Adaptive Approximation and Estimation of Deep Neural Network to Intrinsic Dimensionality

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Abstract

We theoretically prove that the generalization performance of deep neural networks (DNNs) is mainly determined by an intrinsic low-dimensional structure of data. Recently, DNNs empirically provide outstanding performance in various machine learning applications. Motivated by the success, theoretical properties of DNNs (e.g. a generalization error) are actively investigated by numerous studies toward understanding their mechanism. Especially, how DNNs behave with high-dimensional data is one of the most important concerns. However, the problem is not sufficiently investigated from an aspect of characteristics of data, despite it is frequently observed that high-dimensional data have an intrinsic low-dimensionality in practice. In this paper, to clarify a connection between DNNs and such the data, we derive bounds for approximation and generalization errors by DNNs with intrinsic low-dimensional data. To the end, we introduce a general notion of an intrinsic dimension and develop a novel proof technique to evaluate the errors. Consequently, we show that convergence rates of the errors by DNNs do not depend on the nominal high-dimensionality of data, but depend on the lower intrinsic dimension. We also show that the rate is optimal in the minimax sense. Furthermore, we find that DNNs with increasing layers can handle a broader class of intrinsic low-dimensional data. We conduct a numerical simulation to validate (i) the intrinsic dimension of data affects the generalization error of DNNs, and (ii) DNNs outperform other non-parametric estimators which are also adaptive to the intrinsic dimension.

1 Introduction

Theoretical analysis for deep neural networks (DNNs) [29, 17] has attracted a much amount of attention, as motivated by the great success of deep learning in various machine learning applications [10, 12, 20]. One of the representative theoretical results is a universal approximation property [21, 11], which proves that DNNs (or even shallow neural networks)
can approximate a wide class of functions with a sufficient number of nodes. Furthermore, for more precise analysis, rigorous approximation and generalization performances of DNNs are also investigated extensively. Novel studies derive a rate of the approximation error for smooth functions and their variations [2, 46, 47, 31]. Based on the results, a rate of the generalization error of DNNs is also derived in various settings [3, 36, 4, 38, 22, 39].

From the theoretical aspect, the curse of dimensionality is one of the significant interest, which describes that the theoretical rates get worse seriously with high-dimensional data. For a regression (supervised learning) problem as a typical example, the generalization error by DNNs has a convergence rate $O(n^{-2\beta/(2\beta+D)})$, where $n$ is a number of observations, $D$ is a dimension of input data, and $\beta > 0$ is a degree of smoothness of a function which generates the data. It is known that this rate is optimal in the minimax sense in the typical setting [36]. Since $D$ is large in machine learning applications (e.g. a number of pixels of image data), the theoretical bound decays slowly as $n$ increases, and it is quite loose to describe the empirical performance of DNNs. Several studies [33, 35, 39] tackle the problem by introducing a particular structure into the generating function.

In contrast to the studies for the generating function, how the nature of data affects DNNs is not well studied. Empirically, it is frequently observed that high-dimensional data have an implicit structure such as lying around low-dimensional sets (e.g. manifolds) [11, 5], and it is an important fact for the practical performance of DNNs [32, 1]. We numerically confirm that some famous data (e.g. MNIST) have around 30 intrinsic dimension though their nominal dimension is around 1,000 (see Section 3.1). Moreover, for some conventional methods, the intrinsic low-dimensionality is a key factor to relieve the curse of dimensionality [6, 29, 27, 45]. Despite the empirical facts, it is mathematically non-trivial to connect DNNs with an intrinsic dimension of data, hence investigating the property has remained as an important open question.

In this paper, we investigate the performance of DNNs with $D$-dimensional data which have a $d$-dimensional intrinsic structure as $d < D$. To describe the low-dimensionality of data, we introduce the notion for dimensionality such as the Minkowski dimension. Also, we develop a proof technique to adapt DNNs for the low-dimensional structure. Consequently, we derive rates of approximation and generalization by DNNs which depend on only $d$ and $\beta$ but not on $D$, as summarized in Table 1. Namely, we prove that the convergence speed of DNNs is free from the nominal dimension of data, but depends on their intrinsic dimension. We also prove that the derived rate is optimal in the minimax sense. Furthermore, we state that DNNs can achieve the rate easier than other adaptive methods such as kernel methods, since the Minkowski dimension can represent a broader class of low-dimensional sets than other dimensions such as manifolds. We verify the theoretical results by numerical experiments.

We summarize the contributions of this paper as follows:

1. We prove that DNNs with ReLU can relieve the curse of dimensionality by adapting to the intrinsic low-dimensionality of the data.
2. We show that DNNs can achieve the fast convergence with a broader class of distri-
Approximation Generalization

| EXISTING | $O(W^{-\beta/D})$ | $\tilde{O}(n^{-2\beta/(2\beta+D)})$ |
| Ours ($d$-Minkowski dim.) | $O(W^{-\beta/d})$ | $\tilde{O}(n^{-2\beta/(2\beta+d)})$ |

Table 1: Derived rates of approximation and generalization errors by DNNs with $W$ parameters and $n$ observations. $\beta > 0$ denotes smoothness of the generating function, and $D$ is dimension of the observations. In our work, we assume data have intrinsic dimension $d < D$.

butions than other methods that are also adaptive to an intrinsic dimension.
3. For the claim, we derive rates of approximation and generalization errors with $D$-dimensional data which have $d$ intrinsic dimension, and show the rate is minimax optimal.

1.1 Basic Notation
For a vector $b \in \mathbb{R}^d$, $\|b\|_q := (\sum_{j=1}^{d} b_j^q)^{1/q}$ is a $q$-norm for $q \in [0, \infty]$. For a measure $\mu$, the support of $\mu$ is written as $\text{Supp}(\mu)$. For a function $g : \mathbb{R}^D \to \mathbb{R}$, $\|g\|_{L^p(\mu)} := (\int |g|^p \ d\mu)^{1/p}$ is the $L^p(\mu)$ norm with a probability measure $\mu$. $\tilde{O}(\cdot)$ is the Landau’s big O ignoring a logarithmic factor. With $\epsilon > 0$, $N(\Omega, \epsilon)$ is the smallest number of $\epsilon$-balls which cover $\Omega$ in terms of the norm $\|\cdot\|_{\max}$.

2 Preliminaries

Smooth functions: We define a notion of the Hölder spaces as a family of smooth functions. For a function $f : \mathbb{R}^D \to \mathbb{R}$, $\partial_1 f(x)$ is a partial derivative with respect to a $d$-th component, and $\partial^\alpha f := \partial_{x^1}^{\alpha_1} \cdots \partial_{x^D}^{\alpha_D} f$ with a multi-index $\alpha = (\alpha_1, ..., \alpha_D)$.

Definition 1 (Hölder space). Let $\beta > 0$ be a degree of smoothness. For $f : [0,1]^D \to \mathbb{R}$, the Hölder norm is defined as

$$\|f\|_{\mathcal{H}^\beta,D} := \max_{\alpha : |\alpha| < \lceil \beta \rceil} \sup_{x \in [0,1]^D} |\partial^\alpha f(x)| + \max_{\alpha : |\alpha| = \lceil \beta \rceil} \sup_{x, x' \in [0,1]^D, x \neq x'} \frac{|\partial^\alpha f(x) - \partial^\alpha f(x')|}{\|x - x'\|_{\max}^{\beta - \lceil \beta \rceil}}.$$

Then, the Hölder space on $[0,1]^D$ is defined as

$$\mathcal{H}^\beta,D = \{ f \in C^\lceil \beta \rceil([0,1]^D) \|f\|_{\mathcal{H}^\beta,D} < \infty \}.$$

Also, $\mathcal{H}^\beta,D,M = \{ f \in \mathcal{H}^\beta,D \|f\|_{\mathcal{H}^\beta,D} \leq M \}$ denotes the $M$-radius closed ball in $\mathcal{H}^\beta,D$. 

3
The parameter $\beta$ controls a degree of smoothness of functions in $H^{\beta,D}$. The notion is very common in the functional analysis and statistical theory [46, 36].

Deep Neural Network Models: Deep neural networks (DNNs) represent a function by multiple nonlinear transformations with the ReLU activation $\rho(x_1,\ldots,x_p) := (\max\{x_1,0\},\ldots,\max\{x_p,0\})$.

Let $L$ be a number of layers. For each $\ell \in [L]$, $p_\ell$ be a number of nodes, and $A_\ell \in \mathbb{R}^{P_{\ell} \times P_{\ell-1}}$ and $b_\ell \in \mathbb{R}^{P_{\ell}}$ be a parameter matrix and vector. Let $\rho_b := \rho(\cdot + b_\ell)$ be a shifted ReLU activation. The realization of a neural network architecture $\Phi := ((A_L,b_L),\ldots,(A_1,b_1))$ is denoted as $R(\Phi) : \mathbb{R}^{p_0} \to \mathbb{R}^{p_L}$, which has a form

$$R(\Phi)(x) = A_L\rho_{b_{L-1}} \circ \cdots \circ A_2\rho_{b_1}(A_1x) + b_L,$$

for $x \in [0,1]^{p_0}$. $R(\Phi)(x)_i$ denotes the $i$-th output of $R(\Phi)(x)$. For each $\Phi$, a number of layers of $\Phi$ is written as $L(\Phi)$, a number of parameters of $\Phi$ is $W(\Phi) := \sum_{\ell=1}^L \|b_\ell\|_0 + \|\text{vec}(A_\ell)\|_0$, and a scale of parameters of $\Phi$ is $B(\Phi) = \max_{\ell=1,\ldots,L} \max\{\|b_\ell\|_{\text{max}},\|\text{vec}(A_\ell)\|_{\text{max}}\}$. Then, with $W',L'$ and $B'$, we define a functional set by DNNs as

$$\mathcal{F}(W',L',B') = \{ R(\Phi) : [0,1]^{p_0} \to \mathbb{R}^{p_L} \mid L(\Phi) \leq L', W(\Phi) \leq W', B(\Phi) \leq B' \}.$$

3 Introduction to Low-Dimensionality

3.1 Empirical Motivation

As a motivation for the intrinsic low-dimensional data, we provide the empirical analysis for the intrinsic dimensions of real datasets. We analyze the MNIST data [29] and the CIFAR-10 data [28]. Since the data are images, their nominal dimension $D$ is the number of pixels. To measure their intrinsic dimensions, we apply several dimension estimators, such as the local PCA (LPCA) [14, 9], the maximum likelihood (ML) [18], and the expected simplex skewness (ESS) [23]. The results in Table 2 show that the estimated intrinsic dimensions are significantly less than $D$. Though their definitions of intrinsic dimensions are not common, the result provides motivations to investigate the intrinsic low-dimensionality.

| DATA SET | $D$ | INTRINSIC DIMENSION $d$ | LPCA | ML | ESS |
|----------|-----|-------------------------|------|----|-----|
| MNIST    | 784 | 37                      | 13.12| 29.41|
| CIFAR-10 | 1024| 9                       | 25.84| 27.99|

Table 2: Estimated intrinsic dimensions of the MNIST and CIFAR-10 datasets. The dimensions are estimated from 30,000 sub-samples from the original datasets.
3.2 Definition of Dimensionality

We introduce a general notion for dimensionality as follows.

**Definition 2 ((Upper) Minkowski Dimension).** The Minkowski dimension of a compact set \( E \subset [0, 1]^D \) is defined as

\[
\dim_M E := \inf \left\{ d^* \geq 0 \mid \limsup_{\epsilon \downarrow 0} N(E, \epsilon) \epsilon^{d^*} = 0 \right\}.
\]

The dimensionality is measured by how the number of covering balls for \( E \) is affected by the radius of the balls. Intuitively, \( N(\epsilon, E) \approx C\epsilon^{-d} \) holds with \( d = \dim_M E \) with a constant \( C > 0 \). Since the Minkowski dimension does not depend on smoothness, it can measure dimensionality of sets which is highly non-smooth such as fractal sets (e.g. the Koch curve). Figure 1 shows an image of how the Minkowski dimension of \( E \) is measured by max-balls.

![Figure 1: The Koch curve E (red lines) and covering max-balls (green squares) for E. The Minkowski dimension of E is d = log 4 / log 3 ≈ 1.26, while E is a subset of \( \mathbb{R}^D \) with \( D = 2 \).](image)

**Relation to Other Dimensions:** The Minkowski dimension can describe a broader class of low-dimensional sets than several other dimensionalities. For example, a notion of dimension of manifolds describe a dimensionality of sets with smooth structures, and it is often utilized to describe an intrinsic dimensionality [6, 45]. Though manifold dimensions are only available for smooth sets such as circles, the Minkowski dimension is applicable for sets without such restriction. Consequently, for a set \( E \subset [0, 1]^D \), we show that

\[
\{ E \mid \dim_M E \leq d \} \supset \{ E \mid E \text{ is a } d\text{-dimensional manifold} \},
\]

holds (see Lemma A.1 in the supplementary material). On the other hand, a notion of regularity dimensions is also utilized for the intrinsic dimensionality [26, 27]. Similar to the manifold case, the Minkowski dimension is a more general notion than the regularity dimension (see Lemma A.2).
4 Main Results

4.1 Approximation with Low-Dimensionality

We evaluate how well DNNs approximate a function $f_0 \in \mathcal{H}_\beta^D$ when data are intrinsic low-dimensional. To the end, we measure an approximation error by a norm $\| \cdot \|_{L^\infty(\mu)}$ with a measure $\mu$ in cases where $\text{Supp}(\mu)$ has intrinsic low-dimensionality. We utilize the norm since it measures a generalization error by $f$ as $\| f - f_0 \|_{L^2(\mu)} = E_{X \sim \mu}[ (f(X) - f_0(X))^2 ]$.

For analysis, we consider the case where $\text{Supp}(\mu)$ has a $d_{\text{Minkowski}}$ dimension.

