

Deep Network Approximation for Smooth Functions

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Abstract

This paper establishes the optimal approximation error characterization of deep rectified linear unit (ReLU) networks for smooth functions in terms of both width and depth simultaneously. To that end, we first prove that multivariate polynomials can be approximated by deep ReLU networks of width $\mathcal{O}(N)$ and depth $\mathcal{O}(L)$ with an approximation error $\mathcal{O}(N^{-L})$. Through local Taylor expansions and their deep ReLU network approximations, we show that deep ReLU networks of width $\mathcal{O}(N \ln N)$ and depth $\mathcal{O}(L \ln L)$ can approximate $f \in C^s([0, 1]^d)$ with a nearly optimal approximation error $\mathcal{O}(\|f\|_{C^s([0, 1]^d)} N^{-2s/d} L^{-2s/d})$. Our estimate is non-asymptotic in the sense that it is valid for arbitrary width and depth specified by $N \in \mathbb{N}^+$ and $L \in \mathbb{N}^+$, respectively.

Key words. Deep ReLU Network, Smooth Function, Polynomial Approximation, Function Composition, Curse of Dimensionality.

1 Introduction

Deep neural networks have made significant impacts in many fields of computer science and engineering, especially for large-scale and high-dimensional learning problems. Well-designed neural network architectures, efficient training algorithms, and high-performance computing technologies have made neural-network-based methods very successful in real applications. Especially in supervised learning; e.g., image classification and objective detection, the great advantages of neural-network-based methods over traditional learning methods have been demonstrated. Understanding the approximation capacity of deep neural networks has become a key question for revealing the power of deep learning. A large number of experiments in real applications have shown the large capacity of deep network approximation from many empirical points of view, motivating much effort in establishing the theoretical foundation of deep network approximation. One of the fundamental problems is the characterization of the optimal approximation error of deep neural networks of arbitrary depth and width.

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1.1 Main result

Previously, the quantitative characterization of the approximation power of deep feed-forward neural networks (FNNs) with rectified linear unit (ReLU) activation functions was provided in [41]. For ReLU FNNs with width $\mathcal{O}(N)$ and depth $\mathcal{O}(L)$, the deep network approximation of $f \in C([0, 1]^d)$ admits an approximation error $\mathcal{O}(\omega_f(N^{-2/d}L^{-2/d}))$ in the L^p -norm for any $p \in [1, \infty]$, where $\omega_f(\cdot)$ is the modulus of continuity of f . In particular, for the class of Hölder continuous functions, the approximation error is nearly optimal.^① The next question is whether the smoothness of functions can improve the approximation error. In this paper, we investigate the deep network approximation of smaller function space, such as the smooth function space $C^s([0, 1]^d)$.

In Theorem 1.1 below, we prove by construction that ReLU FNNs with width $\mathcal{O}(N \ln N)$ and depth $\mathcal{O}(L \ln L)$ can approximate $f \in C^s([0, 1]^d)$ with a nearly optimal approximation error $\mathcal{O}(\|f\|_{C^s([0, 1]^d)} N^{-2s/d} L^{-2s/d})$, where the norm $\|\cdot\|_{C^s([0, 1]^d)}$ is defined as

$$\|f\|_{C^s([0, 1]^d)} := \max \{ \|\partial^\alpha f\|_{L^\infty([0, 1]^d)} : \|\alpha\|_1 \leq s, \alpha \in \mathbb{N}^d \} \quad \text{for any } f \in C^s([0, 1]^d).$$

Theorem 1.1. *Given a smooth function $f \in C^s([0, 1]^d)$ with $s \in \mathbb{N}^+$, for any $N, L \in \mathbb{N}^+$, there exists a function ϕ implemented by a ReLU FNN with width $C_1(N + 2) \log_2(8N)$ and depth $C_2(L + 2) \log_2(4L) + 2d$ such that*

$$\|\phi - f\|_{L^\infty([0, 1]^d)} \leq C_3 \|f\|_{C^s([0, 1]^d)} N^{-2s/d} L^{-2s/d},$$

where $C_1 = 17s^{d+1}3^d$, $C_2 = 18s^2$, and $C_3 = 85(s + 1)^d 8^s$.

As we can see from Theorem 1.1, the smoothness improves the approximation error in N and L ; e.g., $s \geq d$ implies $N^{-2s/d} L^{-2s/d} \leq N^{-2} L^{-2}$. However, we would like to remark that the improved approximation error is at the price of a prefactor much larger than d^d if $s \geq d$. The proof of Theorem 1.1 will be presented in Section 2.2 and its tightness will be discussed in Section 2.3. In fact, the logarithmic terms in width and depth in Theorem 1.1 can be further reduced if the approximation error is weakened. Given any $\tilde{N}, \tilde{L} \in \mathbb{N}^+$ with

$$\tilde{N} \geq C_1(1 + 2) \log_2(8) = 17s^{d+1}3^{d+2}d \quad \text{and} \quad \tilde{L} \geq C_2(1 + 2) \log_2(4) + 2d = 108s^2 + 2d,$$

there exist $N, L \in \mathbb{N}^+$ such that

$$C_1(N + 2) \log_2(8N) \leq \tilde{N} < C_1((N + 1) + 2) \log_2(8(N + 1))$$

and

$$C_2(L + 2) \log_2(4L) + 2d \leq \tilde{L} < C_2((L + 1) + 2) \log_2(4(L + 1)) + 2d.$$

It follows that

$$N \geq \frac{N + 3}{4} > \frac{\tilde{N}}{4C_1 \log_2(8N + 8)} \geq \frac{\tilde{N}}{4C_1 \log_2(8\tilde{N} + 8)} = \frac{\tilde{N}}{68s^{d+1}3^d d \log_2(8\tilde{N} + 8)}$$

and

$$L \geq \frac{L + 3}{4} > \frac{\tilde{L} - 2d}{4C_2 \log_2(4L + 4)} \geq \frac{\tilde{L} - 2d}{4C_2 \log_2(4\tilde{L} + 4)} = \frac{\tilde{L} - 2d}{72s^2 \log_2(4\tilde{L} + 4)}.$$

Thus, we have an immediate corollary.

^①“nearly optimal” up to a logarithmic factor.

67 **Corollary 1.2.** *Given a function $f \in C^s([0, 1]^d)$ with $s \in \mathbb{N}^+$, for any $\tilde{N}, \tilde{L} \in \mathbb{N}^+$, there*
 68 *exists a function ϕ implemented by a ReLU FNN with width \tilde{N} and depth \tilde{L} such that*

$$69 \quad \|\phi - f\|_{L^\infty([0,1]^d)} \leq \tilde{C}_1 \|f\|_{C^s([0,1]^d)} \left(\frac{\tilde{N}}{\tilde{C}_2 \log_2(8\tilde{N}+8)} \right)^{-2s/d} \left(\frac{\tilde{L}-2d}{\tilde{C}_3 \log_2(4\tilde{L}+4)} \right)^{-2s/d}$$

70 *for any $\tilde{N} \geq 17s^{d+1}3^{d+2}d$ and $\tilde{L} \geq 108s^2 + 2d$, where $\tilde{C}_1 = 85(s+1)^d 8^s$, $\tilde{C}_2 = 68s^{d+1}3^d$, and*
 71 *$\tilde{C}_3 = 72s^2$.*

72 Theorem 1.1 and Corollary 1.2 characterize the approximation error in terms of
 73 total number of neurons (with an arbitrary distribution in width and depth) and the
 74 smoothness of the target function to be approximated. The only result in this direction
 75 we are aware of in the literature is Theorem 4.1 of [46]. It shows that ReLU FNNs with
 76 width $2d + 10$ and depth L achieve a nearly optimal error $\mathcal{O}((\frac{L}{\ln L})^{-2s/d})$ for sufficiently
 77 large L when approximating functions in the unit ball of $C^s([0, 1]^d)$. This result is
 78 essentially a special case of Corollary 1.2 by setting $\tilde{N} = \mathcal{O}(1)$ and \tilde{L} sufficiently large.

79 1.2 Contributions and related work

80 Our key contributions can be summarized as follows.

81 (i) **Upper bound:** We provide a **quantitative** and **non-asymptotic** approximation
 82 error $\mathcal{O}(\|f\|_{C^s([0,1]^d)} N^{-2s/d} L^{-2s/d})$ when the ReLU FNN has width $\mathcal{O}(N \ln N)$ and
 83 depth $\mathcal{O}(L \ln L)$ for functions in $C^s([0, 1]^d)$ in Theorem 1.1. In real applications,
 84 the first question is to decide the network width and depth since they are two
 85 required hyper-parameters. The approximation error as a function of width and
 86 depth in this paper can directly answer this question, while the approximation
 87 results in terms of the total number of parameters in the literature cannot, because
 88 there are many architectures sharing the same number of parameters. Actually, an
 89 immediate corollary of our theorem as we shall discuss can also describe our theory
 90 in terms of the total number of parameters. Furthermore, our results contain
 91 approximation error estimates for both wide networks with fixed finite depth and
 92 deep networks with fixed finite width.

93 (ii) **Lower bound:** Through the Vapnik-Chervonenkis (VC) dimension upper bound
 94 of ReLU FNNs in [22], we prove a lower bound

$$95 \quad C(N^2 L^2 (\ln N)^3 (\ln L)^3)^{-s/d} \quad \text{for some positive constant } C$$

96 for the approximation error of the functions in the unit ball of $C^s([0, 1]^d)$ approx-
 97 imated by ReLU FNNs with width $\mathcal{O}(N \ln N)$ and depth $\mathcal{O}(L \ln L)$ in Section 2.3.
 98 Thus, the approximation error $\mathcal{O}(N^{-2s/d} L^{-2s/d})$ in Theorem 1.1 is nearly optimal
 99 for the unit ball of $C^s([0, 1]^d)$.

100 (iii) **Approximation of polynomials:** It is proved by construction in Proposition 4.1
 101 that ReLU FNNs with width $\mathcal{O}(N)$ and depth $\mathcal{O}(L)$ can approximate polynomials
 102 on $[0, 1]^d$ with an approximation error $\mathcal{O}(N^{-L})$. This is a non-trivial extension of
 103 the result $\mathcal{O}(2^{-L})$ for polynomial approximation by fixed-width ReLU FNNs with
 104 depth L in [44].

(iv) **Uniform approximation:** The approximation error in this paper is measured in the $L^\infty([0,1]^d)$ -norm as a result of Theorem 2.1. To achieve this, given a ReLU FNN approximating the target function f uniformly well on $[0,1]^d$ except for a small region, we develop a technique to construct a new ReLU FNN with a similar size to approximate f **uniformly** well on $[0,1]^d$ in Theorem 2.1. This technique can be applied to improve approximation errors from the L^p -norm to the L^∞ -norm for other function spaces in general, e.g., the continuous function space in [41], which is of independent interest.

In particular, if we denote the best approximation error of functions in $C_u^s([0,1]^d)$ approximated by ReLU FNNs with width \tilde{N} and depth \tilde{L} as

$$\varepsilon_{s,d}(\tilde{N}, \tilde{L}) := \sup_{f \in C_u^s([0,1]^d)} \left(\inf_{\phi \in \mathcal{NN}(\text{width} \leq \tilde{N}; \text{depth} \leq \tilde{L})} \|\phi - f\|_{L^\infty([0,1]^d)} \right) \quad \text{for any } \tilde{N}, \tilde{L} \in \mathbb{N}^+,$$

where $C_u^s([0,1]^d)$ denotes the unit ball of $C^s([0,1]^d)$ defined by

$$C_u^s([0,1]^d) := \{f \in C^s([0,1]^d) : \|\partial^\alpha f\|_{L^\infty([0,1]^d)} \leq 1, \text{ for all } \alpha \in \mathbb{N}^d \text{ with } \|\alpha\|_1 \leq s\}.$$

By combining the upper and lower bounds stated above, we have

$$\underbrace{C_1(s, d) \cdot \left(\tilde{N}^2 \tilde{L}^2 \ln(\tilde{N} \tilde{L}) \right)^{-s/d}}_{\text{proved in Section 2.3}} \leq \varepsilon_{s,d}(\tilde{N}, \tilde{L}) \leq \underbrace{C_2(s, d) \cdot \left(\frac{\tilde{N}^2 \tilde{L}^2}{(\ln \tilde{N} \ln \tilde{L})^2} \right)^{-s/d}}_{\text{shown in Corollary 1.2}},$$

where $C_1(s, d)$ and $C_2(s, d)$ are two positive constants in s and d , and $C_2(s, d)$ can be **explicitly** represented by s and d .

The expressiveness of deep neural networks has been studied extensively from many perspectives, e.g., in terms of combinatorics [34], topology [8], VC-dimension [7, 22, 39], fat-shattering dimension [2, 27], information theory [37], and classical approximation theory [4, 5, 9, 12, 14, 15, 20, 21, 24, 29, 32, 35, 42–45, 47]. In the early works of approximation theory for neural networks, the universal approximation theorem [15, 23, 24] without approximation errors showed that, given any $\varepsilon > 0$, there exists a sufficiently large neural network approximating a target function in a certain function space within an error ε . For one-hidden-layer neural networks and functions with integral representations, Barron [5, 6] showed an asymptotic approximation error $\mathcal{O}(\frac{1}{\sqrt{N}})$ in the L^2 -norm, leveraging an idea that is similar to Monte Carlo sampling for high-dimensional integrals. For very deep ReLU neural networks with width fixed as $\mathcal{O}(d)$ and depth $\mathcal{O}(L)$, Yarotsky [45, 46] showed that the nearly optimal approximation errors for Lipschitz continuous functions and functions in the unit ball of $C^s([0,1]^d)$ are $\mathcal{O}(L^{-2/d})$ and $\mathcal{O}((L/\ln L)^{-2s/d})$, respectively. Note that the results are asymptotic in the sense that L is required to be sufficiently large and the prefactors of these rates are unknown. To obtain a generic result that characterizes the approximation error for arbitrary width and depth with known prefactors to guide applications, the authors of [41] demonstrated that the nearly optimal approximation error for ReLU FNNs with width $\mathcal{O}(N)$ and depth $\mathcal{O}(L)$ to approximate Lipschitz continuous functions on $[0,1]^d$ is $\mathcal{O}(N^{-2/d} L^{-2/d})$. Such a nearly optimal error is further improved to an optimal one, $\mathcal{O}((N^2 L^2 \ln N)^{-1/d})$, in a more recent paper [42]. In this paper, we extend this generic framework to $C^s([0,1]^d)$ with a nearly optimal approximation error $\mathcal{O}(\|f\|_{C^s([0,1]^d)} N^{-2s/d} L^{-2s/d})$.

Most related works are summarized in Table 1 for the comparison of our contributions in this paper and the results in the literature.

Table 1: A summary of existing approximation errors of ReLU FNNs for $\text{Lip}([0, 1]^d)$ (the Lipschitz continuous function space) and $C_u^s([0, 1]^d)$ (the unit ball of $C^s([0, 1]^d)$).

paper	function class	width	depth	approximation error	$L^p([0, 1]^d)$ -norm	tightness	valid for
[44]	polynomial	$\mathcal{O}(1)$	$\mathcal{O}(L)$	$\mathcal{O}(2^{-L})$	$p = \infty$		any $L \in \mathbb{N}^+$
this paper	polynomial	$\mathcal{O}(N)$	$\mathcal{O}(L)$	$\mathcal{O}(N^{-L})$	$p = \infty$		any $N, L \in \mathbb{N}^+$
[40]	$\text{Lip}([0, 1]^d)$	$\mathcal{O}(N)$	3	$\mathcal{O}(N^{-2/d})$	$p \in [1, \infty)$	nearly tight in N	any $N \in \mathbb{N}^+$
[45]	$\text{Lip}([0, 1]^d)$	$2d + 10$	$\mathcal{O}(L)$	$\mathcal{O}(L^{-2/d})$	$p = \infty$	nearly tight in L	large $L \in \mathbb{N}^+$
[41]	$\text{Lip}([0, 1]^d)$	$\mathcal{O}(N)$	$\mathcal{O}(L)$	$\mathcal{O}(N^{-2/d} L^{-2/d})$	$p \in [1, \infty]$	nearly tight in N and L	any $N, L \in \mathbb{N}^+$
[42]	$\text{Lip}([0, 1]^d)$	$\mathcal{O}(N)$	$\mathcal{O}(L)$	$\mathcal{O}((N^2 L^2 \ln N)^{-1/d})$	$p \in [1, \infty]$	tight in N and L	any $N, L \in \mathbb{N}^+$
[46]	$C_u^s([0, 1]^d)$	$2d + 10$	$\mathcal{O}(L)$	$\mathcal{O}((L/\ln L)^{-2s/d})$	$p = \infty$	neatly tight in L	large $L \in \mathbb{N}^+$
this paper	$C_u^s([0, 1]^d)$	$\mathcal{O}(N \ln N)$	$\mathcal{O}(L \ln L)$	$\mathcal{O}(N^{-2s/d} L^{-2s/d})$	$p = \infty$	nearly tight in N and L	any $N, L \in \mathbb{N}^+$
this paper	$C_u^s([0, 1]^d)$	$\mathcal{O}(N)$	$\mathcal{O}(L)$	$\mathcal{O}((N/\ln N)^{-2s/d} (L/\ln L)^{-2s/d})$	$p = \infty$	nearly tight in N and L	any $N, L \in \mathbb{N}^+$

1.3 Discussion

We will discuss the comparison of our theory with existing works and the application scope in machine learning.

Approximation errors in $\mathcal{O}(N)$ and $\mathcal{O}(L)$ versus $\mathcal{O}(W)$

It is fundamental and indispensable to characterize deep network approximation in terms of width $\mathcal{O}(N)$ ^② and depth $\mathcal{O}(L)$ simultaneously in realistic applications, while the approximation in terms of the number of nonzero parameters W is probably only of interest in theory. First, networks used in practice are specified via width and depth and, therefore, Theorem 1.1 can provide an error bound for such networks. However, existing results in W cannot serve this purpose because they may be only valid for networks with other widths and depths. Theories in terms of W essentially have a single variable to control the network size in three types of structures: 1) a fixed width N and a varying depth L ; 2) a fixed depth L and a varying width N ; 3) both the width and depth are controlled by the target error ε (e.g., N is a polynomial of $\frac{1}{\varepsilon^d}$ and L is a polynomial of $\ln(\frac{1}{\varepsilon})$). Therefore, given a network with arbitrary width N and depth L , there might not be a known theory in terms of W to quantify the performance of this structure. Second, the error characterization in terms of N and L is more useful than that in terms of W , because most existing optimization and generalization analyses are based on N and L [1, 3, 10, 13, 17, 18, 25, 26], to the best of our knowledge. Approximation results in terms of N and L are more consistent with optimization and generalization analysis tools to obtain a full error analysis.

Most existing approximation theories for deep neural networks so far focus on the approximation error in the number of parameters W [4, 5, 9, 11, 12, 14, 15, 19–21, 24, 29–33, 35–38, 43–47]. Controlling two variables N and L in our theory is more challenging than controlling one variable W in the literature. The characterization of deep network approximation in terms of N and L can imply an approximation error in terms of W , while this may not be true the other way around, e.g., our theorems cannot be derived from results in [46]. Let us discuss the first type of structure mentioned in the previous paragraph, which includes the best-known result for a nearly optimal approximation error, $\mathcal{O}((W/\ln W)^{-2s/d})$, for functions in the unit ball of $C^s([0, 1]^d)$ using ReLU FNNs with W parameters [46]. As an example to show how Theorem 1.1 in terms of N and

^②For simplicity, we omit $\mathcal{O}(\cdot)$ in the following discussion.

177 L can be applied to show a similar result in terms of W . The main idea is to specify
 178 the value of N and L in Theorem 1.1 to show the desired corollary. For example, if we
 179 let $N = \mathcal{O}(1)$ in Theorem 1.1, then we have the following corollary, which is essentially
 180 equivalent to Theorem 4.1 of [46].

181 **Corollary 1.3.** *Given any function f in the unit ball of $C^s([0,1]^d)$ with $s \in \mathbb{N}^+$, there*
 182 *exists a function ϕ implemented by a ReLU FNN with W parameters such that*

$$183 \quad \|\phi - f\|_{L^\infty([0,1]^d)} \leq \mathcal{O}\left(\left(\frac{W}{\ln W}\right)^{-2s/d}\right) \quad \text{for large } W \in \mathbb{N}^+.$$

184 As we can see in this example, it is simple to derive Corollary 1.3 above and The-
 185 orem 4.1 of [46] using Theorem 1.1 in this paper. However, Theorem 1.1 cannot be
 186 derived from any existing result that characterizes approximation errors in terms of the
 187 number of parameters. Therefore, Theorem 1.1 goes beyond existing results on the
 188 approximation of deep neural networks.

189 Note that the logarithmic term in the approximation error is not significant in the
 190 case of $s > 1$ since it can be cancelled out in the sense that $\left(\frac{W}{\ln W}\right)^{-2s/d} \lesssim W^{-2\tilde{s}/d}$ for
 191 any $\tilde{s} \in (1, s)$. We remark that Theorem 3.3 of [46] provides a better approximation
 192 error by a logarithmic term: ReLU FNNs with W nonzero parameters can approximate
 193 a function f in the unit ball of $C^s([0,1]^d)$ within an error $\mathcal{O}(W^{-2s/d})$. However, the
 194 network architecture therein is relatively complex and s -dependent as stated by the
 195 authors of [46]. In fact, it contains many s -dependent blocks (sub-networks), making
 196 it difficult to implement if s is not known in applications. In contrast, our network
 197 architecture in Corollary 1.2 is simple and can be pre-specified once the width \tilde{N} and
 198 depth \tilde{L} therein are given.

199 Continuity of the weight selection

200 We would like to discuss the continuity of the weight selection as a map $\Sigma : F_{s,d} \rightarrow$
 201 \mathbb{R}^W , where $F_{s,d}$ denotes the unit ball of the d -dimensional Sobolev space with smooth-
 202 ness s . For a fixed network architecture with a fixed number of parameters W , let
 203 $g : \mathbb{R}^W \rightarrow C([0,1]^d)$ be the map of realizing a ReLU FNN from a given set of param-
 204 eters in \mathbb{R}^W to a function in $C([0,1]^d)$. Suppose that the map Σ is continuous such
 205 that $\|f - g(\Sigma(f))\|_{L^\infty([0,1]^d)} \leq \varepsilon$ for all $f \in F_{s,d}$. Then $W \geq c\varepsilon^{-d/s}$ with some constant c
 206 depending only on s . This conclusion is given in Theorem 3 of [44], which is a corollary
 207 of Theorem 4.2 of [16] in a more general form. These theorems mean that the weight
 208 selection map Σ corresponding to our constructive proof in Theorem 1.1 in this paper is
 209 not continuous, since our error is better than $\mathcal{O}(W^{-s/d})$. Theorem 4.2 of [16] is essentially
 210 a min-max criterion to evaluate weight selection maps maintaining continuity: the ap-
 211 proximation error obtained by minimizing over all continuous selections Σ and network
 212 realizations g and maximizing over all target functions is bounded below by $\mathcal{O}(W^{-s/d})$.
 213 In the worst case, a continuous weight selection cannot enjoy an approximation error
 214 beating $\mathcal{O}(W^{-s/d})$. However, Theorem 4.2 of [16] does not exclude the possibility that
 215 most functions of interest in practice may still enjoy a continuous weight selection with
 216 the approximation error in Theorem 1.1. It would be interesting in future work to in-
 217 vestigate whether continuous weight selection is possible for many functions commonly
 218 encountered in real applications.

