$, then $\tilde{f} + \bar{f}$ has the representation $\mathfrak{A} := (A^{(1)}, \ldots, A^{(L)})$ and $\mathfrak{B} := (b^{(1)}, \ldots, b^{(L)})$ defined by

$$A^{(l)} := \begin{pmatrix} \hat{A}^{(l)} & 0 \\ 0 & \underline{A}^{(l)} \end{pmatrix} \in \mathbb{R}^{(\bar{m}_l + \bar{m}_1) \times d}, \quad b^{(l)} := \begin{pmatrix} \hat{b}^{(l)} \\ \underline{b}^{(l)} \end{pmatrix} \in \mathbb{R}^{\bar{m}_l + \bar{m}_1},$$

as well as

$$A^{(l)} := \begin{pmatrix} \hat{A}^{(l)} & 0 \\ 0 & \underline{A}^{(l)} \end{pmatrix} \in \mathbb{R}^{(\bar{m}_l + \bar{m}_1) \times (\bar{m}_{l-1} + \bar{m}_{l-1})}, \quad b^{(l)} := \begin{pmatrix} \hat{b}^{(l)} \\ \underline{b}^{(l)} \end{pmatrix} \in \mathbb{R}^{\bar{m}_l + \bar{m}_l},$$

for all $l = 2, \ldots, L-1$ and

$$A^{(L)} := \begin{pmatrix} \hat{A}^{(L)} & \underline{A}^{(L)} \end{pmatrix} \in \mathbb{R}^{\bar{m}_L + \bar{m}_L}, \quad b^{(L)} := \hat{b}^{(L)} + \underline{b}^{(L)} \in \mathbb{R}.$$

Proof of Lemma D.2. Let $\hat{H}_1, \ldots, \hat{H}_L$ be the layers of $\hat{f}$ and $\bar{H}_1, \ldots, \bar{H}_L$ be the layers of $\bar{f}$. For $l = 1, \ldots, L$, we further introduce the concatenation of layers

$$\hat{W}_l := \hat{H}_1 \circ \cdots \circ \hat{H}_l \quad \text{and} \quad \bar{W}_l := \bar{H}_1 \circ \cdots \circ \bar{H}_1.$$

Moreover, for $l = 1, \ldots, L$, let $\hat{H}_l$ be the layer given by $A^{(l)}$ and $b^{(l)}$ and $W_l := \hat{H}_1 \circ \cdots \circ H_1$. Since the last layers of $\hat{f}$ and $\bar{f}$ do not have an activation function, we then find

$$(\hat{f} + \bar{f})(x) = \hat{A}^{(L)} \cdot \hat{W}_{L-1}(x) + \hat{b}^{(L)} + \underline{A}^{(L)} \cdot \bar{W}_{L-1}(x) + \underline{b}^{(L)}$$

$$= (\hat{A}^{(L)} \underline{A}^{(L)}) \begin{pmatrix} \hat{W}_{L-1}(x) \\ \underline{W}_{L-1}(x) \end{pmatrix} + \hat{b}^{(L)} + \underline{b}^{(L)}$$

$$= A^{(L)} \begin{pmatrix} \hat{W}_{L-1}(x) \\ \underline{W}_{L-1}(x) \end{pmatrix} + b^{(L)}$$

for all $x \in \mathbb{R}^d$. Similarly, for all $l = 2, \ldots, L-1$ and all $x \in \mathbb{R}^d$ we have

$$\begin{pmatrix} \hat{W}_l(x) \\ \underline{W}_l(x) \end{pmatrix} = (\hat{H}_l \circ \hat{W}_{l-1}(x)) = \begin{pmatrix} \hat{A}^{(l)} \cdot \hat{W}_{l-1}(x) + \hat{b}^{(l)} \\ \underline{A}^{(l)} \cdot \hat{W}_{l-1}(x) + \underline{b}^{(l)} \end{pmatrix}$$

$$= \begin{pmatrix} \hat{A}^{(l)} & 0 \\ 0 & \underline{A}^{(l)} \end{pmatrix} \begin{pmatrix} \hat{W}_{l-1}(x) \\ \underline{W}_{l-1}(x) \end{pmatrix} + \begin{pmatrix} \hat{b}^{(l)} \\ \underline{b}^{(l)} \end{pmatrix}$$

$$= A^{(l)} \begin{pmatrix} \hat{W}_{l-1}(x) \\ \underline{W}_{l-1}(x) \end{pmatrix} + b^{(l)}.$$
Finally, for the first layer and all $x \in \mathbb{R}^d$ we obtain
\[
\left(\begin{array}{c}
\hat{W}_1(x) \\
\check{W}_1(x)
\end{array}\right) = \left(\begin{array}{c}
\hat{H}_1(x) \\
\check{H}_1(x)
\end{array}\right) = \left(\begin{array}{c}
\left|\tilde{A}^{(1)} \cdot x + \tilde{b}^{(1)}\right|_+ \\
\left|\bar{A}^{(1)} \cdot x + \bar{b}^{(1)}\right|_+
\end{array}\right) = \left(\begin{array}{c}
\left|\tilde{A}^{(1)}\right|_+ \cdot x + \left|\tilde{b}^{(1)}\right|_+ \\
\left|\bar{A}^{(1)}\right|_+ \cdot x + \left|\bar{b}^{(1)}\right|_+
\end{array}\right) = \left|A^{(1)} \cdot x + b^{(1)}\right|_+ .
\]

Combining these results gives $W_l = (\hat{W}_l, \check{W}_l)^T$ for all $l = 1, \ldots, L$, i.e. we have found the assertion.

\[\square\]

### D.2 Approximating Step Functions by DNNs

In this section we collect the main pieces to approximate histograms with DNNs. The first lemma, which is a longer and more detailed version of Lemma 3.3, shows how to approximate an indicator function on a multidimensional interval by a small ReLU-DNN with two hidden layers.

**Lemma D.3.** Let $d \geq 1$ and let $z_1 = (z_{1,1}, \ldots, z_{1,d}) \in \mathbb{R}^d$ and $z_2 = (z_{2,1}, \ldots, z_{2,d}) \in \mathbb{R}^d$ be two vectors with $z_1 < z_2$. Moreover, let $\varepsilon > 0$ satisfy
\[
\varepsilon < \min\left\{\frac{z_{2,i} - z_{1,i}}{2} : i = 1, \ldots, d\right\}
\]
and define
\[
A^{(1)} := \frac{1}{\varepsilon} \begin{pmatrix}
-I_d \\
I_d
\end{pmatrix}, \quad b^{(1)} := \frac{1}{\varepsilon} \begin{pmatrix}
z_1 + \varepsilon \\
z_2 - \varepsilon
\end{pmatrix}
\]
\[
A^{(2)} := (-1, -1, \ldots, -1) \in \mathbb{R}^{2d}, \quad b^{(2)} := 1
\]
\[
A^{(3)} := 1, \quad b^{(3)} := 0,
\]
where $I_d$ denotes the $d$-dimensional identity matrix, and $A^{(3)}, b^{(2)}, b^{(3)} \in \mathbb{R}$. Then the neural network $f_\varepsilon : \mathbb{R}^d \to \mathbb{R}$ given by the representation $\mathcal{A} := (A^{(1)}, A^{(2)}, A^{(3)})$ and $\mathcal{B} := (b^{(1)}, b^{(2)}, b^{(3)})$ satisfies $f_\varepsilon \in \mathcal{A}_{2d,1}$ and
\[
\{f_\varepsilon > 0\} \subset (z_1, z_2), \quad (52)
\]
\[
\{f_\varepsilon = 1\} = [z_1 + \varepsilon, z_2 - \varepsilon], \quad (53)
\]
\[
\{f_\varepsilon < 0\} = \{f_\varepsilon > 1\} = \emptyset . \quad (54)
\]