**Theorem 4.1** (Approximation with Minkowski dimension). Suppose $d > \dim_M \text{Supp}(\mu)$ holds with $d < D$. Define $\bar{\beta} := (1 \vee \lceil \log_2 \beta \rceil)$. Then, for any $\epsilon \in (0, 1)$ and $f_0 \in \mathcal{H}_\beta^D$, there exist constants $c_1 = c_1(\beta, D, d, M)$, $c_2 = c_2(\beta, D, d, M)$, $c_3 = c_3(\beta, D, d, M)$, $s = s(\beta, D, d, M)$ and a triple $(W, L, B)$ as

\[
W \leq 8(20 + \beta/d)\bar{\beta} + \epsilon^{-d/\bar{\beta}}(4c_1 \log(1/\epsilon) + 3^D(168D + (232 + 8\beta/d)\bar{\beta} + 2c_2(1 + 3^{d/\bar{\beta} - D}))),
\]

\[
L \leq \bar{\beta}(19 + (1 + \beta)/d) + c_1 \log 3 + c_1 \log(1/\epsilon),
\]

\[
B \leq c_3 \epsilon^{-s},
\]

such that an existing $R(\Psi_{\epsilon} f_0) \in \mathcal{F}(W, L, B)$ satisfies

\[
\inf_{R(\Phi) \in \mathcal{F}(W, L, B)} \| R(\Phi) - f_0 \|_{L^\infty(\mu)} \leq \epsilon.
\]

By simplifying Theorem 4.1, the approximation error is written as $\tilde{O}(W^{-\beta/d})$ which depends on $d$ but not $D$. Namely, a rate of the approximation behaves as if data are $d$-dimensional, though they are nominally $D$-dimensional. Also, we note that the number of layers in Theorem 4.2 increases by $\log(1/\epsilon)$, while DNNs require $O(1)$ nodes in an ordinary setting without low-dimensionality.

**Proof Outline:** Firstly, we prepare a set of disjoint hypercubes (max-balls) of $[0, 1]^D$ with a length of its side $1/N$, and approximate $f_0 \in \mathcal{H}_\beta^D$ by sub-networks of DNNs within each of the hypercubes. Since $\dim_M \text{Supp}(\mu) < d$ holds, there are at most $C_{\mu}N^d$ hypercubes for approximating $f_0$ on $\text{Supp}(\mu)$, where $C_{\mu} > 0$ is an existing constant independent of $N$. Within each of the hypercubes, we provide two-step approximation: (i) a Taylor approximation and (ii) "sawtooth" approximation for the Taylor polynomials. By applying the multidimensional binomial theorem, our DNNs can approximate $f_0$ with accuracy $\epsilon$ within each of the hypercubes. Then, we set $N \asymp \epsilon^{-1/\beta}$ and thus obtain the statement of the theorem. An image of the proof is provided in Figure 2.

As the difficulty of this proof, it is a non-trivial task to aggregate the approximators within the hypercubes into an approximator for $f_0$ on $\text{Supp}(\mu)$. This is because each of the approximators in the hypercube affects other approximations in another hypercube. To solve the difficulty, we develop a trapezoid-type approximator which does not affect the other approximations. To control the multiple trapezoid-type approximators, we add several operations to handle them. An image of the whole procedure is provided in Figure 2. 


4.2 Generalization with Low-Dimensionality

We investigate a generalization error of an estimator by DNNs with the low-dimensional settings.

**Regression Problem and Estimator by DNNs:** Let $X_i$ be $D$-dimensional and $Y_i$ be scalar random variables. Suppose we have a set of $n$ observations $\{(X_i, Y_i)\}_{i=1}^n$ which is independently and identically generated from the following data generating process. For $i = 1, ..., n$, $X_i$ marginally follows $X_i \sim \mu$, and $(X_i, Y_i)$ is jointly generated from the model

$$Y_i = f_0(X_i) + \xi_i,$$

(2)

where $f_0 \in \mathcal{H}^{\beta,D,M}$ and $\xi_i$ is an independent noise such as $E[\xi_i] = 0$ and $E[\xi_i^2] = \sigma^2$ with $\sigma > 0$.

By the observations, we introduce an estimator for $f_0$. Here, $\tilde{f}(x) := \max\{-C_B, \min\{C_B, f(x)\}\}$ is a clipping for $f \in \mathcal{F}(W,L,B)$ with a threshold $C_B > 0$. Then, the estimator is defined as

$$\hat{f} \in \arg\min_{f : f \in \mathcal{F}(W,L,B)} \sum_{i=1}^n (Y_i - \tilde{f}(X_i))^2.$$  

(3)

Our goal is evaluate its generalization error as $\|\hat{f} - f_0\|_{L^2(\mu)}$ in terms of $n$.

We note that calculating $\hat{f}$ is not easy since the loss function in (3) is non-convex. Although, we employ the estimator $\hat{f}$ since our aim is to investigate a generalization error in terms of $n$ and it is independent of the difficulty of optimization. Also, we can obtain an approximated version of $\hat{f}$ by various optimization techniques such as the multiple initializations and the Bayesian optimization.

**Generalization Result:** We provide a generalization error of $\hat{f}$ with a setting that $\text{Supp}(\mu)$ has a low Minkowski dimension.
Theorem 4.2 (Generalization with Minkowki dimension). Suppose \( \dim \text{Supp}(\mu) < d \) with \( d < D \). Fix any \( f_0 \in H^{\beta,D,M} \). Set a triple \((W, L, B)\) with the constants \( c_1, c_2, s > 0 \) appearing in the main result 1 as \( W = c_1 n^{d/(2\beta+d)} \), \( L = (2 + \lceil \log_2(1 + \beta) \rceil)(11 + \beta/d) \), and \( B = c_2 n^{2\beta s/(2\beta+d) \log n} \). Then, there exists a constant \( C_1 = C_1(s, \beta, D, d) \) and \( C_2 = C_2(s, \beta, D, d) \) such that

\[
\| \hat{f} - f_0 \|_{L^2(\mu)}^2 \leq C_1 n^{-2\beta/(2\beta+d)}(1 + \log n)^4 + \frac{16}{n},
\]

with probability at least \( 1 - \exp(-C_2/n) \).

The derived generalization error has an order \( \tilde{O}(n^{-2\beta/(2\beta+d)}) \), which is totally released from \( D \). In other words, we show that the rate by DNNs is determined by the dimensionality of \( \text{Supp}(\mu) \) as a manifold. It is much faster than an existing rate \( \tilde{O}(n^{-2\beta/(2\beta+D)}) \) [36] without low-dimensionality. Also, even when data are \( D \)-dimensional, an order of the parameters \((W, L, B)\) are not affected by \( D \) but depend on \( d \). Also, DNNs requires the number of layers to increase by \( \log n \) to adapt to the Minkowski dimension, while an ordinary setting without low-dimensionality requires \( O(1) \) layers.

Proof Outline: Firstly, we decompose the empirical loss into two terms, which are analogously bias and variance. Following the definition of \( \hat{f} \) as (3), a simple calculation leads to

\[
\| \hat{f} - f_0 \|_{n}^2 \leq \| f - f_0 \|_{n}^2 + \frac{2}{n} \sum_{i=1}^{n} \xi_i (\hat{f}(X_i) - f(X_i)),
\]

for any \( f \in F(W, L, B) \). Here, we define an empirical norm as \( \| f \|_{n}^2 := n^{-1} \sum_{i=1}^{n} f(X_i)^2 \).

The first term \( T_B \), which is regarded as a bias, is evaluated by an approximation power of \( F(W, L, B) \). Here, we apply Theorem 4.1 and bound the term. The second term \( T_V \), which describes a variance of the estimator, is evaluated by the technique of the empirical process theory [42]. Namely, by utilizing the notion of the local Rademacher complexity and concentration inequalities [16], we bound \( T_V \) an integration of a covering number of \( F(W, L, B) \). Further, we derive a bound for the covering number by the parameters \((W, L, B)\), thus we can evaluate \( T_V \) in terms of the parameters. Combining the result for \( T_B \) and \( T_V \) and select proper values for \((W, L, B)\), we obtain the claimed result.

4.3 Minimax Rate with Low-Dimensionality

We show the optimality of the obtained rate in Theorem 4.2 by deriving a minimax generalization error of the estimation problem. To the end, we consider an arbitrary probability measure \( \mu \) where \( \text{Supp}(\mu) \) is \( d \)-dimensional measured by covering balls. Then, we obtain the following minimax lower bound.
**Theorem 4.3** (Minimax Rate with Low-Dimensionality). Let \( \mu \) be any probability measure on \([0, 1]^D\). Assume \( N(\epsilon, \text{Supp}(\mu)) = \Omega(\epsilon^{-d}) \). Then, we obtain
\[
\inf \limits_{\tilde{f}} \sup \limits_{f \in \mathcal{H}_{\beta,D,M}} \| \tilde{f} - f_0 \|^2_{L^2(\mu)} \geq C' n^{-2\beta/(2\beta + d)},
\]
where \( \tilde{f} \) is taken from an arbitrary estimator for \( f_0 \).

Namely, any estimator provides an error \( \Omega(n^{-2\beta/(2\beta + d)}) \) in a worse case, then it is regarded as a theoretical limit of efficiency. Since the rate in Theorem 4.2 corresponds to the rate up to logarithmic factors, our rate almost achieves the minimax optimality.

## 5 Comparison

### 5.1 Other Analysis for DNNs

| Study  | Setting        | \( f_0 \)          | \( \mu \)        | Error Approximation | Error Generalization |
|--------|----------------|--------------------|------------------|-------------------|---------------------|
|        |                |                    |                  | \( \tilde{O}(W^{-\beta/D}) \) | \( \tilde{O}(n^{-2\beta/(2\beta + d)}) \) |
|        |                |                    |                  | \( \tilde{O}(W^{-1/2}) \) | \( \tilde{O}(n^{-1}) \) |
|        |                |                    |                  | \( \tilde{O}(W^{-1}) \) | \( \tilde{O}(n^{-2\gamma/(2\gamma + 1)}) \) |
| Ours   | Hölder         |                    | \( d \)-dimensional | \( \tilde{O}(W^{-\beta/d}) \) | \( \tilde{O}(n^{-2\beta/(2\beta + d)}) \) |

Table 3: Comparison of the derived approximation and generalization rates. \( W \) denotes a number of parameters in DNNs, and \( n \) is the number of observations. \( D \) is the dimension of the feature space, and \( d \) is the upper regular dimension of \( \mu \).

There are numerous studies which investigate the approximation and generalization performance of DNNs. Some studies \[46, 36\] clarify the performance of DNNs with ReLU activations when \( f_0 \) is in the Hölder space. Then, they show \( \tilde{O}(W^{-\beta/D}) \) for approximation and \( \tilde{O}(n^{-2\beta/(2\beta + d)}) \) for generalization. To obtain a faster convergence result, a classical approach \[2, 3\] considers a restricted functional class (named the Barron class in this paper) for \( f_0 \) and achieves a very fast rate: \( \tilde{O}(W^{-1/2}) \) for approximation, and \( \tilde{O}(n^{-1}) \) for generalization. Another challenges \[33, 39\] consider a different functional class with mixed smoothness for \( f_0 \) and obtain a novel convergence rate which depends on its peculiar smoothness index \( \gamma \).

Our study assumes \( f_0 \) is an element of the standard Hölder space, and additionally assume that \( \mu \) has an intrinsic low-dimensional structure, namely, \( \text{Supp}(\mu) \) is \( d \)-dimensional in the Minkowski or the manifold sense. Then, we obtain the approximation rate \( \tilde{O}(W^{-\beta/d}) \).
and the generalization rate $\tilde{O}(n^{-2\beta/(2\beta+d)})$. Since $d$ is much less than $D$ empirically (as mentioned in Section 3.1), the rate can relax the curse of dimensionality by large $D$. To the best of our knowledge, this is the first result which succeeds in proving that errors by DNNs converge faster with data equipping general intrinsic low-dimensionality.

5.2 Comparison with Other Adaptive Methods

Except for DNNs, several other estimators can obtain a convergence rate which is adaptive to an intrinsic dimension of a distribution $d$. As typical examples, it is well known that sparse learning methods such as LASSO [19] and tree-based regression methods [8] can select a linear subspace of a sample space by selecting variables in their models. As nonparametric approaches, the local polynomial kernel (LP kernel) regression [6] and the Gaussian process regression (GP) [45] can achieve the rate $O(n^{-2\beta/(2\beta+d)})$ when $\text{Supp}(\mu)$ is a $d$-dimensional manifold with $\beta = 2$. Similarly, the $k$-nearest neighbor (k-NN) regression [26] and the Nadaraya-Watson (NW) kernel regression [27] can achieve the rate with $d$, when $\mu$ has a regularity dimension $d$, which is less general than the Minkowski dimension (Lemma A.2 in the supplementary material).

We show that DNNs with increasing layers can obtain the fast rate $O(n^{-2\beta/(2\beta+d)})$ with a more general situation than the existing adaptive methods. Theorem 4.2 shows that DNNs with $L = O(\log n)$ can obtain the rate when $\dim M \text{Supp}(\mu) < d$, which is less restrictive than the settings with manifolds and the regularity dimension. Intuitively, DNNs can obtain the fast adaptive rate even when $\text{Supp}(\mu)$ does not have a smooth structure like manifolds. Interestingly, when layers it not so many, i.e. $L = O(1)$, DNNs cannot obtain this advantage. Figure 3 shows an overview of the result. This fact potentially has a key point to investigate very deep neural networks.

6 Simulation

6.1 Generalization of DNNs with Different $d$

We calculate generalization errors of DNNs with synthetic data. As a data generating process, we set the true function $f_0$ and the probability measure $\mu$ as follows. About $f_0$, we set it as $f_0(x) := (D - 1)^{-1}\sum_{i=1}^{D-1} x_i x_{i+1} + D^{-1}\sum_{i=1}^{D} 2\sin(2\pi x_i) 1_{x_i \leq 0.5} + D^{-1}\sum_{i=1}^{D} (4\pi(\sqrt{2} - 1)^{-1}(x_i - 2^{-1/2})^2 - \pi(\sqrt{2} - 1)) 1_{x_i > 0.5}$, which belongs to $H^{\beta,D}$ with $\beta = 2$. We plot $f_0$ with $D = 2$ in the supplementary material. Let $\mu$ be a uniform measure on $[0, 1]^D$ and
Supp($\mu$) be a $d$-dimensional sphere embedded in $[0, 1]^D$. Also, let a noise variable $\xi$ follow a Gaussian distribution with zero mean and variance $\sigma^2 = 0.1$. Then, we generate $n$ pairs of $(X_i, Y_i)$ from the regression model (2) and obtain the estimator (3). About the learning process, we employ a DNN architecture with 4 layers, and each layer has $D$ units except an output layer. For optimization, we employ Adam [25] with default hyper-parameters; 0.001 learning rate and $(\beta_1, \beta_2) = (0.9, 0.999)$.