Application scope of our theory in machine learning

In deep learning, given a target function f , the final goal is to train a function $\phi(\mathbf{x}; \boldsymbol{\theta})$ approximating f well, where $\phi(\mathbf{x}; \boldsymbol{\theta})$ is a function in $\mathbf{x} \in \mathcal{X}$ realized by a network architecture parameterized with $\boldsymbol{\theta} \in \mathbb{R}^W$. To get the best solution, one needs to identify the expected risk minimizer

$$\boldsymbol{\theta}_{\mathcal{D}} := \arg \min_{\boldsymbol{\theta} \in \mathbb{R}^W} R_{\mathcal{D}}(\boldsymbol{\theta}), \quad \text{where } R_{\mathcal{D}}(\boldsymbol{\theta}) = \mathbb{E}_{\mathbf{x} \sim U(\mathcal{X})} [\ell(\phi(\mathbf{x}; \boldsymbol{\theta}), f(\mathbf{x}))]$$

with a loss function usually taken as $\ell(y, y') = \frac{1}{2}|y - y'|^2$ and an unknown data distribution $U(\mathcal{X})$.

In practice, only data samples $\{(\mathbf{x}_i, f(\mathbf{x}_i))\}_{i=1}^n$ instead of f and $U(\mathcal{X})$ are available. Thus, the empirical risk minimizer $\boldsymbol{\theta}_{\mathcal{S}}$ is used to model/approximate the expected risk minimizer $\boldsymbol{\theta}_{\mathcal{D}}$, where

$$\boldsymbol{\theta}_{\mathcal{S}} := \arg \min_{\boldsymbol{\theta} \in \mathbb{R}^W} R_{\mathcal{S}}(\boldsymbol{\theta}), \quad \text{where } R_{\mathcal{S}}(\boldsymbol{\theta}) := \frac{1}{n} \sum_{i=1}^n \ell(\phi(\mathbf{x}_i, \boldsymbol{\theta}), f(\mathbf{x}_i)). \quad (1.1)$$

In real applications, only a numerical solution (denoted as $\boldsymbol{\theta}_{\mathcal{N}}$) is achieved when a numerical optimization method is applied to solve (1.1). Hence, the actually learned function generated by the network is $\phi(\mathbf{x}; \boldsymbol{\theta}_{\mathcal{N}})$. Since $R_{\mathcal{D}}(\boldsymbol{\theta}_{\mathcal{N}})$ is the expected inference error over all possible data samples, it can quantify how good $\phi(\mathbf{x}; \boldsymbol{\theta}_{\mathcal{N}})$ is. Note that

$$\begin{aligned} R_{\mathcal{D}}(\boldsymbol{\theta}_{\mathcal{N}}) &= \underbrace{[R_{\mathcal{D}}(\boldsymbol{\theta}_{\mathcal{N}}) - R_{\mathcal{S}}(\boldsymbol{\theta}_{\mathcal{N}})]}_{\text{GE}} + \underbrace{[R_{\mathcal{S}}(\boldsymbol{\theta}_{\mathcal{N}}) - R_{\mathcal{S}}(\boldsymbol{\theta}_{\mathcal{S}})]}_{\text{OE}} + \underbrace{[R_{\mathcal{S}}(\boldsymbol{\theta}_{\mathcal{S}}) - R_{\mathcal{S}}(\boldsymbol{\theta}_{\mathcal{D}})]}_{\leq 0 \text{ by (1.1)}} + \underbrace{[R_{\mathcal{S}}(\boldsymbol{\theta}_{\mathcal{D}}) - R_{\mathcal{D}}(\boldsymbol{\theta}_{\mathcal{D}})]}_{\text{GE}} + \underbrace{R_{\mathcal{D}}(\boldsymbol{\theta}_{\mathcal{D}})}_{\text{AE}} \\ &\leq \underbrace{R_{\mathcal{D}}(\boldsymbol{\theta}_{\mathcal{D}})}_{\text{Approximation error (AE)}} + \underbrace{[R_{\mathcal{S}}(\boldsymbol{\theta}_{\mathcal{N}}) - R_{\mathcal{S}}(\boldsymbol{\theta}_{\mathcal{S}})]}_{\text{Optimization error (OE)}} + \underbrace{[R_{\mathcal{D}}(\boldsymbol{\theta}_{\mathcal{N}}) - R_{\mathcal{S}}(\boldsymbol{\theta}_{\mathcal{N}})] + [R_{\mathcal{S}}(\boldsymbol{\theta}_{\mathcal{D}}) - R_{\mathcal{D}}(\boldsymbol{\theta}_{\mathcal{D}})]}_{\text{Generalization error (GE)}}. \end{aligned} \quad (1.2)$$

Constructive approximation provides an upper bound of $R_{\mathcal{D}}(\boldsymbol{\theta}_{\mathcal{D}})$ in terms of the network size. For example, Theorem 1.1 and its corollaries provide an upper bound $\mathcal{O}(\|f\|_{C^s([0,1]^d)} N^{-2s/d} L^{-2s/d})$ of $R_{\mathcal{D}}(\boldsymbol{\theta}_{\mathcal{D}})$ for $C^s([0,1]^d)$. The second term of (1.2) is bounded by the optimization error of the numerical algorithm applied to solve the empirical loss minimization problem in (1.1). The study of the bounds for the third and fourth terms is referred to as the generalization error analysis of neural networks.

One of the key targets in the area of deep learning is to develop algorithms to reduce $R_{\mathcal{D}}(\boldsymbol{\theta}_{\mathcal{N}})$. Our analysis here provides an upper bound of the approximation error $R_{\mathcal{D}}(\boldsymbol{\theta}_{\mathcal{D}})$ for smooth functions, which is crucial to control $R_{\mathcal{D}}(\boldsymbol{\theta}_{\mathcal{N}})$. Instead of deriving an approximator to attain the error bound, deep learning algorithms aim to identify a solution $\phi(\mathbf{x}; \boldsymbol{\theta}_{\mathcal{N}})$ reducing the generalization and optimization errors in (1.2). Solutions minimizing both generalization and optimization errors will lead to a good solution only if we also have a good upper bound estimate of $R_{\mathcal{D}}(\boldsymbol{\theta}_{\mathcal{D}})$ as shown in (1.2). Independent of whether our analysis here leads to a good approximator, which is an interesting topic to pursue, the theory here does provide a key ingredient in the error analysis of deep learning algorithms.

We would like to emphasize that the introduction of the ReLU activation function to image classification is one of the key techniques that boost the performance of deep learning [28] with surprising generalization, which is the main reason that we focus on ReLU FNNs in this paper.

Organization: The rest of the present paper is organized as follows. In Section 2, we prove Theorem 1.1 by combining two theorems (Theorems 2.1 and 2.2) that will be proved later. We will also discuss the optimality of Theorem 1.1 in Section 2. Next, Theorem 2.1 will be proved in Section 3 while Theorem 2.2 will be shown in Section 4. Several propositions supporting Theorem 2.2 will be presented in Section 5. Finally, Section 6 concludes this paper with a short discussion.

2 Approximation of smooth functions

In this section, we will prove the quantitative approximation error in Theorem 1.1 by construction and discuss its tightness. Notation throughout the proof will be summarized in Section 2.1. The proof of Theorem 1.1 is mainly based on Theorems 2.1 and 2.2, which will be proved in Sections 3 and 4, respectively. To show the tightness of Theorem 1.1, we will introduce the VC-dimension in Section 2.3.

2.1 Notation

Now let us summarize the main notation of this paper as follows.

- Let \mathbb{R} , \mathbb{Q} , and \mathbb{Z} denote the set of real numbers, rational numbers, and integers, respectively.
- Let \mathbb{N} and \mathbb{N}^+ denote the set of natural numbers and positive natural numbers, respectively. That is, $\mathbb{N}^+ = \{1, 2, 3, \dots\}$ and $\mathbb{N} = \mathbb{N}^+ \cup \{0\}$.
- Vectors and matrices are denoted in a bold font. Standard vectorization is adopted in matrix and vector computation. For example, a scalar plus a vector means adding the scalar to each entry of the vector. Additionally, “[” and “]” are used to partition matrices (vectors) into blocks, e.g., $\mathbf{A} = \begin{bmatrix} \mathbf{A}_{11} & \mathbf{A}_{12} \\ \mathbf{A}_{21} & \mathbf{A}_{22} \end{bmatrix}$ and $\mathbf{v} = \begin{bmatrix} v_1 \\ \vdots \\ v_d \end{bmatrix} = [v_1, \dots, v_d]^T \in \mathbb{R}^d$.
- Let $\mathbf{1}_S$ be the characteristic (indicator) function on a set S ; i.e., $\mathbf{1}_S$ is equal to 1 on S and 0 outside S .
- Let $\mathcal{B}(\mathbf{x}, r) \subseteq \mathbb{R}^d$ be the closed ball with a center $\mathbf{x} \in \mathbb{R}^d$ and a radius $r \geq 0$.
- Similar to “min” and “max”, let $\text{mid}(x_1, x_2, x_3)$ be the middle value of three inputs x_1 , x_2 , and x_3 ^③. For example, $\text{mid}(2, 1, 3) = 2$ and $\text{mid}(3, 2, 3) = 3$.
- The set difference of two sets A and B is denoted by $A \setminus B := \{x : x \in A, x \notin B\}$.
- For a real number $p \in [1, \infty)$, the p -norm of $\mathbf{x} = [x_1, x_2, \dots, x_d]^T \in \mathbb{R}^d$ is defined by

$$\|\mathbf{x}\|_p := \left(|x_1|^p + |x_2|^p + \dots + |x_d|^p\right)^{1/p}.$$

^③ “mid” can be defined via $\text{mid}(x_1, x_2, x_3) = x_1 + x_2 + x_3 - \max(x_1, x_2, x_3) - \min(x_1, x_2, x_3)$, which can be implemented by a ReLU FNN.

- For any $x \in \mathbb{R}$, let $\lfloor x \rfloor := \max\{n : n \leq x, n \in \mathbb{Z}\}$ and $\lceil x \rceil := \min\{n : n \geq x, n \in \mathbb{Z}\}$.
- Assume $\mathbf{n} \in \mathbb{N}^d$; then $f(\mathbf{n}) = \mathcal{O}(g(\mathbf{n}))$ means that there exists positive C independent of \mathbf{n} , f , and g such that $f(\mathbf{n}) \leq Cg(\mathbf{n})$ when all entries of \mathbf{n} go to $+\infty$.
- The modulus of continuity of a continuous function $f \in C([0, 1]^d)$ is defined as

$$\omega_f(r) := \sup \{ |f(\mathbf{x}) - f(\mathbf{y})| : \|\mathbf{x} - \mathbf{y}\|_2 \leq r, \mathbf{x}, \mathbf{y} \in [0, 1]^d \} \quad \text{for any } r \geq 0.$$

- A d -dimensional multi-index is a d -tuple $\boldsymbol{\alpha} = [\alpha_1, \alpha_2, \dots, \alpha_d]^T \in \mathbb{N}^d$. Several related notation are listed below.

- $\|\boldsymbol{\alpha}\|_1 = |\alpha_1| + |\alpha_2| + \dots + |\alpha_d|$;
- $\mathbf{x}^{\boldsymbol{\alpha}} = x_1^{\alpha_1} x_2^{\alpha_2} \dots x_d^{\alpha_d}$, where $\mathbf{x} = [x_1, x_2, \dots, x_d]^T$;
- $\boldsymbol{\alpha}! = \alpha_1! \alpha_2! \dots \alpha_d!$;
- $\partial^{\boldsymbol{\alpha}} = \frac{\partial^{\alpha_1}}{\partial x_1^{\alpha_1}} \frac{\partial^{\alpha_2}}{\partial x_2^{\alpha_2}} \dots \frac{\partial^{\alpha_d}}{\partial x_d^{\alpha_d}}$.

- For any closed cube $Q \subseteq \mathbb{R}^d$ and a real number $r > 0$, let rQ denote the closed cube which shares the same center of Q and whose sidelength is the product of r and the sidelength of Q .

- Given any $K \in \mathbb{N}^+$ and $\delta \in (0, \frac{1}{K})$, define a trifling region $\Omega([0, 1]^d, K, \delta)$ of $[0, 1]^d$ as

$$\Omega([0, 1]^d, K, \delta) := \bigcup_{i=1}^d \left\{ \mathbf{x} = [x_1, x_2, \dots, x_d]^T \in [0, 1]^d : x_i \in \cup_{k=1}^{K-1} \left(\frac{k}{K} - \delta, \frac{k}{K} \right) \right\}. \quad (2.1)$$

In particular, $\Omega([0, 1]^d, K, \delta) = \emptyset$ if $K = 1$. See Figure 1 for two examples of the trifling region.

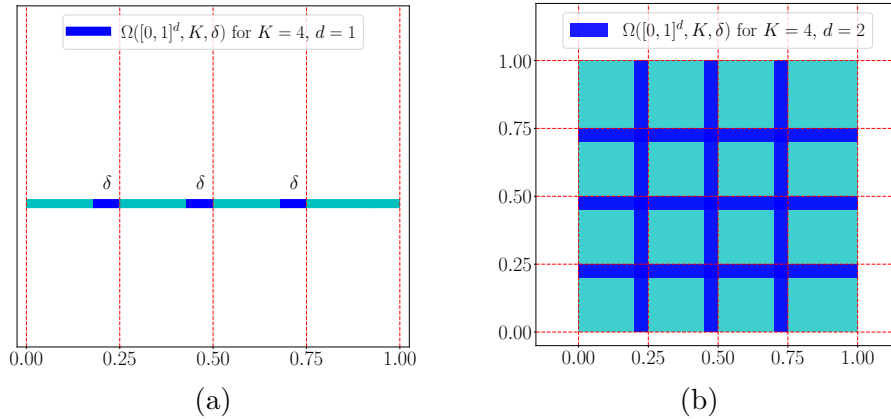


Figure 1: Two examples of the trifling region. (a) $K = 4, d = 1$. (b) $K = 4, d = 2$.

- Given $E \subseteq \mathbb{R}^d$, let $C^s(E)$ denote the set containing all functions, all k -th order partial derivatives of which exist and are continuous on E for any $k \in \mathbb{N}$ with $0 \leq k \leq s$. In particular, $C^0(E)$, also denoted by $C(E)$, is the set of continuous

functions on E . For the case $s = \infty$, $C^\infty(E) = \bigcap_{s=0}^\infty C^s(E)$. The C^s -norm is defined by

$$\|f\|_{C^s(E)} := \max \{ \|\partial^\alpha f\|_{L^\infty(E)} : \alpha \in \mathbb{N}^d \text{ with } \|\alpha\|_1 \leq s \}.$$

Generally, E is assigned as $[0, 1]^d$ in this paper. In particular, the closed unit ball of $C^s([0, 1]^d)$ is denoted by

$$C_u^s([0, 1]^d) := \{f \in C^s([0, 1]^d) : \|f\|_{C^s([0, 1]^d)} \leq 1\}.$$

- We use “ \mathcal{NN} ” to mean “functions implemented by ReLU FNNs” for short and use Python-type notation to specify a class of functions implemented by ReLU FNNs with several conditions. To be precise, we use $\mathcal{NN}(c_1; c_2; \dots; c_m)$ to denote the function set containing all functions implemented by ReLU FNN architectures satisfying m conditions given by $\{c_i\}_{1 \leq i \leq m}$, each of which may specify the number of inputs (#input), the number of outputs (#output), the total number of nodes in all hidden layers (#neuron), the number of hidden layers (depth), the number of total parameters (#parameter), and the width in each hidden layer (widthvec), the maximum width of all hidden layers (width), etc. For example, if $\phi \in \mathcal{NN}(\text{\#input} = 2; \text{widthvec} = [100, 100]; \text{\#output} = 1)$, then ϕ is a function satisfying the following conditions.

- ϕ maps from \mathbb{R}^2 to \mathbb{R} .

- ϕ is implemented by a ReLU FNN with two hidden layers and the number of nodes in each hidden layer being 100.

- Let $\sigma : \mathbb{R} \rightarrow \mathbb{R}$ denote the rectified linear unit (ReLU), i.e. $\sigma(x) = \max\{0, x\}$. With the abuse of notation, we define $\sigma : \mathbb{R}^d \rightarrow \mathbb{R}^d$ as $\sigma(\mathbf{x}) = \begin{bmatrix} \max\{0, x_1\} \\ \vdots \\ \max\{0, x_d\} \end{bmatrix}$ for any $\mathbf{x} = [x_1, \dots, x_d]^T \in \mathbb{R}^d$.
- For a function $\phi \in \mathcal{NN}(\text{\#input} = d; \text{widthvec} = [N_1, N_2, \dots, N_L]; \text{\#output} = 1)$, if we set $N_0 = d$ and $N_{L+1} = 1$, then the architecture of the network implementing ϕ can be briefly described as follows:

$$\mathbf{x} = \tilde{\mathbf{h}}_0 \xrightarrow{\mathbf{W}_0, \mathbf{b}_0} \mathbf{h}_1 \xrightarrow{\sigma} \tilde{\mathbf{h}}_1 \quad \dots \quad \xrightarrow{\mathbf{W}_{L-1}, \mathbf{b}_{L-1}} \mathbf{h}_L \xrightarrow{\sigma} \tilde{\mathbf{h}}_L \xrightarrow{\mathbf{W}_L, \mathbf{b}_L} \mathbf{h}_{L+1} = \phi(\mathbf{x}),$$

where $\mathbf{W}_i \in \mathbb{R}^{N_{i+1} \times N_i}$ and $\mathbf{b}_i \in \mathbb{R}^{N_{i+1}}$ are the weight matrix and the bias vector in the i -th affine linear transform \mathcal{L}_i in ϕ , respectively, i.e.,

$$\mathbf{h}_{i+1} = \mathbf{W}_i \cdot \tilde{\mathbf{h}}_i + \mathbf{b}_i =: \mathcal{L}_i(\tilde{\mathbf{h}}_i) \quad \text{for } i = 0, 1, \dots, L$$

and

$$\tilde{\mathbf{h}}_i = \sigma(\mathbf{h}_i) \quad \text{for } i = 1, 2, \dots, L.$$

In particular, ϕ can be represented in a form of function compositions as follows

$$\phi = \mathcal{L}_L \circ \sigma \circ \mathcal{L}_{L-1} \circ \sigma \circ \dots \circ \sigma \circ \mathcal{L}_1 \circ \sigma \circ \mathcal{L}_0,$$

which has been illustrated in Figure 2.

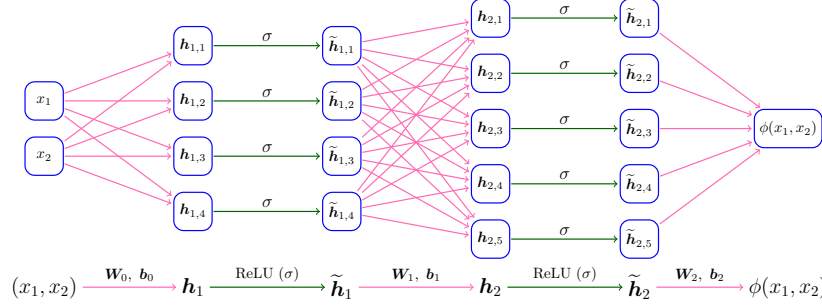


Figure 2: An example of a ReLU FNN with width 5 and depth 2.

- The expression “a network (architecture) with (of) width N and depth L ” means
 - The maximum width of this network (architecture) for all **hidden** layers is no more than N .
 - The number of **hidden** layers of this network (architecture) is no more than L .
- For any $\theta \in [0, 1)$, suppose its binary representation is $\theta = \sum_{\ell=1}^{\infty} \theta_{\ell} 2^{-\ell}$ with $\theta_{\ell} \in \{0, 1\}$. We introduce a special notation $\text{bin}0.\theta_1\theta_2\cdots\theta_L$ to denote the L -term binary representation of θ , i.e., $\text{bin}0.\theta_1\theta_2\cdots\theta_L := \sum_{\ell=1}^L \theta_{\ell} 2^{-\ell} \approx \theta$.

2.2 Proof of Theorem 1.1

The introduction of the trifling region $\Omega([0, 1]^d, K, \delta)$ is due to the fact that ReLU FNNs cannot approximate a step function uniformly well (as the ReLU activation function is continuous), which is also the reason for the main difficulty in obtaining approximation errors in the $L^{\infty}([0, 1]^d)$ -norm in our previous papers [40, 41]. The trifling region is a key technique to simplify the proofs of theories in [40, 41] as well as the proof of Theorem 1.1.

First, we present Theorem 2.1 to show that, as long as good uniform approximation by a ReLU FNN can be obtained outside the trifling region, the uniform approximation error can also be well controlled inside the trifling region when the network size is slightly increased. Second, as a simplified version of Theorem 1.1 ignoring the approximation error in the trifling region $\Omega([0, 1]^d, K, \delta)$, Theorem 2.2 shows the existence of a ReLU FNN approximating a target smooth function uniformly well outside the trifling region. Finally, Theorems 2.1 and 2.2 immediately lead to Theorem 1.1. Theorem 2.1 can be applied to improve the theories in [40, 41] to obtain approximation errors in the $L^{\infty}([0, 1]^d)$ -norm.

Theorem 2.1. *Given any $\varepsilon > 0$, $N, L, K \in \mathbb{N}^+$, and $\delta \in (0, \frac{1}{3K}]$, assume $f \in C([0, 1]^d)$ and $\tilde{\phi}$ is a function implemented by a ReLU FNN with width N and depth L . If*

$$|\tilde{\phi}(\mathbf{x}) - f(\mathbf{x})| \leq \varepsilon \quad \text{for any } \mathbf{x} \in [0, 1]^d \setminus \Omega([0, 1]^d, K, \delta),$$

then there exists a new function ϕ implemented by a ReLU FNN with width $3^d(N + 4)$ and depth $L + 2d$ such that

$$|\phi(\mathbf{x}) - f(\mathbf{x})| \leq \varepsilon + d \cdot \omega_f(\delta) \quad \text{for any } \mathbf{x} \in [0, 1]^d.$$

Theorem 2.2. Assume that $f \in C^s([0, 1]^d)$ satisfies $\|\partial^\alpha f\|_{L^\infty([0, 1]^d)} \leq 1$ for any $\alpha \in \mathbb{N}^d$ with $\|\alpha\|_1 \leq s$. For any $N, L \in \mathbb{N}^+$, there exists a function ϕ implemented by a ReLU FNN with width $16s^{d+1}d(N+2)\log_2(8N)$ and depth $18s^2(L+2)\log_2(4L)$ such that

$$|\phi(\mathbf{x}) - f(\mathbf{x})| \leq 84(s+1)^d 8^s N^{-2s/d} L^{-2s/d} \quad \text{for any } \mathbf{x} \in [0, 1]^d \setminus \Omega([0, 1]^d, K, \delta),$$

where $K = \lfloor N^{1/d} \rfloor^2 \lfloor L^{2/d} \rfloor$ and δ is an arbitrary number in $(0, \frac{1}{3K}]$.

