Neural Scaling Laws of Deep ReLU and Deep Operator Network: A Theoretical Study

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Abstract

Neural scaling laws play a pivotal role in the performance of deep neural networks and have been observed in a wide range of tasks. However, a complete theoretical framework for understanding these scaling laws remains underdeveloped. In this paper, we explore the neural scaling laws for deep operator networks, which involve learning mappings between function spaces, with a focus on the Chen and Chen style architecture. These approaches, which include the popular Deep Operator Network (DeepONet), approximate the output functions using a linear combination of learnable basis functions and coefficients that depend on the input functions. We establish a theoretical framework to quantify the neural scaling laws by analyzing its approximation and generalization errors. We articulate the relationship between the approximation and generalization errors of deep operator networks and key factors such as network model size and training data size. Moreover, we address cases where input functions exhibit low-dimensional structures, allowing us to derive tighter error bounds. These results also hold for deep ReLU networks and other similar structures. Our results offer a partial explanation of the neural scaling laws in operator learning and provide a theoretical foundation for their applications.

Key words: deep operator learning, neural scaling law, approximation theory, generalization theory

1 Introduction

Deep neural networks have demonstrated remarkable performance in a wide range of applications, such as computer vision (He et al., 2016; Creswell et al., 2018), natural language processing (Graves et al., 2013), speech recognition (Hinton et al., 2012), scientific computing (Han et al., 2018; Khoo et al., 2021; Zhang et al., 2023b), etc. In many of these applications, the core problem is to learn an operator between function spaces. For example, in Bhattacharya et al. (2021); Li et al. (2021), deep neural networks are used to represent a solution map of Partial Differential Equations (PDEs), in which the network maps the initial/boundary conditions to PDE solutions. In Ronneberger et al. (2015), deep neural networks are used for image segmentation, in which the network represents an operator from any given image to its segmented counterpart.

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In literature, many network architectures have been proposed to learn operators between function spaces, such as Chen and Chen neural operators (Chen and Chen, 1995, 1993), PCANet (Bhattacharya et al., 2021), Fourier Neural Operator (FNO) (Li et al., 2021), Deep Operator Network (DeepONet) (Lu et al., 2021b), Autoencoder-based Networks (AENet) (Kontolati et al., 2023; Liu et al., 2024b) and Basis Enhanced Learning (BelNet) (Zhang et al., 2023b). Since directly learning an operator is difficult due to the curse of dimensionality, a popular strategy is to use an encoder-decoder framework, i.e., one encodes infinite-dimensional functions into finite-dimensional latent features and then learns a map in the latent space. FNO (Li et al., 2021) uses the Fourier transform to convert computation to the frequency domain and then the map is learned in the frequency domain. PCANet (Bhattacharya et al., 2021) uses Principal Component Analysis (PCA) for encoding and decoding. DeepONet (Lu et al., 2021b; Lin et al., 2023) uses a branch net to convert input functions to a set of coefficients, and a trunk net to learn a set of basis functions in the output space. The resulting neural operator in DeepONet is a linear combination of the bases weighted by the coefficients. A novel training strategy of DeepONet is recently proposed in Lee and Shin (2024).

In the training of deep learning, neural scaling laws are observed in regard to the scaling between the generalization error and the data size/model size/running time (Kaplan et al., 2020). Neural scaling laws between the generalization error and the data size/model size are also empirically observed for operator learning (Lu et al., 2021b; de Hoop et al., 2022; Li et al., 2020; Subramanian et al., 2024). For example, Lu et al. (2021b) reported an exponential convergence of the DeepONet test error as the training data size increases for small training datasets, and a polynomial convergence for moderate and large training datasets. de Hoop et al. (2022) reported a power law between the test error and the training data size on various examples of learning PDE solutions. In the multi-operator learning foundation model for PDE (Liu et al., 2023; Sun et al., 2024), the authors observed a heuristic scaling law of the testing error as the number of distinct families of operators increase (Sun et al., 2024); similar results were noted when scaling up the dataset diversity in climate models (Bodnar et al., 2024), where the authors additionally reported a power scaling law with increasing model size. The difficulty with PDE foundation scaling laws is that they dependent on increasing the dataset heterogeneity, since the data sequences cannot be i.i.d. due to temporal dependencies (Liu et al., 2024e).

Neural scaling laws are often used to quantify the performance of neural networks with respect to the data size/model size/running time. A theoretical understanding of neural scaling laws is of crucial importance, which allows one to analyze and quantify the generalization error in deep learning, and predicts how much the network performance can be improved by increasing the data size, model size, and running time (Hestness et al., 2017; Kaplan et al., 2020). A theoretical understanding of model/data scaling laws (scaling between the generalization error and model/data size) can be related to neural network representation and generalization theory. When feedforward ReLU networks are used for function approximation, the representation theory in Yarotsky (2017); Lu et al. (2021a) quantifies the network approximation error with respect to the model size, which partially explains model scaling laws. Data scaling laws can be justified through the generalization error bound in terms of the data size. It was shown that when feedforward neural networks (Schmidt-Hieber, 2020) and convolutional neural networks (Oono and Suzuki, 2019; Yang et al., 2024) are used for the regression of s-Hölder functions in \mathbb{R}^{D} , the squared generalization error converges on the order of $n^{-\frac{2s}{2s+D}}$ where n denotes the training data size. Similar error bounds are also established for piecewise smooth functions in Petersen and Voigtlaender (2018); Imaizumi and Fukumizu (2019); Liu et al. (2024a) Due to the curse of dimensionality, this rate converges slowly when the data dimension is high (D is large). One way to mitigate the curse of data dimension and improve the rate is by incorporating low-dimensional data structures (Tenenbaum et al., 2000; Pope et al., 2021). Under a manifold hypothesis, one can achieve the same approximation error with a much smaller network size (Chen et al., 2019; Liu et al., 2021), and the squared generalization error is improved to the order of $n^{-\frac{2s}{2s+d}}$ where d is the intrinsic dimension of data (Nakada and Imaizumi, 2020; Dahal et al., 2022; Chen et al., 2022; Liu et al., 2024c).

Compared to regression, theoretical analysis of neural scaling laws for operator learning is less studied. An approximation result for PCANet was established in Bhattacharya et al. (2021) . A thorough study on the approximation error of PCANet was conducted in Lanthaler (2023), which derived both the upper and lower complexity bounds. The generalization error of an encoderdecoder framework for operator learning was studied in Liu et al. (2024d). This encoder-decoder framework assumes that the encoders and decoders are either given or estimated from data, and a network is used to learn the mapping between latent spaces. This encoder-decoder framework includes PCANet as a special case. The generalization error derived in Liu et al. (2024d) consists of a network estimation error and an encoding error. The squared network estimation error for Lipschitz operators is on the order of $n^{-\frac{2}{2+d_U}}$ where d_U is the dimension of the input latent space. Furthermore, if the input functions exhibit a low-dimensional structure and the latent variables are learned by Autoencoder, Liu et al. (2024b) provided a generalization error analysis where the squared generalization error is on the order of $n^{-\frac{1}{2+d_U}}$.

Regarding Chen and Chen (1995, 1993) style neural operators such as the popular DeepONet (Lu et al., 2021a), the first universal approximation theory was established in Chen and Chen (1995, 1993). The authors showed that DeepONet (Lu et al., 2021a,b) can approximate continuous operators with arbitrary accuracy, the authors in Zhang et al. (2023b,a) later extended the theorem to be invariant to the discretization. However, the network size was not specified in Chen and Chen (1995); Lu et al. (2021a) and therefore this theory cannot quantify model scaling laws. A more comprehensive analysis of DeepONet was conducted in Lanthaler et al. (2022), which studied the approximation error of each component in DeepONet with an estimation on the network size. These results were applied to study several concrete problems on the solution operator of differential equations. A generalization error was also studied in Lanthaler et al. (2022), which focused on the stochastic error (variance). The bias-variance trade-off was not addressed and the neural scaling law is not explicitly provided.

In this paper, we study the neural scaling laws of Chen-Chen style neural operators. Specifically, let U and V be two functions sets with domain dimensions d_1 and d_2 respectively, and $G: U \to V$ be a Lipschitz operator between U and V. We consider learning Lipschitz operators by DeepONet and analyze its approximation error and generalization error. Our main results are summarized as follows and in Table 1:

- 1. We show that if the network architecture is properly set, DeepONet can approximate Lipschitz operators with arbitrary accuracy. In particular, if we denote the number of network parameters by $N_{\#}$, the approximation error of DeepONet for Lipschitz operators is on the order of $\left(\frac{\log N_{\#}}{\log \log N_{\#}}\right)^{-\frac{1}{d_1}}$.
- 2. We prove that the squared generalization error of DeepONet for learning Lipschitz operators is on the order of $\left(\frac{\log(nn_y)}{\log\log(nn_y)}\right)^{-\frac{2}{d_1}}$, where *n* is the number of input-output function pairs in the training data, and n_y is the number of sampling points in the output domain *V*.
- 3. Furthermore, we incorporate low-dimensional structures of input functions into our analysis and improve the power law in $\log N_{\#}$ and $\log(nn_y)$ above to a power law in $N_{\#}$ and nn_y

	Approximation Error	Squared Generalization Error
General Case	$\left(\frac{\log N_{\#}}{\log\log N_{\#}}\right)^{-\frac{1}{d_1}}$	$\left(\frac{\log(nn_y)}{\log\log(nn_y)}\right)^{-\frac{2}{d_1}}$
U Expanded by b_U Bases	$N_{\#}^{-\frac{1}{(d_2+1)b_U+d_2}}$	$(nn_y)^{-\frac{2}{2+(d_2+1)b_U+d_2}}$

Table 1: Summary of the orders of our approximation and generalization error bounds of DeepONet for Lipschitz operators. $N_{\#}$ denotes the network model size, n is the number of input-output function pairs in the training data. U is the input set. d_1 and d_2 are the dimension of input domain Ω_U and output domain Ω_V , respectively. n_y is the number of sampling points in the output domain Ω_V .

respectively. Specifically, when all functions in U can be represented by b_U orthogonal bases, the approximation error of DeepONet for Lipschitz operators is on the order of $N_{\#}^{-\frac{1}{(d_2+1)b_U+d_2}}$, and the squared generalization error is on the order of $(nn_y)^{-\frac{2}{2+(d_2+1)b_U}}$ up to some logarithmic factor.

Our results establish novel approximation and generalization error bounds of a class of neural operators originated from Chen and Chen (1995); Lu et al. (2021a), which provide a theoretical justification of neural scaling laws. The slow convergence rate given by the power law in $\log N_{\#}$ and $\log(nn_y)$ in the general case demonstrates the difficulty of learning general Lipschitz operators without additional data structures. This difficulty is also discussed in Mhaskar and Hahm (1997); Lanthaler and Stuart (2023). By utilizing low-dimensional data structures, the neural scaling law is significantly improved to a power law in $N_{\#}$ (model size) and nn_y (data size), which partially explains the observed power scaling laws in many existing works (de Hoop et al., 2022; Lu et al., 2021b).

This paper is organized as follows: We introduce related concepts and notations in Section 2. The problem setup and DeepONet structure are presented in Section 3. We present our main results in Section 4: Section 4.2 for the approximation theory and 4.3 for the generalization theory of learning general Lipschitz operators, and Section 4.4 for an error analysis incorporating low-dimensional data structures. Our main results are proved in Section 5. We conclude this paper in Section 6. All proofs of auxiliary lemmata and theorems are deferred to the appendix.

2 Preliminary

2.1 Neural Network

In this paper, we define a feedforward ReLU network $q: \mathbb{R}^{d_1} \to \mathbb{R}$ as

$$q(\mathbf{x}) = W_L \cdot \operatorname{ReLU}(W_{L-1} \cdots \operatorname{ReLU}(W_1 \mathbf{x} + b_1) + \dots + b_{L-1}) + b_L,$$
(1)

where W_l 's are weight matrices, b_l 's are bias vectors, $\operatorname{ReLU}(a) = \max\{a, 0\}$ is the rectified linear unit activation (ReLU) applied element-wise, and Ω is the domain. We define the network class $\mathcal{F}_{NN} : \mathbb{R}^{d_1} \to \mathbb{R}^{d_2}$:

$$\mathcal{F}_{NN}(d_1, d_2, L, p, K, \kappa, R) = \{ [q_1, q_2, ..., q_{d_2}]^\mathsf{T} \in \mathbb{R}^{d_2} : \text{ for each } k = 1, ..., d_2, \\ q_k : \mathbb{R}^{d_1} \to \mathbb{R} \text{ is in the form of } (1) \text{ with } L \text{ layers, width bounded by } p,$$

$$\|q_k\|_{L^{\infty}} \le R, \ \|W_l\|_{\infty,\infty} \le \kappa, \ \|b_l\|_{\infty} \le \kappa, \ \sum_{l=1}^L \|W_l\|_0 + \|b_l\|_0 \le K, \ \forall l\},$$
(2)

where $||q||_{L^{\infty}(\Omega)} = \sup_{\mathbf{x}\in\Omega} |q(\mathbf{x})|$, $||W_l||_{\infty,\infty} = \max_{i,j} |W_{i,j}|$, $||b||_{\infty} = \max_{i} |b_i|$, and $||\cdot||_0$ denotes the number of nonzero elements of its argument. The network class above has input dimension d_1 , output dimension d_2 , L layers, width p, the number of nonzero parameters no larger than K. All parameters are bounded by κ and each element in the output is bounded by R.

2.2 Cover and Partition of Unity

We define the cover of a set as follows:

Definition 1 (Cover). A collection of sets $\{S_k\}_{k=1}^{C_S}$ is a cover of Ω if $\Omega \subset \bigcup_{k=1}^{C_S} S_k$.

The following lemma shows that, for a compact smooth manifold \mathcal{M} and any given cover of \mathcal{M} , there exists a C^{∞} partition of unity of \mathcal{M} that subordinates to the given cover.

Lemma 1 (Theorem 13.7(ii) of Tu (2011)). Let $\{\Omega_k\}_{k=1}^M$ be an open cover of a compact smooth manifold \mathcal{M} . There exists a C^{∞} partition of unity $\{\omega_k\}_{k=1}^M$ that subordinates to $\{\Omega_k\}_{k=1}^M$ such that $\operatorname{supp}(\omega_k) \subset \Omega_k$ for any k.

2.3 Lipschitz Functional

A Lipschitz functional is defined as follows:

Definition 2 (Lipschitz functional). Given a function set U with domain Ω_U such that $U \subset L^2(\Omega_U)$, we say a functional $f: U \to \mathbb{R}$ is Lipschitz with Lipschitz constant L_f if

$$|f(u_1) - f(u_2)| \le L_f ||u_1 - u_2||_{L^2(\Omega_U)}, \ \forall u_1, u_2 \in U.$$

2.4 Clipping Operation

For a function $f : \mathbb{R} \to \mathbb{R}$, we define the clipping operation:

$$CL_a(f) = \min\{\max\{f, -a\}, a\}$$

for some $a \geq 0$. This clipping operation can be realized by a two-layer ReLU network

$$CL_a(f) = -ReLU(-ReLU(f+a) + 2a) + a.$$
(3)

2.5 Notation

In this paper, we use normal lowercase letters to denote scalars, and bold lowercase letters to denote vectors. Matrices, sets and operators are denoted by upper case letters. We use U to denote the input function set with domain Ω_V , and V to denote the output function set with domain Ω_V . We denote the operator to be learned which maps functions in U to functions in V by G. Express a d-dimensional vector \mathbf{x} as $\mathbf{x} = [x_1, ..., x_d]^{\top}$. The ℓ^{∞} and ℓ^2 norm of a vector \mathbf{x} is defined $\|\mathbf{x}\|_{\infty} = \max_k |x_k|$ and $\|\mathbf{x}\|_2 = \sqrt{\sum_k^d x_k^2}$, respectively. We denote the Euclidean ball with center \mathbf{c} and radius δ by $\mathcal{B}_{\delta}(\mathbf{c})$. The L^{∞} and L^2 norm of a function over domain Ω_U is defined as $\|u\|_{L^{\infty}(\Omega_U)} = \sup_{\mathbf{x}\in\Omega_U} |u(\mathbf{x})|$ and $\|u\|_{L^2(\Omega_U)} = \sqrt{\int_{\Omega_U} [u(\mathbf{x})]^2 d\mathbf{x}}$, respectively. We define the $\|\cdot\|_{\infty,\infty}$ norm of an operator $G: U \to V$ by $\|G\|_{\infty,\infty} = \sup_{\mathbf{v}\in\Omega_V} \sup_{u \in U} |G(u)(\mathbf{y})|$.