We set $D = 128$ and measure the generalization errors of DNNs by the $L^2(\mu)$-norm on sample size $n \in \{100, 200, \ldots, 1000\}$ with different intrinsic dimensions $d = 4, 16, 64, 100$. In each sample size, we replicate the estimation 100 times and calculate the standard deviation of the error. Also, in each replication, 100 initial weights are drawn from the standard normal distribution to avoid local minima.

We plot the errors to log $n$ in Figure 4. From the result, DNNs with small $d$ achieve fewer errors as $d$ decreases. Moreover, since the slopes of the plot correspond to rates of convergence, we can validate that the rates with $d = 4, 16$ are sufficiently faster than $d = 64, 100$.

6.2 Comparison with the Other Estimators

We compare the performances of DNNs with existing methods, such as $k$-nearest neighbor method ($k$-NN) and the Nadaraya-Watson kernel method (NW), that are proved to achieve the fast rate with $d$.

To generate data, we set $D = 3$ and $\mu$ generates $X$ as $X = (Z(\cos(Z) + 1)/2, Z(\sin(Z) + 1)/2, \eta)$, where $Z \sim U[0.1, 1], \eta \sim U[0, 1]$. With this setting, Supp($\mu$) forms a well-known Swiss Roll, hence we have $d = 2$. We set $n \in \{20, 40, \ldots, 300\}$. All the other settings inherit Section 6.1. The learning procedure of DNNs is same as that of Section 6.1. For $k$-NN,
its hyper-parameter $k$ is chosen from \{1, \ldots, 50\}. About NW, we employ the Gaussian kernel whose bandwidth is chosen from \{0.10, 0.11, \ldots, 1.00\}. All the hyper-parameters are selected by the cross-validation.

We plot the generalization error by DNNs and the other methods in Figure 5. It is clearly shown that DNNs outperform the other estimators.

7 Conclusion

We theoretically elucidate that performance deep learning is mainly described by intrinsic low-dimensionality of data. To show the result, we introduce the notion of the Minkowski dimension, then derive the rates of approximation and generalization errors which only depends on the intrinsic dimension but free from the high nominal dimension. Additionally, we find that DNNs with increasing layers can obtain the fast convergence with data which possesses a more complex low-dimensional structure.
A Appendix

Supporting Discussion

Notation: Let \( \|g\|_n := \left\{ (1/n) \sum_{i=1}^{n} g(X_i)^2 \right\}^{1/2} \) be the empirical counterpart of the \( L^2(\mu) \) norm. The closed ball in \( \mathbb{R}^D \) with its center \( x \) and radius \( r \) with norm \( \|\cdot\| \) is described as \( \overline{B}_D(x,r) := \{ x' \in \mathbb{R}^D \mid \|x - x'\| \leq r \} \). The open ball is similarly defined as \( B_D(x,r) \).

The explicit dependence on the norm of the balls is omitted due to the equivalence of norms in \( \mathbb{R}^D \). The closed ball in \( \mathbb{R}^D \) with its center \( x \) and radius \( r \) with the \( \ell^p \)-norm is described as \( \overline{B}_{\ell^p}(x,r) \). An open version of the ball is \( B_{\ell^p}(x,r) \). Also for the max norm \( \|a\|_{\text{max}} := \max_{1 \leq i \leq D} a_i \) for some \( a \in \mathbb{R}^D \), the closed ball \( \overline{B}_{\text{max}} \) and the open ball \( B_{\text{max}} \) are defined similarly. For a set \( \Omega \), \( \mathbb{1}_\Omega(\cdot) \) is an indicator function such that \( \mathbb{1}_\Omega(x) = 1 \) if \( x \in \Omega \), and \( \mathbb{1}_\Omega(x) = 0 \) otherwise.

Definition of Supports: A rigorous definition of a support of measures \( \nu \) is defined as \( \text{Supp}(\nu) := \{x \in \mathcal{X} \mid V \in \mathcal{N}_x \Rightarrow \nu(V) > 0 \} \) where \( \mathcal{N}_x \) is a set of open neighborhoods to which \( x \) belongs.

A.1 Discussion about Notions for Dimensionalities

Firstly, we show the relation between the Minkowski dimension and the dimension of manifolds. We provide the following lemma.

Dimension of Manifolds: The notion of manifolds is common for analyzing low-dimensionality of data \([5, 34, 15]\). The upper Minkowski dimension can describe the dimensionality of manifolds.

Lemma A.1. Let \( \mathcal{M} \) be a compact \( d \)-dimensional manifold in \([0,1]^D\). Assume \( \mathcal{M} = \bigcup_{k=1}^K \mathcal{M}_k \subset [0,1]^D \) for \( K \in \mathbb{N} \). Also assume for any \( 1 \leq k \leq K \), there exists an onto and continuously differentiable map \( \psi_k : [0,1]^{d_k} \to \mathcal{M}_k \) each of which has the input dimension \( d_k \in \mathbb{N} \). Then, \( \dim_{\text{M}} \mathcal{M} \leq \max_{1 \leq k \leq K} d_k \).

Proof. Obviously, if \( \bigcup_{1 \leq k \leq K} \mathcal{M}_k \) satisfies the assumptions, so does each \( \mathcal{M}_k \). Assume the lemma is correct for \( K = 1 \) with \( \mathcal{M} \) replaced by \( \mathcal{M}_k \). Take \( d_k^* > d_k \). Since \( \dim_{\mathcal{M}} \mathcal{M}_k < d_k^* \), there exists a constant \( C > 0 \) such that for any \( \epsilon > 0 \), existing a finite set \( F^k_\epsilon \subset [0,1]^D \) satisfies

1. \( \mathcal{M}_k \subset \bigcup_{x \in F^k_\epsilon} B_2^D(x,\epsilon), \)
2. \( \text{card}(F^k_\epsilon) \leq C_k \epsilon^{-d_k^*}. \)

Let \( F_\epsilon := \bigcup_{k=1}^K F^k_\epsilon \). Then \( \mathcal{M} \subset \bigcup_{x \in F_\epsilon} B_2^D(x,\epsilon) \) and \( N_2(\mathcal{M},\epsilon) \leq \text{card}(F_\epsilon) \leq \left( \sum_{k=1}^K C_k \right) \epsilon^{-\max\{d_k^* \}}. \)

For any \( d^* > d := \max_k d_k \), choosing \( d^*_k > d_k \) such that \( \max_k d^*_k < d^* \) results in \( \limsup_{\epsilon \to 0} N_2(\mathcal{M},\epsilon) \epsilon^{d^*} = 0 \). So the proof is reduced to the case of \( K = 1 \). For simplicity, we omit the subscript \( k \) and write \( \psi = (\psi_1, ..., \psi_D) \).
Recall that $\psi_i$ is continuously differentiable. Define $L_i := \max_{x \in [0,1]^d} \sqrt{\sum_{j=1}^d |\partial \psi_i'(x)/\partial x_j|^2}$.

Applying the mean-value theorem to $\psi_i$ yields $|\psi_i(z) - \psi_i(w)| \leq L_i \|z - w\|_2$. By the Lipschitz continuity of $\psi = (\psi_1, \ldots, \psi_D)$, for any $z, w$, $\|\psi(z) - \psi(w)\|_2 \leq \sqrt{DL} \|z - w\|_2$ where $L := \max_i L_i$. Fix any $\epsilon > 0$ and $d \in \mathbb{N}$. Recall that there exists a constant $C > 0$ so that for any $\delta > 0$, an existing finite set $F_{\delta} \subset [0,1]^d$ (see Example 27.1 in [37]) satisfies

1. $\text{card}(F_{\delta}) \leq C \delta^{-d}$,
2. $[0,1]^d \subset \bigcup_{y \in F_{\delta}} B_{2}^d(y, \delta)$.

Choosing $\delta = \epsilon/(\sqrt{DL})$ yields

$$M \subset \psi \left( \bigcup_{y \in F_{\delta}} B_{2}^d(y, \delta) \cap [0,1]^d \right) = \bigcup_{y \in F_{\delta}} \psi \left( B_{2}^d(y, \delta) \cap [0,1]^d \right) \subset \bigcup_{y \in F_{\delta}} B_{2}^D \left( \psi(y), \epsilon \right)$$

where the last inclusion follows from the Lipschitz continuity of $\psi$. The conclusion is followed by

$$\mathcal{N}_2(M, \epsilon) \leq \text{card}(F_{\delta}) \leq C(\sqrt{DL})^d \epsilon^{-d},$$

and the equivalence of max-norm and 2-norm. \qed

Secondly, we explain the notion of a doubling measure which is another way to describe intrinsic dimensionality. It is employed in several studies [26, 27].

**Definition 3 (Doubling Measure).** A probability measure $\nu$ on $\mathcal{X}$ is called a doubling measure, if there exists a constant $C > 0$ such as

$$\nu(B_D(x, 2r) \cap \mathcal{X}) \leq C \nu(B_D(x, r) \cap \mathcal{X}),$$

for all $x \in \text{Supp}(\nu)$ and $r > 0$.

Then, we can define a dimensionality by the regularity property of doubling measures.

**Definition 4 (Upper Regularity Dimension).** For a doubling measure $\nu$, the upper regularity dimension $\dim_R \nu$ is defined by the infimum of $d^* > 0$ such that there exists a constant $C_\nu > 0$ satisfying

$$\frac{\nu(B_D(x,r) \cap \mathcal{X})}{\nu(B_D(x,\epsilon r) \cap \mathcal{X})} \leq C_\nu \epsilon^{-d^*},$$

for all $x \in \text{Supp}(\nu)$, $\epsilon \in (0,1)$ and $r > 0$.

There also exists a relation between the upper Minkowski dimension and the upper regularity dimension. Intuitively, when $\mathcal{X} \subset \mathbb{R}^D$, a measure $\nu$ with $\dim_R \nu = d$ behaves as if a domain of $\nu$ is $\mathbb{R}^d$, as shown in Figure [2]. The upper regularity dimension of $\nu$ can evaluate the Minkowski dimension of $\text{Supp}(\nu)$. 

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Lemma A.2 (Lemma 3.4 in [24]). Let \((X,B,\nu)\) be a probability space with \(X \subset \mathbb{R}^D\) is bounded. Suppose \(\nu\) is a doubling measure. Then,
\[
\dim_M \text{Supp}(\nu) \leq \dim_R \nu.
\]

B Proof of Main Results

B.1 Proof of Theorem 4.1

Our proof largely owes to the proof of [46, 35]. For convenience, we define the concatenation and parallelization of neural networks.

**Concatenation of Neural Networks**

Given two neural networks \(\Phi^1\) and \(\Phi^2\), we aim to construct a network \(\Phi\) such that \(R(\Phi) = R(\Phi^2) \circ R(\Phi^1)\), which is possible due ReLU activation function has the property \(\rho(x) - \rho(-x) = x\). Write \(\Phi^1 = ((A^1_{L_1}, b^1_{L_1}), \ldots, (A^1_1, b^1_1))\) and \(\Phi^2 = ((A^2_{L_1}, b^2_{L_1}), \ldots, (A^2_1, b^2_1))\). Define
\[
\widetilde{A}^2_1 := \left( \begin{array}{c} A^2_1 \\ -A^2_1 \end{array} \right), \quad \widetilde{b}^2_1 := \left( \begin{array}{c} b^2_1 \\ -b^2_1 \end{array} \right), \quad \widetilde{A}^1_{L_1} := (A^1_{L_1} - A^1_1).
\]

The concatenation of \(\Phi^1\) and \(\Phi^2\) is defined as
\[
\Phi^2 \circ \Phi^1 := ((A^2_{L_2}, b^2_{L_2}), \ldots, (A^2_2, b^2_2), (\widetilde{A}^2_1, \widetilde{b}^2_1), (A^1_{L_1}, b^1_{L_1}), (A^1_{L_1-1}, b^1_{L_1-1}), \ldots, (A^1_1, b^1_1)).
\]

It can be easily shown that
1. \(W(\Phi^2 \circ \Phi^1) \leq 2W(\Phi^2) + 2W(\Phi^1)\),
2. \(L(\Phi^2 \circ \Phi^1) = L(\Phi^2) + L(\Phi^1)\),
3. \(B(\Phi^2 \circ \Phi^1) = \max \{B(\Phi^2), B(\Phi^1)\}\).

Similarly we obtain the following remark.

**Remark 1** (Concatenation).

\[
W(\Phi^k \circ \cdots \circ \Phi^1) \leq 2 \sum_{i=1}^k W(\Phi^i),
\]
\[
L(\Phi^k \circ \cdots \circ \Phi^1) = \sum_{i=1}^k L(\Phi^i),
\]
\[
B(\Phi^k \circ \cdots \circ \Phi^1) = \max_{1 \leq i \leq k} B(\Phi^i).
\]
Parallelization of Neural Networks

Here we define the parallelization of multiple neural networks. Let \( \Phi^i = ((A^i_1, b^i_1), \ldots, (A^i_L, b^i_L)) \) be the neural network with a \( d \)-dimensional input and an \( m_i \)-dimensional output. Since these networks might have a different number of layers, we first have to adjust the layers.

Let \( L = \max_{1 \leq i \leq K} L(\Phi^i) \).