We first prove Theorem 1.1 by assuming Theorems 2.1 and 2.2 are true. The proofs of Theorems 2.1 and 2.2 can be found in Sections 3 and 4, respectively.

Proof of Theorem 1.1. We may assume $\|f\|_{C^s([0, 1]^d)} > 0$ since $\|f\|_{C^s([0, 1]^d)} = 0$ is a trivial case. Define $\tilde{f} := \frac{f}{\|f\|_{C^s([0, 1]^d)}} \in C_u^s([0, 1]^d)$. Set $K = \lfloor N^{1/d} \rfloor^2 \lfloor L^{2/d} \rfloor$ and choose a small $\delta \in (0, \frac{1}{3K}]$ such that

$$d \cdot \omega_{\tilde{f}}(\delta) \leq N^{-2s/d} L^{-2s/d}.$$

Clearly, $\|\partial^\alpha \tilde{f}\|_{L^\infty([0, 1]^d)} \leq 1$ for any $\alpha \in \mathbb{N}^d$ with $\|\alpha\|_1 \leq s$. By Theorem 2.2, there exists a function $\tilde{\phi}$ implemented by a ReLU FNN with width $16s^{d+1}d(N+2)\log_2(8N)$ and depth $18s^2(L+2)\log_2(4L)$ such that

$$|\tilde{\phi}(\mathbf{x}) - \tilde{f}(\mathbf{x})| \leq 84(s+1)^d 8^s N^{-2s/d} L^{-2s/d} =: \varepsilon \quad \text{for any } \mathbf{x} \in [0, 1]^d \setminus \Omega([0, 1]^d, K, \delta).$$

By Theorem 2.1, there exists a new function $\tilde{\phi}$ implemented by a ReLU FNN with width

$$3^d(16s^{d+1}d(N+2)\log_2(8N) + 4) \leq 17s^{d+1}3^d d(N+2)\log_2(8N)$$

and depth $18s^2(L+2)\log_2(4L) + 2d$ such that

$$\begin{aligned} \|\tilde{\phi} - \tilde{f}\|_{L^\infty([0, 1]^d)} &\leq \varepsilon + d \cdot \omega_{\tilde{f}}(\delta) = 84(s+1)^d 8^s N^{-2s/d} L^{-2s/d} + d \cdot \omega_{\tilde{f}}(\delta) \\ &\leq 85(s+1)^d 8^s N^{-2s/d} L^{-2s/d}. \end{aligned}$$

Finally, set $\phi = \|f\|_{C^s([0, 1]^d)} \cdot \tilde{\phi}$; then

$$\begin{aligned} \|\phi - f\|_{L^\infty([0, 1]^d)} &= \|f\|_{C^s([0, 1]^d)} \cdot \|\tilde{\phi} - \tilde{f}\|_{L^\infty([0, 1]^d)} \\ &\leq 85(s+1)^d 8^s \|f\|_{C^s([0, 1]^d)} N^{-2s/d} L^{-2s/d}, \end{aligned}$$

and ϕ can also be implemented by a ReLU FNN with width $17s^{d+1}3^d d(N+2)\log_2(8N)$ and depth $18s^2(L+2)\log_2(4L) + 2d$. So we finish the proof. \square

2.3 Optimality of Theorem 1.1

In this section, we will show that the approximation error in Theorem 1.1 is nearly tight in terms of VC-dimension. The key is the VC-dimension upper bound of ReLU FNNs in [22] will lead to a contradiction if our approximation is not optimal. This idea was used in [44] to prove its tightness for ReLU FNNs of width $\mathcal{O}(d)$ and depth sufficiently large to approximate smooth functions.

Let us first present the definitions of VC-dimension and related concepts. Let H be a class of functions mapping from a general domain \mathcal{X} to $\{0, 1\}$. We say H shatters the set $\{\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_m\} \subseteq \mathcal{X}$ if

$$\left| \left\{ [h(\mathbf{x}_1), h(\mathbf{x}_2), \dots, h(\mathbf{x}_m)]^T \in \{0, 1\}^m : h \in H \right\} \right| = 2^m,$$

where $|\cdot|$ means the size of a set. This equation means, given any $\theta_i \in \{0, 1\}$ for $i = 1, 2, \dots, m$, there exists $h \in H$ such that $h(\mathbf{x}_i) = \theta_i$ for all i . For a general function set \mathcal{F} mapping from \mathcal{X} to \mathbb{R} , we say \mathcal{F} shatters $\{\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_m\} \subseteq \mathcal{X}$ if $\mathcal{T} \circ \mathcal{F}$ does, where

$$\mathcal{T}(t) := \begin{cases} 1, & t \geq 0, \\ 0, & t < 0 \end{cases} \quad \text{and} \quad \mathcal{T} \circ \mathcal{F} := \{\mathcal{T} \circ f : f \in \mathcal{F}\}.$$

For any $m \in \mathbb{N}^+$, we define the growth function of H as

$$\Pi_H(m) := \max_{\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_m \in \mathcal{X}} \left| \left\{ [h(\mathbf{x}_1), h(\mathbf{x}_2), \dots, h(\mathbf{x}_m)]^T \in \{0, 1\}^m : h \in H \right\} \right|.$$

Definition 2.3 (VC-dimension). Let H be a class of functions from \mathcal{X} to $\{0, 1\}$. The VC-dimension of H , denoted by $\text{VCDim}(H)$, is the size of the largest shattered set, namely,

$$\text{VCDim}(H) := \sup \left(\{0\} \cup \{m \in \mathbb{N}^+ : \Pi_H(m) = 2^m\} \right).$$

Let \mathcal{F} be a class of functions from \mathcal{X} to \mathbb{R} . The VC-dimension of \mathcal{F} , denoted by $\text{VCDim}(\mathcal{F})$, is defined by $\text{VCDim}(\mathcal{F}) := \text{VCDim}(\mathcal{T} \circ \mathcal{F})$, where

$$\mathcal{T}(t) := \begin{cases} 1, & t \geq 0, \\ 0, & t < 0 \end{cases} \quad \text{and} \quad \mathcal{T} \circ \mathcal{F} := \{\mathcal{T} \circ f : f \in \mathcal{F}\}.$$

In particular, the expression “VC-dimension of a network (architecture)” means the VC-dimension of the function set that consists of all functions implemented by this network (architecture).

Recall that $C_u^s([0, 1]^d)$ denotes the unit ball of $C^s([0, 1]^d)$. Theorem 2.4 below shows that the best possible approximation error of functions in $C_u^s([0, 1]^d)$ approximated by functions in \mathcal{F} is bounded by a formula characterized by $\text{VCDim}(\mathcal{F})$.

Theorem 2.4. *Given any $s, d \in \mathbb{N}^+$, there exists a (small) positive constant $C_{s,d}$ determined by s and d such that: For any $\varepsilon > 0$ and a function set \mathcal{F} with all elements defined on $[0, 1]^d$, if $\text{VCDim}(\mathcal{F}) \geq 1$ and*

$$\inf_{\phi \in \mathcal{F}} \|\phi - f\|_{L^\infty([0, 1]^d)} \leq \varepsilon \quad \text{for any } f \in C_u^s([0, 1]^d), \quad (2.2)$$

then $\text{VCDim}(\mathcal{F}) \geq C_{s,d} \varepsilon^{-d/s}$.^④

^④In fact, $C_{s,d}$ can be expressed by s and d with a **explicitly** formula as we remark in the proof of this theorem. However, the formula may be very complicated.

This theorem demonstrates the connection between the VC-dimension of \mathcal{F} and the approximation error using elements of \mathcal{F} to approximate functions in $C_u^s([0, 1]^d)$. To be precise, the best possible approximation error is controlled by $\text{VCDim}(\mathcal{F})^{-s/d}$ up to a constant. It is shown in [22] that the VC-dimension of ReLU FNNs with a fixed architecture with W parameters and L layers has an upper bound $\mathcal{O}(WL \ln W)$. It follows that the VC-dimension of ReLU FNNs with width N and depth L is bounded by $\mathcal{O}(N^2 L \cdot L \cdot \ln(N^2 L)) \leq \mathcal{O}(N^2 L^2 \ln(NL))$. That is, $\text{VCDim}(\mathcal{F}) \leq \mathcal{O}(N^2 L^2 \ln(NL))$, where

$$\mathcal{F} = \mathcal{NN}(\# \text{input} = d; \text{width} \leq N; \text{depth} \leq L; \# \text{output} = 1).$$

Hence, the approximation error of functions in $C_u^s([0, 1]^d)$, approximated by ReLU FNNs with width N and depth L , has a lower bound

$$C(s, d) \cdot (N^2 L^2 \ln(NL))^{-s/d}$$

for some positive constant $C(s, d)$ determined by s and d . When the width and depth become $\mathcal{O}(N \ln N)$ and $\mathcal{O}(L \ln L)$, respectively, the lower bound of the approximation error becomes

$$C(s, d) \cdot (N^2 L^2 (\ln N)^3 (\ln L)^3)^{-s/d}$$

for some positive constant $C(s, d)$ determined by s and d . These two lower bounds mean that our approximation errors in Theorem 1.1 and Corollary 1.2 are nearly optimal.

Now let us present the detailed proof of Theorem 2.4.

Proof of Theorem 2.4. To find a subset of \mathcal{F} shattering $\mathcal{O}(\varepsilon^{-d/s})$ points in $[0, 1]^d$, we divided the proof into two steps.

- Construct $\{f_\chi : \chi \in \mathcal{X}\} \subseteq C_u^s([0, 1]^d)$ that scatters $\mathcal{O}(\varepsilon^{-d/s})$ points, where \mathcal{X} is a function set defined later.
- Design $\phi_\chi \in \mathcal{F}$, for each $\chi \in \mathcal{X}$, based on f_χ and Equation (2.2) such that $\{\phi_\chi : \chi \in \mathcal{X}\} \subseteq \mathcal{F}$ also shatters $\mathcal{O}(\varepsilon^{-d/s})$ points.

The details of these two steps can be found below.

Step 1: Construct $\{f_\chi : \chi \in \mathcal{X}\} \subseteq C_u^s([0, 1]^d)$ that scatters $\mathcal{O}(\varepsilon^{-d/s})$ points.

Let $K = \mathcal{O}(\varepsilon^{-1/s})$ be an integer determined later and divide $[0, 1]^d$ into K^d non-overlapping sub-cubes $\{Q_\beta\}_\beta$ as follows:

$$Q_\beta := \{\mathbf{x} = [x_1, x_2, \dots, x_d]^T \in [0, 1]^d : x_i \in [\frac{\beta_i}{K}, \frac{\beta_i+1}{K}] \text{ for } i = 1, 2, \dots, d\}$$

for any index vector $\beta = [\beta_1, \beta_2, \dots, \beta_d]^T \in \{0, 1, \dots, K-1\}^d$.

There exists $\tilde{g} \in C^\infty(\mathbb{R}^d)$ such that $\tilde{g}(\mathbf{0}) = 1$ and $\tilde{g}(\mathbf{x}) = 0$ for $\|\mathbf{x}\|_2 \geq 1/3$.^⑤ Then, $g := \tilde{g}/\tilde{C}_{s,d} \in C_u^s([0, 1]^d)$ by setting $\tilde{C}_{s,d} := \|\tilde{g}\|_{C^s([0, 1]^d)} > 0$.

Define

$$\mathcal{X} := \{\chi : \chi \text{ is a map from } \{0, 1, \dots, K-1\}^d \text{ to } \{-1, 1\}\}$$

^⑤In fact, such a function \tilde{g} is called “bump function”. An example can be attained by setting $\tilde{g}(\mathbf{x}) = C \exp(\frac{1}{\|\mathbf{x}\|_2^2 - 1})$ if $\|\mathbf{x}\|_2 < 1/3$ and $\tilde{g}(\mathbf{x}) = 0$ if $\|\mathbf{x}\|_2 \geq 1/3$, where C is a proper constant such that $\tilde{g}(\mathbf{0}) = 1$.

468 and

$$469 \quad g_\beta := K^{-s}g(K(\mathbf{x} - \mathbf{x}_{Q_\beta})) \quad \text{for each } \beta \in \{0, 1, \dots, K-1\}^d,$$

470 where \mathbf{x}_{Q_β} is the center of Q_β .

471 Next, for each $\chi \in \mathcal{X}$, we can define f_χ via

$$472 \quad f_\chi(\mathbf{x}) := \sum_{\beta \in \{0, 1, \dots, K-1\}^d} \chi(\beta) g_\beta(\mathbf{x}).$$

473 Then $f_\chi \in C_u^s([0, 1]^d)$ for each $\chi \in \mathcal{X}$, since it satisfies the following two conditions.

474 • By the definition of g_β and χ , we have

$$475 \quad \{\mathbf{x} : \chi(\beta) g_\beta(\mathbf{x}) \neq 0\} \subseteq \mathcal{B}(\mathbf{x}_{Q_\beta}, \frac{1}{3K}) \subseteq \frac{2}{3}Q_\beta \quad \text{for each } \beta \in \{0, 1, \dots, K-1\}^d,$$

476 which implies that $f_\chi \in C^\infty([0, 1]^d)$.

477 • For any $\mathbf{x} \in Q_\beta$, $\beta \in \{0, 1, \dots, K-1\}^d$, and $\alpha \in \mathbb{N}^d$ with $\|\alpha\|_1 \leq s$,

$$478 \quad \partial^\alpha f_\chi(\mathbf{x}) = \chi(\beta) \partial^\alpha g_\beta(\mathbf{x}) = K^{-s} \chi(\beta) K^{\|\alpha\|_1} \partial^\alpha g(K(\mathbf{x} - \mathbf{x}_\beta)),$$

479 from which we deduce $|\partial^\alpha f_\chi(\mathbf{x})| = |K^{-(s-\|\alpha\|_1)} \partial^\alpha g(K(\mathbf{x} - \mathbf{x}_\beta))| \leq 1$.

480 It is easy to check that $\{f_\chi : \chi \in \mathcal{X}\} \subseteq C_u^s([0, 1]^d)$ can shatter $K^d = \mathcal{O}(\varepsilon^{-d/s})$ points in
481 $[0, 1]^d$.

482 **Step 2:** Construct $\{\phi_\chi : \chi \in \mathcal{X}\}$ that also scatters $\mathcal{O}(\varepsilon^{-d/s})$ points.

483 By Equation (2.2), for each $\chi \in \mathcal{X}$, there exists $\phi_\chi \in \mathcal{F}$ such that

$$484 \quad \|\phi_\chi - f_\chi\|_{L^\infty([0, 1]^d)} \leq \varepsilon + \varepsilon/2.$$

485 Let $\mu(\cdot)$ denote the Lebesgue measure of a set. Then, for each $\chi \in \mathcal{X}$, there exists
486 $\mathcal{H}_\chi \subseteq [0, 1]^d$ with $\mu(\mathcal{H}_\chi) = 0$ such that

$$487 \quad |\phi_\chi(\mathbf{x}) - f_\chi(\mathbf{x})| \leq \frac{3}{2}\varepsilon \quad \text{for any } \mathbf{x} \in [0, 1]^d \setminus \mathcal{H}_\chi.$$

488 Set $\mathcal{H} = \bigcup_{\chi \in \mathcal{X}} \mathcal{H}_\chi$; then we have $\mu(\mathcal{H}) = 0$ and

$$489 \quad |\phi_\chi(\mathbf{x}) - f_\chi(\mathbf{x})| \leq \frac{3}{2}\varepsilon \quad \text{for any } \chi \in \mathcal{X} \text{ and } \mathbf{x} \in [0, 1]^d \setminus \mathcal{H}. \quad (2.3)$$

490 Clearly, there exists $r \in (0, 1)$ such that

$$491 \quad g_\beta(\mathbf{x}) \geq \frac{1}{2}g_\beta(\mathbf{x}_{Q_\beta}) > 0 \quad \text{for any } \mathbf{x} \in rQ_\beta,$$

492 where \mathbf{x}_{Q_β} is the center of Q_β .

493 Note that $(rQ_\beta) \setminus \mathcal{H}$ is not empty, since $\mu((rQ_\beta) \setminus \mathcal{H}) > 0$ for each β . Then, for any
494 $\chi \in \mathcal{X}$ and $\beta \in \{0, 1, \dots, K-1\}^d$, there exists $\mathbf{x}_\beta \in (rQ_\beta) \setminus \mathcal{H}$ such that

$$495 \quad |f_\chi(\mathbf{x}_\beta)| = |g_\beta(\mathbf{x}_\beta)| \geq \frac{1}{2}|g_\beta(\mathbf{x}_{Q_\beta})| = \frac{1}{2}K^{-s}g(\mathbf{0}) = \frac{1}{2}K^{-s}/\tilde{C}_{s,d} \geq 2\varepsilon, \quad (2.4)$$

496 where the last inequality is attained by setting $K = \lfloor (4\varepsilon\tilde{C}_{s,d})^{-1/s} \rfloor$. Note that it is
497 necessary to verify $K \neq 0$; we do this later in the proof.

By Equations (2.3) and (2.4), we have, for each $\beta \in \{0, 1, \dots, K-1\}^d$ and each $\chi \in \mathcal{X}$,

$$|f_\chi(\mathbf{x}_\beta)| \geq 2\varepsilon > \frac{3}{2}\varepsilon \geq |f_\chi(\mathbf{x}_\beta) - \phi_\chi(\mathbf{x}_\beta)|,$$

implying $f_\chi(\mathbf{x}_\beta)$ and $\phi_\chi(\mathbf{x}_\beta)$ have the same sign. Then $\{\phi_\chi : \chi \in \mathcal{X}\}$ shatters $\{\mathbf{x}_\beta : \beta \in \{0, 1, \dots, K-1\}^d\}$ since $\{f_\chi : \chi \in \mathcal{X}\}$ shatters $\{\mathbf{x}_\beta : \beta \in \{0, 1, \dots, K-1\}^d\}$. Hence,

$$\text{VCDim}(\mathcal{F}) \geq \text{VCDim}(\{\phi_\chi : \chi \in \mathcal{X}\}) \geq K^d = \lfloor (4\varepsilon \tilde{C}_{s,d})^{-1/s} \rfloor^d \geq 2^{-d} (4\varepsilon \tilde{C}_{s,d})^{-d/s},$$

where the last inequality comes from the fact that $\lfloor x \rfloor \geq x/2$ for any $x \in [1, \infty)$.

Finally, by setting

$$C_{s,d} = 2^{-d} (4\tilde{C}_{s,d})^{-d/s} = 2^{-d} (4\|\tilde{g}\|_{C^s([0,1]^d)})^{-d/s},$$

we have

$$\text{VCDim}(\mathcal{F}) \geq 2^{-d} (4\varepsilon \tilde{C}_{s,d})^{-d/s} = 2^{-d} (4\tilde{C}_{s,d})^{-d/s} \varepsilon^{-d/s} = C_{s,d} \varepsilon^{-d/s}$$

and

$$K = \lfloor (4\varepsilon \tilde{C}_{s,d})^{-1/s} \rfloor = \lfloor \varepsilon^{-1/s} (4\tilde{C}_{s,d})^{-1/s} \rfloor = \lfloor \varepsilon^{-1/s} (2^d C_{s,d})^{1/d} \rfloor \geq 1,$$

where the last inequality comes from the assumption $\varepsilon \leq (2^d C_{s,d})^{s/d}$. Such an assumption is reasonable since $\varepsilon > (2^d C_{s,d})^{s/d}$ is a trivial case, which implies

$$\text{VCDim}(\mathcal{F}) \geq 1 \geq 2^{-d} = C_{s,d} \left((2^d C_{s,d})^{s/d} \right)^{-d/s} > C_{s,d} \varepsilon^{-d/s}.$$

So we finish the proof. \square

3 Proof of Theorem 2.1

Intuitively speaking, Theorem 2.1 shows that if a ReLU FNN can implement a function g approximating the target function f well except for the trifling region, then we can design a new ReLU network with a similar size to approximate f well on the whole domain. For example, if g approximates a one-dimensional continuous function f well except for a region in \mathbb{R} with a sufficiently small measure δ , then $\text{mid}(g(x + \delta), g(x), g(x - \delta))$ can approximate f well on the whole domain, where $\text{mid}(\cdot, \cdot, \cdot)$ is a function returning the middle value of three inputs and can be implemented via a ReLU FNN as shown in Lemma 3.1. This key idea is called the horizontal shift (translation) of g in this paper.

Lemma 3.1. *The middle value function $\text{mid}(x_1, x_2, x_3)$ can be implemented by a ReLU FNN with width 14 and depth 2.*

Proof. Recall the fact that

$$x = \sigma(x) - \sigma(-x) \quad \text{and} \quad |x| = \sigma(x) + \sigma(-x) \quad \text{for any } x \in \mathbb{R}. \quad (3.1)$$

Therefore,

$$\begin{aligned} \max(x, y) &= \frac{x + y + |x - y|}{2} \\ &= \frac{1}{2}\sigma(x + y) - \frac{1}{2}\sigma(-x - y) + \frac{1}{2}\sigma(x - y) + \frac{1}{2}\sigma(-x + y), \end{aligned} \quad (3.2)$$

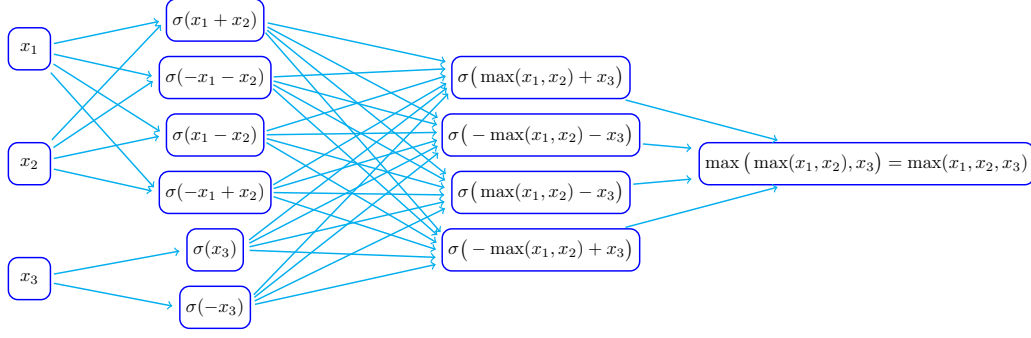


Figure 3: An illustration of the network architecture implementing $\max(x_1, x_2, x_3)$ based on Equations (3.1) and (3.2).

for any $x, y \in \mathbb{R}$. Thus, $\max(x_1, x_2, x_3)$ can be implemented by the network shown in Figure 3.

Clearly,

$$\max(x_1, x_2, x_3) \in \mathcal{NN}(\#input = 3; \text{widthvec} = [6, 4]).$$

Similarly, we have

$$\min(x_1, x_2, x_3) \in \mathcal{NN}(\#input = 3; \text{widthvec} = [6, 4]).$$

It is easy to check that

$$\begin{aligned} \text{mid}(x_1, x_2, x_3) &= x_1 + x_2 + x_3 - \max(x_1, x_2, x_3) - \min(x_1, x_2, x_3) \\ &= \sigma(x_1 + x_2 + x_3) - \sigma(-x_1 - x_2 - x_3) - \max(x_1, x_2, x_3) - \min(x_1, x_2, x_3). \end{aligned}$$

Hence,

$$\text{mid}(x_1, x_2, x_3) \in \mathcal{NN}(\#input = 3; \text{widthvec} = [14, 10]).$$

That is, $\text{mid}(x_1, x_2, x_3)$ can be implemented by a ReLU FNN with width 14 and depth 2. So we finish the proof. \square

The next lemma shows a simple but useful property of the $\text{mid}(x_1, x_2, x_3)$ function that helps to exclude poor approximation in the trifling region.