3 Problem Setup and Deep Operator Learning

3.1 Problem Setup and Examples

This paper studies the operator learning problem where the goal is to learn an unknown Lipschitz operator $G: U \to V$ between two function sets U and V from n training samples $\{(u_i, v_i)\}_{i=1}^n$, where $u_i \in U$ and

$$v_i = G(u_i) + \zeta_i \tag{4}$$

with ζ_i representing noise. We consider Lipschitz operators in the following sense:

Assumption 1. Let Ω_U and Ω_V be the domain of functions in U and V respectively, and $U \subset L^2(\Omega_U)$, $V \subset L^\infty(\Omega_V)$. Assume $G: U \to V$ is a Lipschitz operator: there exists a constant $L_G > 0$ such that

$$||G(u_1) - G(u_2)||_{L^{\infty}(\Omega_V)} \le L_G ||u_1 - u_2||_{L^2(\Omega_U)},$$

for any $u_1, u_2 \in U$.

In Assumption 1, the function distance in the output space is measured by the L^{∞} norm, and the function distance in the input space is measured by the L^2 norm. This condition is needed in our network construction to derive an error bound for the branch net. Assumption 1 is satisfied for the solution operator of many differential equations. We provide some examples below.

The first example is a nonlinear ODE system known as gravity pendulum with external force, which is studied in Lu et al. (2021b); Lanthaler et al. (2022); Reid and King (2009).

Example 1. Consider the following ODE system

$$\begin{cases} \frac{dv_1}{dt} = v_2, \\ \frac{dv_2}{dt} = -\gamma \sin(v_1) + u(t) \end{cases}$$
(5)

with initial condition $v_1(0) = v_2(0) = 0$, and $\gamma > 0$ is a parameter. In (5), v_1, v_2 represent the angle and angular velocity of the pendulum, γ is the frequency parameter and u(t) is an external force controlling the dynamics of the pendulum. For this ODE, we consider the operator: $G: u(t) \rightarrow (v_1(t), v_2(t))$. Let T > 0 the ending time. For any $u_1, u_2 \in L^2([0, T])$, there exists a constant L_G such that

$$\|G(u_1) - G(u_2)\|_{L^{\infty}([0,T])} \le L_G \|u_1 - u_2\|_{L^2([0,T])}$$
(6)

which is proved in Lanthaler et al. (2022, Proof of Lemma 4.1).

In the second example, we consider a transport equation.

Example 2. Let $\Omega \subset \mathbb{R}^d$ be a hyper-cube. Consider the transport equation on $\Omega \times [0,T]$

$$\begin{cases} v_t = \mathbf{c} \cdot \nabla v & \text{on } \Omega \times [0, T] \\ v(\mathbf{x}, 0) = u(\mathbf{x}) & \text{on } \Omega \end{cases}$$

equipped with periodic boundary condition where $\mathbf{c} \in \mathbb{R}^d$ is the velocity. Let G be the solution operator from the initial condition u to the solution $v(\mathbf{x}, T)$ at time T > 0. We set $\Omega_U = \Omega_V = \Omega$. Let $\{w_j\}_{j=1}^J$ be a set of Fourier basis for some positive integer J > 0, and

$$U = \left\{ \sum_{j=1}^{J} a_j w_j : \max_j |a_j| \le C \right\}$$

for some C > 0. Then Assumption 1 is satisfied with $L_G = \sqrt{J}$ (see Section A.1 for a proof).



Figure 1: Illustration of the DeepONet architecture. Here **u** is the discretization of $u \in U$, and $\mathbf{y} \in \Omega_V$.

3.2 Deep Operator Learning

We study the DeepONet (Chen and Chen, 1995; Lu et al., 2021b) architecture which consists of a branch net and a trunk net. The branch net encodes the input function and produces a set of coefficients. The trunk net learns a set of basis functions for the output space. A DeepONet takes an input function together with points in the output function domain. It outputs a scalar which is the output function evaluated at the given points.

Let $\mathcal{F}_1 = \mathcal{F}_{NN}(d_1, 1, L_1, p_1, K_1, \kappa_1, R_1)$ be the network class for the branch net and $\mathcal{F}_2 = \mathcal{F}_{NN}(d_2, 1, L_2, p_2, K_2, \kappa_2, R_2)$ be the network class for the trunk net. We define the network class of DeepONet as

$$\mathcal{G}_{\rm NN} = \left\{ G_{\rm NN}(\mathbf{u})(\mathbf{y}) = \operatorname{CL}_{\beta_V} \left(\sum_{k=1}^N \widetilde{a}_k(\mathbf{u}) \widetilde{q}_k(\mathbf{y}) \right) : \widetilde{q}_k \in \mathcal{F}_1, \widetilde{a}_k \in \mathcal{F}_2 \text{ for } k = 1, .., N \right\},$$
(7)

where **u** is an input vector, which can be thought as a discretization of the input function, and **y** is a point in the domain of output functions. The network architecture is illustrated in Figure 1. A DeepONet takes the discretized function **u** and a point $\mathbf{y} \in \Omega_V$ as input, where **u** is passed to the branch net \tilde{a}_k 's to compute a set of coefficients, and **y** is passed to the trunk net to evaluate each basis function \tilde{q}_k at **y**. The output $G_{NN}(\mathbf{u})(\mathbf{y})$ is the sum of the \tilde{q}_k 's value weighted by the coefficients \tilde{a}_k 's from the branch net.

4 Main Results

4.1 Assumptions

In this section, we make some assumptions on the function sets U and V.

- Assumption 2 (Input space U). Suppose U is a function set such that
 - (i) Any function $u \in U$ is defined on $\Omega_U = [-\gamma_1, \gamma_1]^{d_1}$ for some $\gamma_1 > 0$.
 - (ii) Any function $u \in U$ is Lipschitz with a Lipschitz constant no more than $L_U > 0$:

$$|u(\mathbf{x}_1) - u(\mathbf{x}_2)| \le L_U ||\mathbf{x}_1 - \mathbf{x}_2||_2$$

for any $\mathbf{x}_1, \mathbf{x}_2 \in \Omega_U$.

(iii) Any function $u \in U$ satisfies $||u||_{L^{\infty}(\Omega_U)} \leq \beta_U$ for some $\beta_U > 0$.

The following assumption is made on the output function set V.

Assumption 3 (Output space V). Suppose V is a function space such that

- (i) Any function in V is defined on $\Omega_V = [-\gamma_2, \gamma_2]^{d_2}$ for some $\gamma_2 > 0$,
- (ii) Any function $v \in V$ is Lipschitz with a Lipschitz constant no more than $L_V > 0$:

$$|v(y_1) - v(y_2)| \le L_V ||y_1 - y_2||_2$$

for any $\boldsymbol{y}_1, \boldsymbol{y}_2 \in \Omega_V$.

(iii) Any function $v \in V$ satisfies $||v||_{L^{\infty}(\Omega_V)} \leq \beta_V$ for some $\beta_V > 0$.

Assumption 2 and 3 are mild conditions on U and V and are usually satisfied in applications.

4.2 DeepONet Approximation Error and Model Scaling Law

Our first result is on the approximation error of DeepONet for the representation of Lipschitz operators.

Theorem 1. Let $d_1, d_2 > 0$ be integers, $\gamma_1, \gamma_2, \beta_U, \beta_V, L_U, L_V, L_G > 0$, and U, V be function sets satisfying Assumption 2 and 3 respectively. There exist constants C depending on d_2, L_V, γ_2 and C_{δ} depending on γ_1, d_1, L_f, L_U such that the following holds: For any $\varepsilon > 0$, set $\delta = C_{\delta}\varepsilon$ and $N = C\varepsilon^{-d_2}$. Choose $\{\mathbf{c}_m\}_{m=1}^{c_U} \subset \Omega_U$ so that $\{\mathcal{B}_{\delta}(\mathbf{c}_m)\}_{m=1}^{c_U}$ is a cover of Ω_U . Then there exist two network architectures: $\mathcal{F}_1 = \mathcal{F}_{NN}(d_2, 1, L_1, p_1, \kappa_1, \kappa_1, R_1)$ with

$$L_1 = O\left(\log(\varepsilon^{-1})\right), \ p_1 = O(1), \ K_1 = O\left(\log(\varepsilon^{-1})\right), \ \kappa_1 = O(\varepsilon^{-1}), \ R_1 = 1.$$

and $\mathcal{F}_{2} = \mathcal{F}_{NN}(c_{U}, 1, L_{2}, p_{2}, K_{2}, \kappa_{2}, R_{2})$ with

$$L_{2} = O\left(c_{U}^{2}\log c_{U} + c_{U}^{2}\log(\varepsilon^{-1})\right), \ p_{2} = O(\sqrt{c_{U}}\varepsilon^{-(d_{2}+1)c_{U}})$$
$$K_{2} = O\left(\left(\sqrt{c_{U}}\varepsilon^{-(d_{2}+1)c_{U}}\right)\left(c_{U}^{2}\log c_{U} + c_{U}^{2}\log(\varepsilon^{-1})\right)\right),$$
$$\kappa_{2} = O(c_{U}^{c_{U}/2+1}\varepsilon^{-(d_{2}+1)(c_{U}+1)}), \ R = \beta_{V},$$

such that, for any operator $G: U \to V$ satisfying Assumption 1, there are $\{\widetilde{q}_k\}_{k=1}^N$ with $\widetilde{q}_k \in \mathcal{F}_1$ and $\{\widetilde{a}_k\}_{k=1}^N$ with $\widetilde{a}_k \subset \mathcal{F}_2$ such that

$$\sup_{u \in U} \sup_{\mathbf{y} \in \Omega_V} \left| G(u)(\mathbf{y}) - \sum_{k=1}^N \widetilde{a}_k(\mathbf{u}) \widetilde{q}_k(\mathbf{y}) \right| \le \varepsilon,$$

where $\mathbf{u} = [u(\mathbf{c}_1), u(\mathbf{c}_2), ..., u(\mathbf{c}_{c_U})]^\top$ is a discretization of u. The constant hidden in O depends on $\gamma_1, \gamma_2, \beta_U, \beta_V, d_1, d_2, L_G, L_U, L_V$.

Theorem 1 is proved in Section 5.1. Theorem 1 is a general result that holds for any $\{\mathcal{B}_{\delta}(\mathbf{c}_m)\}_{m=1}^{c_U}$ covering Ω_U . The following lemma (see a proof in Section B.5) shows that for any bounded hypercube, there always exists a cover with Euclidean balls, and an upper bound on the covering number is provided. **Lemma 2.** Let $\Omega = [-\gamma, \gamma]^d$ for some $\gamma > 0$. For any $\delta > 0$, there exists a cover $\{\mathcal{B}_{\delta}(\mathbf{c}_m)\}_{m=1}^M$ of Ω with

$$M \le C\delta^{-d} \tag{8}$$

where C is a constant depending on γ and d.

Combining Theorem 1 and Lemma 2 yields the following corollary, which quantifies c_U in terms of ε and d_1 .

Corollary 1. Let $d_1, d_2 > 0$ be integers, $\gamma_1, \gamma_2, \beta_U, \beta_V, L_U, L_V > 0$, and U, V be function sets satisfying Assumption 2 and 3 respectively. There exist constants C depending on d_2, L_V, γ_2 and C_{δ}, C_1 depending on γ_1, d_1, L_f, L_U , such that the following hold: For any $\varepsilon > 0$, set $\delta = C_{\delta}\varepsilon$, $c_U = C_1 \varepsilon^{-d_1}$ and $N = C \varepsilon^{-d_2}$. There exist $\{\mathbf{c}_m\}_{m=1}^{c_U} \subset \Omega_U$ so that $\{\mathcal{B}_{\delta}(\mathbf{c}_m)\}_{m=1}^{c_U}$ covers Ω_U , and two network architectures: $\mathcal{F}_1 = \mathcal{F}_{NN}(d_2, 1, L_1, p_1, K_1, \kappa_1, R_1)$ and $\mathcal{F}_2 = \mathcal{F}_{NN}(c_U, 1, L_2, p_2, K_2, \kappa_2, R_2)$ with

$$L_1 = O\left(\log(\varepsilon^{-1})\right), \ p_1 = O(1), \ K_1 = O\left(\log(\varepsilon^{-1})\right), \ \kappa_1 = O(\varepsilon^{-1}), \ R_1 = 1.$$

and

$$L_{2} = O\left(\varepsilon^{-2d_{1}}\log\varepsilon^{-1} + \varepsilon^{-2d_{1}}\log(\varepsilon^{-1})\right), \ p_{2} = O(\varepsilon^{-d_{1}/2}\varepsilon^{-C_{1}(d_{2}+1)\varepsilon^{-d_{1}}}),$$

$$K_{2} = O\left(\varepsilon^{-C_{1}(d_{2}+1)\varepsilon^{-d_{1}}-5d_{1}/2}\log\varepsilon^{-1}\right),$$

$$\kappa_{2} = O(\varepsilon^{-C_{1}d_{1}\varepsilon^{-d_{1}}/2+1}\varepsilon^{-(d_{2}+1)(C_{1}\varepsilon^{-d_{1}}+1)}), \ R = \beta_{V},$$

such that, for any operator $G: U \to V$ satisfying Assumption 1, there are $\{\widetilde{q}_k\}_{k=1}^N$ with $\widetilde{q}_k \in \mathcal{F}_1$ and $\{\widetilde{a}_k\}_{k=1}^N$ with $\widetilde{a}_k \in \mathcal{F}_2$ such that

$$\sup_{u \in U} \sup_{\mathbf{y} \in \Omega_V} |G(u)(\mathbf{y}) - \sum_{k=1}^N \widetilde{a}_k(\mathbf{u})\widetilde{q}_k(\mathbf{y})| \le \varepsilon,$$

where $\mathbf{u} = [u(\mathbf{c}_1), u(\mathbf{c}_2), ..., u(\mathbf{c}_{c_U})]^\top$ is a discretization of u. The constant hidden in O depends on $\gamma_1, \gamma_2, \beta_U, \beta_V, d_1, d_2, L_G, L_U, L_V$.

Corollary 1 can be proved by replacing Theorem 6 by Corollary 2 in the proof of Theorem 1. Theorem 1 and Corollary 1 have the following implications:

• Model scaling law. Theorem 1 and Corollary 1 show that if the network architecture is properly set, DeepONet can approximate any Lipschitz operator to arbitrary accuracy. To achieve an accuracy ε , the network size is on the order of $NK_2 = \varepsilon^{-C_1(d_2+1)\varepsilon^{-d_1}-5d_1/2-d_2}\log\varepsilon^{-1}$. In other words, if we denote the total number of network parameters by $N_{\#}$, then the network approximation error is on the order of $\left(\frac{\log N_{\#}}{\log \log N_{\#}}\right)^{-1/d_1}$. This result gives a theoretical estimation of the model scaling law, which depicts the relation between the network approximation error and the network size. Without making additional assumptions on the low-dimensional structures of the input function set, the network approximation error scales poorly (converges at an extremely slow rate) as the model size increases. In Section 4.4, we will show that this scaling law can be improved by utilizing low-dimensional structures.