**Proof of Lemma [D.3]** Let $H_1, H_2, H_3$ be the layers of $f_\varepsilon$. Then we have $H_3 = \text{id}_\mathbb{R}$ and if $h_1^{(1)}, \ldots, h_d^{(1)}, h_1^{(2)}, \ldots, h_d^{(2)}$ denote the $2d$ component functions of $H_1$, that is
\[
H_1(x) = \left(h_1^{(1)}(x), \ldots, h_d^{(1)}(x), h_1^{(2)}(x), \ldots, h_d^{(2)}(x)\right)^T, \quad x \in \mathbb{R}^d,
\]
we thus find
\[
f_\varepsilon(x) = H_3 \circ H_2 \circ H_1(x) = H_2 \circ H_1(x) = \left| -\sum_{i=1}^d h_i^{(1)}(x) - \sum_{i=1}^d h_i^{(2)}(x) + 1 \right|_+
\]
\[
= \left| \sum_{i=1}^d (1 - h_i^{(1)}(x) - h_i^{(2)}(x)) - d + 1 \right|_+ . \quad (55)
\]
for all $x \in \mathbb{R}^d$. Therefore, we first investigate the functions $1 - h_i^{(1)} - h_i^{(2)}$. To this end, let us fix an $i \in \{1, \ldots, d\}$ and an $x = (x_1, \ldots, x_d) \in \mathbb{R}^d$. Then we obviously have

$$h_i^{(1)}(x) = \left| -\frac{x_i}{\varepsilon} + \frac{z_{1,i} + \varepsilon}{\varepsilon} \right| + \begin{cases} \frac{-x_i + z_{1,i} + \varepsilon}{\varepsilon} & \text{if } x_i \leq z_{1,i} + \varepsilon \\ 0 & \text{else,} \end{cases}$$

and

$$h_i^{(2)}(x) = \left| -\frac{x_i}{\varepsilon} + \frac{z_{2,i} - \varepsilon}{\varepsilon} \right| + \begin{cases} \frac{x_i - z_{2,i} + \varepsilon}{\varepsilon} & \text{if } x_i \geq z_{2,i} - \varepsilon \\ 0 & \text{else.} \end{cases}$$

Since $z_{1,i} + \varepsilon < z_{2,i} - \varepsilon$, we consequently find

$$1 - h_i^{(1)}(x) - h_i^{(2)}(x) = \begin{cases} \frac{x_i - z_{1,i}}{\varepsilon} & \text{if } x_i \leq z_{1,i} + \varepsilon \\ 1 & \text{if } x_i \in [z_{1,i} + \varepsilon, z_{2,i} - \varepsilon] \\ \frac{z_{2,i} - x_i}{\varepsilon} & \text{if } x_i \geq z_{2,i} - \varepsilon. \end{cases}$$

In particular, we have

\begin{align*}
\{1 - h_i^{(1)} - h_i^{(2)} > 0\} &= \{(x_1, \ldots, x_d) \in \mathbb{R}^d : x_i \in (z_{1,i}, z_{2,i})\}, \\
\{1 - h_i^{(1)} - h_i^{(2)} = 1\} &= \{(x_1, \ldots, x_d) \in \mathbb{R}^d : x_i \in [z_{1,i} + \varepsilon, z_{2,i} - \varepsilon]\}, \\
\{1 - h_i^{(1)} - h_i^{(2)} > 1\} &= \emptyset. \tag{58}
\end{align*}

Combining our initial equation (55) with (57) and (58) yields

$$\{f_{\varepsilon} = 1\} = \left\{ \left| \sum_{i=1}^{d} (1 - h_i^{(1)} - h_i^{(2)}) - d + 1 \right|_+ = 1 \right\} = \left\{ \sum_{i=1}^{d} (1 - h_i^{(1)} - h_i^{(2)}) = d \right\}
= [z_1 + \varepsilon, z_2 - \varepsilon],$$

i.e. we have found (53). Next we will verify (52) to this end, we first note that (55) gives

$$\{f_{\varepsilon} > 0\} = \left\{ \left| \sum_{i=1}^{d} (1 - h_i^{(1)} - h_i^{(2)}) - d + 1 \right|_+ > 0 \right\}
= \left\{ \sum_{i=1}^{d} (1 - h_i^{(1)} - h_i^{(2)}) > d - 1 \right\}. \tag{59}$$

Our next intermediate goal is to show

$$\left\{ \sum_{i=1}^{d} (1 - h_i^{(1)} - h_i^{(2)}) > d - 1 \right\} \subset \bigcap_{i=1}^{d} \{1 - h_i^{(1)} - h_i^{(2)} > 0\}. \tag{60}$$

To this end, we assume the converse, i.e. there is an $x \in \mathbb{R}^d$ and an $i_0 \in \{1, \ldots, d\}$ with

$$\sum_{i=1}^{d} (1 - h_i^{(1)}(x) - h_i^{(2)}(x)) > d - 1 \quad \text{and} \quad 1 - h_{i_0}^{(1)}(x) - h_{i_0}^{(2)}(x) \leq 0.$$
Without loss of generality we may assume that $i_0 = d$. Then combining both inequalities we find
\[
d - 1 < \sum_{i=1}^{d-1} \left(1 - h_i^{(1)}(x) - h_i^{(2)}(x)\right) + \left(1 - h_d^{(1)}(x) - h_d^{(2)}(x)\right) \leq \sum_{i=1}^{d-1} \left(1 - h_i^{(1)}(x) - h_i^{(2)}(x)\right),
\]
and this shows that there is also an $i \in \{1, \ldots, d - 1\}$ with $1 - h_i^{(1)}(x) - h_i^{(2)}(x) > 1$. This contradicts (58), and hence we have shown (60). Now combining (59) with (60) and (56) we obtain
\[
\{f_\varepsilon > 0\} \subset \bigcap_{i=1}^{d} \{1 - h_i^{(1)} - h_i^{(2)} > 0\} = (z_1, z_2),
\]
i.e. we have found (62). Finally, the equation $\{f_\varepsilon > 1\} = \emptyset$ immediately follows from combining (55) and (58), and $\{f_\varepsilon < 0\} = \emptyset$ is a direct consequence of (55).

Our next goal is to describe how well the function $f_\varepsilon$ found in Lemma D.3 approximates the indicator function $1_{[z_1, z_2]}$. To this end, we first recall a well-known estimate on $\| \cdot \|_\infty$-covering numbers of cuboids in the following lemma. We include its proof for the sake of completeness.

**Lemma D.4.** Let $s_1, \ldots, s_d > 0$, $s_{\text{min}} := \min\{s_1, \ldots, s_d\}$, $z \in \mathbb{R}^d$, and
\[
A := \{x \in \mathbb{R}^d : z_i \leq x_i \leq z_i + s_i\}.
\]
Then for all $\varepsilon \in (0, s_{\text{min}}]$ we have
\[
\mathcal{N}(A, \| \cdot \|_\infty, \varepsilon) \leq \left(\frac{3}{2}\right)^{d} \left(\prod_{i=1}^{d} s_i\right) \cdot \varepsilon^{-d}.
\]

**Proof of Lemma D.4.** Let us fix an $i \in \{1, \ldots, d\}$. Since $\varepsilon \leq s_i$, we then need at most $\left\lceil \frac{s_i}{2\varepsilon} \right\rceil$ closed intervals of length $2\varepsilon$ to cover the interval $[z_i, z_i + s_i]$. From this it is easy to conclude that
\[
\mathcal{N}(A, \| \cdot \|_\infty, \varepsilon) \leq \prod_{i=1}^{d} \left\lceil \frac{s_i}{2\varepsilon} \right\rceil \leq \prod_{i=1}^{d} \left(\frac{s_i}{2\varepsilon} + 1\right) \leq \prod_{i=1}^{d} \left(\frac{s_i}{2\varepsilon} + \frac{s_i}{\varepsilon}\right) = \left(\frac{3}{2}\right)^{d} \left(\prod_{i=1}^{d} s_i\right) \cdot \varepsilon^{-d},
\]
and hence we have shown the assertion.

Now, the next lemma describes the announced description of the approximation error.