Lemma 3.2. *For any $\varepsilon > 0$, if at least two elements of $\{x_1, x_2, x_3\}$ are in $\mathcal{B}(y, \varepsilon)$, then $\text{mid}(x_1, x_2, x_3) \in \mathcal{B}(y, \varepsilon)$.*

Proof. Without loss of generality, we may assume $x_1, x_2 \in \mathcal{B}(y, \varepsilon)$ and $x_1 \leq x_2$. Then the proof can be divided into three cases.

1. If $x_3 < x_1$, then $x_3 < x_1 \leq x_2$, implying $\text{mid}(x_1, x_2, x_3) = x_1 \in \mathcal{B}(y, \varepsilon)$.

2. If $x_1 \leq x_3 \leq x_2$, then $\text{mid}(x_1, x_2, x_3) = x_3 \in \mathcal{B}(y, \varepsilon)$ since $y - \varepsilon \leq x_1 \leq x_3 \leq x_2 \leq y + \varepsilon$.

3. If $x_2 < x_3$, then $x_1 \leq x_2 < x_3$, implying $\text{mid}(x_1, x_2, x_3) = x_2 \in \mathcal{B}(y, \varepsilon)$.

So we finish the proof. \square

Next, given a function g approximating f well on $[0, 1]$ except for the trifling region, Lemma 3.3 below shows how to use the $\text{mid}(x_1, x_2, x_3)$ function to construct a new function ϕ uniformly approximating f well on $[0, 1]$, leveraging the useful property of $\text{mid}(x_1, x_2, x_3)$ in Lemma 3.2.

Lemma 3.3. *Given any $\varepsilon > 0$, $K \in \mathbb{N}^+$, and $\delta \in (0, \frac{1}{3K}]$, assume $f \in C([0, 1])$ and $g : \mathbb{R} \rightarrow \mathbb{R}$ is a general function with*

$$|g(x) - f(x)| \leq \varepsilon, \text{ i.e., } g(x) \in \mathcal{B}(f(x), \varepsilon) \text{ for any } x \in [0, 1] \setminus \Omega([0, 1], K, \delta). \quad (3.3)$$

Then

$$|\phi(x) - f(x)| \leq \varepsilon + \omega_f(\delta) \text{ for any } x \in [0, 1],$$

where

$$\phi(x) := \text{mid}(g(x - \delta), g(x), g(x + \delta)) \text{ for any } x \in \mathbb{R}.$$

Proof. Divide $[0, 1]$ into K small intervals denoted by $Q_k = [\frac{k}{K}, \frac{k+1}{K}]$ for $k = 0, 1, \dots, K-1$. For each $k \in \{0, 1, \dots, K-1\}$, we further divide Q_k into four small closed intervals as shown in Figure 4, i.e.,

$$Q_k = Q_{k,1} \cup Q_{k,2} \cup Q_{k,3} \cup Q_{k,4},$$

where $Q_{k,1} = [\frac{k}{K}, \frac{k}{K} + \delta]$, $Q_{k,2} = [\frac{k}{K} + \delta, \frac{k+1}{K} - 2\delta]$, $Q_{k,3} = [\frac{k+1}{K} - 2\delta, \frac{k+1}{K} - \delta]$, and $Q_{k,4} = [\frac{k+1}{K} - \delta, \frac{k+1}{K}]$.

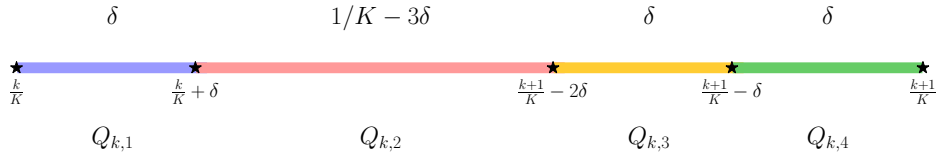


Figure 4: An illustration of $Q_{k,i}$ for $i = 1, 2, 3, 4$.

It is easy to verify that

- $Q_{k,i} \subseteq [0, 1] \setminus \Omega([0, 1], K, \delta)$ for $k = 0, 1, \dots, K-1$ and $i = 1, 2, 3$;
- $Q_{K-1,4} \subseteq [0, 1] \setminus \Omega([0, 1], K, \delta)$.

To estimate the difference between $\phi(x)$ and $f(x)$, we consider the following four cases of x in $[0, 1]$ for each $k \in \{0, 1, \dots, K-1\}$.

Case 1: $x \in Q_{k,1}$.

If $x \in Q_{k,1}$, then $x \in [0, 1] \setminus \Omega([0, 1], K, \delta)$ and

$$x + \delta \in Q_{k,2} \cup Q_{k,3} \subseteq [0, 1] \setminus \Omega([0, 1], K, \delta).$$

It follows from Equation (3.3) that

$$g(x) \in \mathcal{B}(f(x), \varepsilon) \subseteq \mathcal{B}(f(x), \varepsilon + \omega_f(\delta))$$

and

$$g(x + \delta) \in \mathcal{B}(f(x + \delta), \varepsilon) \subseteq \mathcal{B}(f(x), \varepsilon + \omega_f(\delta)).$$

581 By Lemma 3.2, we get

$$582 \quad \text{mid}(g(x - \delta), g(x), g(x + \delta)) \in \mathcal{B}(f(x), \varepsilon + \omega_f(\delta)).$$

583 **Case 2:** $x \in Q_{k,2}$.

584 If $x \in Q_{k,2}$, then

$$585 \quad x - \delta, x, x + \delta \in Q_{k,1} \cup Q_{k,2} \cup Q_{k,3} \subseteq [0, 1] \setminus \Omega([0, 1], K, \delta).$$

586 It follows from Equation (3.3) that

$$587 \quad g(x - \delta) \in \mathcal{B}(f(x - \delta), \varepsilon) \subseteq \mathcal{B}(f(x), \varepsilon + \omega_f(\delta)),$$

$$588 \quad g(x) \in \mathcal{B}(f(x), \varepsilon) \subseteq \mathcal{B}(f(x), \varepsilon + \omega_f(\delta)),$$

590 and

$$591 \quad g(x + \delta) \in \mathcal{B}(f(x + \delta), \varepsilon) \subseteq \mathcal{B}(f(x), \varepsilon + \omega_f(\delta)).$$

592 Then, by Lemma 3.2, we have

$$593 \quad \text{mid}(g(x - \delta), g(x), g(x + \delta)) \in \mathcal{B}(f(x), \varepsilon + \omega_f(\delta)).$$

594 **Case 3:** $x \in Q_{k,3}$.

595 If $x \in Q_{k,3}$, then $x \in [0, 1] \setminus \Omega([0, 1], K, \delta)$ and

$$596 \quad x - \delta \in Q_{k,1} \cup Q_{k,2} \subseteq [0, 1] \setminus \Omega([0, 1], K, \delta).$$

597 It follows from Equation (3.3) that

$$598 \quad g(x) \in \mathcal{B}(f(x), \varepsilon) \subseteq \mathcal{B}(f(x), \varepsilon + \omega_f(\delta))$$

599 and

$$600 \quad g(x - \delta) \in \mathcal{B}(f(x - \delta), \varepsilon) \subseteq \mathcal{B}(f(x), \varepsilon + \omega_f(\delta)).$$

601 By Lemma 3.2, we get

$$602 \quad \text{mid}(g(x - \delta), g(x), g(x + \delta)) \in \mathcal{B}(f(x), \varepsilon + \omega_f(\delta)).$$

603 **Case 4:** $x \in Q_{k,4}$.

604 If $x \in Q_{k,4}$, we can divide this case into two sub-cases.

- 605 • If $k \in \{0, 1, \dots, K - 2\}$, then $x - \delta \in Q_{k,3} \in [0, 1] \setminus \Omega([0, 1], K, \delta)$ and $x + \delta \in Q_{k+1,1} \subseteq$
 606 $[0, 1] \setminus \Omega([0, 1], K, \delta)$. It follows from Equation (3.3) that

$$607 \quad g(x - \delta) \in \mathcal{B}(f(x - \delta), \varepsilon) \subseteq \mathcal{B}(f(x), \varepsilon + \omega_f(\delta))$$

608 and

$$609 \quad g(x + \delta) \in \mathcal{B}(f(x + \delta), \varepsilon) \subseteq \mathcal{B}(f(x), \varepsilon + \omega_f(\delta)).$$

610 By Lemma 3.2, we get

$$611 \quad \text{mid}(g(x - \delta), g(x), g(x + \delta)) \in \mathcal{B}(f(x), \varepsilon + \omega_f(\delta)).$$

• If $k = K - 1$, then $x \in Q_{k,4} = Q_{K-1,4} \subseteq [0, 1] \setminus \Omega([0, 1], K, \delta)$ and $x - \delta \in Q_{k,3} \subseteq [0, 1] \setminus \Omega([0, 1], K, \delta)$. It follows from Equation (3.3) that

$$g(x) \in \mathcal{B}(f(x), \varepsilon) \subseteq \mathcal{B}(f(x), \varepsilon + \omega_f(\delta))$$

and

$$g(x - \delta) \in \mathcal{B}(f(x - \delta), \varepsilon) \subseteq \mathcal{B}(f(x), \varepsilon + \omega_f(\delta)).$$

By Lemma 3.2, we get

$$\text{mid}(g(x - \delta), g(x), g(x + \delta)) \in \mathcal{B}(f(x), \varepsilon + \omega_f(\delta)).$$

Since $[0, 1] = \bigcup_{k=0}^{K-1} \left(\bigcup_{i=1}^4 Q_{k,i} \right)$, we have

$$\text{mid}(g(x - \delta), g(x), g(x + \delta)) \in \mathcal{B}(f(x), \varepsilon + \omega_f(\delta)) \quad \text{for any } x \in [0, 1].$$

Recall that $\phi(x) = \text{mid}(g(x - \delta), g(x), g(x + \delta))$. Then we have

$$|\phi(x) - f(x)| \leq \varepsilon + \omega_f(\delta) \quad \text{for any } x \in [0, 1].$$

So we finish the proof. \square

The next lemma below extend Lemma 3.3 to the multidimensional case.

Lemma 3.4. *Given any $\varepsilon > 0$, $K \in \mathbb{N}^+$, and $\delta \in (0, \frac{1}{3K}]$, assume $f \in C([0, 1]^d)$ and $g : \mathbb{R}^d \rightarrow \mathbb{R}$ is a general function with*

$$|g(\mathbf{x}) - f(\mathbf{x})| \leq \varepsilon, \text{ i.e., } g(\mathbf{x}) \in \mathcal{B}(f(\mathbf{x}), \varepsilon) \quad \text{for any } \mathbf{x} \in [0, 1]^d \setminus \Omega([0, 1]^d, K, \delta).$$

Then

$$|\phi(\mathbf{x}) - f(\mathbf{x})| \leq \varepsilon + d \cdot \omega_f(\delta) \quad \text{for any } \mathbf{x} \in [0, 1]^d,$$

where $\phi := \phi_d$ is defined by induction through

$$\phi_{i+1}(\mathbf{x}) := \text{mid}(\phi_i(\mathbf{x} - \delta \mathbf{e}_{i+1}), \phi_i(\mathbf{x}), \phi_i(\mathbf{x} + \delta \mathbf{e}_{i+1})) \quad \text{for } i = 0, 1, \dots, d-1, \quad (3.4)$$

where $\phi_0 = g$ and $\{\mathbf{e}_i\}_{i=1}^d$ is the standard basis in \mathbb{R}^d .

Proof. For $\ell = 0, 1, \dots, d$, we define

$$E_\ell := \left\{ \mathbf{x} = [x_1, x_2, \dots, x_d]^T : x_i \in \begin{cases} [0, 1], & \text{if } i \leq \ell, \\ [0, 1] \setminus \Omega([0, 1], K, \delta), & \text{if } i > \ell \end{cases} \right\}.$$

Clearly, $E_0 = [0, 1]^d \setminus \Omega([0, 1]^d, K, \delta)$ and $E_d = [0, 1]^d$. See Figure 5 for the illustrations of E_ℓ for $\ell = 0, 1, \dots, d$ when $K = 4$ and $d = 2$.

We would like to construct a sequence of functions $\phi_0, \phi_1, \dots, \phi_d$ by induction, based on Equation (3.4), such that, for each $\ell \in \{0, 1, \dots, d\}$,

$$\phi_\ell(\mathbf{x}) \in \mathcal{B}(f(\mathbf{x}), \varepsilon + \ell \cdot \omega_f(\delta)) \quad \text{for any } \mathbf{x} \in E_\ell. \quad (3.5)$$

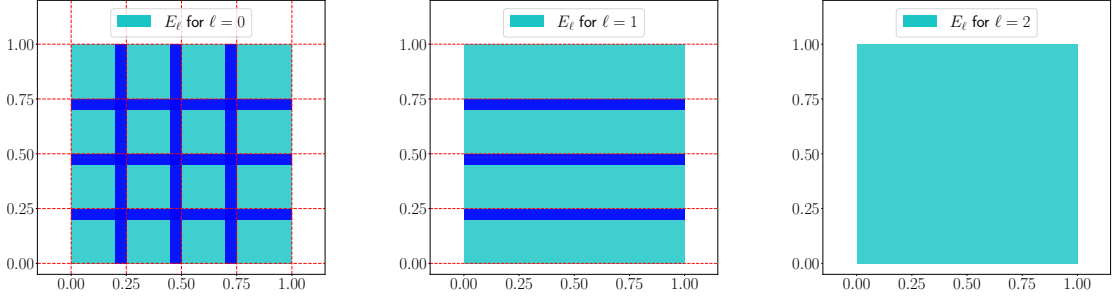


Figure 5: Illustrations of E_ℓ for $\ell = 0, 1, 2$ when $K = 4$ and $d = 2$.

Let us first consider the case $\ell = 0$. Note that $\phi_0 = g$, $E_0 = [0, 1]^d \setminus \Omega([0, 1]^d, K, \delta)$, and $|g(\mathbf{x}) - f(\mathbf{x})| \leq \varepsilon$ for any $\mathbf{x} \in [0, 1]^d \setminus \Omega([0, 1]^d, K, \delta)$. Then we have

$$\phi_0(\mathbf{x}) = g(\mathbf{x}) \in \mathcal{B}(f(\mathbf{x}), \varepsilon) \quad \text{for any } \mathbf{x} \in E_0.$$

That is, Equation (3.5) is true for $\ell = 0$.

Now assume Equation (3.5) is true for $\ell = i$. We will prove that it also holds for $\ell = i + 1$. By the hypothesis of induction, we have

$$\phi_i(x_1, \dots, x_i, t, x_{i+2}, \dots, x_d) \in \mathcal{B}(f(x_1, \dots, x_i, t, x_{i+2}, \dots, x_d), \varepsilon + i \cdot \omega_f(\delta)) \quad (3.6)$$

for any $x_1, \dots, x_i \in [0, 1]$ and $t, x_{i+2}, \dots, x_d \in [0, 1] \setminus \Omega([0, 1], K, \delta)$.

For fixed $x_1, \dots, x_i \in [0, 1]$ and $x_{i+2}, \dots, x_d \in [0, 1] \setminus \Omega([0, 1], K, \delta)$, denote

$$\mathbf{x}^{[i]} := [x_1, \dots, x_i, x_{i+2}, \dots, x_d]^T \in [0, 1]^{d-1}.$$

Then define

$$\psi_{\mathbf{x}^{[i]}}(t) := \phi_i(x_1, \dots, x_i, t, x_{i+2}, \dots, x_d) \quad \text{for any } t \in \mathbb{R}$$

and

$$f_{\mathbf{x}^{[i]}}(t) := f(x_1, \dots, x_i, t, x_{i+2}, \dots, x_d) \quad \text{for any } t \in \mathbb{R}.$$

It follows from Equation (3.6) that

$$\psi_{\mathbf{x}^{[i]}}(t) \in \mathcal{B}(f_{\mathbf{x}^{[i]}}(t), \varepsilon + i \cdot \omega_f(\delta)) \quad \text{for any } t \in [0, 1] \setminus \Omega([0, 1], K, \delta).$$

Then by Lemma 3.3 (set $g = \psi_{\mathbf{x}^{[i]}}$ and $f = f_{\mathbf{x}^{[i]}}$ therein), we get, for any $t \in [0, 1]$,

$$\begin{aligned} \text{mid}(\psi_{\mathbf{x}^{[i]}}(t - \delta), \psi_{\mathbf{x}^{[i]}}(t), \psi_{\mathbf{x}^{[i]}}(t + \delta)) &\in \mathcal{B}(f_{\mathbf{x}^{[i]}}(t), \varepsilon + i \cdot \omega_f(\delta) + \omega_{f_{\mathbf{x}^{[i]}}}(\delta)) \\ &\subseteq \mathcal{B}(f_{\mathbf{x}^{[i]}}(t), \varepsilon + (i + 1)\omega_f(\delta)). \end{aligned}$$

That is, for any $x_{i+1} = t \in [0, 1]$,

$$\begin{aligned} &\text{mid}(\phi_i(x_1, \dots, x_i, x_{i+1} - \delta, x_{i+2}, \dots, x_d), \phi_i(x_1, \dots, x_i, x_{i+1}, x_{i+2}, \dots, x_d), \phi_i(x_1, \dots, x_i, x_{i+1} + \delta, x_{i+2}, \dots, x_d)) \\ &\in \mathcal{B}(f(x_1, \dots, x_d), \varepsilon + (i + 1)\omega_f(\delta)). \end{aligned}$$

Note that $x_1, \dots, x_i \in [0, 1]$, $x_{i+1} = t \in [0, 1]$, and $x_{i+2}, \dots, x_d \in [0, 1] \setminus \Omega([0, 1], K, \delta)$ are arbitrary. Thus, for any $\mathbf{x} \in E_{i+1}$, we have

$$\text{mid}(\phi_i(\mathbf{x} - \delta \mathbf{e}_{i+1}), \phi_i(\mathbf{x}), \phi_i(\mathbf{x} + \delta \mathbf{e}_{i+1})) \in \mathcal{B}(f(\mathbf{x}), \varepsilon + (i+1)\omega_f(\delta)),$$

which implies

$$\phi_{i+1}(\mathbf{x}) \in \mathcal{B}(f(\mathbf{x}), \varepsilon + (i+1)\omega_f(\delta)) \quad \text{for any } \mathbf{x} \in E_{i+1}.$$

So Equation (3.5) is true for $\ell = i+1$, which means we finish the process of mathematical induction.

By the principle of induction, we have

$$\phi(\mathbf{x}) := \phi_d(\mathbf{x}) \in \mathcal{B}(f(\mathbf{x}), \varepsilon + d \cdot \omega_f(\delta)) \quad \text{for any } \mathbf{x} \in E_d = [0, 1]^d.$$

Therefore,

$$|\phi(\mathbf{x}) - f(\mathbf{x})| \leq \varepsilon + d \cdot \omega_f(\delta) \quad \text{for any } \mathbf{x} \in [0, 1]^d,$$

which means we finish the proof. \square

With Lemma 3.4 in hand, we are ready to prove Theorem 2.1.

Proof of Theorem 2.1. Set $\phi_0 = \tilde{\phi}$ and define ϕ_i for $i \in \{1, 2, \dots, d\}$ by induction as follows:

$$\phi_{i+1}(\mathbf{x}) := \text{mid}(\phi_i(\mathbf{x} - \delta \mathbf{e}_{i+1}), \phi_i(\mathbf{x}), \phi_i(\mathbf{x} + \delta \mathbf{e}_{i+1})) \quad \text{for } i = 0, 1, \dots, d-1,$$

where $\{\mathbf{e}_i\}_{i=1}^d$ is the standard basis in \mathbb{R}^d . Then by Lemma 3.4 with $\phi = \phi_d$, we have

$$|\phi(\mathbf{x}) - f(\mathbf{x})| \leq \varepsilon + d \cdot \omega_f(\delta) \quad \text{for any } \mathbf{x} \in [0, 1]^d.$$

It remains to determine the network architecture implementing $\phi = \phi_d$. Clearly, $\phi_0 = \tilde{\phi} \in \mathcal{NN}(\text{width} \leq N; \text{depth} \leq L)$ implies

$$\phi_0(\cdot - \delta \mathbf{e}_1), \phi_0(\cdot), \phi_0(\cdot + \delta \mathbf{e}_1) \in \mathcal{NN}(\text{width} \leq N; \text{depth} \leq L).$$

By defining a vector-valued function $\Phi_0 : \mathbb{R}^d \rightarrow \mathbb{R}^3$ as

$$\Phi_0(\mathbf{x}) := (\phi_0(\mathbf{x} - \delta \mathbf{e}_1), \phi_0(\mathbf{x}), \phi_0(\mathbf{x} + \delta \mathbf{e}_1)) \quad \text{for any } \mathbf{x} \in \mathbb{R}^d,$$

we have $\Phi_0 \in \mathcal{NN}(\# \text{input} = d; \text{width} \leq 3N; \text{depth} \leq L; \# \text{output} = 3)$. Recall that $\text{mid}(\cdot, \cdot, \cdot) \in \mathcal{NN}(\text{width} \leq 14; \text{depth} \leq 2)$ by Lemma 3.1. Therefore, $\phi_1 = \min(\cdot, \cdot, \cdot) \circ \Phi_0$ can be implemented by a ReLU FNN with width $\max\{3N, 14\} \leq 3(N+4)$ and depth $L+2$. Similarly, $\phi = \phi_d$ can be implemented by a ReLU FNN with width $3^d(N+4)$ and depth $L+2d$. So we finish the proof. \square

4 Proof of Theorem 2.2

In this section, we prove Theorem 2.2, a weaker version of the main theorem of this paper (Theorem 1.1) targeting a ReLU FNN constructed to approximate a smooth function outside the trifling region. The main idea is to construct ReLU FNNs through Taylor expansions of smooth functions. We first discuss the proof sketch in Section 4.1 and give the detailed proof in Section 4.2.

693 4.1 Proof sketch of Theorem 2.2

694 Set $K = \mathcal{O}(N^{2/d}L^{2/d})$ and let $\Omega([0,1]^d, K, \delta)$ partition $[0,1]^d$ into K^d cubes Q_β
 695 for $\beta \in \{0, 1, \dots, K-1\}^d$. As we shall see later, the introduction of the trifling region
 696 $\Omega([0,1]^d, K, \delta)$ can reduce the difficulty in constructing ReLU FNNs to achieve the op-
 697 timal approximation error simultaneously in width and depth, since it is only required
 698 to uniformly control the approximation error outside the trifling region and there is
 699 no requirement for the ReLU FNN inside the trifling region. In particular, for each
 700 $\beta = [\beta_1, \beta_2, \dots, \beta_d]^T \in \{0, 1, \dots, K-1\}^d$, we define $\mathbf{x}_\beta := \beta/K$ and

$$701 \quad Q_\beta := \{\mathbf{x} = [x_1, x_2, \dots, x_d]^T : x_i \in [\frac{\beta_i}{K}, \frac{\beta_i+1}{K} - \delta \cdot \mathbf{1}_{\{\beta_i \leq K-2\}}]\} \text{ for } i = 1, 2, \dots, d\}.$$

702 Clearly, $[0,1]^d = \Omega([0,1]^d, K, \delta) \cup (\cup_{\beta \in \{0,1,\dots,K-1\}^d} Q_\beta)$ and \mathbf{x}_β is the vertex of Q_β with
 minimum $\|\cdot\|_1$ norm. See Figure 6 for the illustrations of Q_β and \mathbf{x}_β .