- Optimality. In the proof of Theorem 1, an important ingredient is to approximate Lipschitz functionals, which is given in Theorem 6 and Corollary 2. The network size in Theorem 1 is comparable to that in Corollary 2. As discussed in Remark 1, our network size for approximating Lipschitz functionals is optimal up to a logarithmic factor. Since approximating a Lipschitz operator is more difficult than approximating a Lipschitz functional, we expect the network size in Theorem 1 to be close to the optimal one. Notably, a lower bound of the network complexity of approximating *r*-times Fréchet differentiable operators is analyzed in Lanthaler and Stuart (2023) for several popular network architectures, including DeepONet. The lower bound of the DeepONet size given in Lanthaler and Stuart (2023, Proposition 2.21) for the approximation of Lipschitz functionals is on the order of $\exp(c_1\varepsilon^{-1/(\alpha+1+\delta)})$ where α is a parameter depending on d_1 and δ is a positive number.
- Connection to existing works. Approximation theory of DeepONet has been studied in Chen and Chen (1995) and Lanthaler et al. (2022). The network size in Chen and Chen (1995) was not explicitly specified, which cannot explain model scaling laws. Lanthaler et al. (2022) conducted an in-depth study of DeepONet, in which a DeepONet is decomposed into three components: an encoder, an approximator and a reconstructor. Lanthaler et al. (2022) analyzed the network structure of each component on several concrete examples. Our settings and results are different from those in Lanthaler et al. (2022) in the following aspects: (i) Our approximation error is measured by the L^{∞} norm, while Lanthaler et al. (2022) studied the L^2 error. (ii) Lanthaler et al. (2022) decomposed the DeepONet approximation error into an encoder error, an approximator error and a reconstructor error, and analyzed each of them. The encoder error and reconstructor error are expressed in terms of the eigenvalues of the covariate operator of the input and output function distributions. An explicit relation between the network size and DeepONet approximation error for general operators was not given. In our paper, we analyze the DeepONet approximation error for general Lipschitz operators and explicitly quantify how the error scales with respect to the network size.

4.3 Generalization Error and Data Scaling Law

Let n > 0 be a positive integer. Assume we are given the data set $S = \{u_i, v_i\}_{i=1}^n$ where u_i 's are i.i.d. samples following a distribution ρ_u , and v_i is given by (4). Our setting is summarized below.

Setting 1. Let $\{\mathbf{x}_j\}_{j=1}^{n_x} \subset \Omega_U$ (independent of *i*) be a fixed grid in Ω_U , where n_x is the number of grid points in Ω_U which is to be specified later. For i = 1, ..., n, let $\{\mathbf{y}_{i,j}\}_{j=1}^{n_y} \subset \Omega_V$ be i.i.d. samples following a distribution ρ_y on Ω_V . Assume we are given a set of paired samples $\{\mathbf{u}_i, \mathbf{v}_i\}_{i=1}^n$ with

$$\mathbf{u}_{i} = [u_{i}(\mathbf{x}_{1}), ..., u_{i}(\mathbf{x}_{n_{x}})]^{\top}, \quad \mathbf{v}_{i} = [G(u_{i})(\mathbf{y}_{i,1}) + \xi_{i,1}, ..., G(u_{i})(\mathbf{y}_{i,n_{y}}) + \xi_{i,n_{y}}]^{\top}, \tag{9}$$

where u_i 's are i.i.d. samples from the distribution ρ_u in U, and $\{\xi_{i,j}\}$ follows i.i.d sub-Gaussian distribution with variance proxy σ^2 . We denote $\boldsymbol{\xi}_i = [\zeta(\mathbf{y}_{i,1}), ..., \zeta(\mathbf{y}_{i,n_y})]$. Suppose U, V satisfy Assumption 2 and 3, respectively.

In Setting 1, $\{\mathbf{y}_{i,j}\}_{j=1}^{n_y}$ is the set of discretization grids in Ω_V for the output function v_i . This setting allows output functions in the data set to have different discretization grids in Ω_V .

We consider training DeepONet by minimizing $\frac{1}{nn_y}\sum_{i=1}^n\sum_{j=1}^{n_y}(G_{NN}(\mathbf{u}_i)(\mathbf{y}_{i,j})-v_{i,j})^2$ over $G_{NN} \in \mathcal{G}_{NN}$ to obtain the following minimizer:

$$\widehat{G} = \underset{G_{\rm NN} \in \mathcal{G}_{\rm NN}}{\operatorname{argmin}} \frac{1}{nn_y} \sum_{i=1}^n \sum_{j=1}^{n_y} (G_{\rm NN}(\mathbf{u}_i)(\mathbf{y}_{i,j}) - v_{i,j})^2,$$
(10)

where $v_{i,j} = (\mathbf{v}_i)_j$ an \mathcal{G}_{NN} denotes the DeepONet network class given in (7). In this paper, we study the squared generalization error of DeepONet given by:

Squared Generalization Error :=
$$\mathbb{E}_{\mathcal{S}}\mathbb{E}_{\{\mathbf{y}_j\}_{j=1}^{n_y}\sim\rho_y}\mathbb{E}_{u\sim\rho_u}\left[\frac{1}{n_y}\sum_{j=1}^{n_y}(\widehat{G}(\mathbf{u})(\mathbf{y}_j)-G(u)(\mathbf{y}_j))^2\right],$$

where $\boldsymbol{u} = [u(\mathbf{x}_1), ..., u(\mathbf{x}_{n_x})]^{\top}$. The following theorem gives an upper bound of the generalization error of DeepONet for learning Lipschitz operators.

Theorem 2. Let $d_1, d_2, n_y, n > 0$ be integers, $\gamma_1, \gamma_2, \beta_U, \beta_V, L_U, L_V, L_G > 0$. Suppose $G : U \to V$ satisfy Assumption 1 and consider Setting 1. There exist constants C depending on d_2, L_V and γ_2, C_1 depending on $\gamma_1, d_1, L_f, L_U, C_2$ depending on $\sigma, \gamma_1, \gamma_2, \beta_U, \beta_V, d_1, d_2, L_G, L_U, L_V$, and C_δ depending on γ_1, d_1, L_f, L_U , such that the following holds: Let $\varepsilon \in (0, 1), \delta = C_\delta \varepsilon$ and $N = C\varepsilon^{-d_2}$. Set $n_x = C_1 \varepsilon^{-d_1}$, and then there exist $\{\mathbf{x}_j\}_{j=1}^{n_x}$ such that $\{\mathcal{B}_\delta(\mathbf{x}_j)\}_{j=1}^{n_x}$ is a cover of Ω_U . Consider the DeepONet network (7) with the network architecture $\mathcal{F}_1 = \mathcal{F}_{NN}(d_2, 1, L_1, p_1, K_1, \kappa_1, R_1)$ and $\mathcal{F}_2 = \mathcal{F}_{NN}(C\varepsilon^{-C_1\varepsilon^{-d_1}}, 1, L_2, p_2, K_2, \kappa_2, R_2)$ with

$$L_1 = O\left(\log(\varepsilon^{-1})\right), \ p_1 = O(1), \ K_1 = O\left(\log(\varepsilon^{-1})\right), \ \kappa_1 = O(\varepsilon^{-1}), \ R_1 = 1,$$
(11)

and

$$L_{2} = O\left(\log(\varepsilon^{-1})\right), \ p_{2} = O(\varepsilon^{-C_{1}(d_{2}+1)\varepsilon^{-d_{1}(d_{2}+1)}}), \ K_{2} = O\left(\varepsilon^{-C_{1}(d_{2}+1)\varepsilon^{-d_{1}(d_{2}+1)}}\log(\varepsilon^{-1})\right),$$

$$\kappa_{2} = O(\varepsilon^{-(d_{2}+1)}), \ R_{2} = \beta_{V},$$
(12)

where the constant hidden in O depends on $\sigma, \gamma_1, \gamma_2, \beta_U, \beta_V, d_1, d_2, L_G, L_U, L_V$. Let \widehat{G} be the minimizer in (10). Then we have

$$\mathbb{E}_{\mathcal{S}}\mathbb{E}_{\{\mathbf{y}_j\}_{j=1}^{n_y}\sim\rho_y}\mathbb{E}_{u\sim\rho_u}\left[\frac{1}{n_y}\sum_{j=1}^{n_y}(\widehat{G}(\boldsymbol{u})(\mathbf{y}_j)-G(\boldsymbol{u})(\mathbf{y}_j))^2\right]$$
$$\leq C_2\left(\varepsilon^2+\frac{1}{nn_y}\varepsilon^{-C_1(d_2+1)\varepsilon^{-d_1}-11d_1/2-d_2}\right)\log^3\frac{1}{\varepsilon}.$$
(13)

In particular, setting $\varepsilon = \left(\frac{d_1}{2C_1(d_2+1)} \frac{\log(nn_y)}{\log\log(nn_y)}\right)^{-\frac{1}{d_1}}$ gives rise to

$$\mathbb{E}_{\mathcal{S}}\mathbb{E}_{\{\mathbf{y}_j\}_{j=1}^{n_y}\sim\rho_y}\mathbb{E}_{\mathbf{u}\sim\rho_u}\left[\frac{1}{n_y}\sum_{j=1}^{n_y}(\widehat{G}(\mathbf{u})(\mathbf{y}_j)-G(\mathbf{u})(\mathbf{y}_j))^2\right] \le C_3\left(\frac{\log(nn_y)}{\log\log(nn_y)}\right)^{-\frac{2}{d_1}}.$$
 (14)

for some C_3 depending on $\sigma, \gamma_1, \gamma_2, \beta_U, \beta_V, d_1, d_2, L_G, L_U, L_V$.

Theorem 2 is proved in Section 5.2. To prove Theorem 2, we need to carefully perform a biasvariance trade off. The bias term is related with the approximation error of DeepONet. In practice, one has to train the network to learn the operator from a given data set. The variance term captures the difference between the trained network and the network used in the approximation theory. The network architecture suggested in Theorem 2 is a trade-off by balancing the two error terms.

We have the following discussions:

- Data scaling law. Theorem 2 shows that to learn Lipschitz operators, the generalization error of DeepONet decays in a power law of $\log(nn_y)$. This rate is slower than the empirical observations in Lu et al. (2021b); de Hoop et al. (2022), which suggest a power data scaling law on the order of $n^{-\alpha}$ for some $\alpha > 0$. This slow decay in our theory comes from the intrinsic difficulty of operator learning in infinite-dimensional spaces. Due to the curse of dimensionality, learning an operator is much more difficult than learning a finite-dimensional function, leading to a slower decay of the generalization error. In the next subsection, we will show that when the input function set U has some low-dimensional structures, we can derive an upper bound that matches the empirical power law observed in Lu et al. (2021b); de Hoop et al. (2022).
- Effects of n and n_y . The upper bound in Theorem 2 is expressed as a function of the product nn_y , implying that n and n_y have the same influence on the performance of DeepONet. In other words, one can improve the accuracy by increasing n or n_y or both. This result justifies the empirical observation in Lu et al. (2021b, Section 4.3)
- Connection with existing works. A similar rate was derived in Liu et al. (2024d, Section 4.3) for the encoder-decoder framework of operator learning. In Liu et al. (2024d, Section 4.3), one assumed the input and output functions are C^s functions and Legendre polynomials were used as encoders and decoders. With a fixed grid in Ω_U and Ω_V , it was shown that the squared generalization error decays on the order of $(\log n)^{-s/d_1}$, where n is the number of training samples. The generalization error of DeepONet was also analyzed in Lanthaler et al. (2022), which studied the variance part and did not address the bias-variance trade-off.

4.4 Utilizing low-dimensional structures

Corollary 1 and Theorem 2 give rise to a slow rate of convergence of DeepONet due to the curse of dimensionality. In this subsection, we incorporate low-dimensional structures of input functions and prove a power law convergence which is consistent with empirical observations in Lu et al. (2021b); de Hoop et al. (2022). Specifically, we consider the following assumption on low-dimensional structures of U:

Assumption 4. Suppose the function set U satisfies

(i) There exists a finite orthonormal basis functions $\{\omega_k\}_{k=1}^{b_U}$ so that any $u \in U$ can be expressed as

$$u = \sum_{k=1}^{b_U} \alpha_k \omega_k, \quad \text{with} \quad \alpha_k = \int_{\Omega_U} u(\mathbf{x}) \omega_k(\mathbf{x}) d\mathbf{x}.$$
(15)

(ii) The discretization grid $\{\mathbf{x}_j\}_{j=1}^{n_x}$ satisfies that: there is a matrix $A \in \mathbb{R}^{b_U \times n_x}$ such that for any $u \in U$, we have

$$A\mathbf{u} = [\alpha_1, ..., \alpha_{b_U}]^\top,\tag{16}$$

where $\mathbf{u} = [u(\mathbf{x}_1), \dots, u(\mathbf{x}_{n_x})]^T \in \mathbb{R}^{n_x}$ and the α_k 's are the coefficients of u in (15). We denote $C_A = ||A||_{\infty,\infty}$.

Assumption 4(i) assumes that the input functions in U live in a b_U -dimensional linear subspace. This assumption is commonly used in numerical PDEs. In particular, for some popular bases, such as Legendre polynomials or Fourier bases, Assumption 4(ii) is satisfied by properly choosing $\{\mathbf{x}_j\}_{j=1}^{n_x}$: • Legendre polynomials. Let $\{\omega_k\}_{k=1}^{b_U}$ consist of Legendre polynomials up to degree μ along each dimension. Then $u\omega_k$ is a polynomial with a degree no larger than 2μ along each dimension. By choosing $\{\mathbf{x}_j\}_{j=1}^{n_x}$ so that along each dimension, the points are quadrature points corresponding to Legendre polynomials of degree 2μ , the integral for α_k in (15) can be exactly computed by quadrature rules:

$$\alpha_k = \sum_{j=1}^{n_x} \beta_j u(\mathbf{x}_j) \omega_k(\mathbf{x}_j),$$

where $\{\beta_j\}_{j=1}^{n_x}$ are quadrature weights. Assumption 4(ii) is satisfied by setting $A = [\mathbf{a}_1, ..., \mathbf{a}_{b_U}]$ with $\mathbf{a}_k = [\beta_1 \omega_k(\mathbf{x}_1), ..., \beta_{n_x} \omega_k(\mathbf{x}_{n_x})]^\top$.

• Fourier bases. Let $\{\omega_k\}_{k=1}^{b_U}$ be Fourier bases so that ω_k has period $2/N_k$ along each dimension for some integer $N_k \geq 1$, i.e., $\omega_k = \prod_{j=1}^{d_1} \omega_{k,j}(x_j)$ with $\omega_{k,j} = \sin\left(\frac{N_k \pi}{\gamma_1} x_j\right)$ or $\omega_{k,j} = \cos\left(\frac{N_k \pi}{\gamma_1} x_j\right)$. One can choose $\{\mathbf{x}_j\}_{j=1}^{n_x}$ as uniform grids so that the number of grids along each dimension is $\max_k N_k$. We set $A = [\mathbf{a}_1, ..., \mathbf{a}_{b_U}]$ with $\mathbf{a}_k = [\omega_k(\mathbf{x}_1), ..., \omega_k(\mathbf{x}_{n_x})]^{\top}$. Note A is independent of u as β_j are the quadrature weights.

The following theorem provides an approximation theory of DeepONet under the low dimensional structure in Assumption 4.