**Lemma D.5.** Let $z_1, z_2 \in [-1, 1]^d$, and $\varepsilon > 0$ as in Lemma D.3. Moreover, let $A \subset [-1, 1]^d$ be a subset satisfying $(z_1, z_2) \subset A \subset [z_1, z_2]$. Then the neural network $f_\varepsilon \in A_{2d, 1}$ constructed in Lemma D.3 satisfies
\[
\{f_\varepsilon = 1_A\} = [z_1 + \varepsilon, z_2 - \varepsilon] \cup (X \setminus A).
\]
Moreover, if $A$ is a cube of side length $s > 0$, that is $z_2, i - z_1, i = s$ for all $i = 1, \ldots, d$, and we have a distribution $P_X$ on $[-1, 1]^d$ that satisfies Assumption 2.10 for some $\varphi : \mathbb{R}_+ \to \mathbb{R}_+$, then we further have
\[
P_X(\{f_\varepsilon \neq 1_A\}) \leq 3d \cdot \left(\frac{3s}{2}\right)^{d-1} \cdot \varepsilon^{-d+1} \cdot \varphi(2\varepsilon).
\]
Proof of Lemma [D.5]: By (53) and (52) we find the inclusions \( \{ f_{\varepsilon} = 1 \} = [z_1 + \varepsilon, z_2 - \varepsilon] \subset A \) and \( \{ f_{\varepsilon} > 0 \} \subset (z_1, z_2) \subset A \). Using \( \{ f_{\varepsilon} < 0 \} = \emptyset \), which is known by (54), we then obtain
\[
\{ f_{\varepsilon} = 1_A \} = (A \cap \{ f_{\varepsilon} = 1 \}) \cup ((X \setminus A) \cap \{ f_{\varepsilon} = 0 \}) \\
= (A \cap \{ f_{\varepsilon} = 1 \}) \cup ((X \setminus A) \cap (X \setminus \{ f_{\varepsilon} > 0 \})) \\
= [z_1 + \varepsilon, z_2 - \varepsilon] \cup (X \setminus A),
\]
i.e. we have shown (61). Now, to establish (62), we first note that (61) together with \( A \subset [z_1, z_2] \) implies
\[
\{ f_{\varepsilon} \neq 1_A \} = (X \setminus [z_1 + \varepsilon, z_2 - \varepsilon]) \cap A \subset (z_1 + \varepsilon, z_2 - \varepsilon).
\]
To further bound \([z_1, z_2] \setminus (z_1 + \varepsilon, z_2 - \varepsilon)\) we define
\[
S_i^- := \{ x : x_i \in [z_1, z_1 + \varepsilon] \text{ and } x_j \in [z_1, z_2] \text{ for all } j \neq i \}, \\
S_i^+ := \{ x : x_i \in [z_1, z_2] - \varepsilon, z_2, i] \text{ and } x_j \in [z_1, z_2] \text{ for all } j \neq i \}
\]
Then we have \([z_1, z_2] \setminus (z_1 + \varepsilon, z_2 - \varepsilon) \subset S_i^- \cup \cdots \cup S_d^- \cup S_i^+ \cup \cdots \cup S_d^+ \), and hence we obtain
\[
P_X(\{ f_{\varepsilon} \neq 1_A \}) \leq \sum_{i=1}^{d} P_X(S_i^-) + \sum_{i=1}^{d} P_X(S_i^+).
\]
Now observe that since \( A \) is a cube with side length \( s \), the sets \( S_i^- \) and \( S_i^+ \) are cuboids with side lengths \( s_1, \ldots, s_d \), where \( s_i = \varepsilon \) and \( s_j = s \) for all \( j \neq i \). Applying Lemma [D.4] then shows
\[
\mathcal{N}(S_i^{\pm 1}, || \cdot ||_{\infty}, \varepsilon) \leq \left( \frac{3}{2} \right)^d s^{d-1} \cdot \varepsilon^{-d+1},
\]
and combining with Assumption 2.10 we obtain
\[
P_X(S_i^{\pm 1}) \leq \left( \frac{3}{2} \right)^d s^{d-1} \cdot \varepsilon^{-d+1} \cdot \varphi(2\varepsilon).
\]
Inserting this estimate into (63) yields (62). \(\square\)

As a second step in our construction presented in Subsection 3.1, we combine Lemmas [D.1] and [D.2] with Lemma [D.3] to approximate step-functions on cubic partitions by ReLU-DNNs with two hidden layers.

**Proposition D.6.** Let \( A_1, \ldots, A_k \) be mutually disjoint subsets of \( X := [-1, 1]^d \) such that for each \( i \in \{1, \ldots, k\} \) there exist \( z_i^-, z_i^+ \in X \) with \( z_i^- < z_i^+ \) and \( (z_i^-, z_i^+) \subset A_i \subset [z_i^-, z_i^+] \). Moreover, let \( z_{i,j}^{\pm} \) be the \( j \)-th coordinate of \( z_{i}^{\pm} \). Then for all \( g : X \to \mathbb{R} \) of the form
\[
g = \sum_{i=1}^{k} \alpha_i 1_{A_i}
\]
with \( \alpha_i \in \mathbb{R} \), all \( \varepsilon > 0 \) satisfying
\[
\varepsilon < \min \left\{ \frac{z_{i,j}^{+} - z_{i,j}^{-}}{2} : i = 1, \ldots, k \text{ and } j = 1, \ldots, d \right\}
\]
with \( \alpha_i \in \mathbb{R}, \) all \( \varepsilon > 0 \) satisfying
and all $m_1 \geq 2dk$ and $m_2 \geq k$, there exists a neural network $f_\varepsilon \in A_{m_1,m_2}$ such that

$$\{f_\varepsilon = g\} = \bigcup_{i=1}^{k} [z_i^- + \varepsilon, z_i^+ - \varepsilon] \cup (X \setminus A_i).$$

and $\|f_\varepsilon\|_\infty = \max\{|\alpha_1|, \ldots, |\alpha_k|\}$. In addition, if $A_1, \ldots, A_k$ are cubes of side length $s > 0$, i.e. $z_i^+ - z_i^- = (s, \ldots, s) \in \mathbb{R}^d$ for all $i = 1, \ldots, k$, and $P_X$ is a distribution on $[-1, 1]^d$ that satisfies Assumption 2.10 for some $\varphi : \mathbb{R}_+ \to \mathbb{R}_+$, then we further have

$$P_X(\{f_\varepsilon \neq g\}) \leq 3dk \cdot \left(\frac{3s}{2}\right)^{d-1} \cdot \varepsilon^{-d+1} \cdot \varphi(2\varepsilon).$$

**Proof of Proposition D.6** Since $A_{2dk,k} \subset A_{m_1,m_2}$ it suffices to find an $f_\varepsilon$ with the desired properties in $A_{2dk,k}$ By assumption and Lemma D.3, we find, for all $\varepsilon > 0$ and $i = 1, \ldots, k$, a neural network $f_i^{(e)} \in A_{2d,1}$ and Lemma D.5 shows that

$$\{f_i^{(e)} = 1_{A_i}\} = [z_i^- + \varepsilon, z_i^+ - \varepsilon] \cup (X \setminus A_i).$$

Moreover, for any $\alpha_i \in \mathbb{R}$, Lemma D.1 ensures $\alpha_i f_i^{(e)} \in A_{2d,1}$ with

$$\{\alpha_i f_i^{(e)} = \alpha_i 1_{A_i}\} = [z_i^- + \varepsilon, z_i^+ - \varepsilon] \cup (X \setminus A_i).$$

Now, applying Lemma D.2 shows that

$$f_\varepsilon := \sum_{i=1}^{k} \alpha_i f_i^{(e)}$$

belongs to $A_{2kd,k}$, and since we have

$$\{f_i^{(e)} \neq 0\} \cap \{f_i^{(e)} \neq 0\} = \{f_i^{(e)} > 0\} \cap \{f_i^{(e)} > 0\} \subset (z_i^-, z_i^+) \cap (z_i^-, z_i^+) \subset A_i \cap A_i$$

for all $i \neq l$, our previous considerations give us

$$\{f_\varepsilon = g\} = \bigcup_{i=1}^{k} [z_i^- + \varepsilon, z_i^+ - \varepsilon] \cup (X \setminus A_i).$$

Finally, the identity $\|f_\varepsilon\|_\infty = \max\{|\alpha_1|, \ldots, |\alpha_k|\}$ follows from (65) and $\|f_i^{(e)}\|_\infty = |\alpha_i|$ for all $i = 1, \ldots, k$ and the bound on $P_X(\{f_\varepsilon \neq 1_A\})$ is a direct consequence of (62). \hfill \Box

**D.3 Proof of Main Theorem 3.7**

Throughout this section we assume that the general assumptions of Theorem 3.7 are satisfied. In particular, $D \in (X \times Y)^n$ is an i.i.d. sample of size $n \geq 1$ and $D_X := \{x_1^*, \ldots, x_m^*\} \in \text{Pot}_m(X)$ is the set of input observations. Moreover, $(s_n)_{n \in \mathbb{N}}$ is a sequence with $s_n \to 0$, $s_n^d > 2d/n$ and $\frac{\ln(\eta s_n^d)}{n s_n^d} \to 0$ as $n \to \infty$. In addition, we let $(\rho_n)_{n \in \mathbb{N}}$ be a non-negative sequence with $\rho_n^d \leq 2d/n$ and $\rho_n^{-d} \varphi(\rho_n) \to 0$ for $n \to \infty$. Finally, let $(\varepsilon_n)_{n \in \mathbb{N}}$ and $(\delta_n)_{n \in \mathbb{N}}$ be positive sequences with $\varepsilon_n = \delta_n = \rho_n/2$. 

35
We firstly show our claim for the good interpolating DNN from Example 3.6, having representation
\[ g_{D,s_n,\rho_n}^+ = h_{D,A_D}^+ + \sum_{i=1}^{m} b_i^+ \mathbf{1}_{x_i^+ + tB_\infty} \]
with \( t = \min\{r, \rho_n\} \) and associated \( \mathcal{H}^{(\epsilon)}_{A} \) part
\[ h_{D,A_D}^+ := \sum_{j \in J} c_j^+ \mathbf{1}_{A_j} \].