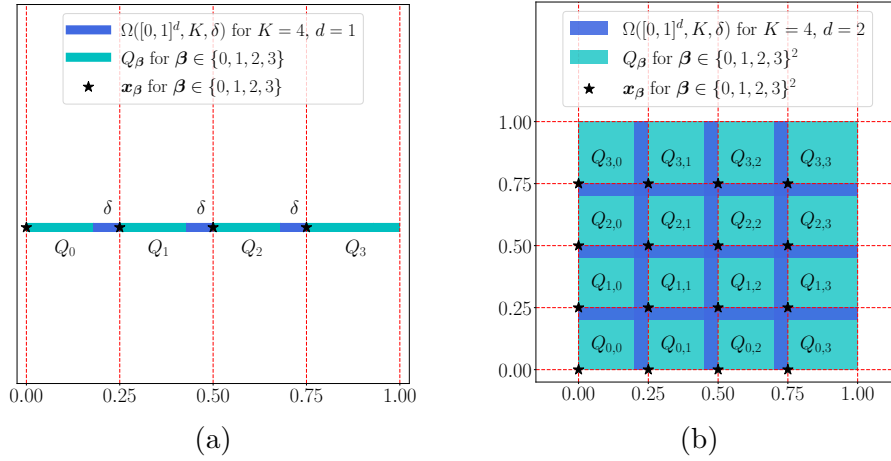


Figure 6: Illustrations of $\Omega([0,1]^d, K, \delta)$, Q_β , and \mathbf{x}_β for $\beta \in \{0, 1, \dots, K-1\}^d$. (a) $K=4$ and $d=1$. (b) $K=4$ and $d=2$.

703 For any $\beta \in \{0, 1, \dots, K-1\}^d$ and $\mathbf{x} \in Q_\beta$, there exists $\xi_{\mathbf{x}} \in (0, 1)$ such that

$$705 \quad f(\mathbf{x}) = \underbrace{\sum_{\|\alpha\|_1 \leq s-1} \frac{\partial^\alpha f(\mathbf{x}_\beta)}{\alpha!} \mathbf{h}^\alpha}_{\mathcal{T}_1} + \underbrace{\sum_{\|\alpha\|_1 = s} \frac{\partial^\alpha f(\mathbf{x}_\beta + \xi_{\mathbf{x}} \mathbf{h})}{\alpha!} \mathbf{h}^\alpha}_{\mathcal{T}_2} =: \mathcal{T}_1 + \mathcal{T}_2, \quad (4.1)$$

706 where $\mathbf{h}(\mathbf{x}) = \mathbf{x} - \mathbf{x}_\beta = \mathbf{x} - \beta/K$. Clearly, the magnitude of \mathcal{T}_2 is bounded by $\mathcal{O}(K^{-s}) =$
 707 $\mathcal{O}(N^{-2s/d}L^{-2s/d})$. So we only need to construct a ReLU FNN with width $\mathcal{O}(N \ln N)$ and
 708 depth $\mathcal{O}(L \ln L)$ to approximate

$$709 \quad \mathcal{T}_1 = \sum_{\|\alpha\|_1 \leq s-1} \frac{\partial^\alpha f(\mathbf{x}_\beta)}{\alpha!} \mathbf{h}^\alpha$$

710 within an error $\mathcal{O}(N^{-2s/d}L^{-2s/d})$. To approximate \mathcal{T}_1 well by ReLU FNNs, we need three
 711 key steps as follows.

^⑥ $\sum_{\|\alpha\|_1=s}$ is short for $\sum_{\|\alpha\|_1=s, \alpha \in \mathbb{N}^d}$. The same notation is used throughout this paper.

- 712 (i) Construct a ReLU FNN to implement a function $P_{\alpha} : \mathbb{R}^d \rightarrow \mathbb{R}$ approximating the
 713 polynomial \mathbf{h}^{α} well for each $\alpha \in \mathbb{N}^d$ with $\|\alpha\|_1 \leq s - 1$.
- 714 (ii) Construct a ReLU FNN to implement a vector-valued function $\Psi : \mathbb{R}^d \rightarrow \mathbb{R}^d$ pro-
 715 jecting the whole cube Q_{β} to a point $\mathbf{x}_{\beta} = \frac{\beta}{K}$, i.e., $\Psi(\mathbf{x}) = \mathbf{x}_{\beta}$ for any $\mathbf{x} \in Q_{\beta}$ and
 716 each $\beta \in \{0, 1, \dots, K - 1\}^d$.
- 717 (iii) Construct a ReLU FNN to implement a function $\phi_{\alpha} : \mathbb{R}^d \rightarrow \mathbb{R}$ approximating $\partial^{\alpha} f$
 718 via solving a point fitting problem, i.e., ϕ_{α} should fit $\partial^{\alpha} f$ well at all points in
 719 $\{\mathbf{x}_{\beta} : \beta \in \{0, 1, \dots, K - 1\}^d\}$ for each $\alpha \in \mathbb{N}^d$ with $\|\alpha\|_1 \leq s - 1$. That is, for each
 720 $\alpha \in \mathbb{N}^d$ with $\|\alpha\|_1 \leq s - 1$, we need to design ϕ_{α} satisfying

$$721 \quad |\phi_{\alpha}(\mathbf{x}_{\beta}) - \partial^{\alpha} f(\mathbf{x}_{\beta})| \leq \mathcal{O}(N^{-2s/d} L^{-2s/d}) \quad \text{for any } \beta \in \{0, 1, \dots, K - 1\}^d. \quad (4.2)$$

722 We will establish three propositions corresponding to these three steps above. They
 723 will be applied to support the construction of the desired ReLU FNNs. Their proofs will
 724 be available in Section 5.

725 First, we establish a general proposition, Proposition 4.1 below, showing how to use
 726 ReLU FNNs to approximate multivariate polynomials. With Proposition 4.1 in hand,
 727 Step (i) is straightforward.

728 **Proposition 4.1.** *Assume $P(\mathbf{x}) = \mathbf{x}^{\alpha} = x_1^{\alpha_1} x_2^{\alpha_2} \dots x_d^{\alpha_d}$ for $\alpha \in \mathbb{N}^d$ with $\|\alpha\|_1 \leq k \in \mathbb{N}^+$.
 729 For any $N, L \in \mathbb{N}^+$, there exists a function ϕ implemented by a ReLU FNN with width
 730 $9(N + 1) + k - 1$ and depth $7k^2 L$ such that*

$$731 \quad |\phi(\mathbf{x}) - P(\mathbf{x})| \leq 9k(N + 1)^{-7kL} \quad \text{for any } \mathbf{x} \in [0, 1]^d.$$

732 Proposition 4.1 shows that ReLU FNNs with width $\mathcal{O}(N)$ and depth $\mathcal{O}(L)$ are
 733 able to approximate polynomials with an error $\mathcal{O}(N^{-L})$. This reveals the power of
 734 depth in ReLU FNNs for approximating polynomials, from the perspective of function
 735 compositions. The starting point of a good approximation of functions is to approximate
 736 polynomials with high accuracy. In classical approximation theory, the approximation
 737 power of any numerical scheme depends on the degree of polynomials that can be locally
 738 reproduced. Being able to approximate polynomials by ReLU FNNs with high accuracy
 739 plays a vital role in the proof of Theorem 1.1. It is interesting to study whether there
 740 is any other function space with reasonable size, besides polynomial space, having an
 741 exponential error $\mathcal{O}(N^{-L})$ when approximated by ReLU FNNs. Obviously, the space of
 742 smooth functions is too big due to the optimality of Theorem 1.1 as shown in Section 2.3.

743 Proposition 4.1 can be generalized to the case of polynomials defined on an arbitrary
 744 hypercube $[a, b]^d$. Let us give an example for the polynomial xy below. Its proof will be
 745 provided later in Section 5.1.

746 **Lemma 4.2.** *For any $N, L \in \mathbb{N}^+$ and $a, b \in \mathbb{R}$ with $a < b$, there exists a function ϕ
 747 implemented by a ReLU FNN with width $9N + 1$ and depth L such that*

$$748 \quad |\phi(x, y) - xy| \leq 6(b - a)^2 N^{-L} \quad \text{for any } x, y \in [a, b].$$

Second, our goal is to construct a step function Ψ mapping $\mathbf{x} \in Q_\beta$ to $\mathbf{x}_\beta = \frac{\beta}{K}$ for any $\beta \in \{0, 1, \dots, K-1\}^d$. We only need to approximate one-dimensional step functions, because in the multidimensional case we can simply set $\Psi(\mathbf{x}) = [\psi(x_1), \psi(x_2), \dots, \psi(x_d)]^T$, where ψ is a one-dimensional step function. Therefore, to implement Step (ii), we need to construct ReLU FNNs with width $\mathcal{O}(N)$ and depth $\mathcal{O}(L)$ to approximate one-dimensional step functions with $\mathcal{O}(K) = \mathcal{O}(N^{2/d}L^{2/d})$ “steps” as shown in Proposition 4.3 below.

Proposition 4.3. *For any $N, L, d \in \mathbb{N}^+$ and $\delta \in (0, \frac{1}{3K}]$ with $K = \lfloor N^{1/d} \rfloor^2 \lfloor L^{2/d} \rfloor$, there exists a one-dimensional function ϕ implemented by a ReLU FNN with width $4\lfloor N^{1/d} \rfloor + 3$ and depth $4L + 5$ such that*

$$\phi(x) = k \quad \text{if } x \in \left[\frac{k}{K}, \frac{k+1}{K} - \delta \cdot \mathbb{1}_{\{k \leq K-2\}}\right] \quad \text{for } k = 0, 1, \dots, K-1.$$

Next, the aim of Step (iii) is to construct ϕ_α implemented by a ReLU FNN such that Equation (4.2) holds for each α . To this end, we establish a proposition, Proposition 4.4 below, to show that ReLU FNNs with width $\mathcal{O}(sN \ln N)$ and depth $\mathcal{O}(L \ln L)$ can be constructed to fit $N^2 L^2$ points within an error $N^{-2s} L^{-2s}$.

Proposition 4.4. *Given any $N, L, s \in \mathbb{N}^+$ and $\xi_i \in [0, 1]$ for $i = 0, 1, \dots, N^2 L^2 - 1$, there exists a function ϕ implemented by a ReLU FNN with width $16s(N+1) \log_2(8N)$ and depth $5(L+2) \log_2(4L)$ such that*

$$(i) \quad |\phi(i) - \xi_i| \leq N^{-2s} L^{-2s} \quad \text{for } i = 0, 1, \dots, N^2 L^2 - 1;$$

$$(ii) \quad 0 \leq \phi(x) \leq 1 \quad \text{for any } x \in \mathbb{R}.$$

The proofs of Propositions 4.1, 4.3, and 4.4 can be found in Sections 5.1, 5.2, and 5.3, respectively. The main ideas of proving Theorem 1.1 are summarized in Table 2.

Table 2: A list of sub-networks for approximating smooth functions. Recall that $\mathbf{h} = \mathbf{x} - \Psi(\mathbf{x}) = \mathbf{x} - \mathbf{x}_\beta$ for $\mathbf{x} \in Q_\beta$.

target function	function implemented by network	width	depth	approximation error
step function	$\Psi(\mathbf{x})$	$\mathcal{O}(N)$	$\mathcal{O}(L)$	no error outside $\Omega([0, 1]^d, K, \delta)$
$x_1 x_2$	$\varphi(x_1, x_2)$	$\mathcal{O}(N)$	$\mathcal{O}(L)$	$\mathcal{E}_1 = 216(N+1)^{-2s(L+1)}$
\mathbf{h}^α	$P_\alpha(\mathbf{h})$	$\mathcal{O}(N)$	$\mathcal{O}(L)$	$\mathcal{E}_2 = 9s(N+1)^{-7sL}$
$\partial^\alpha f(\Psi(\mathbf{x}))$	$\phi_\alpha(\Psi(\mathbf{x}))$	$\mathcal{O}(N \ln N)$	$\mathcal{O}(L \ln L)$	$\mathcal{E}_3 = 2N^{-2s} L^{-2s}$
$\sum_{\ \alpha\ \leq s-1} \frac{\partial^\alpha f(\Psi(\mathbf{x}))}{\alpha!} \mathbf{h}^\alpha$	$\sum_{\ \alpha\ \leq s-1} \varphi\left(\frac{\phi_\alpha(\Psi(\mathbf{x}))}{\alpha!}, P_\alpha(\mathbf{h})\right)$	$\mathcal{O}(N \ln N)$	$\mathcal{O}(L \ln L)$	$\mathcal{O}(\mathcal{E}_1 + \mathcal{E}_2 + \mathcal{E}_3)$
$f(\mathbf{x})$	$\phi(\mathbf{x}) := \sum_{\ \alpha\ \leq s-1} \varphi\left(\frac{\phi_\alpha(\Psi(\mathbf{x}))}{\alpha!}, P_\alpha(\mathbf{x} - \Psi(\mathbf{x}))\right)$	$\mathcal{O}(N \ln N)$	$\mathcal{O}(L \ln L)$	$\mathcal{O}(\ \mathbf{h}\ _2^{-s} + \mathcal{E}_1 + \mathcal{E}_2 + \mathcal{E}_3) \leq \mathcal{O}(K^{-s}) = \mathcal{O}(N^{-2s/d} L^{-2s/d})$

Finally, we would like to compare our analysis with that in [46]. Both [46] and our analysis rely on local Taylor expansions as in Equation (4.1) to approximate the target function f . Both analysis methods construct ReLU FNNs to approximate polynomials and encode the Taylor expansion coefficients into ReLU FNNs. However, the way to localize the Taylor expansion (i.e., defining the local neighborhood such that the expansion is valid) and the approach to constructing ReLU FNNs are different. We will discuss the details as follows.

Localization. In [46], a “two-scale” partition procedure and a standard triangulation divide $[0, 1]^d$ into simplexes and a partition of unity is constructed using compactly supported functions that are linear on each simplex, which implies that these functions in the partition of unity can be represented by ReLU FNNs. Taylor expansions of f are constructed within each support of the functions in the partition of unity. In this paper, we simply divide the domain into small hypercubes of uniform size as visualized in Figure 6. Taylor expansions of f are constructed within each hypercube. The reader can understand our approach as a simple way to construct a partition of unity using piecewise constant functions with binary values. The introduction of the trifling region allows us to simply construct ReLU FNNs to approximate these piecewise constant functions without caring about the approximation error within the trifling region. Hence, our construction can be much simplified and makes it easy to estimate all constant prefactors in our error estimates, which is challenging in [46].

ReLU FNNs for Taylor expansions. In [46], very deep ReLU FNNs with width $\mathcal{O}(1)$ are constructed to approximate polynomials in local Taylor expansions, and hence, the optimal approximation error in width was not explored in [46]. In this paper, we construct ReLU FNNs with arbitrary width and depth to approximate polynomials in local Taylor expansions using Proposition 4.1, which allows us to explore the optimal approximation error in width and is more challenging. In [46], the coefficients of adjacent local Taylor expansions, i.e., $\partial^\alpha f$ in Equation (4.1), are encoded into ReLU FNNs via bit extraction, which is the key to achieving a better approximation error of ReLU FNNs to approximate f than the original local Taylor expansions, since the number of coefficients can be significantly reduced via encoding. Actually, the error in depth by bit extraction is nearly optimal. In this paper, the approximation to $\partial^\alpha f$ is reduced to a point fitting problem that can be solved by constructing ReLU FNNs using bit extraction as sketched out in the previous paragraphs. Hence, we can also achieve the optimal approximation error in depth. The key to achieving the optimal approximation error in width in the above approximation is the application of Lemma 5.4 that essentially fits $\mathcal{O}(N^2)$ samples with ReLU FNNs of width $\mathcal{O}(N)$ and depth 2. Due to the simplicity of our analysis, we can construct ReLU FNNs with arbitrary width and depth to approximate f and specify all constant prefactors in our approximation error.

4.2 Constructive proof

According to the key ideas of proving Theorem 2.2 summarized in Section 4.1, let us present the detailed proof.

Proof of Theorem 2.2. The detailed proof can be divided into four steps as follows.

Step 1: Set up.

Set $K = \lfloor N^{1/d} \rfloor^2 \lfloor L^{2/d} \rfloor$ and let $\Omega([0, 1]^d, K, \delta)$ partition $[0, 1]^d$ into K^d cubes Q_β for $\beta \in \{0, 1, \dots, K-1\}^d$. In particular, for each $\beta = [\beta_1, \beta_2, \dots, \beta_d]^T \in \{0, 1, \dots, K-1\}^d$, we define $\mathbf{x}_\beta := \beta/K$ and

$$Q_\beta := \{\mathbf{x} = [x_1, x_2, \dots, x_d]^T : x_i \in [\frac{\beta_i}{K}, \frac{\beta_i+1}{K} - \delta \cdot \mathbf{1}_{\{\beta_i \leq K-2\}}]\} \text{ for } i = 1, 2, \dots, d\}.$$

Clearly, $[0, 1]^d = \Omega([0, 1]^d, K, \delta) \cup (\cup_{\beta \in \{0, 1, \dots, K-1\}^d} Q_\beta)$ and \mathbf{x}_β is the vertex of Q_β with minimum $\|\cdot\|_1$ norm. See Figure 6 for the illustrations of Q_β and \mathbf{x}_β .

820 By Proposition 4.3, there exists $\psi \in \mathcal{NN}(\text{width} \leq 4N + 3; \text{depth} \leq 4N + 5)$ such that

$$821 \quad \psi(x) = k \quad \text{if } x \in \left[\frac{k}{K}, \frac{k+1}{K} - \delta \cdot \mathbb{1}_{\{k \leq K-2\}}\right] \quad \text{for } k = 0, 1, \dots, K-1.$$

822 Then for each $\beta \in \{0, 1, \dots, K-1\}^d$, $\psi(x_i) = \beta_i$ for all $\mathbf{x} \in Q_\beta$ for $i = 1, 2, \dots, d$.

823 Define

$$824 \quad \Psi(\mathbf{x}) := [\psi(x_1), \psi(x_2), \dots, \psi(x_d)]^T / K \quad \text{for any } \mathbf{x} \in [0, 1]^d,$$

825 then

$$826 \quad \Psi(\mathbf{x}) = \beta / K = \mathbf{x}_\beta \quad \text{if } \mathbf{x} \in Q_\beta \quad \text{for } \beta \in \{0, 1, \dots, K-1\}^d.$$

827 For any $\mathbf{x} \in Q_\beta$ and $\beta \in \{0, 1, \dots, K-1\}^d$, by the Taylor expansion, there exists
828 $\xi_{\mathbf{x}} \in (0, 1)$ such that

$$829 \quad f(\mathbf{x}) = \sum_{\|\alpha\|_1 \leq s-1} \frac{\partial^\alpha f(\Psi(\mathbf{x}))}{\alpha!} \mathbf{h}^\alpha + \sum_{\|\alpha\|_1 = s} \frac{\partial^\alpha f(\Psi(\mathbf{x}) + \xi_{\mathbf{x}} \mathbf{h})}{\alpha!} \mathbf{h}^\alpha, \quad \text{where } \mathbf{h} = \mathbf{x} - \Psi(\mathbf{x}).$$

830 **Step 2:** Construct the desired function ϕ .

831 By Lemma 4.2, there exists

$$832 \quad \varphi \in \mathcal{NN}(\text{width} \leq 9(N+1) + 1; \text{depth} \leq 2s(L+1))$$

833 such that

$$834 \quad |\varphi(x_1, x_2) - x_1 x_2| \leq 216(N+1)^{-2s(L+1)} =: \mathcal{E}_1 \quad \text{for any } x_1, x_2 \in [-3, 3]. \quad (4.3)$$

835 For each $\alpha \in \mathbb{N}^d$ with $\|\alpha\|_1 \leq s$, by Proposition 4.1, there exists

$$836 \quad P_\alpha \in \mathcal{NN}(\text{width} \leq 9(N+1) + s-1; \text{depth} \leq 7s^2 L)$$

837 such that

$$838 \quad |P_\alpha(\mathbf{x}) - \mathbf{x}^\alpha| \leq 9s(N+1)^{-7sL} =: \mathcal{E}_2 \quad \text{for any } \mathbf{x} \in [0, 1]^d. \quad (4.4)$$

839 For each $i \in \{0, 1, \dots, K^d - 1\}$, define

$$840 \quad \boldsymbol{\eta}(i) = [\eta_1, \eta_2, \dots, \eta_d]^T \in \{0, 1, \dots, K-1\}^d$$

841 such that $\sum_{j=1}^d \eta_j K^{j-1} = i$. Such a map $\boldsymbol{\eta}$ is a bijection from $\{0, 1, \dots, K^d - 1\}$ to $\{0, 1, \dots, K-1\}^d$. For each $\alpha \in \mathbb{N}^d$ with $\|\alpha\|_1 \leq s-1$, define

$$843 \quad \xi_{\alpha, i} = (\partial^\alpha f(\frac{\boldsymbol{\eta}(i)}{K}) + 1)/2 \quad \text{for } i \in \{0, 1, \dots, K^d - 1\}.$$

844 Then $\|\partial^\alpha f\|_{L^\infty([0,1]^d)} \leq 1$ implies $\xi_{\alpha, i} \in [0, 1]$ for $i = 0, 1, \dots, K^d - 1$ and each α . Note that
845 $K^d = (\lfloor N^{1/d} \rfloor^2 \lfloor L^{2/d} \rfloor)^d \leq N^2 L^2$. By Proposition 4.4, there exists

$$846 \quad \widetilde{\phi}_\alpha \in \mathcal{NN}(\text{width} \leq 16s(N+1) \log_2(8N); \text{depth} \leq 5(L+2) \log_2(4L))$$

847 such that, for each $\alpha \in \mathbb{N}^d$ with $\|\alpha\|_1 \leq s-1$, we have

$$848 \quad |\widetilde{\phi}_\alpha(i) - \xi_{\alpha, i}| \leq N^{-2s} L^{-2s} \quad \text{for } i = 0, 1, \dots, K^d - 1.$$

For each $\alpha \in \mathbb{N}^d$ with $\|\alpha\|_1 \leq s-1$, define

$$\phi_\alpha(\mathbf{x}) := 2\tilde{\phi}_\alpha\left(\sum_{j=1}^d x_j K^{j-1}\right) - 1 \quad \text{for any } \mathbf{x} = [x_1, x_2, \dots, x_d]^T \in \mathbb{R}^d.$$

It is easy to verify that

$$\phi_\alpha \in \mathcal{NN}(\text{width} \leq 16s(N+1)\log_2(8N); \text{depth} \leq 5(L+2)\log_2(4L)).$$

Then, for each $\alpha \in \mathbb{N}^d$ with $\|\alpha\|_1 \leq s-1$ and each $\eta = \eta(i) = [\eta_1, \eta_2, \dots, \eta_d]^T \in \{0, 1, \dots, K-1\}^d$ corresponding to $i = \sum_{j=1}^d \eta_j K^{j-1} \in \{0, 1, \dots, K^d - 1\}$, we have

$$\begin{aligned} \left| \phi_\alpha\left(\frac{\eta}{K}\right) - \partial^\alpha f\left(\frac{\eta}{K}\right) \right| &= \left| 2\tilde{\phi}_\alpha\left(\sum_{j=1}^d \eta_j K^{j-1}\right) - 1 - (2\xi_{\alpha,i} - 1) \right| \\ &= 2|\tilde{\phi}_\alpha(i) - \xi_{\alpha,i}| \leq 2N^{-2s}L^{-2s}. \end{aligned}$$

Therefore, for each $\beta \in \{0, 1, \dots, K-1\}^d$ and each $\alpha \in \mathbb{N}^d$ with $\|\alpha\|_1 \leq s-1$, we have

$$\left| \phi_\alpha(\mathbf{x}_\beta) - \partial^\alpha f(\mathbf{x}_\beta) \right| = \left| \phi_\alpha\left(\frac{\beta}{K}\right) - \partial^\alpha f\left(\frac{\beta}{K}\right) \right| \leq 2N^{-2s}L^{-2s} =: \mathcal{E}_3. \quad (4.5)$$

Now we can construct the desired function ϕ as

$$\phi(\mathbf{x}) := \sum_{\|\alpha\|_1 \leq s-1} \varphi\left(\frac{\phi_\alpha(\Psi(\mathbf{x}))}{\alpha!}, P_\alpha(\mathbf{x} - \Psi(\mathbf{x}))\right) \quad \text{for any } \mathbf{x} \in \mathbb{R}^d. \quad (4.6)$$

It remains to estimate the approximation error and determine the size of the network implementing ϕ .