Theorem 3. Let $d_1, d_2, b_U, n_x > 0$ be integers, $\gamma_1, \gamma_2, \beta_U, \beta_V, L_U, L_V, C_A > 0$, U satisfy Assumption 2 and 4(i), V satisfy Assumption 3, and the discretization grids $\{\mathbf{x}_j\}_{j=1}^{n_x}$ in Ω_U satisfy Assumption 4(ii). There exist constants C_{δ} depending on γ_1, d_1, L_f, L_U and C depending on d_2, L_V, γ_2 such that the following holds: For any $\varepsilon > 0$, set $N = C\varepsilon^{-d_2}$. There exist two network architectures: $\mathcal{F}_1 = \mathcal{F}_{NN}(d_2, 1, L_1, p_1, K_1, \kappa_1, R_1)$ with

$$L_1 = O\left(\log(\varepsilon^{-1})\right), \ p_1 = O(1), \ K_1 = O\left(\log(\varepsilon^{-1})\right), \ \kappa_1 = O(\varepsilon^{-1}), \ R_1 = 1.$$

and $\mathcal{F}_{2} = \mathcal{F}_{NN}(n_{x}, 1, L_{2}, p_{2}, K_{2}, \kappa_{2}, R_{2})$ with

$$L_{2} = O\left(\log(\varepsilon^{-1})\right), \ p_{2} = O(\varepsilon^{-(d_{2}+1)b_{U}}), \ K_{2} = O\left((\varepsilon^{-(d_{2}+1)b_{U}})(\log(\varepsilon^{-1}) + n_{x})\right),$$

$$\kappa_{2} = O(\varepsilon^{-(d_{2}+1)(b_{U}+1)}), \ R = \beta_{V}.$$

such that, for any operator $G: U \to V$ satisfying Assumption 1, there are $\{\tilde{q}_k\}_{k=1}^N$ with $\tilde{q}_k \in \mathcal{F}_1$ and $\{\tilde{a}_k\}_{k=1}^N$ with $\tilde{a}_k \subset \mathcal{F}_2$ such that

$$\sup_{u \in U} \sup_{\mathbf{y} \in \Omega_V} \left| G(u)(\mathbf{y}) - \sum_{k=1}^N \widetilde{a}_k(\mathbf{u}) \widetilde{q}_k(\mathbf{y}) \right| \le \varepsilon.$$

The constant hidden in O depends on $\gamma_1, \gamma_2, \beta_U, \beta_V, d_1, d_2, L_G, L_U, L_V, b_U, C_A$.

Theorem 3 is proved in Section 5.3. Importantly, Theorem 3 implies a power-law convergence of the DeepONet approximation error.

• Model scaling law. Compared to Corollary 1, Theorem 3 has a significant improvement on the network size: the number of nonzero parameters is improved from the order of $\varepsilon^{-C_1(d_2+1)\varepsilon^{-d_1}-5d_1/2-d_2}$ in Corollary 1 to the order of $\varepsilon^{-(d_2+1)b_U-d_2}$ in Theorem 3 for the C_1 defined in Corollary 1 up to logarithmic factors. If we denote the number of network parameters in Theorem 3 by $N_{\#}$, the approximation error is on the order of $N_{\#}^{-\frac{1}{(d_2+1)b_U+d_2}}$, demonstrating a power model scaling law. Based on Assumption 4, we consider the following setting for learning Lipschitz operators under low-dimensional structures of U:

Setting 2. Let $\{\mathbf{x}_j\}_{j=1}^{n_x} \subset \Omega_U$ be a fixed discretization gird in Ω_U , where n_x is the number of grid points in Ω_U which is to be specified later. For i = 1, ..., n, let $\{\mathbf{y}_{i,j}\}_{j=1}^{n_y} \subset \Omega_V$ be i.i.d. samples following a distribution ρ_y on Ω_V . Assume we are given a set of paired samples $\{\mathbf{u}_i, \mathbf{v}_i\}_{i=1}^n$ with

$$\mathbf{u}_{i} = [u_{i}(\mathbf{x}_{1}), ..., u_{i}(\mathbf{x}_{n_{x}})]^{\top}, \quad \mathbf{v}_{i} = [G(u_{i})(\mathbf{y}_{i,1}) + \xi_{i,1}, ..., G(u_{i})(\mathbf{y}_{i,n_{y}}) + \xi_{i,n_{y}}]^{\top},$$
(17)

where u_i 's are i.i.d. samples from the distribution ρ_u in U, and $\{\xi_{i,j}\}$ follows i.i.d sub-Gaussian distribution with variance proxy σ^2 . We denote $\boldsymbol{\xi}_i = [\zeta(\mathbf{y}_{i,1}), ..., \zeta(\mathbf{y}_{i,n_y})]$. Suppose U satisfies Assumption 2 and 4(i), V satisfies Assumption 3, and $\{\mathbf{x}_j\}_{j=1}^{n_x}$ satisfies Assumption 4(ii).

The generalization error of DeepONet under Setting 2 is given in the following theorem:

Theorem 4. In Setting 2, let $d_1, d_2, n_x, n_y, n, b_U > 0$ be integers, $\gamma_1, \gamma_2, \beta_U, \beta_V, L_U, L_V, L_G, C_A > 0$. Suppose $G : U \to V$ satisfies Assumption 1, and consider Setting 2. There exist constants C depending on d_2, L_V, γ_2 and C_1 depending on $\sigma, \gamma_1, \gamma_2, \beta_U, \beta_V, d_1, d_2, L_G, L_U, L_V$, such that the following holds: Consider the DeepONet network (7) with $N = C(nn_y)^{\frac{d_2}{2+(d_2+1)b_U+d_2}}$, $\mathcal{F}_1 = \mathcal{F}_{NN}(d_2, 1, L_1, p_1, K_1, \kappa_1, R_1)$ and $\mathcal{F}_2 = \mathcal{F}_{NN}(n_x, 1, L_2, p_2, K_2, \kappa_2, R_2)$ where

$$L_1 = O\left(\log(nn_y)\right), \ p_1 = O(1), \ K_1 = O\left(\log(nn_y)\right), \ \kappa_1 = O\left((nn_y)^{\frac{1}{2+(d_2+1)b_U+d_2}}\right), \ R_1 = 1,$$
(18)

and

$$L_{2} = O\left(\log(nn_{y})\right), \ p_{2} = O\left((nn_{y})^{\frac{(d_{2}+1)b_{U}+d_{2}}{2+(d_{2}+1)b_{U}}}\right), \ K_{2} = O\left(\frac{(d_{2}+1)b_{U}}{2+(d_{2}+1)b_{U}+d_{2}}\log(nn_{y})\right),$$

$$\kappa_{2} = O\left((nn_{y})^{\frac{(d_{2}+1)(b_{U}+1)}{2+(d_{2}+1)b_{U}+d_{2}}}\right), \ R_{2} = \beta_{V}.$$
(19)

The constant hidden in O depends on $\sigma, \gamma_1, \gamma_2, \beta_U, \beta_V, d_1, d_2, L_G, L_U, L_V, b_U, C_A$. Then $\widehat{G} \in \mathcal{G}_{NN}$ solving (10) satisfies the following generalization error bound

$$\mathbb{E}_{\mathcal{S}}\mathbb{E}_{\{\mathbf{y}_j\}_{j=1}^{n_y} \sim \rho_y} \mathbb{E}_{u \sim \rho_u} \left[\frac{1}{n_y} \sum_{j=1}^{n_y} (\widehat{G}(\boldsymbol{u})(\mathbf{y}_j) - G(u)(\mathbf{y}_j))^2 \right] \le C_1 (nn_y)^{-\frac{2}{2 + (d_2 + 1)b_U + d_2}} (\log^2(nn_y) + \log n_x)$$
(20)

Theorem 4 is proved in Section 5.4. We have the following discussion:

- Data scaling law. By exploiting low-dimensional structures of U, the squared generalization error is improved from the order of $[\log(nn_y)/\log\log(nn_y)]^{-2/d_1}$ in Theorem 2 to the order of $(nn_y)^{-\frac{2}{2+(d_2+1)b_U}}(\log^2(nn_y) + \log n_x)$ in Theorem 4. This power law decay is consistent with the empirical observations in Lu et al. (2021b); de Hoop et al. (2022), and our theory provides a rigorous justification of the data scaling law.
- Adapting to low-dimensional data structures. By incorporating the low-dimensional structure in Assumption 4, we can derive a faster rate of convergence in comparison with the general case. In our network construction, we do not need to explicitly know or learn the bases $\{\omega_l\}_{k=1}^{b_U}$ by neural networks. The bases are encoded in some functionals which are to be learned by neural networks. Our results show that deep neural networks are automatically adaptive to low-dimensional data structures.



Figure 2: Illustration of the network architecture in Theorem 6. Here **u** is the discretization of $u \in U$.

5 Proof of main Results

5.1 Proof of Theorem 1

The proof of Theorem 1 relies on Theorem 5 and Theorem 6 below. Theorem 5 is an approximation result for Lipschitz functions by deep neural networks.

Theorem 5. Let $d_1 > 0$ be an integer, $\gamma_1, \beta_U, L_U > 0$ and U satisfy Assumption 2. There exists some constant C depending on γ_1, L_U such that the following holds: For any $\varepsilon > 0$, set $N = C\sqrt{d_1}\varepsilon^{-1}$. Let $\{\mathbf{c}_k\}_{k=1}^{N^{d_1}}$ be a uniform grid on Ω_U with spacing $2\gamma_1/N$ along each dimension. There exists a network architecture $\mathcal{F}_{NN}(d_1, 1, L, p, K, \kappa, R)$ and networks $\{\widetilde{q}_k\}_{k=1}^{N^{d_1}}$ with $\widetilde{q}_k \in \mathcal{F}_{NN}(d_1, 1, L, p, K, \kappa, R)$ for $k = 1, ..., N^{d_1}$, such that for any $u \in U$, we have

$$\left\| u - \sum_{k=1}^{N^{d_1}} u(\mathbf{c}_k) \widetilde{q}_k \right\|_{L^{\infty}(\Omega_U)} \le \varepsilon.$$
(21)

Such a network architecture has

$$\begin{split} L &= O\left(d_1^2 \log d_1 + d_1^2 \log(\varepsilon^{-1})\right), p = O(1), K = O\left(d_1^2 \log d_1 + d_1^2 \log(\varepsilon^{-1})\right), \\ \kappa &= O(d_1^{d_1/2 + 1} \varepsilon^{-d_1 - 1}), R = 1. \end{split}$$

The constant hidden in O depends on L_U and γ_1 .

Theorem 5 is proved in Section B.1. Theorem 6 below guarantees the approximation error for Lipschitz functionals.

Theorem 6. Let $d_1 > 0$ be an integer, $\gamma_1, \beta_U, L_U, L_f, R_f > 0$, and U satisfy Assumption 2. There exist constants C depending on $\gamma_1, \beta_U, d_1, L_f, R_f$ and C_{δ} depending on γ_1, d_1, L_f, L_U such that the following holds: For any $\varepsilon > 0$, set $\delta = C_{\delta}\varepsilon$ and let $\{\mathbf{c}_m\}_{m=1}^{c_U} \subset \Omega_U$ so that $\{\mathcal{B}_{\delta}(\mathbf{c}_m)\}_{m=1}^{c_U}$ is a cover of Ω_U for some $c_U > 0$. Let $H = C_V \overline{c_U} \varepsilon^{-c_U}$, and set the network $\mathcal{F}_{NN}(c_U, 1, L, p, K, \kappa, R)$ with

$$L = O\left(c_U^2 \log c_U + c_U^2 \log(\varepsilon^{-1})\right), \ p = O(1), \ K = O\left(c_U^2 \log c_U + c_U^2 \log(\varepsilon^{-1})\right), \\ \kappa = O(c_U^{c_U/2+1} \varepsilon^{-c_U-1}), \ R = 1.$$

There are $\{\widetilde{q}_k\}_{k=1}^H$ with $\widetilde{q}_k \in \mathcal{F}_{NN}(c_U, 1, L, p, K, \kappa, R)$ for any k, such that for any Lipschitz functional f with Lipschitz constant L_f and $||f||_{L^{\infty}(U)} \leq R_f$, we have

$$\sup_{u \in U} \left| f(u) - \sum_{k=1}^{H} a_k \widetilde{q}_k(\mathbf{u}) \right| \le \varepsilon,$$
(22)

where $\mathbf{u} = [u(\mathbf{c}_1), u(\mathbf{c}_2), ..., u(\mathbf{c}_{c_U})]^\top$, a_k 's are coefficients depending on f and satisfying $|a_k| \leq R_f$. The constant hidden in O depends on $\gamma_1, \beta_U, d_1, L_f, L_U$.

Theorem 6 is proved in Section B.2. The network architecture is illustrated in Figure 2. Theorem 6 expresses the functional network as a sum of H parallel branches, and the network architecture of each branch is quantified. In the following, we express the functional network as one large network and quantifies the network architecture of this large network.

We can set the network architecture $\mathcal{F}_{NN}(c_U, 1, L, p, K, \kappa, R)$ as

$$L = O\left(c_U^2 \log c_U + c_U^2 \log(\varepsilon^{-1})\right), \ p = O(\sqrt{c_U}\varepsilon^{-c_U}), \ K = O\left((\sqrt{c_U}\varepsilon^{-c_U})(c_U^2 \log c_U + c_U^2 \log(\varepsilon^{-1}))\right), \\ \kappa = O(c_U^{c_U/2+1}\varepsilon^{-c_U-1}), \ R = R_f.$$
(23)

For any Lipschitz functional f with Lipschitz constant L_f and $||f||_{L^{\infty}(U)} \leq R_f$, there exists $\tilde{f} \in \mathcal{F}_{NN}(c_U, 1, L, p, K, \kappa, R)$ such that

$$\sup_{u \in U} |f(u) - \tilde{f}(\mathbf{u})| \le \varepsilon.$$
(24)

The constant hidden in O in (23) depends on $\gamma_1, \beta_U, d_1, L_f, L_U$ and L_f .

The following corollary gives an estimation of c_U .

Corollary 2. Let $d_1 > 0$ be an integer, $\gamma_1, \beta_U, L_U, L_f, R_f > 0$, and U satisfy Assumption 2. There exist constants C depending on $\gamma_1, \beta_U, d_1, L_U, R_f, L_f$, and C_{δ}, C_1 depending on γ_1, d_1, L_f, L_U such that the following holds: For any $\varepsilon > 0$, set $\delta = C_{\delta}\varepsilon$, $c_U = C_1\varepsilon^{-d_1}$ and $H = C_{\sqrt{c_U}}\varepsilon^{-c_U}$. There exist $\{\mathbf{c}_m\}_{m=1}^{c_U}$ such that $\{\mathcal{B}_{\delta}(\mathbf{c}_m)\}_{m=1}^{c_U}$ is a cover of Ω_U . Set the network $\mathcal{F}_{NN}(c_U, 1, L, p, K, \kappa, R)$ with

$$L = O\left(c_U^2 \log c_U + c_U^2 \log(\varepsilon^{-1})\right), \ p = O(1), \ K = O\left(c_U^2 \log c_U + c_U^2 \log(\varepsilon^{-1})\right), \\ \kappa = O(c_U^{c_U/2+1}\varepsilon^{-c_U-1}), \ R = 1.$$

For any Lipschitz functional f with Lipschitz constant L_f and $||f||_{L^{\infty}(U)} \leq R_f$, there are $\{\widetilde{q}_k\}_{k=1}^H$ with $\widetilde{q}_k \in \mathcal{F}_{NN}(c_U, 1, L, p, K, \kappa, R)$ such that

$$\sup_{u \in U} \left| f(u) - \sum_{k=1}^{H} a_k \widetilde{q}_k(\mathbf{u}) \right| \le \varepsilon,$$
(25)

where $\mathbf{u} = [u(\mathbf{c}_1), u(\mathbf{c}_2), ..., u(\mathbf{c}_{c_U})]^\top$, a_k 's are coefficients depending on f and satisfying $|a_k| \leq R_f$. The constant hidden in O depends on $\gamma_1, \beta_U, d_1, L_f, R_f, L_U$.

Corollary 2 is proved in Section B.4.

Remark 1. The approximation theory for functionals has been studied in Mhaskar and Hahm (1997). It was proved in Mhaskar and Hahm (1997, Theorem 2.2) that, when the activation function is infinitely smooth, the approximation error of a Lipschitz functional by a two-layer network is lower

bounded by $O((\log N)^{-1/d_1})$ where N is the number of computational neurons. In Corollary 2, N is bounded by the total number of weight parameters, thus $N = O(\varepsilon^{-d_1/2}\varepsilon^{-C_1\varepsilon^{-d_1}})(\varepsilon^{-2d_1}\log\varepsilon^{-1})$, which implies $\varepsilon = O\left(\left(\frac{\log N}{\log\log N}\right)^{-\frac{1}{d_1}}\right)$. Rewriting (25) gives $\left\| f(u) - \sum_{k=1}^{H} a_k \widetilde{q}_k(\mathbf{u}) \right\|_{L^{\infty}(U)} \leq C_2 \left(\frac{\log N}{\log\log N}\right)^{-\frac{1}{d_1}}$

for some C_2 depending on $\gamma_1, \beta_U, d_1, L_f, R_f, L_U$. Our result is consistent with the approximation rate in Song et al. (2023) and is optimal up to a $(\log \log N)^{1/d_1}$ factor according to Mhaskar and Hahm (1997).