Define \( I_p \in \mathbb{R}^{p \times p} \) be the identity matrix. For \( L \geq 2 \), let \( \Phi^{id}_{D,L} : \mathbb{R}^D \to \mathbb{R}^D \) be a neural network of identity function

\[
\Phi^{id}_{D,L} := \left( (I_D - I_D), 0), (I_{2D}, 0), \ldots, (I_{2D}, 0), \left( \begin{pmatrix} I_D \\ -I_D \end{pmatrix}, 0 \right) \right).
\]

For \( L = 1 \), let \( \Phi^{id}_{D,L} = ((I_D, 0)). \) We can see \( W(\Phi^{id}_{D,L}) \leq 2DL \), \( L(\Phi^{id}_{D,L}) = L \) and \( B(\Phi^{id}_{D,L}) \leq 1 \) for all \( L \geq 1 \). Define

\[
\Phi^i' = \begin{cases} 
\Phi^i \circ \Phi^{id}_{m_i, L-L(\Phi^i)} & \text{if } L(\Phi^i) < L, \\
\Phi^i & \text{if } L(\Phi^i) = L.
\end{cases}
\]

Then \( L(\Phi^i) = L \) by the previous results. Write \( \Phi^i = ((\tilde{A}^i_1, \tilde{b}^i_1), \ldots, (\tilde{A}^i_L, \tilde{b}^i_L)) \) and define

\[
\tilde{A}_e := \begin{pmatrix} A^1_1 & O & \cdots & O \\ O & A^2_1 & \cdots & O \\ \vdots & \vdots & \ddots & \vdots \\ O & O & \cdots & A^K_1 \end{pmatrix}, \quad \tilde{b}_e := \begin{pmatrix} \tilde{b}^1_1 \\ \vdots \\ \vdots \\ \tilde{b}^K_1 \end{pmatrix}, \quad m := \sum_{i=1}^{K} m_i.
\]

The parallelization of networks \( (\Phi^i)_{i=1}^{K} \) with \( d \)-dimensional input and \( m \)-dimensional output is defined by

\[
[\Phi^1, \Phi^2, \ldots, \Phi^K] := ((\tilde{A}_L, \tilde{b}_L), \ldots, (\tilde{A}_1, \tilde{b}_1)).
\]

Combined with the previous results, the following remark is easily shown.

**Remark 2.** Let \( \Phi^i = ((A^i_1, b^i_1), \ldots, (A^i_L, b^i_L)) \) be the neural network with \( d \)-dimensional input and \( m_i \)-dimensional output for \( i \in \{1, \ldots, K\} \).

\[
W([\Phi^1, \Phi^2, \ldots, \Phi^K]) \leq \sum_{i=1}^{K} \left( 2W(\Phi^i) + 2W(\Phi^{id}_{D,L-L(\Phi^i)}) \right) \leq 2 \sum_{i=1}^{K} W(\Phi^i) + 4KD \max_{1 \leq i \leq K} L(\Phi^i),
\]

\[
L([\Phi^1, \Phi^2, \ldots, \Phi^K]) = \max_{1 \leq i \leq K} L(\Phi^i),
\]

\[
B([\Phi^1, \Phi^2, \ldots, \Phi^K]) \leq \max\{ \max_{1 \leq i \leq K} B(\Phi^i), 1 \}.
\]

Note that if \( L(\Phi^i) = L \) for all \( 1 \leq i \leq K \), then \( W([\Phi^1, \Phi^2, \ldots, \Phi^K]) \leq 2 \sum_{i=1}^{K} W(\Phi^i) \).
Restriction of the output of a neural network

Here restrict the output of a $K$-dimensional neural network into $[-B, B]^K$ for some $B > 0$. Define $\tau_B := \max \{\min \{x, B\}, -B\}$.

**Lemma B.1** (Lemma A.1 in [35]). Let $\Phi$ be a neural network with $K$-dimensional output. Let $\Phi^{R,K,B}$ be a neural network defined by

$$
\Phi^{R,1,B} := ((1, -1), -B) \odot [(1, B), (1, -B)],
\Phi^{R,K,B} := [(\Phi^{R,1,B}, \ldots, \Phi^{R,1,B})_K]
$$

Then, $R(\Phi^{R,K,B}) : \mathbb{R}^K \to \mathbb{R}^K$ satisfies $R(\Phi^{R,K,B})(x) = (\tau_B(x_1), \ldots, \tau_B(x_K))$ for any $x \in \mathbb{R}^K$. By Remark 1 and 2, we obtain

1. $W(\Phi^{R,K,B}) \leq 28K$,
2. $L(\Phi^{R,K,B}) = 2$,
3. $B(\Phi^{R,K,B}) \leq \max \{B, 1\}$.

Division of a domain of $f_0$

Let $N \geq 1$. We divide $[-1/N, 1 + 1/N]^D$ as a domain of $f_0$ into several hypercubes. Define the set of disjoint hypercubes with its size $1/N$ as

$$
\mathcal{I}_N := \{[-1/N, 0), [0, 1/N), [1/N, 2/N), \ldots, [1, 1 + 1/N)\}^D.
$$

For simplicity, we rewrite $\mathcal{I}_N = \{I_\lambda \mid \lambda \in \Lambda_N\}$, where $\Lambda_N$ is the index set with $\Lambda_N = \{1, \ldots, (N + 2)^D\}$. Also define the index set of the hypercubes with positive measure $\Lambda_N^+ \subset \Lambda_N$ as

$$
\Lambda_N^+ := \{\lambda \in \Lambda_N \mid \mu(I_\lambda) > 0\}.
$$

Furthermore, we define the index set $\Lambda_N^* \subset \Lambda_N$ such that for any $\lambda \in \Lambda_N^*$, $I_\lambda$ has positive measure or is neighbouring some hypercube that has positive measure. We rewrite $\Lambda_N^* = \{\lambda^{(1)}, \ldots, \lambda^{(m_N^*)}\}$ where $m_N^* = \text{card } \Lambda_N^*$.

Let $\xi : [0, 1]^D \to \Lambda_N^+$ be a function that receives $x$ and returns the index of a hypercube containing $x$. Also let $\Xi(x) : [0, 1]^D \to 2^{\Lambda_N^+}$ be a function that receives $x$ and returns the indices of hypercubes surrounding $I_{\xi(x)}$.

By definition of the upper Minkowski dimension, for any $d > \dim_M \mu$, $\text{card } \Lambda_N^+ = \mathcal{O}(N^d)$.

For convenience, we propose the following remark.

**Remark 3.** For any $d > \dim_M \text{Supp } \mu$, since there exists a constant $C_{\mu,d}^+ > 0$ such that $\text{card } \Lambda_N^+ \leq C_{\mu,d}^+ N^d$ holds,

$$
m_N^* = \text{card } \Lambda_N^* \leq 3^D C_{\mu,d}^+ N^d =: C_{\mu,d}^* N^d.
$$

Note that $\text{Supp } \mu \subset \bigcup_{\lambda \in \Lambda_N^+} I_\lambda \subset \bigcup_{\lambda \in \Lambda_N^*} I_\lambda$. 

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B.1.1 Simultaneous approximation of multiple Taylor polynomials

[46] approximated the multiplication by a so-called "sawtooth" function [40] with a number of layers depending on the approximation accuracy. [35] introduces the compromise of the number of layers and the number of nonzero weights, which enables a constant number of layers.

Lemma B.2 (Neural Network approximation of multiplication (Lemma A.4 in [35])). Fix any \( l \in \mathbb{N} \). There are constants \( s^{\text{mul}} = s^{\text{mul}}(\beta) \in \mathbb{N} \), \( c_1^{\text{mul}} = c_1^{\text{mul}}(\beta, D, b) \) and \( c_2^{\text{mul}} = c_2^{\text{mul}}(\beta, D, b) \) such that for any \( \epsilon \in (0, 1) \) and \( \alpha \leq \lfloor \beta \rfloor \), there is a neural network \( \Phi^{\text{mul}}_\epsilon \) with \( D \)-dimensional input and \( 1 \)-dimensional output satisfying

1. \( \sup_{x \in [0, 1]^D} |R(\Phi^{\text{mul}}_\epsilon)(x) - x^{\alpha}| \leq \epsilon \),
2. \( W(\Phi^{\text{mul}}_\epsilon) \leq c_1^{\text{mul}} \epsilon^{-D/b} \),
3. \( L(\Phi^{\text{mul}}_\epsilon) \leq (1 + \lceil \log_2 \lfloor \beta \rfloor \rfloor)(10 + b/D) \),
4. \( B(\Phi^{\text{mul}}_\epsilon) \leq c_2^{\text{mul}} \epsilon^{-s^{\text{mul}}} \).

Using this lemma, we construct a neural network approximating multiple taylor polynomials in each output.

[46] constructed a neural network approximating the polynomials by parallelizing networks of multiplication. [35] saved the redundant networks of multiplication using the binomial theorem. Consider approximation of \( m \) Taylor polynomials with the same degree. Along with the previous Lemma B.2 with the substitution \( b \leftarrow (1 + \lfloor \beta \rfloor)D/d \), we modify the Lemma A.5 in [35]. For an \( m \)-dimensional multiple output neural network \( \Phi \), we write \( R(\Phi) = (R(\Phi)_1, \ldots, R(\Phi)_m) \).

Lemma B.3 (Simultaneous approximation of multiple Taylor polynomials). Fix any \( m \in \mathbb{N} \). Let \( \{c_{\ell, \alpha} \} \subset [-B, B] \) for \( 1 \leq \ell \leq m \). Let \( (x_\ell)_{\ell=1}^m \subset [0, 1]^D \). Then there exist constants \( c_1^{\text{pol}} = c_1^{\text{pol}}(\beta, D, d, B) \), \( c_2^{\text{pol}} = c_2^{\text{pol}}(\beta, D, d, B) \) and \( s_1^{\text{pol}} = s_1^{\text{pol}}(\beta, D, d, B) \) such that for any \( \epsilon \in (0, 1) \), there is a neural network \( \Phi^{\text{pol}}_\epsilon \) with

1. \( \max_{\ell=1,\ldots,m} \sup_{x \in [0, 1]^D} |R(\Phi^{\text{pol}}_\epsilon)(x) - \sum_{|\alpha|<\beta} c_{\ell, \alpha}(x - x_\ell)^\alpha| \leq \epsilon \),
2. \( W(\Phi^{\text{pol}}_\epsilon) \leq c_1^{\text{pol}} \epsilon^{-d/\beta} \),
3. \( L(\Phi^{\text{pol}}_\epsilon) \leq 1 + (1 + \lceil \log_2 \beta \rfloor)(11 + \beta/d) \),
4. \( B(\Phi^{\text{pol}}_\epsilon) \leq c_2^{\text{pol}} \epsilon^{-s_1^{\text{pol}}} \).

Proof. By the binomial theorem [13], we have

\[
(x - x_\ell)^\alpha = \sum_{\gamma \leq \alpha} \binom{\alpha}{\gamma} (-x_\ell)^{\alpha - \gamma} x^{\gamma}
\]
Thus

\[
\sum_{|\alpha|<\beta} c_{\ell,\alpha} (x-x_\ell)^\alpha = \sum_{|\alpha|\leq |\beta|} \left\{ \sum_{\gamma \leq \alpha} c_{\ell,\alpha} \left( \frac{\alpha}{\gamma} \right) (-x_\ell)^{\alpha - \gamma} x^\gamma \right\}
\]

\[
= \sum_{|\gamma|\leq |\beta|} \left\{ \sum_{\gamma \leq |\beta|, |\alpha|\leq |\beta|} c_{\ell,\alpha} \left( \frac{\alpha}{\gamma} \right) (-x_\ell)^{\alpha - \gamma} \right\} x^\gamma
\]

\[
=: \sum_{|\gamma|\leq |\beta|} \tilde{c}_{\ell,\gamma} x^\gamma.
\]

Note that $|\tilde{c}_{\ell,\gamma}| \leq c M$ for all $\gamma$ with $|\gamma| \leq |\beta|$ where $c = c(\beta, D)$ is a constant. Since $(\alpha_1, \ldots, \alpha_D)$, we can bound $c M$ by

\[
\sup_{x \in [0,1]^D} \left| \sum_{|\alpha|\leq |\beta|} \sum_{\gamma \leq \alpha} c_{\ell,\alpha} \left( \frac{\alpha}{\gamma} \right) (-x_\ell)^{\alpha - \gamma} \right| \leq M \sum_{|\alpha|\leq |\beta|} \sum_{\gamma \leq |\alpha|} \alpha_{1}^{\gamma_1} \ldots \alpha_{D}^{\gamma_D}
\]

\[
\leq M \sum_{|\alpha|\leq |\beta|} (\alpha_1 + 1) \ldots (\alpha_D + 1) \alpha_{1}^{\gamma_1} \ldots \alpha_{D}^{\gamma_D}
\]

\[
\leq M D^{\beta+1} (1 + \beta)^{D(1+|\beta|)}.
\]

Write \(\{ \gamma \mid |\gamma| \leq |\beta| \} = \{\gamma_1, \ldots, \gamma_K\}\) for some $K = K(\beta)$. Let $\Phi^{\mathrm{dir}, \ell} := (\tilde{c}_{\ell,\gamma_1}, \ldots, \tilde{c}_{\ell,\gamma_K}, 0)$. The number of parameters in Lemma [B.2] has the exponential decay with exponent $-D/b$.