Step 3: Estimate approximation error.

Fix $\beta \in \{0, 1, \dots, K-1\}^d$, let us estimate the approximation error for a fixed $\mathbf{x} \in Q_\beta$. See Table 2 for a summary of the approximation errors. Recall that $\Psi(\mathbf{x}) = \mathbf{x}_\beta$ and $\mathbf{h} = \mathbf{x} - \Psi(\mathbf{x}) = \mathbf{x} - \mathbf{x}_\beta$. It is easy to check that $|f(\mathbf{x}) - \phi(\mathbf{x})|$ is bounded by

$$\begin{aligned} &\left| \sum_{\|\alpha\|_1 \leq s-1} \frac{\partial^\alpha f(\Psi(\mathbf{x}))}{\alpha!} \mathbf{h}^\alpha + \sum_{\|\alpha\|_1 = s} \frac{\partial^\alpha f(\Psi(\mathbf{x}) + \xi_{\mathbf{x}} \mathbf{h})}{\alpha!} \mathbf{h}^\alpha - \sum_{\|\alpha\|_1 \leq s-1} \varphi\left(\frac{\phi_\alpha(\Psi(\mathbf{x}))}{\alpha!}, P_\alpha(\mathbf{x} - \Psi(\mathbf{x}))\right) \right| \\ &\leq \underbrace{\sum_{\|\alpha\|_1 = s} \left| \frac{\partial^\alpha f(\mathbf{x}_\beta + \xi_{\mathbf{x}} \mathbf{h})}{\alpha!} \mathbf{h}^\alpha \right|}_{\mathcal{I}_1} + \underbrace{\sum_{\|\alpha\|_1 \leq s-1} \left| \frac{\partial^\alpha f(\mathbf{x}_\beta)}{\alpha!} \mathbf{h}^\alpha - \varphi\left(\frac{\phi_\alpha(\mathbf{x}_\beta)}{\alpha!}, P_\alpha(\mathbf{h})\right) \right|}_{\mathcal{I}_2} =: \mathcal{I}_1 + \mathcal{I}_2. \end{aligned}$$

Recall the fact that

$$\sum_{\|\alpha\|_1 = s} 1 = |\{\alpha \in \mathbb{N}^d : \|\alpha\|_1 = s\}| \leq (s+1)^{d-1} \quad \textcircled{7}$$

and

$$\sum_{\|\alpha\|_1 \leq s-1} 1 = \sum_{i=0}^{s-1} \left(\sum_{\|\alpha\|_1 = i} 1 \right) \leq \sum_{i=0}^{s-1} (i+1)^{d-1} \leq s \cdot (s-1+1)^{d-1} = s^d.$$

$\textcircled{7}$ In fact, we have $|\{\alpha \in \mathbb{N}^d : \|\alpha\|_1 = s\}| = \binom{s+d-1}{d-1}$, implying $(s/d+1)^{d-1} \leq \sum_{\|\alpha\|_1 = s} 1 \leq (s+1)^{d-1}$. Thus, the lower bound of the estimate is still exponentially large in d . To the best of our knowledge, we cannot avoid a constant prefactor that is exponentially large in d when Taylor expansion is used in the analysis.

871 For the first part \mathcal{J}_1 , we have

$$872 \quad \mathcal{J}_1 = \sum_{\|\alpha\|_1=s} \left| \frac{\partial^\alpha f(\mathbf{x}_\beta + \xi \mathbf{h})}{\alpha!} \mathbf{h}^\alpha \right| \leq \sum_{\|\alpha\|_1=s} \left| \frac{1}{\alpha!} \mathbf{h}^\alpha \right| \leq (s+1)^{d-1} K^{-s}.$$

873 For the second part \mathcal{J}_2 , we have

$$874 \quad \mathcal{J}_2 = \sum_{\|\alpha\|_1 \leq s-1} \underbrace{\left| \frac{\partial^\alpha f(\mathbf{x}_\beta)}{\alpha!} \mathbf{h}^\alpha - \varphi\left(\frac{\phi_\alpha(\mathbf{x}_\beta)}{\alpha!}, P_\alpha(\mathbf{h})\right) \right|}_{\mathcal{J}_2(\alpha)} =: \sum_{\|\alpha\|_1 \leq s-1} \mathcal{J}_2(\alpha).$$

875 Fix $\alpha \in \mathbb{N}^d$ with $\|\alpha\|_1 \leq s-1$, we have

$$\begin{aligned} \mathcal{J}_2(\alpha) &= \left| \frac{\partial^\alpha f(\mathbf{x}_\beta)}{\alpha!} \mathbf{h}^\alpha - \varphi\left(\frac{\phi_\alpha(\mathbf{x}_\beta)}{\alpha!}, P_\alpha(\mathbf{h})\right) \right| \\ 876 \quad &\leq \underbrace{\left| \frac{\partial^\alpha f(\mathbf{x}_\beta)}{\alpha!} \mathbf{h}^\alpha - \varphi\left(\frac{\partial^\alpha f(\mathbf{x}_\beta)}{\alpha!}, P_\alpha(\mathbf{h})\right) \right|}_{\mathcal{J}_{2,1}(\alpha)} + \underbrace{\left| \varphi\left(\frac{\partial^\alpha f(\mathbf{x}_\beta)}{\alpha!}, P_\alpha(\mathbf{h})\right) - \varphi\left(\frac{\phi_\alpha(\mathbf{x}_\beta)}{\alpha!}, P_\alpha(\mathbf{h})\right) \right|}_{\mathcal{J}_{2,2}(\alpha)} \\ &=: \mathcal{J}_{2,1}(\alpha) + \mathcal{J}_{2,2}(\alpha). \end{aligned}$$

877 Note that $\mathcal{E}_2 = 9s(N+1)^{-7sL} \leq 9s(2)^{-7s} \leq 2$. By $\mathbf{h}^\alpha \in [0, 1]$ and Equation (4.4), we
878 have $P_\alpha(\mathbf{h}) \in [-2, 3] \subseteq [-3, 3]$. Then by $\partial^\alpha f(\mathbf{x}_\beta) \in [-1, 1]$ and Equations (4.3) and (4.4),
879 we have

$$\begin{aligned} \mathcal{J}_{2,1}(\alpha) &= \left| \frac{\partial^\alpha f(\mathbf{x}_\beta)}{\alpha!} \mathbf{h}^\alpha - \varphi\left(\frac{\partial^\alpha f(\mathbf{x}_\beta)}{\alpha!}, P_\alpha(\mathbf{h})\right) \right| \\ &\leq \left| \frac{\partial^\alpha f(\mathbf{x}_\beta)}{\alpha!} \mathbf{h}^\alpha - \frac{\partial^\alpha f(\mathbf{x}_\beta)}{\alpha!} P_\alpha(\mathbf{h}) \right| + \underbrace{\left| \frac{\partial^\alpha f(\mathbf{x}_\beta)}{\alpha!} P_\alpha(\mathbf{h}) - \varphi\left(\frac{\partial^\alpha f(\mathbf{x}_\beta)}{\alpha!}, P_\alpha(\mathbf{h})\right) \right|}_{\leq \mathcal{E}_1 \text{ by Eq. (4.3)}} \\ 880 \quad &\leq \frac{1}{\alpha!} \underbrace{|\mathbf{h}^\alpha - P_\alpha(\mathbf{h})|}_{\leq \mathcal{E}_2 \text{ by Eq. (4.4)}} + \mathcal{E}_1 \leq \frac{1}{\alpha!} \mathcal{E}_2 + \mathcal{E}_1 \leq \mathcal{E}_1 + \mathcal{E}_2. \end{aligned}$$

881 To estimate $\mathcal{J}_{2,2}(\alpha)$, we need the following fact derived from Equation (4.3):

$$\begin{aligned} |\varphi(x_1, x_2) - \varphi(\tilde{x}_1, x_2)| &\leq \underbrace{|\varphi(x_1, x_2) - x_1 x_2|}_{\leq \mathcal{E}_1 \text{ by Eq. (4.3)}} + \underbrace{|\varphi(\tilde{x}_1, x_2) - \tilde{x}_1 x_2|}_{\leq \mathcal{E}_1 \text{ by Eq. (4.3)}} + |x_1 x_2 - \tilde{x}_1 x_2| \\ 882 \quad &\leq 2\mathcal{E}_1 + 3|x_1 - \tilde{x}_1|, \end{aligned} \tag{4.7}$$

883 for any $x_1, \tilde{x}_1, x_2 \in [-3, 3]$.

884 Since $\mathcal{E}_3 = 2N^{-2s}L^{-2s} \leq 2$ and $\partial^\alpha f(\mathbf{x}_\beta) \in [-1, 1]$, we have $\phi_\alpha(\mathbf{x}_\beta) \in [-3, 3]$ by
885 Equation (4.5). Then by $P_\alpha(\mathbf{h}) \in [-3, 3]$ and Equations (4.7) and (4.5), we have

$$\begin{aligned} \mathcal{J}_{2,2}(\alpha) &= \left| \varphi\left(\frac{\partial^\alpha f(\mathbf{x}_\beta)}{\alpha!}, P_\alpha(\mathbf{h})\right) - \varphi\left(\frac{\phi_\alpha(\mathbf{x}_\beta)}{\alpha!}, P_\alpha(\mathbf{h})\right) \right| \\ 886 \quad &\leq 2\mathcal{E}_1 + 3 \underbrace{\left| \frac{\partial^\alpha f(\mathbf{x}_\beta)}{\alpha!} - \frac{\phi_\alpha(\mathbf{x}_\beta)}{\alpha!} \right|}_{\leq \mathcal{E}_3 \text{ by Eq. (4.5)}} \leq 2\mathcal{E}_1 + 3\mathcal{E}_3. \end{aligned}$$

Therefore, we get

$$\begin{aligned}
|f(\mathbf{x}) - \phi(\mathbf{x})| &\leq \mathcal{I}_1 + \mathcal{I}_2 \leq \mathcal{I}_1 + \sum_{\|\alpha\|_1 \leq s-1} \mathcal{I}_2(\alpha) \leq \mathcal{I}_1 + \sum_{\|\alpha\|_1 \leq s-1} \left(\mathcal{I}_{2,1}(\alpha) + \mathcal{I}_{2,2}(\alpha) \right) \\
&\leq (s+1)^{d-1} K^{-s} + s^d \left((\mathcal{E}_1 + \mathcal{E}_2) + (2\mathcal{E}_1 + 3\mathcal{E}_3) \right) \\
&\leq (s+1)^d (K^{-s} + 3\mathcal{E}_1 + \mathcal{E}_2 + 3\mathcal{E}_3).
\end{aligned}$$

Since $\beta \in \{0, 1, \dots, K-1\}^d$ and $\mathbf{x} \in Q_\beta$ are arbitrary and

$$[0, 1]^d = \Omega([0, 1]^d, K, \delta) \cup \left(\cup_{\beta \in \{0, 1, \dots, K-1\}^d} Q_\beta \right),$$

we have, for any $\mathbf{x} \in [0, 1]^d \setminus \Omega([0, 1]^d, K, \delta)$,

$$|f(\mathbf{x}) - \phi(\mathbf{x})| \leq (s+1)^d (K^{-s} + 3\mathcal{E}_1 + \mathcal{E}_2 + 3\mathcal{E}_3).$$

Recall that $K = \lfloor N^{1/d} \rfloor^2 \lfloor L^{2/d} \rfloor \geq \frac{N^{2/d} L^{2/d}}{8}$ and

$$(N+1)^{-7sL} \leq (N+1)^{-2s(L+1)} \leq (N+1)^{-2s} 2^{-2sL} \leq N^{-2s} L^{-2s}.$$

Then we have

$$\begin{aligned}
&(s+1)^d (K^{-s} + 3\mathcal{E}_1 + \mathcal{E}_2 + 3\mathcal{E}_3) \\
&= (s+1)^d \left(K^{-s} + 648(N+1)^{-2s(L+1)} + 9s(N+1)^{-7sL} + 6N^{-2s} L^{-2s} \right) \\
&\leq (s+1)^d \left(8^s N^{-2s/d} L^{-2s/d} + (654 + 9s) N^{-2s} L^{-2s} \right) \\
&\leq (s+1)^d (8^s + 654 + 9s) N^{-2s/d} L^{-2s/d} \leq 84(s+1)^d 8^s N^{-2s/d} L^{-2s/d}.
\end{aligned}$$

Step 4: Determine the size of the network implementing ϕ .

It remains to estimate the width and depth of the network implementing ϕ . Recall that, for $\alpha \in \mathbb{N}^d$ with $\|\alpha\|_1 \leq s-1$,

$$\begin{cases} \Psi \in \mathcal{NN}(\text{width} \leq d(4N+3); \text{depth} \leq 4L+5), \\ \phi_\alpha \in \mathcal{NN}(\text{width} \leq 16s(N+1)\log_2(8N); \text{depth} \leq 5(L+2)\log_2(4L)), \\ P_\alpha \in \mathcal{NN}(\text{width} \leq 9(N+1)+s-1; \text{depth} \leq 7s^2L), \\ \varphi \in \mathcal{NN}(\text{width} \leq 9(N+1)+1; \text{depth} \leq 2s(L+1)). \end{cases}$$

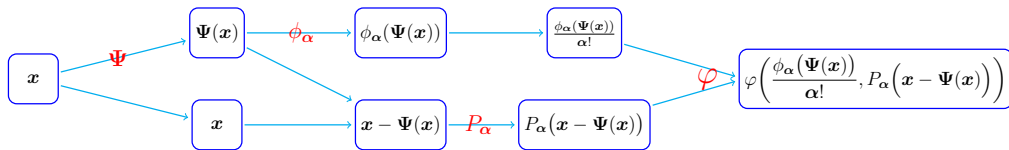


Figure 7: An illustration of the sub-network architecture implementing each component of ϕ , $\varphi\left(\frac{\phi_\alpha(\Psi(\mathbf{x}))}{\alpha!}, P_\alpha(\mathbf{x} - \Psi(\mathbf{x}))\right)$ for each $\alpha \in \mathbb{N}^d$ with $\|\alpha\|_1 \leq s-1$.

By Equation (4.6) and Figure 7, it easy to verify that ϕ can be implemented by a ReLU FNN with width

$$\sum_{\|\alpha\|_1 \leq s-1} 16sd(N+2)\log_2(8N) \leq s^d \cdot 16sd(N+2)\log_2(8N) \\ = 16s^{d+1}d(N+2)\log_2(8N)$$

and depth

$$(4L+5) + 2s(L+1) + 7s^2L + 5(L+2)\log_2(4L) + 3 \leq 18s^2(L+2)\log_2(4L)$$

as desired. So we finish the proof. \square

5 Proofs of Propositions in Section 4.1

In this section, we will prove all propositions in Section 4.1.

5.1 Proof of Proposition 4.1 for polynomial approximation

To prove Proposition 4.1, we will construct ReLU FNNs to approximate multivariate polynomials following the four steps below.

- $f(x) = x^2$. We approximate $f(x) = x^2$ by the combinations and compositions of “sawtooth” functions as shown in Figures 8 and 9.
- $f(x, y) = xy$. To approximate $f(x, y) = xy$, we use the result of the previous step and the fact that $xy = 2\left(\left(\frac{x+y}{2}\right)^2 - \left(\frac{x}{2}\right)^2 - \left(\frac{y}{2}\right)^2\right)$.
- $f(x_1, x_2, \dots, x_k) = x_1x_2 \dots x_k$. We approximate $f(x_1, x_2, \dots, x_k) = x_1x_2 \dots x_k$ for any $k \geq 2$ via mathematical induction based on the result of the previous step.
- A general polynomial $P(\mathbf{x}) = \mathbf{x}^\alpha = x_1^{\alpha_1}x_2^{\alpha_2} \dots x_d^{\alpha_d}$ with $\|\alpha\|_1 \leq k$. Any one-term polynomial of degree $\leq k$ can be written as $Cz_1z_2 \dots z_k$ with some entries equaling 1, where C is a constant and $\mathbf{z} = [z_1, z_2, \dots, z_k]^T$ can be attained via an affine linear map with \mathbf{x} as the input. Then use the result of the previous step.

The idea of using “sawtooth” functions (see Figure 8) was first raised in [44] for approximating x^2 using FNNs with width 6 and depth $\mathcal{O}(L)$ and achieving an error $\mathcal{O}(2^{-L})$; our construction is different from and more general than that in [44], working for ReLU FNNs of width $\mathcal{O}(N)$ and depth $\mathcal{O}(L)$ for any N and L , and achieving an error $\mathcal{O}(N^{-L})$. As discussed below Proposition 4.1, this $\mathcal{O}(N^{-L})$ approximation error of polynomial functions shows the power of depth in ReLU FNNs via function composition.

First, let us show how to construct ReLU FNNs to approximate $f(x) = x^2$.

Lemma 5.1. *For any $N, L \in \mathbb{N}^+$, there exists a function ϕ implemented by a ReLU FNN with width $3N$ and depth L such that*

$$|\phi(x) - x^2| \leq N^{-L} \quad \text{for any } x \in [0, 1].$$

932 *Proof.* Define a set of “sawtooth” functions $T_i : [0, 1] \rightarrow [0, 1]$ by induction as follows.
 933 Set

$$934 \quad T_1(x) = \begin{cases} 2x, & \text{if } x \in [0, \frac{1}{2}], \\ 2(1-x), & \text{if } x \in (\frac{1}{2}, 1], \end{cases}$$

935 and

$$936 \quad T_i = T_{i-1} \circ T_1 \quad \text{for } i = 2, 3, \dots.$$

937 It is easy to check that T_i has 2^{i-1} “sawteeth” and

$$938 \quad T_{m+n} = T_m \circ T_n \quad \text{for any } m, n \in \mathbb{N}^+.$$

See Figure 8 for illustrations of T_i for $i = 1, 2, 3, 4$.

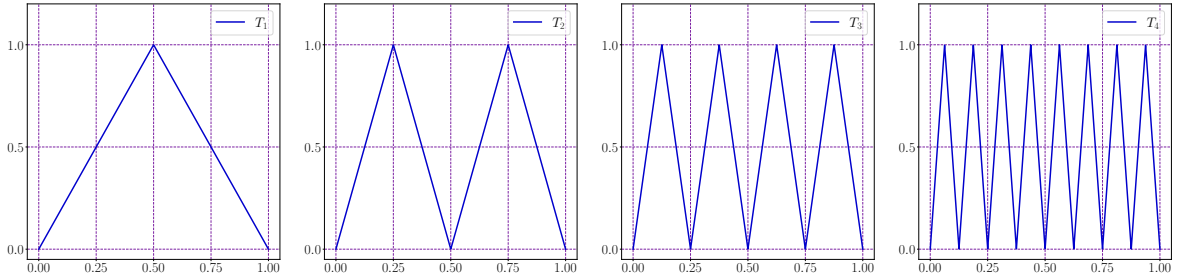


Figure 8: Examples of “sawtooth” functions T_1 , T_2 , T_3 , and T_4 .

939

940 Define piecewise linear functions $f_s : [0, 1] \rightarrow [0, 1]$ for $s \in \mathbb{N}^+$ satisfying the following
 941 two requirements (see Figure 9 for several examples of f_s).

- 942 • $f_s(\frac{j}{2^s}) = (\frac{j}{2^s})^2$ for $j = 0, 1, 2, \dots, 2^s$.
- 943 • $f_s(x)$ is linear between any two adjacent points of $\{\frac{j}{2^s} : j = 0, 1, 2, \dots, 2^s\}$.

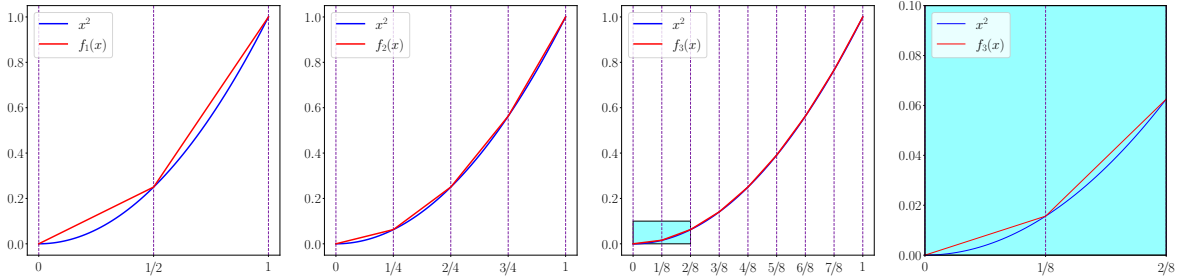


Figure 9: Illustrations of f_1 , f_2 , and f_3 for approximating x^2 .