Remark 2. A simple set of $\{\mathbf{c}_m\}_{m=1}^{c_U}$ satisfying the condition in Corollary 2 is the uniform grid in Ω_U with grid spacing $\frac{\varepsilon}{4\sqrt{d_1}(2\gamma_1)^{d_1/2}L_fL_U}$.

Now we are ready to prove Theorem 1.

Proof of Theorem 1. By Theorem 5, for any $\varepsilon_1 > 0$, there exists a constant $N = C\varepsilon_1^{-d_2}$ for some constant C depending on d_2 , L_V and γ_2 , and a network architecture $\mathcal{F}_1 = \mathcal{F}_{NN}(d_2, 1, L_1, p_1, K_1, \kappa_1, R_1)$ and $\{\widetilde{q}_k\}_{k=1}^N$ with $\widetilde{q}_k \in \mathcal{F}_1$, and $\{\mathbf{c}_k\}_{k=1}^N \subset \Omega_V$ such that for any $u \in U$, we have

$$\sup_{\mathbf{y}\in\Omega_V} \left| G(u)(\mathbf{y}) - \sum_{k=1}^N G(u)(\mathbf{c}_k)\widetilde{q}_k(\mathbf{y}) \right| \le \varepsilon_1.$$
(26)

Such a network has parameters

$$L_1 = O\left(\log(\varepsilon_1^{-1})\right), \ p_1 = O(1), \ K_1 = O\left(\log(\varepsilon_1^{-1})\right), \ \kappa_1 = O(\varepsilon_1^{-d_2 - 1}), \ R_1 = 1,$$

where the constant hidden in O depends on d_2, L_V and γ_2 .

For each k, define the functional $f_k: V \to R$ such that

$$f_k(G(u)) = G(u)(\mathbf{c}_k). \tag{27}$$

For any $u_1, u_2 \in U$, we have $|f_k(G(u_1))| \leq \beta_V$, $|f_k(G(u_2))| \leq \beta_V$ and

$$|f_{k}(G(u_{1})) - f_{k}(G(u_{2}))| = |G(u_{1})(\mathbf{c}_{k}) - G(u_{2})(\mathbf{c}_{k})|$$

$$\leq \sup_{\mathbf{y} \in \Omega_{V}} |G(u_{1})(\mathbf{y}) - G(u_{2})(\mathbf{y})|$$

$$\leq L_{G} ||u_{1} - u_{2}||_{L^{2}(\Omega_{U})}, \qquad (28)$$

where the last inequality follows from Assumption 1.

By Theorem 6, for any $\varepsilon_2 > 0$, there exists a network architecture $\mathcal{F}_2 = \mathcal{F}_{NN}(c_U, 1, L_2, p_2, K_2, \kappa_2, R_2)$ with

$$L_{2} = O\left(c_{U}^{2}\log c_{U} + c_{U}^{2}\log(\varepsilon_{2}^{-1})\right), \ p_{2} = O(\sqrt{c_{U}}\varepsilon_{2}^{-c_{U}}), \ K_{2} = O\left((\sqrt{c_{U}}\varepsilon_{2}^{-c_{U}})(c_{U}^{2}\log c_{U} + c_{U}^{2}\log(\varepsilon^{-1}))\right), \\ \kappa_{2} = O(c_{U}^{c_{U}/2+1}\varepsilon_{2}^{-c_{U}-1}), \ R = \beta_{V},$$
(29)

such that, for every functional f_k defined in (27), this network architecture gives a network \tilde{f}_k satisfying

$$\sup_{u \in U} |f_k(G(u)) - \widetilde{f}_k(\mathbf{u})| \le \varepsilon_2.$$

The constant hidden in O of (29) depends on $\gamma_1, \beta_U, \beta_V, d_1, L_G, L_U$. Since $|\tilde{q}_k(\mathbf{y})| \leq 1$ for any $\mathbf{y} \in \Omega_V$, we deduce

$$\sup_{\mathbf{y}\in\Omega_{V}}\left|\sum_{k=1}^{N}f_{k}(G(u))\widetilde{q}_{k}(\mathbf{y})-\sum_{k=1}^{N}\widetilde{f}_{k}(\mathbf{u})\widetilde{q}_{k}(\mathbf{y})\right|$$
$$=\sup_{\mathbf{y}\in\Omega_{V}}\left|\sum_{k=1}^{N}\left(f_{k}(G(u))-\widetilde{f}_{k}(\mathbf{u})\right)\widetilde{q}_{k}(\mathbf{y})\right|$$
$$\leq\sum_{k=1}^{N}\left\|f_{k}(G(u))-\widetilde{f}_{k}(\mathbf{u})\right\|_{L^{\infty}(U)}=N\varepsilon_{2}.$$
(30)

Putting (26) and (30) together, we have

$$\sup_{u \in U} \sup_{\mathbf{y} \in \Omega_{V}} \left| G(u)(\mathbf{y}) - \sum_{k=1}^{N} \widetilde{f}_{k}(\mathbf{u}) \widetilde{q}_{k}(\mathbf{y}) \right|$$

$$\leq \sup_{u \in U} \sup_{\mathbf{y} \in \Omega_{V}} \left| G(u)(y) - \sum_{k=1}^{N} f_{k}(G(u)) \widetilde{q}_{k}(y) \right| + \sup_{u \in U} \sup_{\mathbf{y} \in \Omega_{V}} \left| \sum_{k=1}^{N} f_{k}(G(u)) \widetilde{q}_{k}(y) - \sum_{k=1}^{N} \widetilde{a}_{k}(\mathbf{u}) \widetilde{q}_{k}(y) \right|$$

$$\leq \varepsilon_{1} + N \varepsilon_{2}.$$

Set $\varepsilon_2 = \varepsilon_1/(2N), \varepsilon_1 = \frac{\varepsilon}{2}$, we have

$$\sup_{u \in U} \sup_{\mathbf{y} \in \Omega_V} \left| G(u)(\mathbf{y}) - \sum_{k=1}^N \widetilde{a}_k(\mathbf{u}) \widetilde{q}_k(\mathbf{y}) \right| \le \varepsilon.$$

The resulting network architectures have $N = O(\varepsilon^{-d_2})$,

$$L_1 = O\left(\log(\varepsilon^{-1})\right), \ p_1 = O(1), \ K_1 = O\left(\log(\varepsilon^{-1})\right), \ \kappa_1 = O(\varepsilon^{-1}), \ R_1 = 1,$$

and

$$L_{2} = O\left(c_{U}^{2}\log c_{U} + c_{U}^{2}\log(\varepsilon^{-1})\right), \ p_{2} = O(\sqrt{c_{U}}\varepsilon^{-(d_{2}+1)c_{U}}),$$

$$K_{2} = O\left(\left(\sqrt{c_{U}}\varepsilon^{-(d_{2}+1)c_{U}}\right)\left(c_{U}^{2}\log c_{U} + c_{U}^{2}\log(\varepsilon^{-1})\right)\right),$$

$$\kappa_{2} = O(c_{U}^{c_{U}/2+1}\varepsilon^{-(d_{2}+1)(c_{U}+1)}), \ R = \beta_{V}.$$

The constant hidden in O depends on $\gamma_1, \gamma_2, \beta_U, \beta_V, d_1, d_2, L_G, L_U, L_V$.

5.2 Proof of Theorem 2

Proof of Theorem 2. We rewrite the error as

$$\mathbb{E}_{\mathcal{S}} \mathbb{E}_{\{\mathbf{y}_j\}_{j=1}^{n_y} \sim \rho_y} \mathbb{E}_{u \sim \rho_u} \left[\frac{1}{n_y} \sum_{j=1}^{n_y} (\widehat{G}(\mathbf{u})(\mathbf{y}_j) - G(u)(\mathbf{y}_j))^2 \right]$$
$$= \underbrace{2\mathbb{E}_{\mathcal{S}} \left[\frac{1}{n} \sum_{i=1}^n \frac{1}{n_y} \sum_{j=1}^{n_y} (\widehat{G}(\mathbf{u}_i)(\mathbf{y}_{i,j}) - G(u_i)(\mathbf{y}_{i,j}))^2 \right]}_{\mathrm{T}_1}$$

where u_i and $\mathbf{y}_{i,j}$ are given in the training dataset \mathcal{S} . • Bounding T₁. For T₁, we have

$$\begin{split} & \mathbf{T}_{1} = 2\mathbb{E}_{\mathcal{S}} \left[\frac{1}{n} \sum_{i=1}^{n} \frac{1}{n_{y}} \sum_{j=1}^{n_{y}} (\hat{G}(\mathbf{u}_{i})(\mathbf{y}_{i,j}) - G(u)(\mathbf{y}_{i,j}))^{2} \right] \\ &= 2\mathbb{E}_{\mathcal{S}} \left[\frac{1}{n} \sum_{i=1}^{n} \frac{1}{n_{y}} \sum_{j=1}^{n_{y}} (\hat{G}(\mathbf{u}_{i})(\mathbf{y}_{i,j}) - v_{i,j} + \xi_{i,j})^{2} \right] \\ &= 2\mathbb{E}_{\mathcal{S}} \left[\frac{1}{n} \sum_{i=1}^{n} \frac{1}{n_{y}} \sum_{j=1}^{n_{y}} \left[(\hat{G}(\mathbf{u}_{i})(\mathbf{y}_{i,j}) - v_{i,j})^{2} + 2(\hat{G}(\mathbf{u}_{i})(\mathbf{y}_{i,j}) - v_{i,j})\xi_{i,j} + \xi_{i,j}^{2} \right] \right] \\ &= 2\mathbb{E}_{\mathcal{S}} \left[\frac{1}{n} \sum_{i=1}^{n} \frac{1}{n_{y}} \sum_{j=1}^{n_{y}} (\hat{G}(\mathbf{u}_{i})(\mathbf{y}_{i,j}) - v_{i,j})^{2} + 2(\hat{G}(\mathbf{u}_{i})(\mathbf{y}_{i,j}) - v_{i,j})\xi_{i,j} + \xi_{i,j}^{2} \right] \\ &= 2\mathbb{E}_{\mathcal{S}} \left[\frac{1}{n} \sum_{i=1}^{n} \frac{1}{n_{y}} \sum_{j=1}^{n_{y}} (\hat{G}(\mathbf{u}_{i})(\mathbf{y}_{i,j}) - v_{i,j})\xi_{i,j} \right] + 2\mathbb{E}_{\mathcal{S}} \left[\frac{1}{n} \sum_{i=1}^{n} \frac{1}{n_{y}} \sum_{j=1}^{n_{y}} \xi_{i,j}^{2} \right] \\ &= 2\mathbb{E}_{\mathcal{S}} \inf_{GNN \in \mathcal{G}_{NN}} \left[\frac{1}{n} \sum_{i=1}^{n} \frac{1}{n_{y}} \sum_{j=1}^{n_{y}} (G(\mathbf{u}_{i})(\mathbf{y}_{i,j}) - G(u_{i})(\mathbf{y}_{i,j}) - \xi_{i,j})\xi_{i,j} \right] + 2\mathbb{E}_{\mathcal{S}} \left[\frac{1}{n} \sum_{i=1}^{n} \frac{1}{n_{y}} \sum_{j=1}^{n_{y}} \xi_{i,j}^{2} \right] \\ &= 2\mathbb{E}_{\mathcal{S}} \inf_{GNN \in \mathcal{G}_{NN}} \mathbb{E}_{\mathcal{S}} \left[\frac{1}{n} \sum_{i=1}^{n} \frac{1}{n_{y}} \sum_{j=1}^{n_{y}} (G(\mathbf{u}_{i})(\mathbf{y}_{i,j}) - G(u_{i})(\mathbf{y}_{i,j}) - \xi_{i,j})\xi_{i,j} \right] + 2\mathbb{E}_{\mathcal{S}} \left[\frac{1}{n} \sum_{i=1}^{n} \frac{1}{n_{y}} \sum_{j=1}^{n_{y}} \xi_{i,j}^{2} \right] \\ &= 2 \inf_{GNN \in \mathcal{G}_{NN}} \mathbb{E}_{\mathcal{S}} \left[\frac{1}{n} \sum_{i=1}^{n} \frac{1}{n_{y}} \sum_{j=1}^{n_{y}} (G(\mathbf{u}_{i})(\mathbf{y}_{i,j}) - G(u_{i})(\mathbf{y}_{i,j}) - \xi_{i,j})^{2} - 2\mathbb{E}_{\mathcal{S}} \left[\frac{1}{n} \sum_{i=1}^{n} \frac{1}{n_{y}} \sum_{j=1}^{n_{y}} \xi_{i,j}^{2} \right] \\ &= 2 \inf_{GNN \in \mathcal{G}_{NN}} \mathbb{E}_{\mathcal{S}} \left[\frac{1}{n} \sum_{i=1}^{n} \frac{1}{n_{y}} \sum_{j=1}^{n_{y}} (\widehat{G}(\mathbf{u}_{i})(\mathbf{y}_{i,j}) - G(u_{i})(\mathbf{y}_{i,j}) - G(u_{i})(\mathbf{y}_{j,j})^{2} - \xi_{i,j}^{2} \right] \\ &= 2 \inf_{GNN \in \mathcal{G}_{NN}} \mathbb{E}_{\mathcal{G}_{NN}} \mathbb{E}_{\mathcal{G}_{N}} \left[\frac{1}{n_{y}} \sum_{j=1}^{n_{y}} (G(\mathbf{u}_{N})(\mathbf{u}_{i,j}) - G(u_{i})(\mathbf{y}_{j,j}) - G(u_{i})(\mathbf{y}_{j,j})^{2} \right] \\ &= 2 \inf_{GNN \in \mathcal{G}_{NN}} \mathbb{E}_{\mathcal{G}_{NN}} \mathbb{E}_{\mathcal{G}_{N}} \left[\frac{1}{n_{y}} \sum_{j=1}^{n_{y}} (\widehat{G}(\mathbf{u}_{N})(\mathbf{y}_{i,j}) - G(u_{i})(\mathbf{y}_{i,j}) - G($$

$$+ 4\mathbb{E}_{\mathcal{S}}\left[\frac{1}{n}\sum_{i=1}^{n}\frac{1}{n_{y}}\sum_{j=1}^{n_{y}}\widehat{G}(\mathbf{u}_{i})(\mathbf{y}_{i,j})\xi_{i,j}\right]$$
(32)

The first term in (32) can be bounded by Corollary 1. More specifically, for any $\varepsilon > 0$, we choose $n_x = C_1 \varepsilon^{-d_1}$ so that $\{\mathcal{B}_{\delta}(\mathbf{c}_m)\}_{m=1}^{n_x}$ is a cover of Ω_U with $\delta = C_{\delta}\varepsilon$ for some C_1, C_{δ} depending on γ_1, d_1, L_f and L_U . According to Corollary 1, we can set network architecture $\mathcal{F}_1 = \mathcal{F}_{NN}(d_2, 1, L_1, p_1, K_1, \kappa_1, R_1)$ and $\mathcal{F}_2 = \mathcal{F}_{NN}(n_x, 1, L_2, p_2, K_2, \kappa_2, R_2)$ with

$$L_1 = O\left(\log(\varepsilon^{-1})\right), \ p_1 = O(1), \ K_1 = O\left(\log(\varepsilon^{-1})\right), \ \kappa_1 = O(\varepsilon^{-1}), \ R_1 = 1.$$
(33)

and

$$L_{2} = O\left(\varepsilon^{-2d_{1}}\log\varepsilon^{-1} + \varepsilon^{-2d_{1}}\log(\varepsilon^{-1})\right), \ p_{2} = O(\varepsilon^{-d_{1}/2}\varepsilon^{-C_{1}(d_{2}+1)\varepsilon^{-d_{1}}}),$$

$$K_{2} = O\left(\varepsilon^{-C_{1}(d_{2}+1)\varepsilon^{-d_{1}+5d_{1}/2}}\log\varepsilon^{-1}\right),$$

$$\kappa_{2} = O(\varepsilon^{-C_{1}d_{1}\varepsilon^{-d_{1}/2+1}}\varepsilon^{-(d_{2}+1)(C_{1}\varepsilon^{-d_{1}+1})}), \ R = \beta_{V}.$$
(34)