We split the excess risk into three different terms
\[
\mathcal{R}_{L,P}(g_{D,s_n,\rho_n}^+) - \mathcal{R}_{L,P}^* = \mathcal{R}_{L,P}(g_{D,s_n,\rho_n}^+) - \mathcal{R}_{L,P}(h_{D,A_D}^+) + \mathcal{R}_{L,P}(h_{D,A_D}^+) - \mathcal{R}_{L,P}^* . \tag{66}
\]
Convergence of the first term follows from Lemma C.2 and by exploiting Assumption 2.10. We obtain
\[
\mathcal{R}_{L,P}(g_{D,s_n,\rho_n}^+) - \mathcal{R}_{L,P}(h_{D,A_D}^+) \leq 4 \mathbb{P}(\{g_{D,s_n,\rho_n}^+ \neq h_{D,A_D}^+\}) \leq 4 \mathbb{P}(D_{X}^+) \leq 4 \mathbb{P}(D_{X}^+ \rho_n) \leq 4n\varphi(\rho_n) \leq 4 \cdot 2^d \rho_n^{-d} \varphi(\rho_n) . \tag{67}
\]
Hence, by our assumption on \( \rho_n \) may we conclude
\[
\mathcal{R}_{L,P}(g_{D,s_n,\rho_n}^+) - \mathcal{R}_{L,P}(h_{D,A_D}^+) \to 0 ,
\]
in probability for \( |D| \to \infty \).

For bounding the second term in (66) we remind that \(|J| \leq \left( \frac{2}{s_n} \right)^d \). Lemma C.2 and Proposition D.6 yield\(^3\)
\[
\mathcal{R}_{L,P}(h_{D,A_D}^+) - \mathcal{R}_{L,P}(h_{D,A_D}^+) \leq 12 \cdot d |J| \cdot \left( \frac{3s_n}{2} \right)^{d-1} \varepsilon_n^{-d+1} \cdot \varphi(2\varepsilon_n) \leq 12 \cdot d \left( \frac{2}{s_n} \right)^d \cdot \left( \frac{3s_n}{2} \right)^{d-1} \varepsilon_n^{-d+1} \cdot \varphi(2\varepsilon_n) \leq 4 \cdot d \cdot 6^d \cdot \rho_n^{-d} \cdot \varphi(\rho_n) . \tag{68}
\]
Hence, our assumption on \( \rho_n \) ensures
\[
\mathcal{R}_{L,P}(h_{D,A_D}^+) - \mathcal{R}_{L,P}(h_{D,A_D}^+) \to 0 ,
\]
\(^3\)This is justified since \( \varepsilon_n = \rho_n/2 \leq n^{-1/d} < s_n/2 \).
in probability for $|D| \to \infty$. Finally, convergence of the last term in (68) is easily derived with the help of Proposition E.5 and we conclude that

$$\|g_{D,s_n,\rho_n}^+ - f_{L,P}^*\|_{L^2(P_X)}^2 = \mathcal{R}_{L,P}(g_{D,s_n,\rho_n}^+) - \mathcal{R}_{L,P}^* \to 0,$$

in probability for $|D| \to \infty$.

We now turn to considering the bad interpolating DNN from Example 3.6. Since we have $g_{D,s_n,\rho_n}(x) \in [-1,1]$ and $f_{L,P}^1(x) \in [-1,1]$ for all $x \in X$, Assumption 2.10 gives

$$\int_{D_X^+}(g_{D,s_n,\rho_n}(x) - f_{L,P}^1(x))^2 \, dP_X \leq 4P_X(D_X^{+\rho_n}) \leq 4n\varphi(\rho_n) \leq 4\rho_n^{-d}\varphi(\rho_n). \quad (69)$$

Moreover, for all $x \in X \setminus D_X^+$ we have $g_{D,s_n,\rho_n}(x) = -h_{D,A_D}^{+,\varepsilon_n}$ and $f_{L,P}^1(x) = -f_{L,P}^*$. Hence

$$\int_{X \setminus D_X^+}(g_{D,s_n,\rho_n}(x) - f_{L,P}^1(x))^2 \, dP_X \leq \mathcal{R}_{L,P}(h_{D,A_D}^{+,\varepsilon_n}) - \mathcal{R}_{L,P}^*.$$

Combining both considerations with the first part of the proof shows then in probability for $|D| \to \infty$

$$\|g_{D,s_n,\rho_n}^+ - f_{L,P}^*\|_{L^2(P_X)} \to 0.$$

Finally, since $|J| \leq (\frac{2}{\alpha})^d \leq n$, Proposition D.6 shows that $g_{D,s_n,\rho_n}^+ \in A_{4dn,2n}$.

D.4 Proof of Main Theorem 3.8

Let all assumptions of Theorem 3.8 be satisfied. Moreover, we let $(\varepsilon_n)_{n \in \mathbb{N}}$ and $(\delta_n)_{n \in \mathbb{N}}$ be positive sequences with $\varepsilon_n = \delta_n = \rho_n/2$. We prove the result for the good interpolating DNN by reconsidering (66). Indeed, by our assumption $\rho_n^{-d}\varphi(\rho_n) \leq \ln(n)n^{-2/3}$ and thus (67) leads to

$$\mathcal{R}_{L,P}(g_{D,s_n,\rho_n}^+) - \mathcal{R}_{L,P}(h_{D,A_D}^{+,\varepsilon_n}) \leq 4\rho_n^{-d}\varphi(\rho_n) \leq 4\ln(n)n^{-2/3} \leq 4\ln(n)n^{-2\alpha\gamma}.$$

Moreover, (68) gives

$$\mathcal{R}_{L,P}(h_{D,A_D}^{+,\varepsilon_n}) - \mathcal{R}_{L,P}(h_{D,A_D}^{+,\varepsilon_n}) \leq 4 \cdot d \cdot 6^d \cdot \rho_n^{-d} \cdot \varphi(\rho_n) \leq 16 \cdot d \cdot 6^d \ln(n)n^{-2\alpha\gamma}.$$

Finally, (51) shows with probability $P^n$ at least $1 - 2^d n^{1+d}e^{-n^{d\gamma}}$

$$\mathcal{R}_{L,P}(h_{D,A_D}^{+,\varepsilon_n}) - \mathcal{R}_{L,P}^* \leq c_{d,\alpha} \ln(n)n^{-2\alpha\gamma}, \quad (70)$$

where $c_{d,\alpha} > 0$ is a constant only depending on $d, \alpha$, and $|f_L^*|_\alpha$. Collecting the above considerations shows the first part of the theorem.

Now, coming to the bad interpolating DNN, we derive from (69)

$$\int_{D_X^+}(g_{D,s_n,\rho_n}(x) - f_{L,P}^1(x))^2 \, dP_X \leq 4P_X(D_X^{+\rho_n}) \leq 4\ln(n)n^{-2\alpha\gamma}.$$

Moreover, combining the results from (68) and (70) gives with probability $P^n$ at least $1 - 2^d n^{1+d}e^{-n^{d\gamma}}$

$$\mathcal{R}_{L,P}(h_{D,A_D}^{+,\varepsilon_n}) - \mathcal{R}_{L,P}^* \leq 4 \cdot d \cdot 6^d \cdot \ln(n)n^{-2/3} + c_{d,\alpha} \ln(n)n^{-2\alpha\gamma} \leq c_{d,\alpha} \ln(n)n^{-2\alpha\gamma},$$

37
where \( c'_{d,\alpha} = 4 \cdot d \cdot 6^d + c_{d,\alpha} \). Thus, with probability \( P^n \) at least \( 1 - 2^d n^{1+d} e^{-n^{2\gamma}} \)
\[
\| g_{D,s_n,\rho_n} - f_{L,P}^1 \|_{L_2(P_X)}^2 \leq c''_{d,\alpha} \ln(n) n^{-2\alpha\gamma},
\]
where \( c''_{d,\alpha} = 4 + c'_{d,\alpha} \).

Finally, we have \( |J| \leq (2/n)^d = 2^d n^{2d+1} \leq n \), provided \( n \geq n_{d,\alpha} \), for some \( n_{d,\alpha} \in \mathbb{N} \), depending on \( d \) and \( \alpha \). Proposition D.6 shows then that \( g_{D,s_n,\rho_n} \in A_{4dn,2n} \).