944 Recall the fact

$$945 \quad 0 \leq tx_1^2 + (1-t)x_2^2 - (tx_1 + (1-t)x_2)^2 \leq \frac{(x_2 - x_1)^2}{4} \quad \text{for any } t, x_1, x_2 \in [0, 1].$$

946 Thus, we have

$$947 \quad 0 \leq f_s(x) - x^2 \leq \frac{(2^{-s})^2}{4} = 2^{-2(s+1)} \quad \text{for any } x \in [0, 1] \text{ and } s \in \mathbb{N}^+. \quad (5.1)$$

948 Note that $f_{i-1}(x) = f_i(x) = x^2$ for $x \in \{\frac{j}{2^{i-1}} : j = 0, 1, 2, \dots, 2^{i-1}\}$ and the graph of $f_{i-1} - f_i$
 949 is a symmetric “sawtooth” between any two adjacent points of $\{\frac{j}{2^{i-1}} : j = 0, 1, 2, \dots, 2^{i-1}\}$.
 950 It is easy to verify that

$$951 \quad f_{i-1}(x) - f_i(x) = \frac{T_i(x)}{2^{2i}} \quad \text{for any } x \in [0, 1] \text{ and } i = 2, 3, \dots.$$

952 Therefore, for any $x \in [0, 1]$ and $s \in \mathbb{N}^+$, we have

$$953 \quad f_s(x) = f_1(x) + \sum_{i=2}^s (f_i - f_{i-1}) = x - (x - f_1(x)) - \sum_{i=2}^s \frac{T_i(x)}{2^{2i}} = x - \sum_{i=1}^s \frac{T_i(x)}{2^{2i}}.$$

954 Given $N \in \mathbb{N}^+$, there exists a unique $k \in \mathbb{N}^+$ such that $(k-1)2^{k-1} + 1 \leq N \leq k2^k$.
 955 For this k , using $s = Lk$, we can construct a ReLU FNN as shown in Figure 10 to
 956 implement a function $\phi = f_{Lk}$ approximating x^2 well. Note that T_i can be implemented
 957 by a one-hidden-layer ReLU FNN with width 2^i . Hence, the network in Figure 10 has
 958 width $k2^k + 1 \leq 3N$ ^⑧ and depth $2L$.

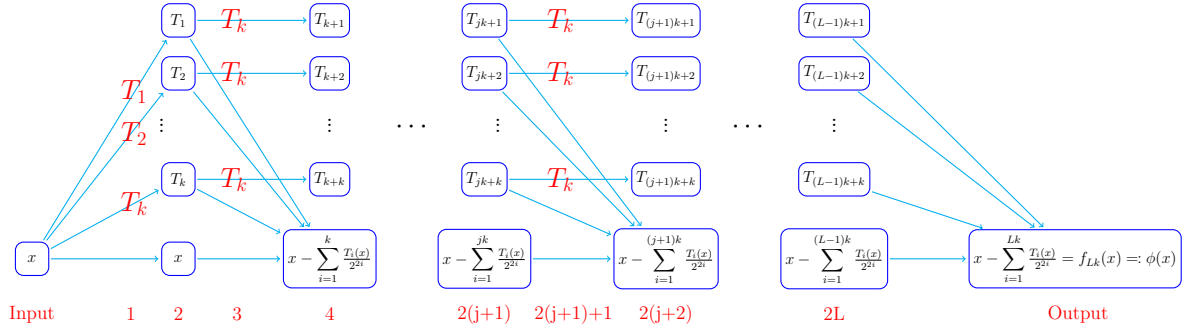


Figure 10: An illustration of the target network architecture for approximating x^2 on $[0, 1]$. T_i can be implemented by a one-hidden-layer ReLU FNN with width 2^i for $i = 1, 2, \dots, K$. The red numbers below the architecture indicate the order of hidden layers.

959 As shown in Figure 10, the (2ℓ) -th hidden layer of the network has the identify
 960 function as activation functions for $\ell = 1, 2, \dots, L$. Thus, the network in Figure 10 can
 961 be interpreted as a ReLU FNN with width $3N$ and depth L . In fact, if all activation
 962 functions in a certain hidden layer are identity maps, the depth can be reduced by one via
 963 combining two adjacent linear transforms into one. For example, suppose $\mathbf{W}_1 \in \mathbb{R}^{N_1 \times N_2}$,
 964 $\mathbf{W}_2 \in \mathbb{R}^{N_2 \times N_3}$, and ϱ is an identity map that can be applied to vectors or matrices
 965 elementwisely; then $\mathbf{W}_1 \varrho(\mathbf{W}_2 \mathbf{x}) = \mathbf{W}_3 \mathbf{x}$ for any $\mathbf{x} \in \mathbb{R}^{N_3}$, where $\mathbf{W}_3 = \mathbf{W}_1 \cdot \mathbf{W}_2 \in \mathbb{R}^{N_1 \times N_3}$.

966 It remains to estimate the approximation error of $\phi(x) \approx x^2$. By Equation (5.1), for
 967 any $x \in [0, 1]$, we have

$$968 \quad |\phi(x) - x^2| = |f_{Lk}(x) - x^2| \leq 2^{-2(Lk+1)} \leq 2^{-2Lk} \leq N^{-L},$$

969 where the last inequality comes from $N \leq k2^k \leq 2^{2k}$. So we finish the proof. \square

^⑧This inequality is clear for $k = 1, 2, 3, 4$. In the case $k \geq 5$, we have $k2^k + 1 \leq \frac{k2^k+1}{N}N \leq \frac{(k+1)2^k}{(k-1)2^{k-1}}N \leq 2\frac{k+1}{k-1}N \leq 3N$.

We have constructed a ReLU FNN to approximate $f(x) = x^2$. By the fact that $xy = 2\left(\left(\frac{x+y}{2}\right)^2 - \left(\frac{x}{2}\right)^2 - \left(\frac{y}{2}\right)^2\right)$, it is easy to construct a new ReLU FNN to approximate $f(x, y) = xy$ as follows.

Lemma 5.2. *For any $N, L \in \mathbb{N}^+$, there exists a function ϕ implemented by a ReLU FNN with width $9N$ and depth L such that*

$$|\phi(x, y) - xy| \leq 6N^{-L} \quad \text{for any } x, y \in [0, 1].$$

Proof. By Lemma 5.1, there exists a function ψ implemented by a ReLU FNN with width $3N$ and depth L such that

$$|x^2 - \psi(x)| \leq N^{-L} \quad \text{for any } x \in [0, 1].$$

Inspired by the fact

$$xy = 2\left(\left(\frac{x+y}{2}\right)^2 - \left(\frac{x}{2}\right)^2 - \left(\frac{y}{2}\right)^2\right) \quad \text{for any } x, y \in \mathbb{R},$$

we construct the desired function ϕ as

$$\phi(x, y) := 2\left(\psi\left(\frac{x+y}{2}\right) - \psi\left(\frac{x}{2}\right) - \psi\left(\frac{y}{2}\right)\right) \quad \text{for any } x, y \in \mathbb{R}. \quad (5.2)$$

Then ϕ can be implemented by the network architecture in Figure 11.

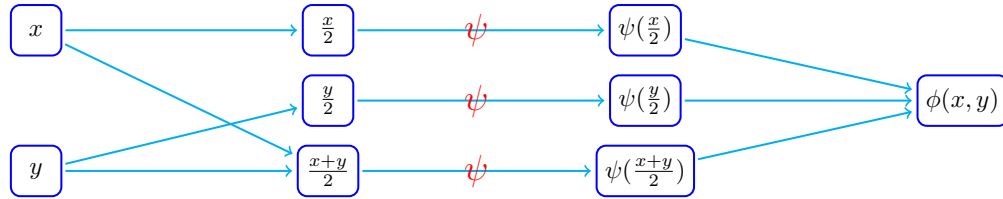


Figure 11: An illustration of the network architecture implementing ϕ for approximating xy on $[0, 1]^2$.

It follows from $\psi \in \mathcal{NN}(\text{width} \leq 3N; \text{depth} \leq L)$ that the network in Figure 11 is with width $9N$ and depth $L + 2$. Similar to the discussion in the proof of Lemma 5.1, the network in Figure 11 can be interpreted as a ReLU FNN with width $9N$ and depth L , since two of the hidden layers have the identity function as their activation functions. Moreover, for any $x, y \in [0, 1]$,

$$\begin{aligned} |xy - \phi(x, y)| &= \left| 2\left(\left(\frac{x+y}{2}\right)^2 - \left(\frac{x}{2}\right)^2 - \left(\frac{y}{2}\right)^2\right) - 2\left(\psi\left(\frac{x+y}{2}\right) - \psi\left(\frac{x}{2}\right) - \psi\left(\frac{y}{2}\right)\right) \right| \\ &\leq 2\left|\left(\frac{x+y}{2}\right)^2 - \psi\left(\frac{x+y}{2}\right)\right| + 2\left|\left(\frac{x}{2}\right)^2 - \psi\left(\frac{x}{2}\right)\right| + 2\left|\left(\frac{y}{2}\right)^2 - \psi\left(\frac{y}{2}\right)\right| \leq 6N^{-L}. \end{aligned}$$

Therefore, we have finished the proof. \square

Now let us prove Lemma 4.2, which shows how to construct a ReLU FNN to approximate $f(x, y) = xy$ on $[a, b]^2$ with arbitrary $a < b$, i.e., a rescaled version of Lemma 5.2.

993 *Proof of Lemma 4.2.* By Lemma 5.2, there exists a function ψ implemented by a ReLU
 994 FNN with width $9N$ and depth L such that

$$995 \quad |\psi(\tilde{x}, \tilde{y}) - \tilde{x}\tilde{y}| \leq 6N^{-L} \quad \text{for any } \tilde{x}, \tilde{y} \in [0, 1].$$

996 By setting $\tilde{x} = \frac{x-a}{b-a}$ and $\tilde{y} = \frac{y-a}{b-a}$ for any $x, y \in [a, b]$, we have $\tilde{x}, \tilde{y} \in [0, 1]$, implying

$$997 \quad \left| \psi\left(\frac{x-a}{b-a}, \frac{y-a}{b-a}\right) - \frac{x-a}{b-a} \frac{y-a}{b-a} \right| \leq 6N^{-L} \quad \text{for any } x, y \in [a, b].$$

998 It follows that, for any $x, y \in [a, b]$,

$$999 \quad \left| (b-a)^2 \psi\left(\frac{x-a}{b-a}, \frac{y-a}{b-a}\right) + a(x+y) - a^2 - xy \right| \leq 6(b-a)^2 N^{-L}.$$

1000 Define, for any $x, y \in \mathbb{R}$,

$$1001 \quad \phi(x, y) := (b-a)^2 \psi\left(\frac{x-a}{b-a}, \frac{y-a}{b-a}\right) + a \cdot \sigma(x+y+2|a|) - a^2 - 2a|a|.$$

1002 Then ϕ can be implemented by the network architecture in Figure 12.

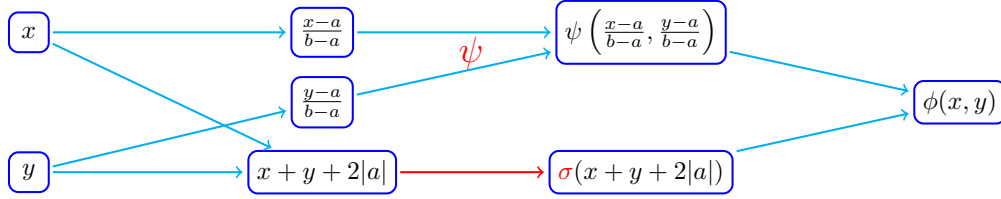


Figure 12: An illustration of the network architecture implementing ϕ for approximating xy on $[a, b]^2$. Two of the hidden layers have the identify function as their activation functions, since the red “ σ ” comes from the red arrow “ \rightarrow ”, where the red arrow “ \rightarrow ” is a ReLU FNN with width 1 and depth L .

1003 It follows from $\psi \in \mathcal{NN}(\text{width} \leq 9N; \text{depth} \leq L)$ that the network in Figure 12 is
 1004 with width $9N+1$ and depth $L+2$. Similar to the discussion in the proof of Lemma 5.1,
 1005 the network in Figure 12 can be interpreted as a ReLU FNN with width $9N+1$ and
 1006 depth L , since two of the hidden layers have the identify function as their activation
 1007 functions.

1008 Note that $x+y+2|a| \geq 0$ for any $x, y \in [a, b]$, implying

$$1009 \quad \phi(x, y) = (b-a)^2 \psi\left(\frac{x-a}{b-a}, \frac{y-a}{b-a}\right) + a(x+y) - a^2 \quad \text{for any } x, y \in [a, b].$$

1010 Hence,

$$1011 \quad |\phi(x, y) - xy| \leq 6(b-a)^2 N^{-L} \quad \text{for any } x, y \in [a, b].$$

1012 So we finish the proof. □

1013 The next lemma shows how to construct a ReLU FNN to approximate a multivariate
 1014 function $f(x_1, x_2, \dots, x_k) = x_1 x_2 \dots x_k$ on $[0, 1]^k$.

1015 **Lemma 5.3.** For any $N, L, k \in \mathbb{N}^+$ with $k \geq 2$, there exists a function ϕ implemented by
 1016 a ReLU FNN with width $9(N+1) + k - 1$ and depth $7kL(k-1)$ such that

$$1017 \quad |\phi(\mathbf{x}) - x_1 x_2 \dots x_k| \leq 9(k-1)(N+1)^{-7kL} \quad \text{for any } \mathbf{x} = [x_1, x_2, \dots, x_k]^T \in [0, 1]^k.$$

1018 *Proof.* By Lemma 4.2, there exists a function ϕ_1 implemented by a ReLU FNN with
 1019 width $9(N+1)+1$ and depth $7kL$ such that

$$1020 \quad |\phi_1(x, y) - xy| \leq 6(1.2)^2(N+1)^{-7kL} \leq 9(N+1)^{-7kL} \quad \text{for any } x, y \in [-0.1, 1.1]. \quad (5.3)$$

1021 Next, we construct a sequence of functions $\phi_i : [0, 1]^{i+1} \rightarrow [0, 1]$ for $i \in \{1, 2, \dots, k-1\}$ by
 1022 induction such that

1023 (i) ϕ_i can be implemented by a ReLU FNN with width $9(N+1)+i$ and depth $7kLi$
 1024 for each $i \in \{1, 2, \dots, k-1\}$.

1025 (ii) For any $i \in \{1, 2, \dots, k-1\}$ and $x_1, x_2, \dots, x_{i+1} \in [0, 1]$, it holds that

$$1026 \quad |\phi_i(x_1, \dots, x_{i+1}) - x_1 x_2 \dots x_{i+1}| \leq 9i(N+1)^{-7kL}. \quad (5.4)$$

1027 First, let us consider the case $i = 1$, it is obvious that the two required conditions
 1028 are true: 1) $9(N+1)+i = 9(N+1)+1$ and $7kLi = 7kL$ if $i = 1$; 2) Equation (5.3) implies
 1029 Equation (5.4) for $i = 1$.

1030 Now assume ϕ_i has been defined; we then define

$$1031 \quad \phi_{i+1}(x_1, \dots, x_{i+2}) := \phi_1(\phi_i(x_1, \dots, x_{i+1}), \sigma(x_{i+2})) \quad \text{for any } x_1, \dots, x_{i+2} \in \mathbb{R}.$$

1032 Note that $\phi_i \in \mathcal{NN}$ (width $\leq 9(N+1)+i$; depth $\leq 7kLi$) and $\phi_1 \in \mathcal{NN}$ (width $\leq 9(N+1)+$
 1033 1 ; depth $\leq 7kL$). Then ϕ_{i+1} can be implemented via a ReLU FNN with width

$$1034 \quad \max\{9(N+1)+i+1, 9(N+1)+1\} = 9(N+1)+(i+1)$$

1035 and depth $7kLi + 7kL = 7kL(i+1)$.

1036 By the hypothesis of induction, we have

$$1037 \quad |\phi_i(x_1, \dots, x_{i+1}) - x_1 x_2 \dots x_{i+1}| \leq 9i(N+1)^{-7kL}. \quad (5.5)$$

1038 Recall the fact that $9i(N+1)^{-7kL} \leq 9k2^{-7k} \leq 9k\frac{2^{-7}}{k} \leq 0.1$ for any $N, L, k \in \mathbb{N}^+$ and
 1039 $i \in \{1, 2, \dots, k-1\}$. It follows that

$$1040 \quad \phi_i(x_1, \dots, x_{i+1}) \in [-0.1, 1.1] \quad \text{for any } x_1, \dots, x_{i+1} \in [0, 1].$$

1041 Therefore, by Equations (5.3) and (5.5), we have

$$\begin{aligned} & |\phi_{i+1}(x_1, \dots, x_{i+2}) - x_1 x_2 \dots x_{i+2}| \\ &= |\phi_1(\phi_i(x_1, \dots, x_{i+1}), \sigma(x_{i+2})) - x_1 x_2 \dots x_{i+2}| \\ 1042 &\leq |\phi_1(\phi_i(x_1, \dots, x_{i+1}), x_{i+2}) - \phi_i(x_1, \dots, x_{i+1})x_{i+2}| + |\phi_i(x_1, \dots, x_{i+1})x_{i+2} - x_1 x_2 \dots x_{i+2}| \\ &\leq 9(N+1)^{-7kL} + 9i(N+1)^{-7kL} = 9(i+1)(N+1)^{-7kL}, \end{aligned}$$

1043 for any $x_1, x_2, \dots, x_{i+2} \in [0, 1]$, which means we finish the process of induction.

1044 Now let $\phi := \phi_{k-1}$, by the principle of induction, we have

$$1045 \quad |\phi(x_1, \dots, x_k) - x_1 x_2 \dots x_k| \leq 9(k-1)(N+1)^{-7kL} \quad \text{for any } x_1, \dots, x_k \in [0, 1].$$

1046 So ϕ is the desired function implemented by a ReLU FNN with width $9(N+1)+k-1$
 1047 and depth $7kL(k-1)$, which means we finish the proof. \square

With Lemma 5.3 in hand, we are ready to prove Proposition 4.1 for approximating general multivariate polynomials by ReLU FNNs.

Proof of Proposition 4.1. The case $k = 1$ is trivial, so we assume $k \geq 2$ below. Set $\tilde{k} = \|\boldsymbol{\alpha}\|_1 \leq k$, denote $\boldsymbol{\alpha} = [\alpha_1, \alpha_2, \dots, \alpha_d]^T$, and let $[z_1, z_2, \dots, z_{\tilde{k}}]^T \in \mathbb{R}^{\tilde{k}}$ be the vector such that

$$z_\ell = x_j \quad \text{if} \quad \sum_{i=1}^{j-1} \alpha_i < \ell \leq \sum_{i=1}^j \alpha_i \quad \text{for } j = 1, 2, \dots, d.$$

That is,

$$[z_1, z_2, \dots, z_{\tilde{k}}]^T = \left[\overbrace{x_1, \dots, x_1}^{\alpha_1 \text{ times}}, \overbrace{x_2, \dots, x_2}^{\alpha_2 \text{ times}}, \dots, \overbrace{x_d, \dots, x_d}^{\alpha_d \text{ times}} \right]^T \in \mathbb{R}^{\tilde{k}}.$$

Then we have $P(\mathbf{x}) = \mathbf{x}^\alpha = z_1 z_2 \dots z_{\tilde{k}}$.

We construct the target ReLU FNN in two steps. First, there exists an affine linear map $\mathcal{L} : \mathbb{R}^d \rightarrow \mathbb{R}^k$ that duplicates \mathbf{x} to form a new vector $[z_1, z_2, \dots, z_{\tilde{k}}, 1, \dots, 1]^T \in \mathbb{R}^k$, i.e., $\mathcal{L}(\mathbf{x}) = [z_1, z_2, \dots, z_{\tilde{k}}, 1, \dots, 1]^T \in \mathbb{R}^k$. Second, by Lemma 5.3, there exists a function $\psi : \mathbb{R}^k \rightarrow \mathbb{R}$ implemented by a ReLU FNN with width $9(N+1) + k - 1$ and depth $7kL(k-1)$ such that ψ maps $[z_1, z_2, \dots, z_{\tilde{k}}, 1, \dots, 1]^T \in \mathbb{R}^k$ to $z_1 z_2 \dots z_{\tilde{k}}$ within an error $9(k-1)(N+1)^{-7kL}$. Hence, we can construct the desired function via $\phi := \psi \circ \mathcal{L}$. Then ϕ can be implemented by a ReLU FNN with width $9(N+1) + k - 1$ and depth $7kL(k-1) \leq 7k^2L$, and

$$\begin{aligned} |\phi(\mathbf{x}) - P(\mathbf{x})| &= |\phi(\mathbf{x}) - \mathbf{x}^\alpha| = |\psi \circ \mathcal{L}(\mathbf{x}) - x_1^{\alpha_1} x_2^{\alpha_2} \dots x_d^{\alpha_d}| \\ &= |\psi(z_1, z_2, \dots, z_{\tilde{k}}, 1, \dots, 1) - z_1 z_2 \dots z_{\tilde{k}}| \\ &\leq 9(k-1)(N+1)^{-7kL} \leq 9k(N+1)^{-7kL} \end{aligned}$$

for any $x_1, x_2, \dots, x_d \in [0, 1]$. So, we finish the proof. \square

5.2 Proof of Proposition 4.3 for step function approximation

To prove Proposition 4.3 in this sub-section, we will discuss how to pointwisely approximate step functions by ReLU FNNs except for the trifling region. Before proving Proposition 4.3, let us first introduce a basic lemma about fitting $\mathcal{O}(N_1 N_2)$ samples using a two-hidden-layer ReLU FNN with $\mathcal{O}(N_1 + N_2)$ neurons.

Lemma 5.4. *For any $N_1, N_2 \in \mathbb{N}^+$, given $N_1(N_2 + 1) + 1$ samples $(x_i, y_i) \in \mathbb{R}^2$ with $x_0 < x_1 < \dots < x_{N_1(N_2+1)}$ and $y_i \geq 0$ for $i = 0, 1, \dots, N_1(N_2+1)$, there exists $\phi \in \mathcal{NN}(\#input = 1; \text{widthvec} = [2N_1, 2N_2 + 1])$ satisfying the following conditions:*

1. $\phi(x_i) = y_i$ for $i = 0, 1, \dots, N_1(N_2 + 1)$.
2. ϕ is linear on each interval $[x_{i-1}, x_i]$ for $i \notin \{(N_2 + 1)j : j = 1, 2, \dots, N_1\}$.

The above lemma is Lemma 2.2 of [40]; and the reader is referred to [40] for its proof. Essentially, this lemma shows the equivalence of one-hidden-layer ReLU FNNs of size $\mathcal{O}(N^2)$ and two-hidden-layer ones of size $\mathcal{O}(N)$ to fit $\mathcal{O}(N^2)$ samples.

The next lemma below shows that special shallow and wide ReLU FNNs can be represented by deep and narrow ones. This lemma was proposed as Proposition 2.2 in [41].

1083 **Lemma 5.5.** *For any $N, L, d \in \mathbb{N}^+$, it holds that*

$$1084 \quad \begin{aligned} & \mathcal{NN}(\#input = d; \text{widthvec} = [N, NL]; \#output = 1) \\ & \subseteq \mathcal{NN}(\#input = d; \text{width} \leq 2N + 2; \text{depth} \leq L + 1; \#output = 1). \end{aligned}$$

1085 With Lemmas 5.4 and 5.5 in hand, let us present the detailed proof of Proposi-
1086 tion 4.3.

1087 *Proof of Proposition 4.3.* We divide the proof into two cases: $d = 1$ and $d \geq 2$.

1088 **Case 1:** $d = 1$.