The constant in O depends on $\gamma_1, \gamma_2, \beta_U, \beta_V, d_1, d_2, L_G, L_U, L_V$. Set $N = C\varepsilon^{-d_2}$ for some constant C depending on d_2, L_V and γ_2 . There are $\{\widetilde{q}_k\}_{k=1}^N$ with $\widetilde{q}_k \in \mathcal{F}_1$ and $\{\widetilde{a}_k\}_{k=1}^N$ with $\widetilde{a}_k \in \mathcal{F}_2$ such that

$$\sup_{u \in U} \sup_{\mathbf{y} \in \Omega_V} \left| G(u)(\mathbf{y}) - \sum_{k=1}^N \widetilde{a}_k(\mathbf{u}) \widetilde{q}_k(\mathbf{y}) \right| \le \varepsilon.$$

The first term in (32) is bounded by

$$2\inf_{G_{\rm NN}\in\mathcal{G}_{\rm NN}}\mathbb{E}_{\boldsymbol{u}\sim\rho_{\boldsymbol{u}}}\mathbb{E}_{\{\mathbf{y}_j\}_{j=1}^{n_y}}\left[\frac{1}{n_y}\sum_{j=1}^{n_y}\left(G_{\rm NN}(\mathbf{u})(\mathbf{y}_j)-G(\boldsymbol{u})(\mathbf{y}_j)\right)^2\right] \le 2\varepsilon^2.$$
(35)

The second term in (32) is bounded by the following lemma (see proof in Section B.6):

Lemma 3. Under the condition of Theorem 2, the second term in (32) is bounded as

$$\mathbb{E}_{\mathcal{S}}\left[\frac{1}{n}\sum_{i=1}^{n}\frac{1}{n_{y}}\sum_{j=1}^{n_{y}}\widehat{G}(\mathbf{u}_{i})(\mathbf{y}_{i,j})\xi_{i,j}\right]$$

$$\leq 2\sigma\left(\sqrt{\mathbb{E}_{\mathcal{S}}\left[\|\widehat{G}-G\|_{n}^{2}\right]}+\theta\right)\sqrt{\frac{4\log\mathcal{N}(\theta,\mathcal{G}_{\mathrm{NN}},\|\cdot\|_{\infty,\infty})+6}{nn_{y}}}+\sigma\theta.$$
(36)

Let \hat{G} be the network specified in (33) and (34). Substituting (35) and (36) into (32) gives rise to

$$T_{1} = 2\mathbb{E}_{\mathcal{S}}\left[\frac{1}{n}\sum_{i=1}^{n}\frac{1}{n_{y}}\sum_{j=1}^{n_{y}}(\widehat{G}(\mathbf{u}_{i})(\mathbf{y}_{i,j}) - G(u_{i})(\mathbf{y}_{i,j}))^{2}\right]$$
$$\leq 2\varepsilon^{2} + 8\sigma\left(\sqrt{\mathbb{E}_{\mathcal{S}}\left[\|\widehat{G} - G\|_{n}^{2}\right]} + \theta\right)\sqrt{\frac{4\log\mathcal{N}(\theta,\mathcal{G}_{\mathrm{NN}},\|\cdot\|_{\infty,\infty}) + 6}{nn_{y}}} + 4\sigma\theta.$$
(37)

Denote

$$\eta = \sqrt{\mathbb{E}_{\mathcal{S}} \left[\|\widehat{G} - G\|_{n}^{2} \right]},$$

$$a = \varepsilon^{2} + 2\sigma\theta + 4\sigma\theta\sqrt{\frac{4\log\mathcal{N}(\theta, \mathcal{G}_{\mathrm{NN}}, \|\cdot\|_{\infty,\infty}) + 6}{nn_{y}}},$$

$$b = 2\sigma\sqrt{\frac{4\log\mathcal{N}(\theta, \mathcal{G}_{\mathrm{NN}}, \|\cdot\|_{\infty,\infty}) + 6}{nn_{y}}}.$$

Then (37) can be rewritten as

$$\eta^2 \le a + 2b\eta,$$

from which we deduce that

$$(\eta - b)^2 \le a + b^2 \quad \Rightarrow \quad \eta \le \sqrt{a + b^2} + b \quad \Rightarrow \quad \eta^2 \le 2a + 4b^2.$$

Thus we have

$$T_{1} = 2\eta^{2}$$

$$\leq 4\varepsilon^{2} + 8\sigma\theta + 16\sigma\theta\sqrt{\frac{4\log\mathcal{N}(\theta,\mathcal{G}_{NN},\|\cdot\|_{\infty,\infty}) + 6}{nn_{y}}} + 16\sigma^{2}\frac{4\log\mathcal{N}(\theta,\mathcal{G}_{NN},\|\cdot\|_{\infty,\infty}) + 6}{nn_{y}}.$$
 (38)

Bounding T₂. An upper bound of T₂ is given by the following lemma (see a proof in Section B.7)
Lemma 4. Under the condition of Theorem 2, we have

$$T_{2} \leq \frac{19\beta_{V}^{2}}{nn_{y}} \log \mathcal{N}\left(\frac{\theta}{4\beta_{V}}, \mathcal{G}_{NN}, \|\cdot\|_{\infty,\infty}\right) + 6\theta.$$
(39)

• Putting T_1, T_2 together.

Substituting (38) and (84) into (31) gives rise to

$$\mathbb{E}_{\mathcal{S}}\mathbb{E}_{\{\mathbf{y}_{j}\}_{j=1}^{n_{y}}\sim\rho_{y}}\mathbb{E}_{u\sim\rho_{u}}\left[\frac{1}{n_{y}}\sum_{j=1}^{n_{y}}(\widehat{G}(\mathbf{u};\mathbf{y}_{j}))-G(\mathbf{u};\mathbf{y}_{j}))^{2}\right] \\
\leq 4\varepsilon^{2}+8\sigma\theta+16\sigma\theta\sqrt{\frac{4\log\mathcal{N}(\theta,\mathcal{G}_{\mathrm{NN}},\|\cdot\|_{\infty,\infty})+6}{nn_{y}}}+16\sigma^{2}\frac{4\log\mathcal{N}(\theta,\mathcal{G}_{\mathrm{NN}},\|\cdot\|_{\infty,\infty})+6}{nn_{y}} \\
+\frac{19\beta_{V}^{2}}{nn_{y}}\log\mathcal{N}\left(\frac{\theta}{4\beta_{V}},\mathcal{G}_{\mathrm{NN}},\|\cdot\|_{\infty,\infty}\right)+6\theta \\
\leq 4\varepsilon^{2}+\frac{64\sigma^{2}+19\beta_{V}^{2}+96}{nn_{y}}\log\mathcal{N}\left(\frac{\theta}{4\beta_{V}},\mathcal{G}_{\mathrm{NN}},\|\cdot\|_{\infty,\infty}\right) \\
+16\sigma\theta\sqrt{\frac{4\log\mathcal{N}(\frac{\theta}{4\beta_{V}},\mathcal{G}_{\mathrm{NN}},\|\cdot\|_{\infty,\infty})+6}{nn_{y}}}+(8\sigma+6)\theta.$$
(40)

The following lemma (see a proof in Section B.8) gives an upper bound of $\mathcal{N}(\theta, \mathcal{G}_{NN}, \|\cdot\|_{\infty,\infty})$:

Lemma 5. Let $\mathcal{F}_1 = \mathcal{F}_{NN}(d_1, 1, L_1, p_1, K_1, \kappa_1, R_1)$ and $\mathcal{F}_2 = \mathcal{F}_{NN}(d_2, 1, L_2, p_2, K_2, \kappa_2, R_2)$. We have

$$\mathcal{N}(\theta, \mathcal{G}_{\mathrm{NN}}, \|\cdot\|_{\infty,\infty}) \le \left(\frac{2L_1 p_1^2 \kappa_1 H}{\theta}\right)^{NK_1} \left(\frac{2L_2 p_2^2 \kappa_2 H}{\theta}\right)^{NK_2},$$

with $H = N \left(R_1 L_1 (p_1 \gamma_2 + 2) (\kappa_1 p_1)^{L_1 - 1} + R_2 L_2 (p_2 \beta_U + 2) (\kappa_2 p_2)^{L_2 - 1} \right).$

Substituting (33) and (34) into Lemma 5 gives rise to

$$\log \mathcal{N}(\theta, \mathcal{G}_{\mathrm{NN}}, \|\cdot\|_{\infty,\infty})$$

$$= NK_{1}(\log 2 + \log L_{1} + 2\log p_{1} + \log \kappa_{1} + \log H + \log \frac{1}{\theta})$$

$$+ NK_{2}(\log 2 + \log L_{2} + 2\log p_{2} + \log \kappa_{2} + \log H + \log \frac{1}{\theta})$$

$$\leq C_{4}N(K_{1} + K_{2})(\log H + \log \frac{1}{\theta})$$

$$\leq C_{4}N(K_{1} + K_{2})(\log N + L_{2}(\log L_{2} + \log p_{2} + \log \kappa_{2}) + \log \frac{1}{\theta})$$

$$\leq C_{4}\varepsilon^{-C_{1}(d_{2}+1)\varepsilon^{-d_{1}} - 5d_{1}/2 - d_{2}}\log \frac{1}{\varepsilon} \left(\log \frac{1}{\varepsilon} + \varepsilon^{-2d_{1}}\log \frac{1}{\varepsilon} \left(\log \frac{1}{\varepsilon} + \varepsilon^{-d_{1}}\log \frac{1}{\varepsilon}\right) + \log \frac{1}{\theta}\right)$$

$$\leq C_{4}\varepsilon^{-C_{1}(d_{2}+1)\varepsilon^{-d_{1}} - 11d_{1}/2 - d_{2}}\log \frac{1}{\varepsilon} (\log^{2} \frac{1}{\varepsilon} + \log \frac{1}{\theta})$$

$$(41)$$

where C_4 is a constant depending on $\gamma_1, \gamma_2, \beta_U, \beta_V, d_1, d_2, L_G, L_U, L_V$.

Substituting (41) into (40) gives rise to

$$\mathbb{E}_{\mathcal{S}} \mathbb{E}_{\{\mathbf{y}_{j}\}_{j=1}^{n_{y}} \sim \rho_{y}} \mathbb{E}_{u \sim \rho_{u}} \left[\frac{1}{n_{y}} \sum_{j=1}^{n_{y}} (\widehat{G}(\mathbf{u})(\mathbf{y}_{j}) - G(u)(\mathbf{y}_{j}))^{2} \right] \\
\leq 4\varepsilon^{2} + \frac{64\sigma^{2} + 19\beta_{V}^{2} + 96}{nn_{y}} C_{4}\varepsilon^{-C_{1}(d_{2}+1)\varepsilon^{-d_{1}-11d_{1}/2-d_{2}}} \log \frac{1}{\varepsilon} (\log^{2} \frac{1}{\varepsilon} + \log \frac{1}{\theta}) \\
+ 16\sigma\theta \sqrt{\frac{4C_{4}\varepsilon^{-C_{1}(d_{2}+1)\varepsilon^{-d_{1}-11d_{1}/2-d_{2}} \log \frac{1}{\varepsilon} (\log^{2} \frac{1}{\varepsilon} + \log \frac{1}{\theta}) + 6}{nn_{y}}} + (8\sigma + 6)\theta. \quad (42)$$

Set $\theta = (nn_y)^{-1}$. We have

$$\mathbb{E}_{\mathcal{S}}\mathbb{E}_{\{\mathbf{y}_j\}_{j=1}^{n_y} \sim \rho_y} \mathbb{E}_{u \sim \rho_u} \left[\frac{1}{n_y} \sum_{j=1}^{n_y} (\widehat{G}(\mathbf{u})(\mathbf{y}_j) - G(\mathbf{u})(\mathbf{y}_j))^2 \right] \\
\leq C_2 \left(\varepsilon^2 + \frac{1}{nn_y} \varepsilon^{-C_1(d_2+1)\varepsilon^{-d_1} - 11d_1/2 - d_2} \right) \log^3 \frac{1}{\varepsilon},$$
(43)

for some C_2 depending on $\sigma, \gamma_1, \gamma_2, \beta_U, \beta_V, d_1, d_2, L_G, L_U, L_V$ In particular, set $\varepsilon = \left(\frac{d_1}{2C_1(d_2+1)} \frac{\log(nn_y)}{\log\log(nn_y)}\right)^{-\frac{1}{d_1}}$. After taking logarithm, ε^2 is of $O(-\log\log(nn_y))$, $\frac{1}{nn_y}\varepsilon^{-C_1(d_2+1)\varepsilon^{-d_1}-11d_1/2-d_2}$ is of $O(-\log(nn_y))$. Thus the error inside the parenthesis of (43) is dominated by ε^2 . We have

$$\mathbb{E}_{\mathcal{S}}\mathbb{E}_{\{\mathbf{y}_j\}_{j=1}^{n_y}\sim\rho_y}\mathbb{E}_{u\sim\rho_u}\left[\frac{1}{n_y}\sum_{j=1}^{n_y}(\widehat{G}(\mathbf{u})(\mathbf{y}_j)-G(\mathbf{u})(\mathbf{y}_j))^2\right] \le C_3\left(\frac{\log(nn_y)}{\log\log(nn_y)}\right)^{-\frac{2}{d_1}}.$$
 (44)
constant C_3 depending on $\sigma, \gamma_1, \gamma_2, \beta_U, \beta_V, d_1, d_2, L_C, L_U, L_V.$

for some constant C_3 depending on $\sigma, \gamma_1, \gamma_2, \beta_U, \beta_V, d_1, d_2, L_G, L_U, L_V$.

5.3 Proof of Theorem 3

To prove Theorem 3, we need the following approximation result for functionals defined on U satisfying Assumption 4.

Theorem 7. Let $d_1, n_x, b_U > 0$ be integers, $\gamma_1, \beta_U, L_U, L_f, R_f > 0$, and U satisfy Assumption 2 and 4 (i), the discretization grids $\{\mathbf{x}_j\}_{j=1}^{n_x}$ satisfy Assumption 4 (ii). There exist constant C depending on $\gamma_1, \beta_U, d_1, L_f, R_f, b_U$ and C_1 depending on γ_1, d_1, β_U such that the following holds: For any $\varepsilon > 0$, set $H = C\sqrt{b_U}\varepsilon^{-b_U}$ and the network $\mathcal{F}_{NN}(n_x, 1, L, p, K, \kappa, R)$ with

$$L = O\left(\log(\varepsilon^{-1})\right), \ p = O(1), \ K = O\left(\log(\varepsilon^{-1})\right),$$

$$\kappa = O(\varepsilon^{-b_U-1}), \ R = 1.$$

There are

$$\sup_{u \in U} \left| f(u) - \sum_{k=1}^{H} a_k \widetilde{q}_k(\mathbf{u}) \right| \le \varepsilon,$$
(45)

where $\mathbf{u} = [u(\mathbf{x}_1), u(\mathbf{x}_2), ..., u(\mathbf{x}_{n_x})]^\top$, a_k 's are coefficients depending on f and satisfying $|a_k| \leq C_1$. The constant hidden in O depends on $\gamma_1, \beta_U, d_1, L_f, L_U, b_U, C_A$.