### E Uniform bounds for histograms based on data-dependent partitions

The main purpose of this section is to firstly present a general variance improved oracle inequality for bounding the excess risk with respect to a broad class of loss functions. We apply this result to the special case of the least squares loss and to histogram rules that choose their cubic partitions in a certain, data-dependent way. In particular, we give an optimized uniform bound that crucially relies on an explicit capacity bound, expressed in terms of the covering number. This is a necessary step to provide in Section E.2 the learning properties of histograms based on data-dependent cubic partitions.

### E.1 A Generic Oracle Inequality for Empirical Risk Minimization

If not stated otherwise, we assume throughout this subsection that \( X \) is an arbitrary non-empty set that is equipped with some \( \sigma \)-algebra. We write \( L_\infty \) for the corresponding set of all bounded, measurable functions \( f : X \to \mathbb{R} \). Moreover, \( Y \subset \mathbb{R} \) is assumed to be measurable.

Following [19, Definition 2.18] we say that a measurable loss \( L : X \times Y \times \mathbb{R} \to [0, \infty) \) is locally Lipschitz continuous if for all \( a \geq 0 \) there exists a constant \( c_a \geq 0 \) such that
\[
\sup_{x \in X, y \in Y} \left| L(x, y, t) - L(x, y, t') \right| \leq c_a |t - t'|, \quad t, t' \in [-a, a].
\]

Moreover, for \( a \geq 0 \), the smallest such constant \( c_a \) is denoted by \( |L|_{a,1} \).

In addition, we need to recall the notion of covering numbers, which is recalled in the following definition.

**Definition E.1.** Let \( (T,d) \) be a metric space and \( \varepsilon > 0 \). We call \( S \subset T \) an \( \varepsilon \)-net of \( T \) if for all \( t \in T \) there exists an \( s \in S \) with \( d(s,t) \leq \varepsilon \). Moreover, the \( \varepsilon \)-covering number of \( T \) is defined by
\[
\mathcal{N}(T,d,\varepsilon) := \inf \left\{ n \geq 1 : \exists s_1, \ldots, s_n \in T \text{ such that } T \subset \bigcup_{i=1}^n B_d(s_i,\varepsilon) \right\},
\]
where \( \inf \emptyset := \infty \) and \( B_d(s,\varepsilon) := \{ t \in T : d(t,s) \leq \varepsilon \} \) denotes the closed ball with center \( s \in T \) and radius \( \varepsilon \).

Moreover, if \( (T,d) \) is a subspace of a normed space \( (E,\|\cdot\|) \) and the metric is given by \( d(x,x') = \|x - x'\| \), \( x, x' \in T \), we write \( \mathcal{N}(T,\|\cdot\|,\varepsilon) := \mathcal{N}(T,d,\varepsilon) \).

Finally, we need to fix some notation related to empirical risk minimization. To this end, we fix a loss function \( L : X \times Y \times \mathbb{R} \to [0,\infty) \) and an \( \mathcal{F} \subset L_\infty(X) \). Given a distribution
\( P \) on \( X \times Y \), we denote the smallest possible risk attained by functions in \( \mathcal{F} \) by \( \mathcal{R}^*_L,p,\mathcal{F} \), that is
\[
\mathcal{R}^*_L,p,\mathcal{F} := \inf_{f \in \mathcal{F}} \mathcal{R}_L,f(p) .
\]

Finally, following [19, Definition 6.2], we say that an ERM method \( D \mapsto f_D \) with respect to \( L \) and \( \mathcal{F} \) is measurable, if for all \( n \geq 1 \) the map
\[
(X \times Y)^n \times X \to \mathbb{R} \\
(D, x) \mapsto f_D(x)
\]
is measurable with respect to the universal completion of the product \( \sigma \)-algebra of the product space \( (X \times Y)^n \times X \). Recall from [19, Lemma 6.17] that for closed, separable \( \mathcal{F} \subset \mathcal{L}_\infty(X) \) for which there exists an ERM, there also exists a measurable ERM. Moreover, in this case the map
\[
(X \times Y)^n \to [0, \infty] \\
(D, x) \mapsto \mathcal{R}_L,p(f_D)
\]
is also measurable with respect to the universal completion of the product \( \sigma \)-algebra of \( (X \times Y)^n \), see [19, Lemma 6.3]. In the following, we thus assume that \( (X \times Y)^n \) is equipped with this universal completion.

With the help of these notions we can now state the generic oracle inequality for empirical risk minimizers.

**Theorem E.2.** Let \( L : X \times Y \times \mathbb{R} \to [0, \infty) \) be a locally Lipschitz continuous loss, \( \mathcal{F} \subset \mathcal{L}_\infty(X) \) be a closed, separable set satisfying \( \| f \|_\infty \leq M \) for a suitable constant \( M > 0 \) and all \( f \in \mathcal{F} \), and \( P \) be a distribution on \( X \times Y \) that has a Bayes decision function \( f^*_L,p \) with \( \mathcal{R}_L,p(f^*_L,p) < \infty \). Assume that there exist constants \( B > 0 \), \( \vartheta \in [0, 1] \), and \( V \geq B^{2-\vartheta} \) such that for all measurable \( f : X \to [-M, M] \) we have
\[
\| L \circ f - L \circ f^*_L,p \|_\infty \leq B , \tag{72}
\]
\[
\mathbb{E}_P(L \circ f - L \circ f^*_L,p)^2 \leq V \cdot (\mathbb{E}_P(L \circ f - L \circ f^*_L,p))^{\vartheta} . \tag{73}
\]

Then, for all measurable empirical risk minimization algorithms \( D \mapsto f_D \), all \( n \geq 1 \), \( \tau > 0 \), and all \( \varepsilon > 0 \) we have
\[
\mathcal{R}_L,p(f_D) - \mathcal{R}^*_L,p,\mathcal{F} \leq 4(\mathcal{R}^*_L,p,\mathcal{F} - \mathcal{R}^*_L,p) + 5 |L|_{M,1} \cdot \varepsilon \\
+ 2 \left( \frac{16V(\tau + 1 + \ln \mathcal{N}(\mathcal{F}, \| \cdot \|_\infty, \varepsilon))}{n} \right)^{\frac{1}{\vartheta}}
\]
with probability \( P^n \) not less than \( 1 - e^{-\tau} \).

**Proof.** We first note that (72) ensures \( \mathcal{R}_L,p(f_D) - \mathcal{R}^*_L,p,\mathcal{F} \leq B \) and since we have additionally assumed \( V \geq B^{2-\vartheta} \), we see that it suffices to consider sample sizes \( n \geq 16\tau \).

Given an \( f \in \mathcal{F} \), we define \( h_f := L \circ f - L \circ f^*_L,p \). Let us now fix an \( f_0 \in \mathcal{F} \) and a data set \( D \in (X \times Y)^n \). Since \( f_D \) is an empirical risk minimizer, we have \( \mathcal{R}_{L,D}(f_D) \leq \mathcal{R}_{L,D}(f_0) \), and hence we find \( \mathbb{E}_D h_{f_D} \leq \mathbb{E}_D h_{f_0} \). As a consequence, we obtain
\[
\mathcal{R}_L,p(f_D) - \mathcal{R}_L,p(f_0) = \mathbb{E}_p h_{f_D} - \mathbb{E}_p h_{f_0} \leq \mathbb{E}_p h_{f_D} - \mathbb{E}_D h_{f_D} + \mathbb{E}_D h_{f_0} - \mathbb{E}_p h_{f_0} . \tag{74}
\]
To bound the first difference in (74) we first observe that for \( f, f' \in \mathcal{F}, x \in X, \) and \( y \in Y \) the local Lipschitz continuity of \( L \) gives

\[
|h_f(x, y) - h_{f'}(x, y)| = |L(x, y, f(x)) - L(x, y, f'(x))| \leq |L|_{M, 1} \cdot |f(x) - f'(x)|,
\]

and thus we have \( \|h_f - h_{f'}\|_\infty \leq |L|_{M, 1} \cdot \|f - f'\|_\infty \) for all \( f, f' \in \mathcal{F} \). Now, let \( \mathcal{C} \subset \mathcal{F} \) be a minimal \( \varepsilon \)-net of \( \mathcal{F} \) with respect to \( \|\cdot\|_\infty \). For a data set \( D \in (X \times Y)^n \) there then exists an \( f \in \mathcal{C} \) such that \( \|f - f_D\|_\infty \leq \varepsilon \), and hence \( \|h_{f_D} - h_f\|_\infty \leq |L|_{M, 1} \cdot \varepsilon \). This yields

\[
\max\left\{|E_p h_{f_D} - E_P h_f|, |E_D h_{f_D} - E_D h_f|\right\} \leq \max\left\{|E_P| h_{f_D} - h_f|, |E_D| h_{f_D} - h_f|\right\} \\
\leq \|h_{f_D} - h_f\|_\infty \\
\leq |L|_{M, 1} \cdot \varepsilon. \tag{75}
\]