In order to decrease the rate of parameters, we define the neural network $\Phi^{\mathrm{mul},\gamma_k}_{\ell}$ as the one constructed by Lemma [B.2] with substitution $\epsilon \leftarrow \epsilon/(cK M)$, $b \leftarrow (1 + |\beta|) D/d$ and $\alpha \leftarrow \gamma_k$ for $k \in \{1, \ldots, K\}$. Then, there exist constants $c^{\mathrm{pol}}_3 = c^{\mathrm{pol}}_3 (\beta, D, d, M)$ and $c^{\mathrm{pol}}_4 = c^{\mathrm{pol}}_4 (\beta, D, d, M)$ such that

1. $W(\Phi^{\mathrm{mul},\gamma_k}_{\ell}) \leq c^{\mathrm{pol}}_3 \epsilon^{-d/(1 + |\beta|)}$,

2. $L(\Phi^{\mathrm{mul},\gamma_k}_{\ell}) \leq (1 + \lceil \log_2 \beta \rceil)(10 + (1 + \beta)/d)$,

3. $B(\Phi^{\mathrm{mul},\gamma_k}_{\ell}) \leq c^{\mathrm{pol}}_4 \epsilon^{-s^{\mathrm{mul}}}$,

holds for all $k \in \{1, \ldots, K\}$. Note that since $K \leq D^0 + D^1 + \cdots + D^{|\beta|} \leq (1 + |\beta|) D^{|\beta|+1}$, it is easily shown that

\[
c_{3}^{\mathrm{pol}} \leq c_{3}^{\mathrm{mul}} D^{2d(1 + |\beta|)} D^{d+d/(1 + |\beta|)} M^{d/(1 + |\beta|)}
\]

\[
c_{4}^{\mathrm{pol}} \leq c_{4}^{\mathrm{mul}} D^{s^{\mathrm{mul}}+d/(1 + |\beta|)+s^{\mathrm{mul}}(1 + |\beta|)(c M)^{s^{\mathrm{mul}}(1 + |\beta|)^{s^{\mathrm{mul}}+d(1 + |\beta|)+s^{\mathrm{mul}}}.
\]

Finally, define

\[
\Phi^{\mathrm{pol},1}_{\ell} := [\Phi^{\mathrm{mul},\gamma_1}_{\ell}, \Phi^{\mathrm{mul},\gamma_2}_{\ell}, \ldots, \Phi^{\mathrm{mul},\gamma_K}_{\ell}],
\]

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\[
\Phi_{\epsilon}^{\text{pol},2} := [\Phi_{\epsilon}^{\text{tlr},1}, \Phi_{\epsilon}^{\text{tlr},2}, \ldots, \Phi_{\epsilon}^{\text{tlr},m}], \\
\Phi_{\epsilon}^{\text{pol}} := \Phi_{\epsilon}^{\text{pol},2} \odot \Phi_{\epsilon}^{\text{pol},1}.
\]

Thus,
\[
\sup_{x \in [0,1]^D} \left| \sum_{|\gamma| \leq \lfloor \beta \rfloor} \tilde{c}_{\ell,\gamma} x^\gamma - R(\Phi_{\epsilon}^{\text{pol}})_{\ell}(x) \right| \leq cMK \frac{\epsilon}{cMK} = \epsilon.
\]

Note that by Remark 1 and Remark 2,
\[
W(\Phi_{\epsilon}^{\text{pol}}) \leq 2W(\Phi_{\epsilon}^{\text{pol},2}) + 2W(\Phi_{\epsilon}^{\text{pol},1}) \\
\leq 2Km + 2(2Ke_3^{\text{pol}} \epsilon^{-d/(1+\lfloor \beta \rfloor)}) + 4KD(1 + \lfloor \log_2 \beta \rfloor)(10 + (1 + \beta)/d), \\
L(\Phi_{\epsilon}^{\text{pol}}) = L(\Phi_{\epsilon}^{\text{pol},2}) + L(\Phi_{\epsilon}^{\text{pol},1}) \leq 1 + (1 + \lfloor \log_2 \beta \rfloor)(10 + (1 + \beta)/d), \\
B(\Phi_{\epsilon}^{\text{pol}}) \leq \max \left\{ cM, c_4^{\text{pol}} \epsilon^{-s_{\gamma}^{\text{pol}}} \right\}.
\]

This confirms the desired property of \(\Phi_{\epsilon}^{\text{pol}}\). \(\Box\)

### B.1.2 Approximation of \(f_0\).

Here we introduce a neural network construction of the partition of unity on \([0,1]^D\).

Define a function \(u_{a,b}(x) : \mathbb{R} \to [0,1]\) by
\[
u_{a,b}(x) = \begin{cases} 
1 - a|x - b| & \text{if } x \in \left[b - \frac{1}{a}, b + \frac{1}{a}\right], \\
0 & \text{otherwise}.
\end{cases}
\]

**Lemma B.4** (Neural network version of the partition of unity). Let \(a, b \in \mathbb{R}\). Define a neural network \(\Phi_{U,a,b}^{U,a,b}\) as,
\[
\Phi_{U,a,b}^{U,a,b} := ((1, -2, 1), 0) \odot [(a, -ab + 1), (a, -ab), (a, -ab - 1)].
\]

Then \(R(\Phi_{U,a,b}^{U,a,b}) : \mathbb{R} \to [0,1]\) is a neural network version of a function \(u_{a,b} : \mathbb{R} \to [0,1]\).

With Remark 1, it can be easily verified that
1. \(W(\Phi_{U,a,b}^{U,a,b}) \leq 18\),
2. \(L(\Phi_{U,a,b}^{U,a,b}) = 2\),
3. \(B(\Phi_{U,a,b}^{U,a,b}) \leq \max \{2, |a|, |ab - 1|, |ab + 1|\}\).

We first approximate the Taylor polynomials of the Hölder class functions with controlled accuracy.
Lemma B.5 (Lemma A.8 in [35]). Fix any \( f_0 \in F^{\beta,D,M} \) and \( x_\ell \in [0,1]^D \). Let \( f_\ell(x) \) be the Taylor polynomial of degree \( \lfloor \beta \rfloor \) of \( f_0 \) around \( x_\ell \), namely,

\[
f_\ell(x) := \sum_{|\alpha| \leq \lfloor \beta \rfloor} \frac{\partial^\alpha f(x_\ell)}{\alpha!} (x-x_\ell)\alpha.
\]

Then, \( |f_0(x) - f_\ell(x)| \leq CM|x-x_\ell|^\beta \) for any \( x \in [0,1]^D \).

Note that \( \sup_{|\alpha| \leq \lfloor \beta \rfloor} |\partial^\alpha f(x_\ell)/\alpha!| < CM \) for some constant \( C = C(\beta,D,M) \). For \( \lambda \in \Lambda_N \) and any arbitrary point \( x_\lambda \in I_\lambda \), take \( f_\lambda(x) \) as in the Lemma B.5 with \( x_\ell \leftarrow x_\lambda \).

Define \( u_\lambda : \mathbb{R}^D \to [0,1] \) by \( u_\lambda(x) := \prod_{j=1}^D u_{N,(2j^2-1)/(2N)}(x_i) \).

Since \( \{u_\lambda \mid \lambda \in \Lambda_N^*\} \) is a partition of unity on \( \text{Supp} \mu \), \( u_\xi(x) + \sum_{\lambda \in \Xi(x)} u_\lambda(x) = 1 \) for any \( x \in \text{Supp} \mu \).

Recall that for a continuous function \( g \), \( \|g\|_{L^\infty(\mu)} = \sup_{x \in \text{Supp} \mu} |g(x)| \). Observe

\[
\left\| f_0 - \sum_{\lambda \in \Lambda_N^*} f_\lambda \otimes u_\lambda \right\|_{L^\infty(\mu)} = \left\| \sum_{\lambda \in \Lambda_N^*} (f_0 - f_\lambda) \otimes u_\lambda \right\|_{L^\infty(\mu)}
\]

\[
= \sup_{x \in \text{Supp} \mu} \left| \sum_{\lambda \in \Lambda_N^*} (f_0(x) - f_\lambda(x)) u_\lambda(x) \right|
\]

\[
\leq \sup_{x \in \text{Supp} \mu} \left( CM \left( \frac{1}{N} \right)^\beta u_\xi(x) + \sum_{\lambda \in \Xi(x)} CM \left( \frac{2}{N} \right)^\beta u_\lambda(x) \right)
\]

\[
\leq 3^D CM \left( \frac{2}{N} \right)^\beta.
\]

The last inequality follows since \( \text{card}(\{\xi(x)\} \cup \Xi(x)) = 3^D \).

Choose \( N \) as

\[
N = \left\lceil (3^{D+1}CM2^\beta)^{1/\beta} \epsilon^{-1/\beta} \right\rceil.
\]

Then,

\[
\left\| f_0 - \sum_{\lambda \in \Lambda_N^*} f_\lambda \otimes u_\lambda \right\|_{L^\infty(\mu)} \leq 3^D CM \left( \frac{2}{N} \right)^\beta
\]

\[
\leq 3^D CM2^\beta \frac{\epsilon}{3^{D+1}CM2^\beta}
\]

\[
\leq \frac{\epsilon}{3}.
\]
Let $\Phi^\text{pol}_{\epsilon/3}$ be a neural network constructed in Lemma B.3 with $\epsilon \leftarrow \epsilon/3$, $(x_\ell)_{\ell=1}^{m_N^*} \leftarrow (x_\ell)_{\ell=1}^{m_N^*} \in I_{\psi(1)} \times I_{\psi(m_N^*)}$, $(c_\ell, a_\ell)_{\ell=1}^{m_N^*} \leftarrow (\partial^a f(x_\ell)/\alpha_\ell)_{\ell=1}^{m_N^*}$, $m \leftarrow m_N^*$ and $B \leftarrow CM$. Then

\[
\left\| \sum_{\lambda \in \Lambda_N^*} f_\lambda \otimes u_\lambda - \sum_{\ell=1}^{m_N^*} R(\Phi^\text{pol}_{\epsilon/3})_\ell \otimes u_\psi(\ell) \right\|_{L^\infty(\mu)} \leq \frac{\epsilon}{3},
\]

since $\{u_\lambda \mid \lambda \in \Lambda_N^*\}$ is a partition of unity on $\text{Supp } \mu$.

Next, we approximate $\sum_{\ell=1}^{m_N^*} R(\Phi^\text{pol}_{\epsilon/3})_\psi(\ell) u_\psi(\ell)$. By chaining the argument of Proposition 3 in [46], we obtain the following lemma.

**Lemma B.6.** For any $B > 0$, there is a neural network $\Phi^x,K : \mathbb{R}^K \rightarrow \mathbb{R}$ with constants $c'_1 = c'_1(K, B)$, $c'_2 = c'_2(K, B)$ and $c'_3 = c'_3(B)$ such that

1. $|x_1 \times \cdots \times x_K - R(\Phi^x,K)(x)| \leq \epsilon$ for any $x = (x_1, \ldots, x_K) \in [-B, B]^K$,
2. $x_1 \times \cdots \times x_K = 0 \Rightarrow R(\Phi^x,K)(x) = 0$,
3. $L(\Phi^x,K) = c'_1 \log(1/\epsilon)$,
4. $W(\Phi^x,K) = c'_2 \log(1/\epsilon)$,
5. $B(\Phi^x,K) \leq c'_3$.

We can assume the hypercube $I_\lambda$ is open without loss of generality. Write $I_\lambda$ as

\[
I_\lambda = \prod_{i=1}^{D} \left( \frac{j_i^\lambda - 1}{N}, \frac{j_i^\lambda}{N} \right) = B_{\max}^D \left( \left( \frac{2j_i^\lambda - 1}{2N}, \ldots, \frac{2j_i^\lambda - 1}{2N} \right), \frac{1}{2N} \right),
\]

where $j_i^\lambda \in \{1, \ldots, N\}$ and $i \in \{1, \ldots, D\}$.

Let $\Phi^{U,N,(2j_i^\lambda - 1)/(2N)}$ be a neural network constructed in Lemma B.4 with $a \leftarrow N$ and $b \leftarrow (2j_i^\lambda - 1)/(2N)$. Consider the following network $\Phi$ with $D$-dimensional inputs and $m(D + 1)$-dimensional outputs.

\[
\Phi^U,\ell := \left[ \Phi^{U,N,(2j_i^\epsilon - 1)/(2N)} \otimes (e_1^T, 0), \ldots, \Phi^{U,N,(2j_i^{D-1} - 1)/(2N)} \otimes (e_D^T, 0) \right],
\]

\[
\Phi := \left[ \Phi^\text{pol}_{\epsilon/3}, \Phi^{U,1}, \ldots, \Phi^{U,m_N^*} \right],
\]

where $e_i \in \mathbb{R}^D$ is a unit vector with $i$-th element 1. Then, for $x = (x_1, \ldots, x_D) \in \mathbb{R}^D$,

\[
R(\Phi)(x) = (R(\Phi^\text{pol}_{\epsilon/3})(x_1), \ldots, R(\Phi^\text{pol}_{\epsilon/3})(x_m), u_{N,(2j_1^\lambda - 1)/(2N)}(x_1), \ldots, u_{N,(2j_D^\lambda - 1)/(2N)}(x_D), \ldots,
\]

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\[ u_{N,(2j^{\lambda}-1)/(2N)}(x_1), \ldots, u_{N,(2j^{\lambda}-1)/(2N)}(xD) \].

To aggregate the outputs of \( \Phi \), construct a neural network \( \Phi^{\text{filter},i} : \mathbb{R}^{m(D+1)} \rightarrow \mathbb{R}^{D+1} \) that filters the \( i \)-th input and \( D(i+1) \)-th, \( D(i+1)+1 \)-th, \ldots, \( D(i+2) - 1 \)-th input as

\[
\Phi^{\text{filter},i} := \left( \begin{array}{cccc}
\frac{e_i}{I_D} & 0 & 0 & 0 \\
0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0
\end{array} \right), 0_{D+1}.
\]

Take a neural network \( \Phi^{x,D+1}_{\epsilon/3} \) constructed in Lemma B.6 with \( \epsilon \leftarrow \epsilon/2 \) and \( K \leftarrow D+1 \). Define \( \Phi^{\text{sum}} := \left((1, \ldots, 1, 0)\right) \). Define

\[
\Psi_{\epsilon}^{f_0} := \Phi^{R,1,M} \circ \Phi^{\text{sum}} \circ \left[ \Phi^{x,D+1}_{\epsilon/3} \circ \Phi^{R,D+1,M} \circ \Phi^{\text{filter},1}, \ldots, \Phi^{x,D+1}_{\epsilon/3} \circ \Phi^{R,D+1,M} \circ \Phi^{\text{filter},m_N^{*}} \right] \circ \Phi,
\]

where \( \Phi^{R,1,M} \) and \( \Phi^{R,D+1,M} \) is the neural networks constructed in Lemma B.1 with \( K \leftarrow 1 \) or \( K \leftarrow D+1 \) and \( B \leftarrow M \), respectively. Then \( \Psi_{\epsilon}^{f_0} \) approximates \( \sum_{\ell=1}^{m_N^{*}} R(\Phi_{\epsilon/3}^{\text{pol}})(\psi(\ell) \Phi^{\text{pol}}(\ell))u_{\psi(\ell)}(x) \), with the error bounded by

\[
\left\| R(\Psi_{\epsilon}^{f_0})(x) - \sum_{\ell=1}^{m_N^{*}} R(\Phi_{\epsilon/3}^{\text{pol}})(\psi(\ell) \Phi^{\text{pol}}(\ell))u_{\psi(\ell)}(x) \right\|_{L^\infty} \leq \epsilon/3
\]