Theorem 7 is proved in Section B.3. Theorem 7 expresses the functional network as a sum of H parallel branches, and the network architecture of each branch is quantified. In the following, we express the functional network as one large network and quantify the network architecture of this large network.

If we set the network architecture $\mathcal{F}_{NN}(n_x, 1, L, p, K, \kappa, R)$ as

$$L = O\left(\log(\varepsilon^{-1})\right), \ p = O(\varepsilon^{-b_U}), \ K = O\left(\varepsilon^{-b_U}\log(\varepsilon^{-1})\right), \ \kappa = O(\varepsilon^{-b_U-1}), \ R = R_f,$$
(46)

for any Lipschitz functional f with Lipschitz constant no more than L_f and $||f||_{L^{\infty}(U)} \leq R_f$, there exists $\tilde{f} \in \mathcal{F}_{NN}(n_x, 1, L, p, K, \kappa, R)$ such that we have

$$\sup_{u \in U} |f(u) - \widetilde{f}(\mathbf{u})| \le \varepsilon.$$
(47)

The constant hidden in O in (46) depends on $\gamma_1, \beta_U, d_1, L_f, L_U, L_f, b_U, C_A$.

Now we are ready to prove Theorem 3.

Proof of Theorem 3. We follow the proof of Theorem 1 until (28). By Theorem 7, there exists a network architecture $\mathcal{F}_2 = \mathcal{F}_{NN}(n_x, 1, L_2, p_2, K_2, \kappa_2, R_2)$ with

$$L_2 = O\left(\log(\varepsilon_2^{-1})\right), \ p_2 = O(\varepsilon_2^{-b_U}), \ K_2 = O\left(\varepsilon_2^{-b_U}\log(\varepsilon_2^{-1}) + n_x\right), \ \kappa_2 = O(\varepsilon_2^{-b_U-1}), \ R_2 = 1.$$

such that for every functional f_k defined in (27), this network architecture gives a network \tilde{f}_k satisfying

$$\sup_{u \in U} |f_k(G(u)) - \widetilde{f}_k(\mathbf{u})| \le \varepsilon_2.$$

The constant hidden in O depends on $\gamma_1, \beta_U, \beta_V, d_1, L_G, L_U, C_A, b_U$. Since $|\tilde{q}_k(\mathbf{y})| \leq 1$ for any $\mathbf{y} \in \Omega_V$, we deduce

$$\sup_{\mathbf{y}\in\Omega_V}\left|\sum_{k=1}^N f_k(G(u))\widetilde{q}_k(\mathbf{y}) - \sum_{k=1}^N \widetilde{f}_k(\mathbf{u})\widetilde{q}_k(\mathbf{y})\right|$$

$$= \sup_{\mathbf{y}\in\Omega_{V}} \left| \sum_{k=1}^{N} \left(f_{k}(G(u)) - \widetilde{f}_{k}(\mathbf{u}) \right) \widetilde{q}_{k}(\mathbf{y}) \right|$$
$$\leq \sum_{k=1}^{N} \left\| f_{k}(G(u)) - \widetilde{f}_{k}(\mathbf{u}) \right\|_{L^{\infty}(U)} = N\varepsilon_{2}.$$
(48)

Putting (26) and (48) together, we have

$$\sup_{u \in U} \sup_{\mathbf{y} \in \Omega_{V}} \left| G(u)(\mathbf{y}) - \sum_{k=1}^{N} \widetilde{f}_{k}(\mathbf{u}) \widetilde{q}_{k}(\mathbf{y}) \right|$$

$$\leq \sup_{u \in U} \sup_{\mathbf{y} \in \Omega_{V}} \left| G(u)(y) - \sum_{k=1}^{N} f_{k}(G(u)) \widetilde{q}_{k}(y) \right| + \sup_{u \in U} \sup_{\mathbf{y} \in \Omega_{V}} \left| \sum_{k=1}^{N} f_{k}(G(u)) \widetilde{q}_{k}(y) - \sum_{k=1}^{N} \widetilde{a}_{k}(\mathbf{u}) \widetilde{q}_{k}(y) \right|$$

$$\leq \varepsilon_{1} + N \varepsilon_{2}.$$

Set $\varepsilon_2 = \varepsilon_1/(2N), \varepsilon_1 = \frac{\varepsilon}{2}$, we have

$$\sup_{u \in U} \sup_{\mathbf{y} \in \Omega_V} \left| G(u)(\mathbf{y}) - \sum_{k=1}^N \widetilde{a}_k(\mathbf{u}) \widetilde{q}_k(\mathbf{y}) \right| \le \varepsilon.$$

The resulting network architecture has $N = O(\varepsilon^{-d_2})$ branch and trunk sub-networks. Each branch sub-network has parameters

$$L_1 = O\left(\log(\varepsilon^{-1})\right), \ p_1 = O(1), \ K_1 = O\left(\log(\varepsilon^{-1})\right), \ \kappa_1 = O(\varepsilon^{-1}), \ R_1 = 1,$$

and each trunk sub-network has parameters

$$L_{2} = O\left(\log(\varepsilon^{-1})\right), \ p_{2} = O(\varepsilon^{-(d_{2}+1)b_{U}}), \ K_{2} = O\left((\varepsilon^{-(d_{2}+1)b_{U}})(\log(\varepsilon^{-1}) + n_{x})\right),$$

$$\kappa_{2} = O(\varepsilon^{-(d_{2}+1)(b_{U}+1)}), \ R = \beta_{V}.$$

The constant hidden in O depends on $\gamma_1, \gamma_2, \beta_U, \beta_V, d_1, d_2, L_G, L_U, L_V, C_A, b_U$.

5.4 Proof of Theorem 4

Proof of Theorem 4. We follow the proof of Theorem 2 until (40) and replace Corollary 1 by Theorem 3 and \mathcal{F}_2 by $\mathcal{F}_2 = \mathcal{F}_{NN}(n_x, 1, L_2, p_2, K_2, \kappa_2, R_2)$ with

$$L_{2} = O\left(\log(\varepsilon^{-1})\right), \ p_{2} = O(\varepsilon^{-(d_{2}+1)b_{U}}), \ K_{2} = O\left((\varepsilon^{-(d_{2}+1)b_{U}})(\log(\varepsilon^{-1}) + n_{x})\right),$$
(49)

$$\kappa_2 = O(\varepsilon^{-(d_2+1)(b_U+1)}), \ R = \beta_V.$$
(50)

Substituting (33) and (50) into Lemma 5 gives rise to

$$\log \mathcal{N}(\theta, \mathcal{G}_{\mathrm{NN}}, \|\cdot\|_{\infty,\infty})$$

= $NK_1(\log 2 + \log L_1 + 2\log p_1 + \log \kappa_1 + \log H + \log \frac{1}{\theta})$
+ $NK_2(\log 2 + \log L_2 + 2\log p_2 + \log \kappa_2 + \log H + \log \frac{1}{\theta})$
 $\leq C_4(K_1 + K_2)(\log H + \log \frac{1}{\theta})$

$$\leq C_4(K_1 + K_2)(\log N + L_2(\log L_2 + \log p_2 + \log \kappa_2) + \log \frac{1}{\theta})$$

$$\leq C_4 \varepsilon^{-(d_2+1)b_U - d_2} \left(\log^2 \frac{1}{\varepsilon} + \log n_x + \log \frac{1}{\theta}\right)$$
(51)

where C_4 is a constant depending on $\gamma_1, \gamma_2, \beta_U, \beta_V, d_1, d_2, L_G, L_U, L_V, b_U, C_A$.

Substituting (51) into (40) gives rise to

$$\mathbb{E}_{\mathcal{S}}\mathbb{E}_{\{\mathbf{y}_{j}\}_{j=1}^{n_{y}}\sim\rho_{y}}\mathbb{E}_{u\sim\rho_{u}}\left[\frac{1}{n_{y}}\sum_{j=1}^{n_{y}}(\widehat{G}(\mathbf{u})(\mathbf{y}_{j})-G(u)(\mathbf{y}_{j}))^{2}\right]$$

$$\leq 4\varepsilon^{2} + \frac{64\sigma^{2}+19\beta_{V}^{2}+96}{nn_{y}}C_{4}\varepsilon^{-(d_{2}+1)b_{U}-d_{2}}(\log^{2}\frac{1}{\varepsilon}+\log n_{x}+\log\frac{1}{\theta})$$

$$+16\sigma\theta\sqrt{\frac{4C_{4}\varepsilon^{-(d_{2}+1)b_{U}-d_{2}}(\log^{2}\frac{1}{\varepsilon}+\log n_{x}+\log\frac{1}{\theta})+6}{nn_{y}}} + (8\sigma+6)\theta.$$
(52)

Set $\theta = (nn_y)^{-1}$ and $\varepsilon = (nn_y)^{-\frac{1}{2+(d_2+1)b_U+d_2}}$, we have

$$\mathbb{E}_{\mathcal{S}}\mathbb{E}_{\{\mathbf{y}_j\}_{j=1}^{n_y}\sim\rho_y}\mathbb{E}_{u\sim\rho_u}\left[\frac{1}{n_y}\sum_{j=1}^{n_y}(\widehat{G}(\mathbf{u})(\mathbf{y}_j)-G(\mathbf{u})(\mathbf{y}_j))^2\right] \le C_2(nn_y)^{-\frac{2}{2+(d_2+1)b_U+d_2}}(\log^2\frac{1}{\varepsilon}+\log n_x),$$
(53)

for some C_2 depending on $\sigma, \gamma_1, \gamma_2, \beta_U, \beta_V, d_1, d_2, L_G, L_U, L_V, b_U, C_A$.

6 Conclusion

In this paper, we have developed mathematical and statistical theories to justify neural scaling laws of DeepONet by analyzing its approximation and generalization error. Our approximation theory can be used to quantify the model scaling law of DeepONet, depicting the scaling between the DeepONet approximation error and the model size. Our generalization theory can be used to quantify the data scaling law of DeepONet, depicting the scaling between the DeepONet generalization error and the training data size. Our general results for learning Lipschitz operators give rise to a slow rate of convergence of the DeepONet error as the model/data size increases. Furthermore, we incorporate low-dimensional structures of the input functions into consideration, and improve the rate of convergence to a power law, which is consistent with the empirical observations in Lu et al. (2021b); de Hoop et al. (2022). Our results provide theoretical foundations of DeepONet, to partially explain the empirical success and neural scaling laws of DeepONet. In the future, we will investigate the optimality of our error bound, and improve it if possible. Another interesting future direction is to incorporate more complicated low-dimensional structures under the framework of DeepONet.

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Appendix

A Proof of Examples in Section 3

A.1 Proof of Example 2

Proof of Example 2. The exact solution is given as

$$v(\mathbf{x}, T) = u(\mathbf{x} + T\mathbf{c}).$$

For any $u, \bar{u} \in U$ with $u = \sum_{j=1}^{J} a_j w_j, \bar{u} = \sum_{j=1}^{J} \bar{a}_j w_j$, we have

$$\|G(u) - G(\bar{u})\|_{L^{\infty}(\Omega_{V})} = \left\|\sum_{j=1}^{J} |a_{j} - \bar{a}_{j}|w_{j}(\mathbf{x} + T\mathbf{c})\right\|_{L^{\infty}(\Omega_{V})} \le \|\mathbf{a} - \bar{\mathbf{a}}\|_{\ell^{1}}$$
$$\le \sqrt{J} \|\mathbf{a} - \bar{\mathbf{a}}\|_{\ell^{2}} = \sqrt{J} \|u - \bar{u}\|_{L^{2}(\Omega_{U})}.$$

B Proof of Theorems and Lemmata in Section 5

B.1 Proof of Theorem 5

Proof of Theorem 5. We partition Ω_U into N^{d_1} subcubes for some N to be specified later. We are going to approximate u on each cube by a constant function and then assemble them together to get an approximation of u on Ω_U . Denote the centers of the subcubes by $\{\mathbf{c}_k\}_{k=1}^{N^{d_1}}$ with $\mathbf{c}_k = [c_{k,1}, c_{k,2}, ..., c_{k,d_1}]^{\mathsf{T}}$.

Let $\{\mathbf{c}_k\}_{k=1}^{N^{d_1}}$ be a uniform grid on Ω_U so that each $\mathbf{c}_k \in \left\{-\gamma_1, -\gamma_1 + \frac{2\gamma_1}{N-1}, ..., \gamma_1\right\}^{d_1}$ for each k. Define

$$\psi(a) = \begin{cases} 1, |a| < 1, \\ 0, |a| > 2, \\ 2 - |a|, 1 \le |a| \le 2, \end{cases}$$
(54)

with $a \in \mathbb{R}$, and

$$\phi_{\mathbf{c}_{k}}(\mathbf{x}) = \prod_{j=1}^{d_{1}} \psi\left(\frac{3(N-1)}{2\gamma_{1}}(x_{j} - c_{k,j})\right).$$
(55)

In this definition, we have $\operatorname{supp}(\phi_{\mathbf{c}_k}) = \left\{ \mathbf{x} : \|\mathbf{x} - \mathbf{c}_k\|_{\infty} \leq \frac{4\gamma_1}{3(N-1)} \right\} \subset \left\{ \mathbf{x} : \|\mathbf{x} - \mathbf{c}_k\|_{\infty} \leq \frac{2\gamma_1}{(N-1)} \right\}$ and

$$\|\phi_{\mathbf{c}_k}\|_{L^{\infty}(\Omega_U)} = 1, \quad \sum_{k=1}^{N^{a_1}} \phi_{\mathbf{c}_k} = 1.$$

For any $u \in U$, we construct a piecewise constant approximation to u as

$$\bar{u}(\mathbf{x}) = \sum_{k=1}^{N^{d_1}} u(\mathbf{c}_k) \phi_{\mathbf{c}_k}(\mathbf{x}).$$

By utilizing the partition of unity property given by $\sum_{k=1}^{N^{d_1}} \phi_{\mathbf{c}_k} = 1$, it follows that for any $\mathbf{x} \in \Omega_U$,

$$|u(\mathbf{x}) - \bar{u}(\mathbf{x})| = \left| \sum_{k=1}^{N^{d_1}} \phi_{\mathbf{c}_k}(\mathbf{x})(u(\mathbf{x}) - u(\mathbf{c}_k)) \right|$$

$$\leq \sum_{k=1}^{N^{d_1}} \phi_{\mathbf{c}_k}(\mathbf{x})|u(\mathbf{x}) - u(\mathbf{c}_k)|$$

$$= \sum_{k:\|\mathbf{c}_k - \mathbf{x}\|_{\infty} \leq \frac{2\gamma_1}{(N-1)}} \phi_{\mathbf{c}_k}(\mathbf{x})|(u(\mathbf{x}) - u(\mathbf{c}_k))|$$

$$\leq \max_{k:\|\mathbf{c}_k - \mathbf{x}\|_{\infty} \leq \frac{2\gamma_1}{(N-1)}} |(u(\mathbf{x}) - u(\mathbf{c}_k))|$$

$$\leq \max_{k:\|\mathbf{c}_k - \mathbf{x}\|_{\infty} \leq \frac{2\gamma_1}{(N-1)}} |(u(\mathbf{x}) - u(\mathbf{c}_k))|$$

$$\leq \frac{2\sqrt{d_1}\gamma_1 L_U}{N-1},$$
(56)

where we use the Lipschitz assumption of U in the last inequality. Setting $N = \left\lceil \frac{4\sqrt{d_1}\gamma_1 L_U}{\varepsilon} \right\rceil + 1$ gives rise to

$$|u(\mathbf{x}) - \bar{u}(\mathbf{x})| \le \frac{\varepsilon}{2}, \quad \forall \mathbf{x} \in \Omega_U.$$
 (57)

We then show that $\phi_{\mathbf{c}_k}$ can be approximated by a network with arbitrary accuracy. Note that $\phi_{\mathbf{c}_k}$ is the product of d_1 functions, each of which is piecewise linear and can be realized by 4-layer ReLU networks.