For \( f \in \mathcal{C} \) and \( r > 0 \) we now define the function

\[
g_{f,r} := \frac{E_P h_f - h_f}{E_P h_f + r}.
\]

It is easy to see that both \( E_P g_{f,r} = 0 \) and \( \|g_{f,r}\|_\infty \leq 2B r^{-1} \) hold. In addition, in the case \( \vartheta > 0 \) and \( b := E_P h_f \neq 0 \), setting \( q := \frac{2}{2 - \vartheta}, q' := \frac{2}{\vartheta}, \) and \( a := r \) in the second inequality of [19] Lemma 7.1] shows

\[
E_P g_{f,r}^2 \leq \frac{E_P h_f^2}{(E_P h_f + r)^2} \leq \frac{(2 - \vartheta)^2 - \vartheta a^2 E_P h_f^2}{4r^2 - \vartheta (E_P h_f)^2} \leq V r^{\vartheta - 2}.
\]

Furthermore, in the case \( \vartheta > 0 \) and \( E_P h_f = 0 \), the variance bound (73) gives \( E_P h_f^2 = 0 \), and hence we have \( E_P g_{f,r}^2 \leq V r^{\vartheta - 2} \). Finally, in the case \( \vartheta = 0 \), we have \( E_P g_{f,r}^2 \leq E_P h_f^2 r^{-2} \leq V r^{\vartheta - 2} \). In summary, we have thus found

\[
E_P g_{f,r}^2 \leq V r^{\vartheta - 2}
\]

in all cases. By applying Bernstein’s inequality in the form of [19] Theorem 6.12 in combination with a union bound we thus find

\[
P^n \left(D \in (X \times Y)^n : \sup_{f \in \mathcal{C}} E_D g_{f,r} < \sqrt{\frac{2V \tau}{n^{r^2 - \vartheta}} + \frac{4B \tau}{3nr}} \right) \geq 1 - |\mathcal{C}| e^{-\gamma} \tag{76}
\]

for all \( r > 0 \). Let us now pick a data set \( D \in (X \times Y)^n \) that satisfies the above inequality, that is

\[
\sup_{f \in \mathcal{C}} E_D g_{f,r} < \sqrt{\frac{2V \tau}{n^{r^2 - \vartheta}} + \frac{4B \tau}{3nr}}.
\]

For an \( f \in \mathcal{C} \) with \( \|f - f_D\|_\infty \leq \varepsilon \), Inequality (75) together with the definition of \( g_{f,r} \) then gives

\[
E_P h_{f_D} - E_D h_{f_D} \leq E_P h_f - E_D h_f + 2 |L|_{M, 1} \cdot \varepsilon \\
< E_P h_f \left( \sqrt{\frac{2V \tau}{n^{r^2 - \vartheta}} + \frac{4B \tau}{3nr}} \right) + \sqrt{\frac{2V \tau r^\vartheta}{n} + \frac{4B \tau}{3n} + 2 |L|_{M, 1} \cdot \varepsilon} \\
\leq (E_P h_f + \varepsilon) \left( \sqrt{\frac{2V \tau}{n^{r^2 - \vartheta}} + \frac{4B \tau}{3nr}} \right) + \sqrt{\frac{2V \tau r^\vartheta}{n} + \frac{4B \tau}{3n} + 2 |L|_{M, 1} \cdot \varepsilon}. \tag{77}
\]
Our next goal is to estimate the second difference (74), that is $E_P h_f - E_P h_f_0$. Let us first consider case $\vartheta > 0$. Here, we have both $\|h_f - E_P h_f_0\|_{\infty} \leq 2B$ and

$$E_P(h_f - E_P h_f_0)^2 \leq E_P h_f^2 \leq V(E_P h_f)^{\vartheta}.$$  

Furthermore, setting $q := \frac{2}{2-\vartheta}$, $q' := \frac{2}{\vartheta}$, $a := \left(\frac{2^{1-\vartheta}\vartheta V_{\tau}}{n}\right)^{1/2}$, and $b := \left(\frac{2E_P h_{f_0}}{\vartheta}\right)^{\vartheta/2}$ in Lemma 7.1 yields

$$\sqrt{\frac{2\tau V(E_P h_f)^{\vartheta}}{n}} \leq \left(1 - \frac{\vartheta}{2}\right) \left(\frac{2^{1-\vartheta}\vartheta V_{\tau}}{n}\right)^{\frac{1}{2-\vartheta}} + E_P h_f_0 \leq \left(\frac{2V_{\tau}}{n}\right)^{\frac{1}{2}} + E_P h_f.$$  

By another application of Bernstein’s inequality we consequently find that

$$E_P h_f - E_P h_f_0 < E_P h_f_0 + \left(\frac{2V_{\tau}}{n}\right)^{\frac{1}{2}} + \frac{4B_{\tau}}{3n}$$  

holds with probability $P^n$ not less than $1 - e^{-\tau}$. Finally, in the case $\vartheta = 0$, Hoeffding’s inequality in combination with $\|h_f\|_{\infty} \leq B \leq \sqrt{V}$ also yields (78).

To finish the proof, we now combine (74), (76), (77), and (78). As a result we see that

$$E_P h_{f_D} < 2E_P h_f_0 + \left(E_P h_f_0 + \varepsilon\right) \left(\sqrt{\frac{2V_{\tau}}{nr^{2-\vartheta}}} + \frac{4B_{\tau}}{3n}\right) + \sqrt{\frac{2V_{\tau}r^{\vartheta}}{n}}$$  

holds with probability $P^n$ not less than $1 - (1 + |C|)e^{-\tau}$. In the following, we fix a data set $D$, for which this inequality holds. Defining

$$r := \left(\frac{16V_{\tau}}{n}\right)^{1/(2-\vartheta)},$$  

a simple calculation then shows both

$$\sqrt{\frac{2V_{\tau}}{nr^{2-\vartheta}}} = \frac{1}{\sqrt{8}}$$  

and $$\sqrt{\frac{2V_{\tau}r^{\vartheta}}{n}} = \frac{r}{\sqrt{8}}. $$

Moreover, $V \geq B^{2-\vartheta}$ together with $n \geq 16\tau$ gives

$$\frac{4B_{\tau}}{3nr} = \frac{1}{12} \cdot \frac{16\tau}{n} \cdot \frac{B}{r} \leq \frac{1}{12} \cdot \left(\frac{16\tau}{n}\right)^{\frac{1}{2-\vartheta}} \cdot \frac{V^{\frac{1}{2}}}{r} = \frac{1}{12} \quad \text{and} \quad \frac{8B_{\tau}}{3n} \leq \frac{r}{6}.$$  

Finally, we have

$$\left(\frac{2V_{\tau}}{n}\right)^{\frac{1}{2-\vartheta}} = 8^{-\frac{1}{2-\vartheta}} \left(\frac{16V_{\tau}}{n}\right)^{\frac{1}{2}} \leq \frac{r}{\sqrt{8}}.$$  

Inserting these estimates in our inequality on $E_P h_{f_D}$ gives

$$E_P h_{f_D} < 2E_P h_f_0 + \left(E_P h_f_0 + \varepsilon\right) \left(\frac{1}{\sqrt{8}} + \frac{1}{12}\right) + \frac{r}{\sqrt{8}} + \frac{r}{6} + 2 |L|_{M,1} \cdot \varepsilon$$  

$$= 2E_P h_f_0 + \frac{6 + \sqrt{2}}{12\sqrt{2}} \cdot E_P h_f_0 + \frac{6 + \sqrt{2}}{6\sqrt{2}} \cdot r + \frac{6 + 25\sqrt{2}}{12\sqrt{2}} \cdot |L|_{M,1} \cdot \varepsilon,$$  

41
and by elementary transformations we thus conclude that
\[
\mathcal{R}_{L,P}(f_D) - \mathcal{R}_{L,P}^* = \mathbb{E}_{P}h_{f_D} - \mathbb{E}_{P}h_{f_0} + \frac{12}{11\sqrt{2} - 6} \cdot r + \frac{6 + 2\sqrt{2}}{11\sqrt{2} - 6} \cdot |L|_{M,1} \cdot \varepsilon
\]
\[
< 4 \mathbb{E}_{P}h_{f_0} + 2r + 5 |L|_{M,1} \cdot \varepsilon
\]
\[
= 4(\mathcal{R}_{L,P}(f_0) - \mathcal{R}_{L,P}^*) + 2 \left(\frac{16Vr}{n}\right)^{1/(2-\vartheta)} + 5 |L|_{M,1} \cdot \varepsilon
\]

Now the assertion follows by a simple algebraic transformation of \(\tau\) and taking the infimum over all \(f_0 \in \mathcal{F}\).