1089 In this case, $K = \lfloor N^{1/d} \rfloor^2 \lfloor L^{2/d} \rfloor = N^2 L^2$. Denote $M = N^2 L$ and consider the sample
1090 set

$$1091 \quad \begin{aligned} & \{(1, M-1), (2, 0)\} \cup \left\{ \left(\frac{m}{M}, m \right) : m = 0, 1, \dots, M-1 \right\} \\ & \cup \left\{ \left(\frac{m+1}{M} - \delta, m \right) : m = 0, 1, \dots, M-2 \right\}. \end{aligned}$$

1092 Its size is $2M + 1 = N \cdot ((2NL - 1) + 1) + 1$. By Lemma 5.4 (set $N_1 = N$ and $N_2 = 2NL - 1$
1093 therein), there exists

$$1094 \quad \begin{aligned} \phi_1 & \in \mathcal{NN}(\text{widthvec} = [2N, 2(2NL - 1) + 1]) \\ & = \mathcal{NN}(\text{widthvec} = [2N, 4NL - 1]) \end{aligned}$$

1095 such that

- 1096 • $\phi_1(\frac{M-1}{M}) = \phi_1(1) = M - 1$ and $\phi_1(\frac{m}{M}) = \phi_1(\frac{m+1}{M} - \delta) = m$ for $m = 0, 1, \dots, M - 2$;
- 1097 • ϕ_1 is linear on $[\frac{M-1}{M}, 1]$ and each interval $[\frac{m}{M}, \frac{m+1}{M} - \delta]$ for $m = 0, 1, \dots, M - 2$.

1098 Then

$$1099 \quad \phi_1(x) = m \quad \text{if } x \in \left[\frac{m}{M}, \frac{m+1}{M} - \delta \cdot \mathbf{1}_{\{m \leq M-2\}} \right] \quad \text{for } m = 0, 1, \dots, M - 1. \quad (5.6)$$

1100 Now consider another sample set

$$1101 \quad \begin{aligned} & \left\{ \left(\frac{1}{M}, L-1 \right), (2, 0) \right\} \cup \left\{ \left(\frac{\ell}{ML}, \ell \right) : \ell = 0, 1, \dots, L-1 \right\} \\ & \cup \left\{ \left(\frac{\ell+1}{ML} - \delta, \ell \right) : \ell = 0, 1, \dots, L-2 \right\}. \end{aligned}$$

1102 Its size is $2L + 1 = 1 \cdot ((2L - 1) + 1) + 1$. By Lemma 5.4 (set $N_1 = 1$ and $N_2 = 2L - 1$
1103 therein), there exists

$$1104 \quad \begin{aligned} \phi_2 & \in \mathcal{NN}(\text{widthvec} = [2, 2(2L - 1) + 1]) \\ & = \mathcal{NN}(\text{widthvec} = [2, 4L - 1]) \end{aligned}$$

1105 such that

- 1106 • $\phi_2(\frac{L-1}{ML}) = \phi_2(\frac{1}{M}) = L - 1$ and $\phi_2(\frac{\ell}{ML}) = \phi_2(\frac{\ell+1}{ML} - \delta) = \ell$ for $\ell = 0, 1, \dots, L - 2$;
- 1107 • ϕ_2 is linear on $[\frac{L-1}{ML}, \frac{1}{M}]$ and each interval $[\frac{\ell}{ML}, \frac{\ell+1}{ML} - \delta]$ for $\ell = 0, 1, \dots, L - 2$.

1108 It follows that, for $m = 0, 1, \dots, M-1$ and $\ell = 0, 1, \dots, L-1$,

$$1109 \quad \phi_2(x - \frac{m}{M}) = \ell \quad \text{for } x \in [\frac{mL+\ell}{ML}, \frac{mL+\ell+1}{ML} - \delta \cdot \mathbb{1}_{\{\ell \leq L-2\}}]. \quad (5.7)$$

1110 $K = ML$ implies that any $k \in \{0, 1, \dots, K-1\}$ can be unique represented by $k = mL + \ell$
 1111 for $m \in \{0, 1, \dots, M-1\}$ and $\ell \in \{0, 1, \dots, L-1\}$. Then the desired function ϕ can be
 1112 implemented by ReLU FNN as shown in Figure 13.

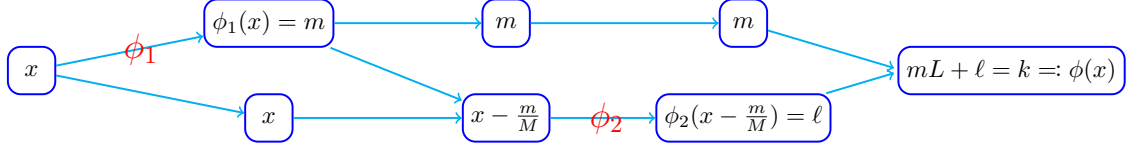


Figure 13: An illustration of the network architecture implementing ϕ based on Equations (5.6) and (5.7) with $x \in [\frac{k}{K}, \frac{k+1}{K} - \delta \cdot \mathbb{1}_{\{k \leq K-2\}}] = [\frac{mL+\ell}{ML}, \frac{mL+\ell+1}{ML} - \delta \cdot \mathbb{1}_{\{m \leq M-2 \text{ or } \ell \leq L-2\}}]$, where $k = mL + \ell$ for $m = 0, 1, \dots, M-1$ and $\ell = 0, 1, \dots, L-1$.

1113 Clearly,

$$1114 \quad \phi(x) = k \quad \text{if } x \in [\frac{k}{K}, \frac{k+1}{K} - \delta \cdot \mathbb{1}_{\{k \leq K-2\}}] \quad \text{for } k \in \{0, 1, \dots, K-1\}.$$

1115 By Lemma 5.5, $\phi_1 \in \mathcal{NN}(\text{widthvec} = [2N, 4NL - 1]) \subseteq \mathcal{NN}(\text{width} \leq 4N + 2; \text{depth} \leq$
 1116 $2L + 1)$ and $\phi_2 \in \mathcal{NN}(\text{widthvec} = [2, 4L - 1]) \subseteq \mathcal{NN}(\text{width} \leq 6; \text{depth} \leq 2L + 1)$, implying
 1117 $\phi \in \mathcal{NN}(\text{width} \leq \max\{4N + 2 + 1, 6 + 1\} = 4N + 3; \text{depth} \leq (2L + 1) + 2 + (2L + 1) + 1 = 4L + 5)$.
 1118 So we finish the proof for the case $d = 1$

1119 **Case 2:** $d \geq 2$.

1120 Now we consider the case when $d \geq 2$. Consider the sample set

$$1121 \quad \{(1, K-1), (2, 0)\} \cup \{(\frac{k}{K}, k) : k = 0, 1, \dots, K-1\} \\ \cup \{(\frac{k+1}{K} - \delta, k) : k = 0, 1, \dots, K-2\},$$

1122 whose size is $2K + 1 = \lfloor N^{1/d} \rfloor ((2\lfloor N^{1/d} \rfloor \lfloor L^{2/d} \rfloor - 1) + 1) + 1$. By Lemma 5.4 (set $N_1 = \lfloor N^{1/d} \rfloor$
 1123 and $N_2 = 2\lfloor N^{1/d} \rfloor \lfloor L^{2/d} \rfloor - 1$ therein), there exists

$$1124 \quad \phi \in \mathcal{NN}(\text{widthvec} = [2\lfloor N^{1/d} \rfloor, 2(2\lfloor N^{1/d} \rfloor \lfloor L^{2/d} \rfloor - 1) + 1]) \\ = \mathcal{NN}(\text{widthvec} = [2\lfloor N^{1/d} \rfloor, 4\lfloor N^{1/d} \rfloor \lfloor L^{2/d} \rfloor - 1])$$

1125 such that

- 1126 • $\phi(\frac{K-1}{K}) = \phi(1) = K-1$, and $\phi(\frac{k}{K}) = \phi(\frac{k+1}{K} - \delta) = k$ for $k = 0, 1, \dots, K-2$;
- 1127 • ϕ is linear on $[\frac{K-1}{K}, 1]$ and each interval $[\frac{k}{K}, \frac{k+1}{K} - \delta]$ for $k = 0, 1, \dots, K-2$.

1128 Then

$$1129 \quad \phi(x) = k \quad \text{if } x \in [\frac{k}{K}, \frac{k+1}{K} - \delta \cdot \mathbb{1}_{\{k \leq K-2\}}] \quad \text{for } k = 0, 1, \dots, K-1.$$

1130 By Lemma 5.5,

$$1131 \quad \phi \in \mathcal{NN}(\text{widthvec} = [2\lfloor N^{1/d} \rfloor, 4\lfloor N^{1/d} \rfloor \lfloor L^{2/d} \rfloor - 1]) \\ \subseteq \mathcal{NN}(\text{width} \leq 4\lfloor N^{1/d} \rfloor + 2; \text{depth} \leq 2\lfloor L^{2/d} \rfloor + 1) \\ \subseteq \mathcal{NN}(\text{width} \leq 4\lfloor N^{1/d} \rfloor + 3; \text{depth} \leq 4L + 5).$$

1132 which means we have finished the proof for the case $d \geq 2$. □

5.3 Proof of Proposition 4.4 for point fitting

In this sub-section, we will discuss how to use ReLU FNNs to fit a collection of points in \mathbb{R}^2 .^⑨ It is trivial to fit n points via one-hidden-layer ReLU FNNs with $\mathcal{O}(n)$ parameters. However, to prove Proposition 4.4, we need to fit $\mathcal{O}(n)$ points with much fewer parameters, which is the main difficulty of our proof. Our proof below is mainly based on the “bit extraction” technique and the composition architecture of neural networks.

Let us first introduce a basic lemma based on the “bit extraction” technique, which is actually Lemma 2.6 of [41].

Lemma 5.6. *For any $N, L \in \mathbb{N}^+$, any $\theta_{m,\ell} \in \{0, 1\}$ for $m = 0, 1, \dots, M-1$ and $\ell = 0, 1, \dots, L-1$, where $M = N^2L$, there exists a function ϕ implemented by a ReLU FNN with width $4N + 3$ and depth $3L + 3$ such that*

$$\phi(m, \ell) = \sum_{j=0}^{\ell} \theta_{m,j} \quad \text{for } m = 0, 1, \dots, M-1 \text{ and } \ell = 0, 1, \dots, L-1.$$

Next, let us introduce Lemma 5.7, a variant of Lemma 5.6 for a different mapping for the “bit extraction”. Its proof is based on Lemmas 5.4, 5.5, and 5.6.

Lemma 5.7. *For any $N, L \in \mathbb{N}^+$ and any $\theta_i \in \{0, 1\}$ for $i = 0, 1, \dots, N^2L^2 - 1$, there exists a function ϕ implemented by a ReLU FNN with width $8N + 6$ and depth $5L + 7$ such that*

$$\phi(i) = \theta_i \quad \text{for } i = 0, 1, \dots, N^2L^2 - 1.$$

Proof. The case $L = 1$ is clear. We assume $L \geq 2$ below.

Denote $M = N^2L$, for each $i \in \{0, 1, \dots, N^2L^2 - 1\}$, there exists a unique representation $i = mL + \ell$ for $m \in \{0, 1, \dots, M-1\}$ and $\ell \in \{0, 1, \dots, L-1\}$. Thus, we can define, for $m = 0, 1, \dots, M-1$ and $\ell = 0, 1, \dots, L-1$,

$$a_{m,\ell} := \theta_i, \quad \text{where } i = mL + \ell.$$

Then, for $m = 0, 1, \dots, M-1$, we set $b_{m,0} = 0$ and $b_{m,\ell} = a_{m,\ell-1}$ for $\ell = 1, 2, \dots, L-1$.

By Lemma 5.6, there exist $\phi_1, \phi_2 \in \mathcal{NN}(\text{width} \leq 4N + 3; \text{depth} \leq 3L + 3)$ such that

$$\phi_1(m, \ell) = \sum_{j=0}^{\ell} a_{m,j} \quad \text{and} \quad \phi_2(m, \ell) = \sum_{j=0}^{\ell} b_{m,j}$$

for $m = 0, 1, \dots, M-1$ and $\ell = 0, 1, \dots, L-1$.

We consider the sample set

$$\{(mL, m) : m = 0, 1, \dots, M\} \cup \{((m+1)L - 1, m) : m = 0, 1, \dots, M-1\}.$$

Its size is $2M + 1 = N \cdot ((2NL - 1) + 1) + 1$. By Lemma 5.4 (set $N_1 = N$ and $N_2 = 2NL - 1$ therein), there exists

$$\begin{aligned} \psi &\in \mathcal{NN}(\text{widthvec} = [2N, 2(2NL - 1) + 1]) \\ &= \mathcal{NN}(\text{widthvec} = [2N, 4NL - 1]) \end{aligned}$$

such that

^⑨Fitting a collection of points $\{(x_i, y_i)\}_i$ in \mathbb{R}^2 means that the target ReLU FNN takes a value close to y_i at the location x_i .

- $\psi(ML) = M$ and $\psi(mL) = \psi((m+1)L - 1) = m$ for $m = 0, 1, \dots, M-1$;
- ψ is linear on each interval $[mL, (m+1)L - 1]$ for $m = 0, 1, \dots, M-1$.

It follows that

$$\psi(x) = m \quad \text{if } x \in [mL, (m+1)L - 1] \quad \text{for } m = 0, 1, \dots, M-1,$$

implying

$$\psi(mL + \ell) = m \quad \text{for } m = 0, 1, \dots, M-1 \text{ and } \ell = 0, 1, \dots, L-1.$$

For $i = 0, 1, \dots, N^2L^2 - 1$, by representing $i = mL + \ell$ for $m = 0, 1, \dots, M-1$ and $\ell = 0, 1, \dots, L-1$, we have $\psi(i) = \psi(mL + \ell) = m$ and $i - L\psi(i) = \ell$, from which we deduce

$$\begin{aligned} & \phi_1(\psi(i), i - L\psi(i)) - \phi_2(\psi(i), i - L\psi(i)) \\ &= \phi_1(m, \ell) - \phi_2(m, \ell) = \sum_{j=0}^{\ell} a_{m,j} - \sum_{j=0}^{\ell} b_{m,j} \\ &= \sum_{j=0}^{\ell} a_{m,j} - \sum_{j=1}^{\ell} a_{m,j-1} - b_0 = a_{m,\ell} = \theta_i. \end{aligned} \tag{5.8}$$

Therefore, the desired function ϕ can be implemented by the network architecture described in Figure 14.

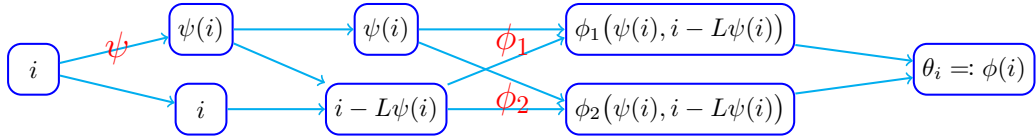


Figure 14: An illustration of the network architecture implementing the desired function ϕ based on Equation (5.8).

Note that

$$\phi_1, \phi_2 \in \mathcal{NN}(\text{width} \leq 4N + 3; \text{depth} \leq 3L + 3).$$

And by Lemma 5.5,

$$\begin{aligned} \psi &\in \mathcal{NN}(\text{widthvec} = [2N, 4NL - 1]) \\ &\subseteq \mathcal{NN}(\text{width} \leq 4N + 2; \text{depth} \leq 2L + 1). \end{aligned}$$

Hence, the network architecture shown in Figure 14 is with width $\max\{4L + 2 + 1, 2(4L + 3)\} = 8N + 6$ and depth $(2L + 1) + 2 + (3L + 3) + 1 = 5L + 7$, implying $\phi \in \mathcal{NN}(\text{width} \leq 8N + 6; \text{depth} \leq 5L + 7)$. So we finish the proof. \square

With Lemma 5.7 in hand, we are now ready to prove Proposition 4.4.

Proof of Proposition 4.4. Set $J = \lceil 2s \log_2(NL + 1) \rceil \in \mathbb{N}^+$. For each $\xi_i \in [0, 1]$, there exist $\xi_{i,1}, \xi_{i,2}, \dots, \xi_{i,J} \in \{0, 1\}$ such that

$$|\xi_i - \text{bin}_{0.\xi_{i,1}\xi_{i,2}\dots\xi_{i,J}}| \leq 2^{-J} \quad \text{for } i = 0, 1, \dots, N^2L^2 - 1.$$

By Lemma 5.7, there exist

$$\phi_1, \phi_2, \dots, \phi_J \in \mathcal{NN}(\text{width} \leq 8N + 6; \text{depth} \leq 5L + 7)$$

such that

$$\phi_j(i) = \xi_{i,j} \quad \text{for } i = 0, 1, \dots, N^2 L^2 - 1 \text{ and } j = 1, 2, \dots, J.$$

Define

$$\tilde{\phi}(x) := \sum_{j=1}^J 2^{-j} \phi_j(x) \quad \text{for any } x \in \mathbb{R}.$$

It follows that, for $i = 0, 1, \dots, N^2 L^2 - 1$,

$$\begin{aligned} |\tilde{\phi}(i) - \xi_i| &= \left| \sum_{j=1}^J 2^{-j} \phi_j(i) - \xi_i \right| = \left| \sum_{j=1}^J 2^{-j} \xi_{i,j} - \xi_i \right| \\ &= |\text{bin}_{0,\xi_{i,1}\xi_{i,2}\dots\xi_{i,J}} - \xi_i| \leq 2^{-J} \leq N^{-2s} L^{-2s}, \end{aligned}$$

where the last inequality comes from

$$2^{-J} = 2^{-\lceil 2s \log_2(NL+1) \rceil} \leq 2^{-2s \log_2(NL+1)} = (NL+1)^{-2s} \leq N^{-2s} L^{-2s}.$$

Now let us estimate the width and depth of the network implementing $\tilde{\phi}$. Recall that

$$\begin{aligned} J = \lceil 2s \log_2(NL+1) \rceil &\leq 2s(1 + \log_2(NL+1)) \leq 2s(1 + \log_2(2N) + \log_2 L) \\ &\leq 2s(1 + \log_2(2N))(1 + \log_2 L) \leq 2s \lceil \log_2(4N) \rceil \lceil \log_2(2L) \rceil, \end{aligned}$$

and $\phi_j \in \mathcal{NN}(\text{width} \leq 8N + 6; \text{depth} \leq 5L + 7)$ for each j .

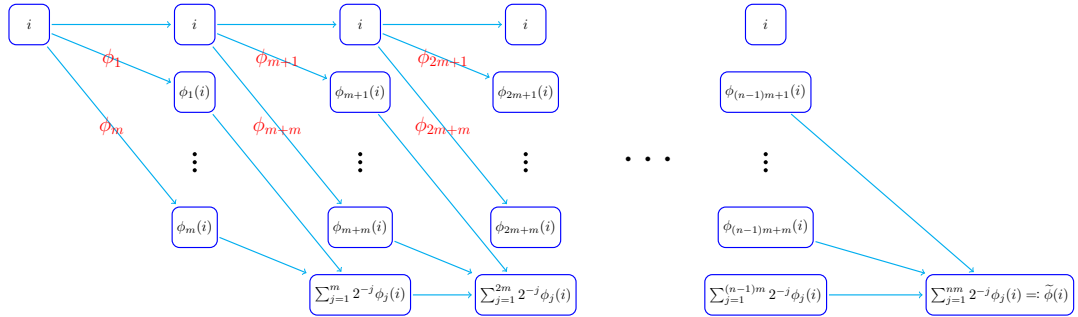


Figure 15: An illustration of the network architecture implementing $\tilde{\phi} = \sum_{j=1}^J 2^{-j} \phi_j$ for any $i \in \{0, 1, \dots, N^2 L^2 - 1\}$. We assume $J = mn$, where $m = 2s \lceil \log_2(4N) \rceil$ and $n = \lceil \log_2(2L) \rceil$, since we can set $\phi_{J+1} = \dots = \phi_{nm} = 0$ if $J < nm$.

As we can see from Figure 15, $\tilde{\phi} = \sum_{j=1}^J 2^{-j} \phi_j$ can be implemented by a ReLU FNN with width

$$\begin{aligned} (8N + 6)m + (1 + m + 1) &= (8N + 6)2s \lceil \log_2(4N) \rceil + 2s \lceil \log_2(4N) \rceil + 2 \\ &\leq 16s(N + 1) \log_2(8N) \end{aligned}$$

and depth

$$((5L + 7) + 1)n = (5L + 8) \lceil \log_2(2L) \rceil \leq (5N + 8) \log_2(4L).$$

Finally, we define

$$\phi(x) := \min \{ \sigma(\tilde{\phi}(x)), 1 \} = \min \{ \max \{ 0, \tilde{\phi}(x) \}, 1 \} \quad \text{for any } x \in \mathbb{R}.$$

Then $0 \leq \phi(x) \leq 1$ for any $x \in \mathbb{R}$ and ϕ can be implemented by a ReLU FNN with width $16s(N+1)\log_2(8N)$ and depth $(5L+8)\log_2(4L)+3 \leq 5(L+2)\log_2(4L)$. See Figure 16 for the network architecture implementing ϕ . Note that

$$\tilde{\phi}(i) = \sum_{j=1}^J 2^{-j} \phi_j(i) = \sum_{j=1}^J 2^{-j} \xi_{i,j} \in [0, 1] \quad \text{for } i = 0, 1, \dots, N^2 L^2 - 1.$$

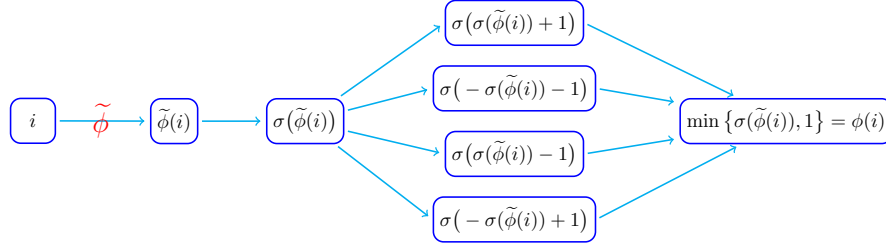


Figure 16: An illustration of the network architecture implementing the desired function ϕ based on the fact that $\min\{x_1, x_2\} = \frac{x_1+x_2-|x_1-x_2|}{2} = \frac{\sigma(x_1+x_2)-\sigma(-x_1-x_2)-\sigma(x_1-x_2)-\sigma(-x_1+x_2)}{2}$.

It follows that

$$|\phi(i) - \xi_i| = \left| \min \{ \max \{ 0, \tilde{\phi}(i) \}, 1 \} - \xi_i \right| = |\tilde{\phi}(i) - \xi_i| \leq N^{-2s} L^{-2s},$$

for $i = 0, 1, \dots, N^2 L^2 - 1$. The proof is complete. \square

6 Conclusions

This paper has established a nearly optimal approximation error of ReLU FNNs in terms of both width and depth to approximate smooth functions. It is shown that ReLU FNNs with width $\mathcal{O}(N \ln N)$ and depth $\mathcal{O}(L \ln L)$ can approximate functions in the unit ball of $C^s([0, 1]^d)$ with an approximation error $\mathcal{O}(N^{-2s/d} L^{-2s/d})$. Through VC-dimension, it is also proved that this approximation error is asymptotically nearly tight for the closed unit ball of $C^s([0, 1]^d)$.

We would like to remark that our analysis is for the fully connected feed-forward neural networks with the ReLU activation function. It would be an interesting direction for further study to generalize our results to neural networks with other architectures (e.g., convolutional neural networks and ResNet) and activation functions (e.g., tanh and sigmoid functions). These will be subjects of future work.

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