Recall that \( m_N^{*} \leq C_{\mu,d}N^d \) by Remark 3. Combined with Remark 1 and 2 \( \Psi_{\epsilon}^{f_0} \) has the property that

\[
W(\Psi_{\epsilon}^{f_0}) \leq 2W(\Phi^{R,1,M}) + 2W(\Phi^{\text{sum}}) + 2m_N^{*}W(\Phi^{x,D+1}_{\epsilon/3} \circ \Phi^{R,D+1,M} \circ \Phi^{\text{filter},1}) + 2W(\Phi)
\]

\[
\leq 56 + 2m_N^{*} + 4m_N^{*}(c_2 \log(1/\epsilon) + 28(D + 1) + (D + 1)) + 2W(\Phi)
\]

\[
\leq 56 + m_N^{*}(4c_2 \log(1/\epsilon) + 116D + 118)
\]

\[
+ 2W(\Phi_{\epsilon/3}^{\text{pol}}) + 2m_N^{*}W(\Phi^{U,1}) + 4(m_N^{*} + 1) \max \left\{ L(\Phi_{\epsilon/3}^{\text{pol}}), L(\Phi^{U,1}) \right\}
\]

\[
\leq 56 + m_N^{*}(4c_2 \log(1/\epsilon) + 116D + 118)
\]

\[
+ 2(c_1^{\text{pol}}(\epsilon^{-d/\beta}3^{d/\beta} + m_N^{*})) + 152Dm_N^{*} + 4(m_N^{*} + 1) \max \left\{ 1 + (1 + [\log_2 \beta])(11 + \beta/d), 3 \right\}
\]

\[
\leq c_1 + c_2 \epsilon^{-d/\beta} \log(1/\epsilon),
\]

\[
L(\Psi_{\epsilon}^{f_0}) \leq 2 + 1 + c_1 L(\Phi_{\epsilon/3}^{x,D+1}) + 2 + 1 + L(\Phi)
\]

\[
\leq 6 + c_1 \log 3 + c_1 \log(1/\epsilon) + \max \left\{ L(\Phi_{\epsilon/2}^{\text{pol}}), 3 \right\}
\]

\[
\leq 9 + c_1 \log 3 + c_1 \log(1/\epsilon) + (1 + [\log_2 \beta])(10 + (1 + \beta)/d)
\]
\[ \begin{aligned} &= c_3 + c_4 \log(1/\epsilon), \\ B(\Psi_{\epsilon} f_0) &\leq \max \left\{ 2, cM, N, c'_3, c'_4 \epsilon^{\frac{-s}{2} \rho} \right\} =: c'\epsilon^{-s'}, \end{aligned} \]

where \( c'_1 = c'_1(D + 1, M) \), \( c'_2 = c'_2(D + 1, M) \), \( c'_3 = c'_3(D + 1, M) \), \( c'_4 \rho \) and \( s^2 \) are the constants appearing in Lemma [B.6] and [B.3].

Finally, we bound \( \| f_0 - R(\Psi_{\epsilon} f_0) \|_{L^{\infty}(\mu)} \). By the triangle inequality,

\[ \begin{aligned} \| f_0 - R(\Psi_{\epsilon} f_0) \|_{L^{\infty}(\mu)} &\leq \left\| f_0 - \sum_{\lambda \in \Lambda^*_N} f_{\lambda} \otimes u_{\lambda} \right\|_{L^{\infty}(\mu)} + \left( \sum_{\lambda \in \Lambda^*_N} f_{\lambda} \otimes u_{\lambda} - \sum_{\ell=1}^{m_N} R(\Phi_{\epsilon/3}^\rho f_{\ell}) \otimes u_{\psi(\ell)} \right)_{L^{\infty}(\mu)} \\
&\quad + \left( \sum_{\ell=1}^{m_N} R(\Phi_{\epsilon/3}^\rho f_{\ell}) \otimes u_{\psi(\ell)} - R(\Psi_{\epsilon} f_{0}) \right)_{L^{\infty}(\mu)} \\
&\leq \frac{\epsilon}{3} + \frac{\epsilon}{3} + \frac{\epsilon}{3} = \epsilon. \end{aligned} \]

\( \square \)

### B.2 Proof of Theorem 4.2

We basically follows the proof of [38, 36, 22]. By definition of \( \hat{f} \), \( \| Y - \hat{f} \|^2_n \leq \| Y - f \|^2_n \) for any \( f \in F(W, L, D) \). By substituting \( Y_i = f_0(X_i) + \xi_i \), we obtain

\[ \begin{aligned} \| \hat{f} - f_0 \|^2_n &\leq \| f - f_0 \|^2_n + \frac{2}{n} \sum_{i=1}^n \xi_i \left( \hat{f}(X_i) - f(X_i) \right) \end{aligned} \]

We divide the proof into 3 steps.

**Step 1.** Derive the upper bound of \( \| \hat{f} - f_0 \|^2_{L^2(\mu)} \) using \( \| \hat{f} - f_0 \|^2_n \).

**Step 2.** Evaluate \( (1/n) \sum_{i=1}^n \xi_i \left( \hat{f}(X_i) - f(X_i) \right) \).

**Step 3.** Combine the results of step 1 and step 2.

Let \( \Psi_{\epsilon} f_0 \) be the neural network approximation of \( f_0 \) constructed by Theorem 4.1 with the triple \((W, L, B)\) set as in Theorem 4.1 with accuracy \( \epsilon \leftarrow n^{d/(2\beta + d)} \). Denote \( f^* = R(\Psi_{\epsilon} f_0) \). Let \( G_\delta := \{ g : \mathbb{R}^D \to \mathbb{R} \mid g = f - f^*, \| f - f^* \|_n \leq \delta, f \in F \} \).
B.2.1 Step 1.

Before going into the detailed proof, we prepare the rough evaluation of the entropy number bound. Let \( N(\epsilon, \mathcal{F}, \|\cdot\|) \) be the minimum \( \epsilon \)-covering number of \( \mathcal{F} \) by a norm \( \|\cdot\| \).

**Lemma B.7** (Covering entropy bound for \( \mathcal{F} \)). Let \( \mathcal{F} = \mathcal{F}(W, L, B) \) be a space of neural networks with the number of nonzero weights, the number of layers, and the maximum absolute value of weights are respectively bounded by \( W, L \) and \( B \). Then,

\[
\log N(\epsilon, \mathcal{F}(W, L, B), \|\cdot\|_{\text{max}}) \leq W \log \left( \frac{2LB^L(W+1)^L}{\epsilon} \right).
\]

Before presenting the proof, we need the following preliminary result, which makes it possible to regard neural networks in \( \mathcal{F}(W, L, B) \) share the same dimensional parameter space.

**Lemma B.8.** Let \( \mathcal{F}(W, L, B) \) be a class of neural networks. Define

\[
S_B(p, q) := \{(A, b) \mid A \in [-B, B]^{p \times q}, b \in [-B, B]^p\},
\]

\[
\mathcal{G}(W, L, B) := S_B(1, W) \times S_B(W, W) \times \cdots \times S_B(W, D).
\]

Then there exists a map \( Q: \mathcal{F}(W, L, B) \rightarrow \mathcal{G}(W, L, B) \) such that

\[
R(\Phi)(x) = A^Q_L \rho_{b^Q_L-1} \circ \cdots \circ A^Q_1 \rho_{b^Q_1}(A^Q_1 x) + b^Q_L,
\]

where \((A^Q_L, b^Q_L), \ldots, (A^Q_1, b^Q_1)) = Q(R(\Phi)) \in \mathcal{G}(W, L, B).

**Proof.** Take any \( R(\Phi) \in \mathcal{F}(W, L, B) \). Write \( \Phi = ((A_L, b_L), \ldots, (A_1, b_1)) \) and assume \( A_l \in \mathbb{R}^{p_l \times p_{l-1}} \) and \( b_l \in \mathbb{R}^{p_l} \). Consider \((A_{l-1}, b_{l-1})\) for \( l = 2, \ldots, L \). Since the number of nonzero parameters are bounded by \( W \), the number of nonzero parameters in \( A_{l-1} x + b_{l-1} \) for any \( x \in \mathbb{R}^{p_{l-2}} \) is at most \( W \). For \( p_{l-1} > W \), without loss of generality, we can assume the \( W \)-th, \ldots, \( p_{l-1} \)-th element of \( A_{l-1} x + b_{l-1} \) are 0. Let \( A'_{l-1} \in \mathbb{R}^{W \times p_{l-1}} \) be the upper-left part of \( A_{l-1} \) and \( A'_l \in \mathbb{R}^{p_l \times W} \) be the upper-left part of \( A_l \). Also let \( b'_{l-1} \in \mathbb{R}^{p_{l-1}} \) be the first \( W \) elements of \( b_{l-1} \). Then \( A'_l x + b'_{l-1} = A_l (A_{l-1} x + b_{l-1}) \). For \( p_{l-1} < W \), we can simply extend \( A_l, A_{l-1}, b_{l-1} \) to be in \( \mathbb{R}^{p_l \times W}, \mathbb{R}^{W \times p_{l-2}}, \mathbb{R}^W \), respectively. Applying this procedure repeatedly yields the conclusion.\( \square \)

**Proof of Lemma C.6.** Take \( R(\Phi), R(\Phi') \in \mathcal{F}(W, L, B) \). Write \( \Phi = Q(R(\Phi)) = ((A_L, B_L), \ldots, (A_1, b_1)) \) and \( \Phi' = Q(R(\Phi')) = ((A'_L, B'_L), \ldots, (A'_1, b'_1)) \), such that for each \( l = 1, \ldots, L \), \( (A'_l, b'_l) \) has elements at most \( \epsilon \) apart from \( (A_l, b_l) \). Write \( (A_l, b_l) = ((a^l_{ij}), (b^l_i)) \) and \( (A'_l, b'_l) = ((a'^l_{ij}), (b'^l_i)) \). Define

\[
h^l(x) := (h^l_{11}(x), \ldots, h^l_{p_l}(x))^\top := A_l x + b_l,
\]

\[
h'^l(x) := (h'^l_{11}(x), \ldots, h'^l_{p_l}(x))^\top := A'_l x + b'_l.
\]
\[ g'(x) := (g'_1(x), \ldots, g'_{p_l}(x))^\top := h^l(x) - h'^l(x). \]

Then,
\[
\sup_{x \in [-E, E]^{p_l-1}} |g'_i(x)| \leq \sum_{j=1}^{p_l-1} |a_{ij} - a'_{ij}| |x_j| + |b_i - b'_i|
\leq p_{l-1} \epsilon E + \epsilon
\leq (WE + 1) \epsilon
\leq (W + 1) E \epsilon.
\]

Also note that
\[
\sup_{x \in [-E, E]^{p_l-1}} |h'_i(x)| \leq \sum_{j=1}^{p_l-1} |a_{ij}| |x_j| + |b_i|
\leq p_{l-1} BE + B
\leq (WE + 1) B
\leq (W + 1) EB.
\]

Since the Lipschitz constant of ReLU function is 1 for each coordinate, applying this inequality repeatedly to obtain
\[
\sup_{x \in [0, 1]^D} |R(\Phi) - R(\Phi')|.
\]

\[
= \left| h^L \circ \rho \circ h^{L-1} \circ \rho \circ \cdots \circ \rho \circ h^2 \circ \rho \circ h^1(x) - h'^L \circ \rho \circ h'^{L-1} \circ \rho \circ \cdots \circ \rho \circ h'^2 \circ \rho \circ h'^1(x) \right|
\leq \left| h^L \circ \rho \circ h^{L-1} \circ \rho \circ \cdots \circ \rho \circ h^2 \circ \rho \circ h^1(x) - h'^L \circ \rho \circ h'^{L-1} \circ \rho \circ \cdots \circ \rho \circ h'^2 \circ \rho \circ h'^1(x) \right|
+ \left| h^L \circ \rho \circ h^{L-1} \circ \rho \circ \cdots \circ \rho \circ h^2 \circ \rho \circ h^1(x) - h'^L \circ \rho \circ h'^{L-1} \circ \rho \circ \cdots \circ \rho \circ h'^2 \circ \rho \circ h'^1(x) \right|
\vdots
+ \left| h^L \circ \rho \circ h'^{L-1} \circ \rho \circ \cdots \circ \rho \circ h'^2 \circ \rho \circ h'^1(x) - h'^L \circ \rho \circ h'^{L-1} \circ \rho \circ \cdots \circ \rho \circ h'^2 \circ \rho \circ h'^1(x) \right|
\leq L(W + 1)^L B^{L-1} \epsilon
\]

Discretize \( W \) parameters with \( \epsilon/L(W + 1)^L B^{L-1} \) grid size yields the covering number bound
\[
\mathcal{N}(\epsilon, \mathcal{F}(W, L, B), \| \cdot \|_{\text{max}}) \leq \left( \frac{2BL(W + 1)^L B^{L-1}}{\epsilon} \right)^W = \left( \frac{2L(W + 1)^L B^L}{\epsilon} \right)^W
\]
\[
\square
\]

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Next we bound the generalization error $\|\hat{f} - f_0\|_{L^2(\mu)}$ by $\|\hat{f} - f\|_n$ and $\|f - f_0\|_{L^2(\mu)}$.