If we have an upper bound on the covering numbers occurring in Theorem \[\text{E.2}\], then we can optimize the right hand side of its oracle inequality with respect to \(\varepsilon\). The following corollary executes this idea for the least squares loss and histogram rules that choose their cubic partitions in a certain, data-dependent way.

**Corollary E.3.** Let \(Y = [-M, M]\) and let \(L\) be the least squares loss. For \(K < \infty\) and \(A < \infty\) let \(A_1, \ldots, A_K\) be finite Partitions of \(X\), satisfying \(|A_i| \leq A\) for any \(i = 1, \ldots, K\). Moreover, let \(D \mapsto h_{D,A_D}\) be an algorithm, that first chooses a partition \(A_D\) from \(A_1, \ldots, A_K\) and then computes the corresponding \(A_D\)-histogram. Then, for all \(n \geq 1\) and \(\tau > 0\), we have
\[
\mathcal{R}_{L,P}(h_{D,A_D}) - \mathcal{R}_{L,P}^* \leq 4 \sup_{i=1,\ldots,K} (\mathcal{R}_{L,P,A_i}^* - \mathcal{R}_{L,P}^*) + 1024 \frac{\tau M^2}{n} + 512 \frac{AM^2}{n} \left(1 + \ln\left(\frac{n}{A}\right)\right)
\]
with probability \(P^n\) not less than \(1 - Ke^{-\tau}\).

**Proof of Corollary E.3.** Since \(L\) is the least squares loss, the assumptions \[\text{E.2}\] and \[\text{E.2}\] of Theorem \[\text{E.2}\] are satisfied with \(\vartheta = 1\), \(B = 4M^2\), and \(V = 16M^2\). Moreover, our assumption \(Y \subset [-M, M]\) ensures that \(L\) is locally Lipschitz continuous with \(|L|_{M,1} \leq 4M\).

Now, for a fixed \(i \in \{1, \ldots, K\}\) we recall that the histogram rule \(D \mapsto h_{D,A_i}\) is an empirical risk minimizer over the hypotheses class
\[
\mathcal{H}_{A_i} = \left\{ \sum_{j \in J} c_j 1_{A_j} : c_j \in Y \right\},
\]
where \(A_i = (A_j)_{j \in J}\). Moreover, for any \(\varepsilon > 0\), the \(\varepsilon\)-covering number of \(\mathcal{H}_{A_i}\) satisfies
\[
N(\mathcal{H}_{A_i}, \|\cdot\|_{\infty}, \varepsilon) \leq (2M/\varepsilon)^{|A_i|} \leq (2M/\varepsilon)^A. \tag{79}
\]
For \(n \geq 1\), \(\tau > 0\), and \(\varepsilon > 0\) Theorem \[\text{E.2}\] thus gives
\[
\mathcal{R}_{L,P}(h_{D,A_i}) - \mathcal{R}_{L,P}^* \leq 4(\mathcal{R}_{L,P,A_i}^* - \mathcal{R}_{L,P}^*) + 20M \cdot \varepsilon + \frac{512M^2 (2\tau + A \ln(2M/\varepsilon))}{n}
\]
with probability \(P^n\) not less than \(1 - e^{-\tau}\).

Next we optimize this bound over \(\varepsilon > 0\). To this end, we consider the strongly convex function
\[
h(\varepsilon) = \alpha \varepsilon + \beta \ln(\gamma/\varepsilon),
\]

42
where \( \alpha := 20M \), \( \beta := \frac{512AM^2}{n} \), and \( \gamma := 2M \). Then a simple calculation shows that \( h \) has a minimum at \( \varepsilon^* := \frac{\beta}{\alpha} \), giving
\[
h(\varepsilon^*) = \beta \left( 1 + \ln \left( \frac{\alpha \gamma}{\beta} \right) \right) = \frac{512AM^2}{n} \left( 1 + \ln \left( \frac{40nM^2}{512AM^2} \right) \right) \leq \frac{512AM^2}{n} \left( 1 + \ln \left( \frac{n}{A} \right) \right).
\]

Inserting this estimate in our above oracle inequality obtained from Theorem E.2, using the fact that
\[
R_{L,P}(h_{D,A}) - R^*_L \leq \sup_{i=1,\ldots,K} R_{L,P}(h_{D,A_i}) - R^*_L,
\]
and finally applying a simple union bound then gives the assertion.

**E.2 Learning Properties of Histograms**

The first lemma describes how well the infinite sample histogram rules defined in (7) can approximate the least squares Bayes risk.

**Lemma E.4 (Approximation Error).** Let \( L \) be the least squares loss, \( X := [-1,1]^d \), \( Y = [-1,1] \), and \( P \) be a distribution on \( X \times Y \). Then, for all \( \varepsilon > 0 \), there exists an \( s_\varepsilon > 0 \) such that for any cubic partition \( A \) of \( X \) with width \( s \in (0,s_\varepsilon] \) one has
\[
R_{L,P}(h_{P,A}) - R^*_L < \varepsilon.
\]
Moreover, if \( f^*_L \) is \( \alpha \)-Hölder continuous for some \( \alpha \in (0,1] \), then for all \( s \in (0,1] \) and all cubic partitions \( A \) of \( X \) with width \( s \) we have
\[
R_{L,P}(h_{P,A}) - R^*_L \leq |f^*_L|^2 \cdot s^{2\alpha}.
\]

**Proof of Lemma E.4:** For the proof of the first assertion we fix an \( \varepsilon > 0 \). Then recall that there exists a continuous function \( f : \mathbb{R}^d \to \mathbb{R} \) with compact support such that
\[
\|f^*_L - f\|_2 \leq \varepsilon,
\]see e.g. [3, Theorem 29.14 and Lemma 26.2]. Moreover, since \( \|f^*_L\|_\infty \leq 1 \), we can assume without loss of generality that \( \|f\|_\infty \leq 1 \). Now, since \( f \) is continuous and has compact support, \( f \) is uniformly continuous, and hence there exists a \( \delta \in (0,1] \) such that for all \( x, x' \in X \) with \( \|x - x'\|_\infty \leq \delta \) we have
\[
|f(x) - f(x')| \leq \varepsilon.
\]
We define \( s_\varepsilon := \delta \). Now, we fix a cubic partition \( A = (A_j)_{j \in J} \) of width \( s > 0 \) for some \( s \in (0,s_\varepsilon] \). For \( x \in X \) with \( P_X(A(x)) > 0 \) we then have
\[
h_{P,A}(x) = \frac{1}{P_X(A(x))} \int_{A(x)} f^*_L dP_X.
\]
For such \( x \) we then define
\[
\hat{f}(x) := \frac{1}{P_X(A(x))} \int_{A(x)} f dP_X.
\]
For the remaining $x \in X$ we simply set $\bar{f}(x) := 0$. With these preparations we then have
\[
\|h_{P,A} - f^*_{L,P}\|_2 \leq \|h_{P,A} - \bar{f}\|_2 + \|\bar{f} - f\|_2 + \|f - f^*_{L,P}\|_2.
\] (83)

Clearly, (80) shows that the third term is bounded by $\varepsilon$. Let us now consider the second term. Here we first note that for an $x \in X$ with $P_X(A(x)) > 0$ we have
\[
|f(x) - \bar{f}(x)| = \frac{1}{P_X(A(x))} \left| \int_{A(x)} f(x) - f(x') dP_X(x') \right|
\leq \frac{1}{P_X(A(x))} \int_{A(x)} |f(x) - f(x')| dP_X(x')
\leq \varepsilon,
\] (84)

where in the last step we used (81). Consequently, we obtain
\[
\|f - \bar{f}\|_2^2 = \sum_{j \in J : P_X(A_j) > 0} \int_{A_j} |f(x) - \bar{f}(x)|^2 dP_X(x')
\leq \sum_{j \in J : P_X(A_j) > 0} \varepsilon^2 \cdot P_X(A_j)
\leq \varepsilon^2.
\] (85)

In other words, the second term is bounded by $\varepsilon$, too. Let us finally consider the first term. Here we have
\[
\|h_{P,A} - \bar{f}\|_2^2 = \sum_{j \in J : P_X(A_j) > 0} \int_{A_j} \left| h_{P,A} - \bar{f} \right|^2 dP_X
\leq \sum_{j \in J : P_X(A_j) > 0} \left( \sum_{j \in J : P_X(A_j) > 0} \left| \int_{A_j} f^*_{L,P} dP_X - \int_{A_j} f dP_X \right|^2 \right)\]
\leq \left( \sum_{j \in J : P_X(A_j) > 0} \left| \int_{A_j} f^*_{L,P} dP_X - \int_{A_j} f dP_X \right| \right)^2
\leq \left( \sum_{j \in J : P_X(A_j) > 0} \left| \int_{A_j} |f^*_{L,P} - f| dP_X \right| \right)^2
\leq \varepsilon^2.
\]