By generalized Bennett’s inequality in [7],

**Theorem B.9.** Let $(\mathcal{G}, \|\cdot\|)$ be a separable set of measurable and square-integrable functions from $\mathbb{R}^D$ to $\mathbb{R}$. Assume $\sup_{g \in \mathcal{G}} \|g\|^2 \leq M < \infty$. Define $\tau^2 := \sup_{g \in \mathcal{G}} E[g^4]$ and $Z := \sup_{g \in \mathcal{G}} \left(\frac{1}{n} \sum_{i=1}^n \{g(X_i)\}^2 - E[g^2]\right)$. Then

$$P\left(Z \geq E[Z] + \sqrt{\frac{2\tau_1 M^2}{n}} (n\tau^2 + 2E[Z]) + \frac{r_1 M}{3n}\right) \leq e^{-r_1}.$$

Thus there exist a constant $C > 0$ not depending on $n$ such that

$$Z \leq C \left(E[Z] + \sqrt{\frac{2\tau_1 M^2}{n}} + \frac{r_1 M}{n}\right)$$

with probability at least $1 - e^{-r_1}$. Next, we bound the right hand side. Let $\{\varepsilon_i\}$ be independent Rademacher variables. By symmetrization inequality in Lemma 2.3.1 of [42],

$$E[Z] \leq 2E\left[\sup_{g \in \mathcal{G}} \left|\frac{1}{n} \sum_{i=1}^n \varepsilon_i \{g(X_i)\}^2\right|\right].$$

Also by contraction inequality in Theorem 4.12 of [30],

$$E\left[\sup_{g \in \mathcal{G}} \left|\frac{1}{n} \sum_{i=1}^n \varepsilon_i \{g(x_i)\}^2\right|\right] \leq 4Me\left[\sup_{g \in \mathcal{G}} \left|\frac{1}{n} \sum_{i=1}^n \varepsilon_i g(x_i)\right|\right].$$

By covering number bound in [16]

$$E\left[\sup_{g \in \mathcal{G}} \left|\frac{1}{n} \sum_{i=1}^n \varepsilon_i g(X_i)\right|\right] \leq \frac{8\sqrt{2\tau}}{\sqrt{n}} \int_0^{\delta/2} \sqrt{\log(2N(\epsilon, \mathcal{G}, \|\cdot\|_n))} \, d\epsilon.$$

With $\mathcal{G} = \mathcal{G}_\delta$ and Lemma [B.7], the right hand side can be evaluated. Finally we obtain

$$\sup_{g \in \mathcal{G}} \left|\frac{1}{n} \sum_{i=1}^n \{g(X_i)\}^2 - E[g^2]\right| \leq \frac{4\tau \sqrt{2W\delta}}{\sqrt{n}} \log \left(\frac{L(W + 1)B^L}{\delta} \right) \log \left(\frac{L(W + 1)B^L}{\delta} + 1\right),$$

with probability at least $1 - e^{-r_1}$.

Now, we have

$$\|\hat{f} - f_0\|_{L^2(\mu)}^2 \leq 2\|\hat{f} - f\|_{L^2(\mu)}^2 + 2\|f - f_0\|_{L^2(\mu)}^2.$$
\[ \leq 2 \| \hat{f} - f \|_n^2 + 2 \| f - f_0 \|_{L^2(\mu)}^2 + 2 \left| \| \hat{f} - f \|_n^2 - \| \hat{f} - f \|_{L^2(\mu)}^2 \right|. \]

To bound the term \( \left| \| \hat{f} - f \|_n^2 - \| \hat{f} - f \|_{L^2(\mu)}^2 \right| \), we apply Theorem B.9 with \( g = \hat{f} - f \in G \).

\[ \left| \| g \|_n^2 - \| g \|_{L^2(\mu)}^2 \right| \leq \frac{4\tau \sqrt{2W \delta}}{\sqrt{n}} \log \left( \frac{L(W + 1)LB}{\delta} + 1 \right), \]

with probability \( 1 - e^{-r_1} \). Hence we have

\[ \| \hat{f} - f_0 \|_{L^2(\mu)}^2 \leq 2 \| \hat{f} - f \|_n^2 + 2 \| f - f_0 \|_{L^2(\mu)}^2 + \frac{4\tau \sqrt{2W \delta}}{\sqrt{n}} \log \left( \frac{L(W + 1)LB}{\delta} + 1 \right), \]

Substitute \( \delta \leftarrow \sqrt{\frac{W}{n}} \), then

\[ \| \hat{f} - f_0 \|_{L^2(\mu)}^2 \leq 2 \| \hat{f} - f \|_n^2 + 2 \| f - f_0 \|_{L^2(\mu)}^2 + \frac{4\sqrt{2}\tau W}{n} \log \left( \sqrt{n}L(W + 1)LW^{-1/2}B + 1 \right). \]

**B.2.2 Step 2.**

Let \( W_n \coloneqq \sup_{g \in G} \left| (1/n) \sum_{i=1}^n \xi_i g(X_i) \right| \). By Gaussian concentration inequality (Theorem 2.5.8 in [16]),

\[ P(W_n \geq E[W_n] + r_2) \leq \exp \left\{ -\frac{nr_2^2}{2\sigma^2 \| G \|_n^2} \right\} \leq \exp \left\{ -\frac{nr_2^2}{2\sigma^2 B_f^2} \right\} \]

where \( \| G \|_n^2 = \sup_{g \in G} \| g \|_n^2 \). Also By covering entropy bound in [16] combined with \( \log \mathcal{N}(\epsilon, \mathcal{G}, \| \cdot \|_n) \leq \log \mathcal{N}(\epsilon, \mathcal{F}, \| \cdot \|_{\text{max}}) \), we obtain

\[ E[W_n] \leq \frac{4\sqrt{2}\sigma}{\sqrt{n}} \int_0^{2\delta} \sqrt{\log(2\mathcal{N}(\epsilon, \mathcal{G}, \| \cdot \|_n))} d\epsilon \leq \frac{4\sigma \sqrt{2W \delta}}{\sqrt{n}} \log \left( \frac{L(W + 1)LB}{\delta} + 1 \right). \]

Finally, we obtain

\[ W_n \leq \frac{4\sigma \sqrt{2W \delta}}{\sqrt{n}} \log \left( \frac{L(W + 1)LB}{\delta} + 1 \right) + r_2 \]

for any \( g \in \mathcal{G}_\delta \) with probability at least \( 1 - \exp(-nr_2^2/(2\sigma^2 B_f^2)) \).
B.2.3 Step 3.

Recall that for the empirical risk minimizer $\hat{f} \in \mathcal{F}(W, L, B)$, the inequality
\[
\|\hat{f} - f_0\|_n^2 \leq \|f - f_0\|_n^2 + \frac{2}{n} \sum_{i=1}^{n} \xi_i \left( \hat{f}(X_i) - f(X_i) \right)
\]
holds for all $f \in \mathcal{F}(W, L, B)$. Combined with the trivial inequality $\|\hat{f} - f_0\|_n^2 \leq 2\|\hat{f} - f_0\|_n^2 + 2\|f - f_0\|_n^2$, we obtain
\[
\|\hat{f} - f\|_n^2 \leq 3\|f - f_0\|_n^2 + \frac{4}{n} \sum_{i=1}^{n} \xi_i \left( \hat{f}(X_i) - f(X_i) \right).
\]

Let $V_n = \frac{16\sigma\sqrt{2W}}{\sqrt{n}}$. From the conclusion of step 2,
\[
\frac{4}{n} \sum_{i=1}^{n} \xi_i \left( \hat{f}(X_i) - f(X_i) \right) \leq \delta V_n \log \left( \frac{L(W + 1)LB}{\delta} + 1 \right) + 4r_2
\]
\[
\leq 2\delta^2 + 2V_n^2 \left( \log \left( \frac{L(W + 1)LB}{\delta} + 1 \right) \right)^2 + 4r_2,
\]
where the last inequality follows from the inequality $xy \leq 2x^2 + 2y^2$. Substitute $\delta \leftarrow \max \left\{ \|\hat{f} - f\|_n, V_n \right\}/2$, we obtain
\[
\frac{4}{n} \sum_{i=1}^{n} \xi_i \left( \hat{f}(X_i) - f(X_i) \right) \leq \frac{1}{2} \max \left\{ \|\hat{f} - f\|_n^2, V_n^2 \right\} + 2V_n^2 \left( \log \left( \frac{2L(W + 1)LB}{V_n} + 1 \right) \right)^2 + 4r_2.
\]

If $V_n \leq \|\hat{f} - f\|_n$, then
\[
\|\hat{f} - f\|_n^2 \leq 3\|f - f_0\|_n^2 + \frac{4}{n} \sum_{i=1}^{n} \xi_i \left( \hat{f}(X_i) - f(X_i) \right)
\]
\[
\leq 3\|f - f_0\|_n^2 + \frac{1}{2} \|\hat{f} - f\|_n^2 + 2V_n^2 \left( \log \left( \frac{2L(W + 1)LB}{V_n} + 1 \right) \right)^2 + 4r_2.
\]
Thus
\[
\|\hat{f} - f\|_n^2 \leq 6\|f - f_0\|_n^2 + 4V_n^2 \left( \log \left( \frac{2L(W + 1)LB}{V_n} + 1 \right) \right)^2 + 8r_2.
\]

If $V_n > \|\hat{f} - f\|_n$, then the same inequality trivially holds.
Combined with the inequality of conclusion in Step 1,
\[
\|\hat{f} - f_0\|_{L^2(\mu)}^2 \leq 2\|\hat{f} - f\|_n^2 + 2\|f - f_0\|_{L^2(\mu)}^2 + \frac{4\sqrt{2}\tau W}{n} \log \left( \sqrt{n} L(W + 1)^L W^{-1/2} B^L + 1 \right)
\]
\[
\leq 12\|f - f_0\|_n^2 + 2\|f - f_0\|_{L^2(\mu)}^2 + 8V_n^2 \left( \log \left( \frac{2L(W + 1)^L B^L}{V_n} + 1 \right) \right)^2 + 16r_2
\]
\[
+ \frac{4\sqrt{2}\tau W}{n} \log \left( \sqrt{n} L(W + 1)^L W^{-1/2} B^L + 1 \right),
\]
with probability at least \(1 - \exp(-nr_3^2/(2\sigma^2 B^2)) - \exp(-r_1)\).

Under the assumption of proper choice of triples \((W, L, B)\), our first main result shows there exists a neural network \(f^* \in \mathcal{F}(W, L, B)\) satisfying \(\|f^* - f_0\|_{L^2(\mu)} \leq n^{-\beta/(2\beta + d)}\). Note that by construction, \(f^* \in [-M, M]\). By Hoeffding’s inequality
\[
P\left( \|f^* - f_0\|_n^2 - \|f^* - f_0\|_{L^2(\mu)}^2 > r_3 \right) \leq 2\exp\left(-\frac{nr_3^2}{4M^2}\right).
\]
Thus the inequality
\[
\|f^* - f_0\|_n^2 \leq \|f^* - f_0\|_{L^2(\mu)}^2 + r_3
\]
holds with probability at least \(1 - 2\exp\left(-\frac{nr_3^2}{4M^2}\right)\). Substitute \(f \leftarrow f^*, r_2 \leftarrow 1/n, r_1 \leftarrow 1/n\) and \(r_3 \leftarrow 1/n\) to obtain
\[
\|\hat{f} - f_0\|_{L^2(\mu)}^2 \leq 14\|f^* - f_0\|_{L^2(\mu)}^2 + 8V_n^2 \left( \log \left( \frac{2L(W + 1)^L B^L}{V_n} + 1 \right) \right)^2
\]
\[
+ \frac{16}{n} + \frac{4\sqrt{2}\tau W}{n} \log \left( \sqrt{n} L(W + 1)^L W^{-1/2} B^L + 1 \right).\]

Combining the result by Theorem 4.1 and \(W, B\) as the setting, we obtain
\[
\|\hat{f} - f_0\|_{L^2(\mu)}^2 \leq 14\epsilon^2 n^{-2\beta/(2\beta + d)} + 256 \sigma^2 n^{-2\beta/(2\beta + d)} (\log n) \left( 1 + C_2(s, L, \beta, d) \log n \right)^2
\]
\[
+ \frac{16}{n} + 4\sqrt{2}\tau Cn^{-2\beta/(2\beta + d)} \log(1 + C_3(s, L, \beta, d) n \log n) \log n,
\]
with probability at least \(1 - \exp(-1/n) - \exp\left(-1/(2n\sigma^2 B^2)\right) - 2\exp\left(-1/(4nM^2)\right)\). \(C_2(s, L, \beta, d)\) and \(C_3(s, L, \beta, d)\) are some constants.

**B.3 Proof of theorem 4.3**

Here we prove Theorem 4.3 [11] showed that the minimax optimal rate of estimating some class of functions is tied with the covering entropy of the class.
Lemma B.10 (Proposition 1 from Yang and Barron(1992)). Let $\mathcal{F}$ be any class of functions $f$ with $\sup_{f \in \mathcal{F}} |f| < \infty$. For the regression model $Y_i = f_0(X_i) + \xi_i$, assume $X$ and $\xi$ are independent, where $X_i \sim \mathcal{N}(0, \sigma^2)$. Assume $M \leq \log(\mathcal{N}(\epsilon_n^2, \mathcal{F}, \|\cdot\|_{L^2(\mu)}) M$. Let $\epsilon_n$ be the solution of $\epsilon_n^2 = \log(\mathcal{N}(\epsilon_n^2, \mathcal{F}, \|\cdot\|_{L^2(\mu)})$. Then

$$\inf \sup_{f \neq f_0} \|\hat{f} - f_0\|_{L^2(\mu)} = \Theta(\epsilon_n),$$

where $\hat{f}$ is any estimator based on $n$ independent and identically distributed observations $(X_1, Y_1), \ldots, (X_n, Y_n)$.

To apply Lemma B.10 to $\mathcal{H}^{\beta,D,M}$, we need to evaluate the covering entropy number of the smooth function class $\mathcal{H}^{\beta,D,M}$. For a tight evaluation of the covering entropy of the $\mathcal{H}^{\beta,D,M}$, we introduce the following condition.

**Definition 5 (Concentration Condition).** We say $E$ satisfy the Concentration Condition, when there exist constants $C_1 > 0$ and $C_2 > 0$ such that for any $\epsilon > 0$, an $\epsilon$-cover $\{B^D_{\max}(x, \epsilon)\}_{i=1}^T$ of $E$ satisfies the following property. There exists a map $g : \{x_1, \ldots, x_T\} \rightarrow \{1, \ldots, U\}$ for some $U$ such that for all $j \in \{1, \ldots, U\}$, and for all $X \in 2\sigma^{-1}(j) \setminus \{0, g^{-1}(j)\}$, some $y = y \in g^{-1}(j) \setminus X$ satisfy $\min_{x \in X} \|x - y\|_{\max} \leq \epsilon$. Also $T \leq C_1 \mathcal{N}(\epsilon, E, \|\cdot\|_{\max})$ and $U \log(1/\epsilon) \leq C_2 \mathcal{N}(\epsilon, E, \|\cdot\|_{\max})$.

In short, this condition requires the existence of some nearly minimal $\epsilon$-cover of $E$ that can be grouped into properly concentrated parts. To make clear this condition, we introduce the following lemma.

**Lemma B.11.** Assume $\mathcal{M}$ is a compact $d$-dimensional manifold in $[0, 1]^D$, namely, assume $\mathcal{M} = \bigcup_{k=1}^K \mathcal{M}_k \subset [0, 1]^D$ for some $K \in \mathbb{N}$. Also assume for any $1 \leq k \leq K$, there exists an onto and continuously differentiable map $\psi_k : [0, 1]^d \rightarrow \mathcal{M}_k$ each of which has the input dimension $d_k \in \mathbb{N}$. Then, $\mathcal{M}$ satisfies the Concentration Condition.

**Proof.** If $\mathcal{M}_k \subset [0, 1]^D$ satisfy the Concentration Condition, it is easily shown that $\bigcup_{k=1}^K \mathcal{M}_k$ satisfies the Concentration Condition. So the problem is reduced to showing that for any $k \in \{1, \ldots, K\}$, $\mathcal{M}_k$ satisfies the Concentration Condition.

Fix any $k \in \{1, \ldots, K\}$. For simplicity, we omit the subscript $k$ from $\psi_k, d_k$ and $\mathcal{M}_k$. Write $\psi = (\psi_1, \ldots, \psi_D)$. Define $L_i := \max_{x \in [0, 1]^D} \sqrt{\sum_{j=1}^d |\partial \psi_j(x)/\partial x_j|^2}$. Applying the mean-value theorem to $\psi_i$ along with Cauchy-Schwartz inequality yields $|\psi_i(x) - \psi_i(y)| \leq L_i \|x - y\|_2$ for any $x, y \in [0, 1]^d$. By the Lipschitz continuity of $\psi = (\psi_1, \ldots, \psi_D)$, for any $z, w \in [0, 1]^d$, $\|\psi(x) - \psi(y)\|_{\max} \leq \sqrt{DL} \|x - y\|_{\max}$ where $L := \max_i L_i$.

Note that $[0, 1]^d$ satisfies Concentration Condition, since for any $\delta > 0$, the $\delta$-cover $\{B^D_{\max}(x, \delta)\}_{i=1}^T$ constructed by expanding the minimal $\delta/2$-cover $\{B^D_{\max}(x, \delta/2)\}_{i=1}^T$ to radius $\delta$ always satisfy the property of the condition with $U = 1$.

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Fix any $\epsilon > 0$. Since $[0,1]^d$ satisfies Concentration condition, we can take an $\epsilon/(\sqrt{DL})$-cover \( \{B_{\max}^d(x_i, \epsilon/(\sqrt{DL}))\}_{i=1}^N \) of $[0,1]^d$ such that for any $x \in 2^{\{x_1,\ldots,x_T\}} \setminus \{\emptyset, \{x_1,\ldots,x_T\}\}$, there exists some $y \in \{x_1,\ldots,x_T\} \setminus X$ such that $\min_{x \in X} \|x - y\|_{\max} \leq \epsilon/(\sqrt{DL})$. Let $C := \{B_{\max}^D(\psi(x_1), \epsilon), \ldots, B_{\max}^D(\psi(x_T), \epsilon)\}$. We first verify that $C$ is an $\epsilon$-cover of $\mathcal{M}$. Since $\psi$ is onto, for any $z \in \mathcal{M}$, there exists some $x \in [0,1]^d$ such that $z = \psi(x)$. For this $x$, some $y \in \{x_1,\ldots,x_T\}$ satisfies $\|x - y\|_{\max} \leq \epsilon/(\sqrt{DL})$. Thus

$$\|z - \psi(y)\|_{\max} = \|\psi(x) - \psi(y)\|_{\max} \leq \sqrt{DL} \|x - y\|_{\max} \leq \sqrt{DL} \frac{\epsilon}{\sqrt{DL}} = \frac{\epsilon}{2}.$$ 

This verifys that $C$ is an $\epsilon/2$-cover of $\mathcal{M}$ and thus an $\epsilon$-cover of $\mathcal{M}$.

Take any $X' \in 2^{\{\psi(x_1),\ldots,\psi(x_T)\}} \setminus \{\emptyset, \{\psi(x_1),\ldots,\psi(x_T)\}\}$. Write $X' = \{\psi(x_{j_1}), \ldots, \psi(x_{j_k})\}$. By assumption, there exists some $y \in \{x_1,\ldots,x_T\} \setminus \psi^{-1}(X')$ such that $\min_{x \in \psi^{-1}(X')} \|x - y\|_{\max} \leq \epsilon/(\sqrt{DL})$ holds. Hence, for this $y$,

$$\min_{\psi(x) \in X'} \|\psi(x) - \psi(y)\|_{\max} \leq \sqrt{DL} \min_{x \in \psi^{-1}(X')} \|x - y\|_{\max} \leq \sqrt{DL} \frac{\epsilon}{\sqrt{DL}} = \epsilon.$$ 

This concludes the proof.

**Lemma B.12** (Minimax optimal rate under Concentration Condition). Let $\mu$ be a probability measure on $[0,1]^D$. Assume $N(\epsilon, \text{Supp} \mu, ||\cdot||_{\max}) = \Theta(\epsilon^{-d})$ for some $d > 0$. Also assume that $\text{Supp} \mu$ satisfy the Concentration Condition. Then,

$$\inf_{f} \sup_{f_0 \in \mathcal{F}} \left\| \tilde{f} - f_0 \right\|_{L^2(\mu)} = \Theta(\epsilon^{-\beta/(2\beta+d)}).$$

Note that if $\mu$ satisfies $N(\epsilon, \text{Supp} \mu, ||\cdot||_{\max}) = \Theta(\epsilon^{-d})$, then $\mu$ is a probability measure with $\dim \mu = d$. From Lemma A.1, any compact $d$-dimensional manifold is included in the set of measures with Minkowski dimension greater or equal to $d$. Also from the proof of Lemma A.1, for compact $d$-dimensional manifold, it holds that $N(\epsilon, \text{Supp} \mu, ||\cdot||_{\max}) = O(\epsilon^{-d})$. Thus we obtain the following corollary as an immediate consequence of Lemma B.11.

**Corollary B.12.1** (Minimax Optimal rate for compact smooth manifolds). Let $\mu$ be a probability measure on $[0,1]^D$ with $\dim \text{Supp} \mu \geq d$. Assume $N(\epsilon, \text{Supp} \mu, ||\cdot||_{\max}) = \Omega(\epsilon^{-d})$. Then,

$$\inf_{f} \sup_{f_0 \in \mathcal{F}} \left\| \tilde{f} - f_0 \right\|_{L^2(\mu)} = \Omega(\epsilon^{-\beta/(2\beta+d)}).$$

Finally, we prove Lemma B.12.

**Proof.** In order to utilize Lemma B.10, we here aim to evaluate the covering entropy of $\mathcal{H}^{\beta,D,M}$. For the lower bound of $N(\epsilon, \mathcal{H}^{\beta,D,M}, ||\cdot||_{L^2(\mu)})$, we basically follow [123]. We first
construct a packing \( \{ f_\gamma \mid \gamma \in \{-1, 1\}^S \} \) for some \( S \in \mathbb{N} \). Define
\[
\phi(y) := \begin{cases} 
  e^{2\beta D} \prod_{j=1}^{D} (1/2 - y_j)^\beta (1/2 + y_j)^\beta & \text{if } y \in [-1/2, 1/2]^D \\
  0 & \text{if } y \not\in [-1/2, 1/2]^D 
\end{cases}
\]
where \( c = c(\beta, D, M) \) is chosen small enough so that \( \phi \in \mathcal{H}^{\beta, D, M} \).

For any \( \epsilon > 0 \), set \( \delta = (\epsilon/2c)^{1/\beta} \). Consider \( \delta/2 \)-packing of \( \text{Supp} \mu \) as \( \{ x_i \}_{i=1}^S \subset \text{Supp} \mu \).

Recall that \( \mathcal{N}(\delta, \text{Supp} \mu, \|\cdot\|_{\text{max}}) \leq S \leq \mathcal{N}(\delta/2, \text{Supp} \mu, \|\cdot\|_{\text{max}}) \).

For each \( \gamma \in \{-1, 1\}^S \), define
\[
f_\gamma(x) = \sum_{i=1}^{S} \gamma_i \delta^\beta \phi \left( \frac{x - x_i}{\delta} \right)
\]
If \( \gamma \neq \gamma' \), then for \( x \in (x_{i1} - \delta/2, x_{i1} + \delta/2) \times \cdots \times (x_{iD} - \delta/2, x_{iD} + \delta/2) \),
\[
|f_\gamma(x) - f_{\gamma'}(x)| = 2\delta^\beta \phi \left( \frac{x - x_i}{\delta} \right).
\]
Setting \( x \leftarrow x_i \) yields
\[
|f_\gamma(x) - f_{\gamma'}(x)| = 2\delta^\beta c = \epsilon
\]
So \( \{ f_\gamma \mid \gamma \in \{-1, 1\}^S \} \) is an \( \epsilon \)-packing of \( \mathcal{H}^{\beta, D, M} \) and thus,
\[
\log \mathcal{N}(\epsilon, \mathcal{H}^{\beta, D, M}, \|\cdot\|_{L^\infty(\mu)}) \geq \log 2^S \geq \mathcal{N}(2(\epsilon/2c)^{1/\beta}, [0, 1]^D, \|\cdot\|_{\text{max}}) \log 2 \geq \epsilon^{-d/\beta},
\]
where the last inequality follows from the assumption \( \mathcal{N}(\epsilon, \text{Supp} \mu, \|\cdot\|_{\text{max}}) = \Theta(\epsilon^{-d}) \).

For the upper bound of \( \mathcal{N}(\epsilon, \mathcal{H}^{\beta, D, M}, \|\cdot\|_{L^\infty(\mu)}) \). We modify the Theorem 2.7.1 in [42].

Take the minimal \( \delta \)-cover \( \{ x_i \}_{i=1}^T \subset \text{Supp} \mu \), where \( T = \mathcal{N}(\delta, \text{Supp} \mu, \|\cdot\|_{\text{max}}) \). Note that by assumption \( T = \Theta(\delta^{-d}) \). For a multi-index \( k = (k_1, \ldots, k_D) \) with \( k \leq \beta \), define the operators \( A_k, B_k \) by
\[
A_k f := ([D^k f(x_1)/\delta^\beta - |k|], \ldots, [D^k f(x_T)/\delta^\beta - |k|]),
\]
\[
B_k f := \delta^\beta - |k| A_k f.
\]
If \( A_k f = A_k g \) for all \( k \) with \( |k| \leq \beta \), then \( \| f - g \|_{L^\infty(\mu)} \lesssim \epsilon \).

Define
\[
Af := \begin{pmatrix}
A_{0,0}, \ldots, 0f \\
A_{1,0}, \ldots, 0f \\
A_{0,1}, \ldots, 0f \\
\vdots \\
A_{0,0}, \ldots, \beta f
\end{pmatrix} \in \mathbb{R}^{r \times T}.
\]

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Note that we can bound the number of row $r$ of $Af$ as $r \leq \binom{D}{0} + \binom{D}{1} + \cdots + \binom{D}{\beta} \leq (\beta + 1)^D$. Since $|D^k f(x)| \leq M$ for all $x \in [0, 1]^D$, each element in $A_k f$ takes at most $2M/\delta^{\beta - |k|} + 1 \leq 2M\delta^{-\beta} + 1$ values.

Suppose $\|x_i - x'_i\|_{\max} \leq \delta$ for some $i, i'$. Since $D^k f(x_i) = \sum_{|k| + |l| \leq \beta} B_{k+l} f(x_i') \frac{(x_i - x'_i)^l}{l!} + R$ with $|R| \leq \|x_i - x'_i\|_{\max}^{\beta - |k|}$.

$$\left| D^k f(x_i) - \sum_{|k| + |l| \leq \beta} B_{k+l} f(x_i') \frac{(x_i - x'_i)^l}{l!} \right| \leq \sum_{|k| + |l| \leq \beta} \left| D^k f(x_i) - B_{k+l} f(x_i') \right| \frac{(x_i - x'_i)^l}{l!} + \delta^{\beta - |k|}$$

$$\leq \sum_{|k| + |l| \leq \beta} \delta^{\beta - |k| - |l|} \frac{\delta^{|l|}}{l!} + \delta^{\beta - |k|} \lesssim \delta^{\beta - |k|}.$$

Given the $i'$-th column, $i$-th column ranges over $\Theta(\delta^{\beta - |k|} / \delta^{\beta - |k|}) = \Theta(1)$.

By assumption, $\text{Supp } \mu$ satisfy the Concentration Condition. Thus there exist disjoint sets $X_1, \ldots, X_U$ such that $X := \{x_1, \ldots, x_T\} = \bigcup_{u=1}^U X_u$ and that $X_u = \{x_1, \ldots, x_{T_u}\}$ with $\|x_{i+1} - x_i\|_{\max} \leq \delta$ for any $i = 1, \ldots, T_u - 1$. Thus

$$\text{card } \{Af \mid f \in \mathcal{H}^{\beta, D, M} \} \leq (2M\delta^{-\beta} + 1)^U(\beta + 1)^D C^{T-U},$$

for some constant $C > 0$. Substitute $\delta \leftarrow \epsilon^{1/\beta}$, we obtain

$$\log(\text{card } \{Af \mid f \in \mathcal{H}^{\beta, D, M} \}) \lesssim \max \left\{ U \log \left( \frac{1}{\epsilon} \right), T - U \right\}.$$ 

Since $U \log(1/\epsilon) = \mathcal{O}(T)$,

$$\log \mathcal{N}(\epsilon, \mathcal{H}^{\beta, D, M}, \| \cdot \|_{L^{\infty}(\mu)}) \lesssim \epsilon^{-d/\beta}.$$

Since it is shown that $\log \mathcal{N}(\epsilon, \mathcal{H}^{\beta, D, M}, \| \cdot \|_{L^{\infty}(\mu)}) = \Theta(\epsilon^{-d/\beta})$, applying Lemma B.10 yields the conclusion that

$$\inf_{f_0} \sup_{f} \| \hat{f} - f_0 \|_{L^2(\mu)} = \Theta \left( n^{-\beta/(2\beta + d)} \right).$$

\[\square\]
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