Consequently, the first term is bounded by $\varepsilon$, too, and hence we conclude by (83) that the excess risk satisfies
\[
\mathcal{R}_{L,P}(h_{P,A}) - \mathcal{R}_{L,P}^* = \|h_{P,A} - f^*_{L,P}\|_2^2 \leq 9\varepsilon^2.
\]

A simple variable transformation then yields the first assertion.
To show the second assertion we first note that for all \( x, x' \in X \) we have

\[
|f^*_L,P(x) - f^*_L,P(x')| \leq |f^*_L,P|_{\alpha} \cdot ||x - x'||_{\infty}^\alpha.
\]

For \( s \in (0, 1], \varepsilon := |f^*_L,P|_{\alpha} \cdot s^\alpha \), and \( x, x' \in X \) with \( ||x - x'||_{\infty} \leq s \) we thus find

\[
|f^*_L,P(x) - f^*_L,P(x')| \leq \varepsilon.
\]

Now consider \( f := f^*_L,P \) and fix an arbitrary cubic partition \( A \) of width \( s \). Then \( f \) defined by \((82)\) is given by \( f = h_{P,A} \). Moreover, we have

\[
\mathcal{R}_{L,P}(h_{P,A}) - \mathcal{R}_{L,P}^* = \|f^*_L,P - h_{P,A}\|_2^2 \leq \varepsilon^2,
\]

where in the last step we used \((84)\) and \((85)\).

Based on the previous results we can now establish universal consistency of the empirical histogram rule \( D \mapsto h_{D,A_D} \) for regression based on a cubic data-dependent partition \( A_D \) from \( \mathcal{P}(X) \).

**Proposition E.5** (Universal Consistency). Let \( L \) be the least squares loss, \( X := [-1, 1]^d \), \( Y = [-1, 1] \), \( P \) be a distribution on \( X \times Y \), and \( D \in (X \times Y)^n \) be an i.i.d. sample of size \( n \geq 1 \) drawn from \( P \) with \( |D_X| = m_n \). Suppose that \((s_n)_{n \in \mathbb{N}}\) is a sequence with \( s_n \to 0 \) as well as \( \frac{\ln(n/s_n^d)}{ns_n^d} \to 0 \) as \( n \to \infty \). Assume further that \( \pi_{m_n,s_n} \) is an \( m_n \)-sample cubic partitioning rule of width \( s_n \in (0, 1] \), satisfying \( |\text{Im}(\pi_{m_n,s_n})| \leq cn^d \), for some \( c < \infty \) and some \( \beta > 0 \) that are independent of \( n \). Denoting \( A_D := \pi_{m_n,s_n}(D_X) \), we have

\[
\mathcal{R}_{L,P}(h_{D,A_D}) \to \mathcal{R}_{L,P}^*
\]

in probability as \( n \to \infty \).

**Proof of Proposition E.5.** Note that for any \( \varepsilon > 0 \) and for any \( A \in \text{Im}(\pi_{m_n,s_n}) \), the \( \varepsilon \)-covering number of \( \mathcal{H}_A \) satisfies

\[
\mathcal{N}(\mathcal{H}_A, || \cdot ||_{\infty}, \varepsilon) \leq (2/\varepsilon)^{|A|},
\]

with \(|A| \leq (2/s_n)^d\). Let us write \( P_n := \text{Im}(\pi_{1,s_n}) \cup \cdots \cup \text{Im}(\pi_{n,s_n}) \). Applying Corollary E.3 with \( A := (2/s_n)^d \) and \( K := |P_n| \leq cn^{1+\beta} \) gives, for all \( \tau \geq 1 \) and \( n \geq 1 \), with probability \( P^n \) at least \( 1 - 2cn^{1+\beta}e^{-\tau} \) that

\[
\mathcal{R}_{L,P}(h_{D,A_D}) - \mathcal{R}_{L,P}^* \leq 4 \sup_{A \in \mathcal{P}_n} (\mathcal{R}_{L,P,H_A}^* - \mathcal{R}_{L,P}^*)
\]

\[
+ 1024 \frac{\tau}{n} + 512 \frac{2^d}{ns_n^d} \left( 1 + \ln \left( \frac{ns_n^d}{2d} \right) \right).
\]

Now, for all \( \varepsilon > 0 \), Lemma 2.4 guarantees the existence of an \( s_\varepsilon > 0 \) such that for any cubic partition \( A \) of width \( s_n \in (0, s_\varepsilon] \) we have

\[
\mathcal{R}_{L,P}(h_{P,A}) - \mathcal{R}_{L,P}^* < \varepsilon.
\]

Since we assumed \( s_n \to 0 \) we conclude that the latter inequality holds for all sufficiently large \( n \). Combining both bounds we find for all sufficiently large \( n \) that with probability \( P^n \) at least \( 1 - 2cn^{1+\beta}e^{-\tau} \) it holds

\[
\mathcal{R}_{L,P}(h_{D,A_D}) - \mathcal{R}_{L,P}^* \leq 4\varepsilon + 1024 \frac{\tau}{n} + c_d \frac{\ln(ns_n^d)}{ns_n^d},
\]

45
where \(c_d = 1024 \cdot 2^d\). Finally, choosing \(\tau = (\beta + 2) \log(n)\), the result follows by remembering that by assumption \(\frac{\ln(n s_n^d)}{n s_n^d} \to 0\). 

We now come to our second main contribution of this section, namely the derivation of learning rates for the empirical histogram rule \(D \mapsto h_{D,A_D}\) for regression based on a cubic data-dependent partition \(A_D\) from \(\mathcal{P}(X)\).

**Proposition E.6 (Learning Rates).** Let \(L\) be the least squares loss, \(X := [-1,1]^d\), \(Y = [-1,1]\), \(P\) be a distribution on \(X \times Y\), and \(D \in (X \times Y)^n\) be an i.i.d. sample of size \(n \geq 1\) drawn from \(P\) with \(|D_X| = m_n\). Assume the Bayes decision function \(f^*_L,P\) is \(\alpha\)-Hölder continuous for some \(\alpha \in (0,1]\). Suppose further that \((s_n)_{n \in \mathbb{N}}\) is a sequence satisfying

\[
s_n = n^{-\gamma}, \quad \gamma = \frac{1}{2\alpha + d},
\]

Assume further that \(\pi_{m_n,s_n}\) is an \(m_n\)-sample cubic partitioning rule of width \(s_n \in (0,1]\), satisfying \(|\text{Im}(\pi_{m_n,s_n})| \leq cn^\beta\), for some \(c < \infty\) and some \(\beta > 0\) that are independent of \(n\). Denoting \(A_D := \pi_{m_n,s_n}(D_X)\), the excess risk then satisfies for all \(n \geq 1\) the inequality

\[
R_{L,P}(h_{D,A_D}) - R^*_L,P \leq c_{d,\alpha} \ln(n) \left(\frac{1}{n}\right)^{2\alpha \gamma}
\]

with probability \(P^n\) at least \(1 - cn^{1+\beta}e^{-n^\gamma}\), where \(c_{d,\alpha} > 0\) is a constant only depending on \(d, \alpha,\) and \(|f^*_L,P|_\alpha\).

**Proof of Proposition E.6.** If the Bayes decision function \(f^*_L,P\) is \(\alpha\)-Hölder continuous, Lemma E.4 gives us for all \(n \geq 1\) that

\[
R_{L,P}(h_{P,A}) - R^*_L,P < |f^*_L,P|_\alpha s_n^{2\alpha}.
\]

(88)

Repeating the proof of Proposition E.5 by replacing (87) with (88) shows that for all \(\tau \geq 1\) and \(n \geq 1\) we have

\[
R_{L,P}(h_{D,A_D}) - R^*_L,P \leq 4|f^*_L,P|_\alpha s_n^{2\alpha} + 1024 \frac{\tau}{n} + 1024 \cdot 2^d \frac{\ln(ns_n^d)}{ns_n^d}.
\]

(89)

with probability \(P^n\) not less than \(1 - 2cn^{1+\beta}e^{-\tau}\). Using the definition of \(s_n\) and setting \(\tau_n := n s_n^{2\alpha} = n^{\frac{d}{2\alpha + d}}\) then gives the assertion. 

\[\square\]