The following lemma shows that a function of the product can be approximated by a network with arbitrary accuracy.

Lemma 6 (Proposition 3 of Yarotsky (2017)). Given M > 0 and $\varepsilon > 0$, there is a ReLU network $\widetilde{\times} : \mathbb{R}^2 \to \mathbb{R}$ in $\mathcal{F}_{NN}(2, 1, L, p, K, \kappa, R)$ such that for any $|x| \leq M, |y| \leq M$, we have

$$|\widetilde{\times}(x,y) - xy| < \varepsilon$$

The network architecture has

$$L = O(\log \varepsilon^{-1}), \ p = 6, \ K = O(\log \varepsilon^{-1}), \ \kappa = O(\varepsilon^{-1}), \ R = M^2.$$
 (58)

The constant hidden in O depends on M.

Let $\tilde{\times}$ be the network defined in Lemma 6 with accuracy δ . We approximate $\phi_{\mathbf{c}_k}$ by \tilde{q}_k defined as,

$$\widetilde{q}_k(\mathbf{x}) = \widetilde{\times} \left(\psi \left(\frac{3(N-1)}{2\gamma_1} (x_1 - c_{k,1}) \right), \widetilde{\times} \left(\psi \left(\frac{3(N-1)}{2\gamma_1} (x_2 - c_{k,2}) \right), \cdots \right) \right).$$

For each $k, \, \widetilde{q}_k \in \mathcal{F}_{NN}(d_1, 1, L, p, K, \kappa, R)$ with

$$L = O(d_1 \log \delta^{-1}), p = O(1), K = O(d_1 \log \delta^{-1}), \kappa = O(\delta^{-1} + N), R = 1.$$

For any $\mathbf{x} \in \Omega_U$, we have

$$\begin{aligned} &|\widetilde{q}_{k}(\mathbf{x}) - \phi_{\mathbf{c}_{k}}(\mathbf{x})| \\ \leq & \left| \widetilde{\times} \left(\psi \left(\frac{3(N-1)}{2\gamma_{1}} (x_{1} - c_{k,1}) \right), \widetilde{\times} \left(\psi \left(\frac{3(N-1)}{2\gamma_{1}} (x_{2} - c_{k,2}) \right), \cdots \right) \right) - \phi_{\mathbf{c}_{k}}(\mathbf{x}) \right| \\ \leq & \left| \widetilde{\times} \left(\psi \left(\frac{3(N-1)}{2\gamma_{1}} (x_{1} - c_{k,1}) \right), \widetilde{\times} \left(\psi \left(\frac{3(N-1)}{2\gamma_{1}} (x_{2} - c_{k,2}) \right), \cdots \right) \right) \right) \\ & - \psi \left(\frac{3(N-1)}{2\gamma_{1}} (x_{1} - c_{k,1}) \right) \widetilde{\times} \left(\psi \left(\frac{3(N-1)}{2\gamma_{1}} (x_{2} - c_{k,2}) \right), \cdots \right) \right) \\ & + \left| \psi \left(\frac{3(N-1)}{2\gamma_{1}} (x_{1} - c_{k,1}) \right) \widetilde{\times} \left(\psi \left(\frac{3(N-1)}{2\gamma_{1}} (x_{2} - c_{k,2}) \right), \cdots \right) - \phi_{\mathbf{c}_{k}}(\mathbf{x}) \right| \\ \leq \delta + \mathcal{E}_{2}, \end{aligned}$$

where

$$\mathcal{E}_{2} = \left| \psi \left(\frac{3(N-1)}{2\gamma_{1}} (x_{1} - c_{k,1}) \right) \widetilde{\times} \left(\psi \left(\frac{3(N-1)}{2\gamma_{1}} (x_{2} - c_{k,2}) \right), \cdots \right) - \phi_{\mathbf{c}_{k}}(\mathbf{x}) \right|$$
$$= \left| \psi \left(\frac{3(N-1)}{2\gamma_{1}} (x_{1} - c_{k,1}) \right) \right\| \widetilde{\times} \left(\psi \left(\frac{3(N-1)}{2\gamma_{1}} (x_{2} - c_{k,2}) \right), \cdots \right) - \prod_{j=2}^{d_{1}} \psi \left(\frac{3(N-1)}{2\gamma_{1}} (x_{j} - c_{k,j}) \right) \right|$$

Repeat this process to estimate $\mathcal{E}_2, \mathcal{E}_3, ..., \mathcal{E}_{d_1+1}$, where $\mathcal{E}_{d_1+1} = \prod_{k=1}^{d_1} \psi \left(\frac{3(N-1)}{2\gamma_1} (x_2 - c_{k,2}) \right) - \phi_{\mathbf{c}_k} = 0$. This implies that $\|\phi_{\mathbf{c}_k} - \widetilde{q}_k\|_{L^{\infty}(\Omega_U)} \leq d_1 \delta$. It follows that,

$$\left\| \sum_{k=1}^{N^{d_1}} u(\mathbf{c}_k) \widetilde{q}_k - \overline{u} \right\|_{L^{\infty}(\Omega_U)} = \left\| \sum_{k=1}^{N^{d_1}} u(\mathbf{c}_k) \widetilde{q}_k - \sum_{k=1}^{N^{d_1}} u(\mathbf{c}_k) \phi_{\mathbf{c}_k} \right\|_{L^{\infty}(\Omega_U)}$$
$$\leq \sum_{k=1}^{N^{d_1}} |u(\mathbf{c}_k)| \| \widetilde{q}_k - \phi_{\mathbf{c}_k} \|_{L^{\infty}(\Omega_U)}$$
$$\leq d_1 N^{d_1} \beta_U \delta. \tag{59}$$

Setting $\delta = \frac{\varepsilon}{2d_1 N^{d_1} \beta_U}$ and putting (57) and (59) together, we have

$$\left\| u - \sum_{k=1}^{N^{d_1}} u(\mathbf{c}_k) \widetilde{q}_k \right\|_{L^{\infty}(\Omega_U)} \le \| u - \bar{u} \|_{L^{\infty}(\Omega_U)} + \left\| \bar{u} - \sum_{k=1}^{N^{d_1}} u(\mathbf{c}_k) \widetilde{q}_k \right\|_{L^{\infty}(\Omega_U)} \le \frac{\varepsilon}{2} + \frac{\varepsilon}{2} = \varepsilon.$$
(60)

The network architecture is specified in the theorem.

B.2 Proof of Theorem 6

Proof of Theorem 6. We let $\{\mathcal{B}_{\delta}(\mathbf{c}_m)\}_{m=1}^{c_U}$ be a finite cover of Ω_U by c_U Euclidean balls, where c_U can be further estimated in Corollary 2. By Lemma 1, there exists a partition of unity $\{\omega_m(\mathbf{x})\}_{m=1}^{c_U}$ subordinate to the cover $\{\mathcal{B}_{\delta}(\mathbf{c}_m)\}_{m=1}^{c_U}$. For any $\mathbf{z} = [z_1, ..., z_{c_U}]^{\top} \in (-\beta_U, \beta_U)^{c_U}$, we can then define a function $z_{\omega}(\mathbf{x}) : \Omega_U \to \mathbb{R}$ such that

$$z_{\omega}(\mathbf{x}) = \sum_{m=1}^{c_U} \mathbf{z}_m \omega_m(\mathbf{x}) \quad \forall \mathbf{x} \in \Omega_U.$$
(61)

Note that for $u \in U$ and $\mathbf{u} = [u(\mathbf{c}_1), ..., u(\mathbf{c}_{c_U})]^{\top}$, if we set $\mathbf{z} = \mathbf{u}$, it follows that $u_{\omega} = z_{\omega}$ is an approximation of u with the point-wise error estimation:

$$|u(\mathbf{x}) - u_{\omega}(\mathbf{x})| \leq \sum_{m=1}^{c_U} |u(\mathbf{x}) - u(\mathbf{c}_m)| |\omega_m(\mathbf{x})|$$
$$= \sum_{m: \|\mathbf{x} - \mathbf{c}_m\|_2 \leq \delta} |u(\mathbf{x}) - u(\mathbf{c}_m)| |\omega_m(\mathbf{x})| \leq L_U \delta$$

for any $\mathbf{x} \in \Omega_U$. Setting $\delta = \frac{\varepsilon}{2(2\gamma_1)^{d_1/2}L_fL_U}$ and using the Lipschtiz property of f, we have

$$|f(u) - f(u_{\omega})| \le L_f ||u - u_{\omega}||_{L^2(\Omega_U)} \le L_f (2\gamma_1)^{d_1/2} L_U \delta = \frac{\varepsilon}{2}$$

We next define a function $g: (-\beta_U, \beta_U)^{c_U} \to \mathbb{R}$ such that $g(\mathbf{z}) = f(z_{\omega})$, i.e., $g(\mathbf{z}) = f(u_{\omega})$. We claim that g is Lipschitz in the following sense: For any $u, \bar{u} \in U$, define u_{ω} and \bar{u}_{ω} as in (61) where $\mathbf{u} = [u(\mathbf{c}_1), ..., u(\mathbf{c}_{c_U})]^{\top}$ and $\bar{\mathbf{u}} = [\bar{u}(\mathbf{c}_1), ..., \bar{u}(\mathbf{c}_{c_U})]^{\top}$. Then we have

$$\begin{split} |g(\mathbf{u}) - g(\bar{\mathbf{u}})| &= |f(u_{\omega}) - f(\bar{u}_{\omega})| \\ &\leq L_{f} ||u_{\omega} - \bar{u}_{\omega}||_{L^{2}(\Omega_{U})} \\ &= L_{f} \sqrt{\int_{\Omega_{U}} \left(\sum_{m=1}^{c_{U}} \left(u(\mathbf{c}_{m}) - \bar{u}(\mathbf{c}_{m}) \right) \omega_{m}(\mathbf{x}) \right)^{2} d\mathbf{x}} \\ &= L_{f} \sqrt{\int_{\Omega_{U}} \sum_{m=1}^{c_{U}} \left(u(\mathbf{c}_{m}) - \bar{u}(\mathbf{c}_{m}) \right)^{2} \sum_{m=1}^{c_{U}} \left(\omega_{m}(\mathbf{x}) \right)^{2} d\mathbf{x}} \\ &\leq L_{f} \sqrt{\int_{\Omega_{U}} \sum_{m=1}^{c_{U}} \left(u(\mathbf{c}_{m}) - \bar{u}(\mathbf{c}_{m}) \right)^{2} \sum_{m=1}^{c_{U}} \omega_{m}(\mathbf{x}) d\mathbf{x}} \\ &\leq L_{f} \sqrt{\int_{\Omega_{U}} \sum_{m=1}^{c_{U}} \left(u(\mathbf{c}_{m}) - \bar{u}(\mathbf{c}_{m}) \right)^{2} d\mathbf{x}} \\ &\leq L_{f} \sqrt{\int_{\Omega_{U}} \sum_{m=1}^{c_{U}} \left(u(\mathbf{c}_{m}) - \bar{u}(\mathbf{c}_{m}) \right)^{2} d\mathbf{x}} \\ &= L_{f} |\Omega_{U}|^{\frac{1}{2}} ||\mathbf{u} - \bar{\mathbf{u}}||_{2} \\ &= L_{f} (2\gamma_{1})^{d_{1}/2} ||\mathbf{u} - \bar{\mathbf{u}}||_{2} \end{split}$$

where the third equality follows from the property that $\{\omega_m\}_{m=1}^{c_U}$ is a partition of unity. The claim is proved.

By Theorem 5, for $\varepsilon > 0$, if we set $H = C\sqrt{c_U}\varepsilon^{-c_U}$ for some C depending on d_1, γ_1, β_U and L_f , then there exists a network architecture $\mathcal{F}_{NN}(c_U, 1, L, p, K, \kappa, R)$ and $\{\widetilde{q}_k\}_{k=1}^H$ with $\widetilde{q}_k \in \mathcal{F}_{NN}(c_U, 1, L, p, K, \kappa, R)$ for $k = 1, \ldots, H$ such that

$$\sup_{u \in U} \left| g(\mathbf{u}) - \sum_{k=1}^{H} a_k \widetilde{q}_k(\mathbf{u}) \right| \le \frac{\varepsilon}{2},$$

where a_k are constants depending on f with $|a_k| \leq R_f$. Such an architecture has

$$L = O(c_U^2 + c_U \log(\varepsilon^{-1})), \ p = O(1), \ K = O(c_U^2 \log c_U + c_U^2 \log(\varepsilon^{-1})),$$

$$\kappa = O(c_U^{c_U/2+1}\varepsilon^{-c_U-1}), \ R = 1.$$

The constant hidden in O depends on d_1, γ_1, β_U and L_f . We have, for any $u \in U$ and $\mathbf{u} =$ $[u(\mathbf{c}_1), ..., u(\mathbf{c}_{c_U})]^\top$

$$\sup_{u \in U} \left| f(u) - \sum_{k=1}^{H} a_k \widetilde{q}_k(\mathbf{u}) \right| \leq \sup_{u \in U} |f(u) - g(\mathbf{u})| + \sup_{u} \left| g(\mathbf{u}) - \sum_{k=1}^{H} a_k \widetilde{q}_k(\mathbf{u}) \right|$$
$$\leq \frac{\varepsilon}{2} + \frac{\varepsilon}{2} = \varepsilon.$$

Proof of Theorem 7 **B.3**

Proof of Theorem 7. Under Assumption 3 and Assumption 4(ii), for each $u \in U$, we have $|\alpha_k| \leq C_{\alpha}$ for $k = 1, \ldots, b_U$ where $C_{\alpha} = (2\gamma_1)^{d_1/2} \beta_U$. For any $\mathbf{z} = [z_1, \ldots, z_{b_U}]^{\top} \in [-C_{\alpha}, C_{\alpha}]^{b_U}$, we define the function $z_{\omega}: \Omega_U \to \mathbb{R}$ such that

$$z_{\omega}(\mathbf{x}) = \sum_{m=1}^{b_U} \mathbf{z}_m \omega_m(\mathbf{x}), \ \forall \mathbf{x} \in \Omega_U,$$
(62)

where $\{\omega_m\}_{m=1}^{b_U}$ are the orthonormal basis in Assumption 4(i). For $u \in U$ and $\mathbf{u} = [u(\mathbf{x}_1), ..., u(\mathbf{x}_{n_x})]^{\top}$, if $\mathbf{z} = A\mathbf{u}$ then we have $u = z_{\omega}$. Let us define the function $g: [-C_{\alpha}, C_{\alpha}]^{b_U} \to \mathbb{R}$ such that $g(\mathbf{z}) = f(z_{\omega})$ (i.e., $g(A\mathbf{u}) = f(u)$). Then g is Lipschitz in the following sense: For any $u, \bar{u} \in U$, let $\mathbf{u} = [u(\mathbf{x}_1), ..., u(\mathbf{x}_{n_x})]^{\top}$, $\bar{\mathbf{u}} = [\bar{u}(\mathbf{x}_1), ..., \bar{u}(\mathbf{x}_{n_x})]^{\top}$, and then we have

$$\begin{split} |g(\mathbf{z}) - g(\bar{\mathbf{z}})| &= |f(z_{\omega}) - f(\bar{z}_{\omega})| \\ &\leq L_{f} ||z_{\omega} - \bar{z}_{\omega}||_{L^{2}(\Omega_{U})} \\ &= L_{f} \sqrt{\int_{\Omega_{U}} (z_{\omega} - \bar{z}_{\omega})^{2} d\mathbf{x}} \\ &\leq L_{f} \sqrt{\int_{\Omega_{U}} \left(\sum_{m=1}^{b_{U}} |\mathbf{z}_{m} - \bar{\mathbf{z}}_{m}| \omega_{m}(\mathbf{x})\right)^{2} d\mathbf{x}} \\ &\leq L_{f} \sqrt{\int_{\Omega_{U}} \sum_{m=1}^{b_{U}} |\mathbf{z}_{m} - \bar{\mathbf{z}}_{m}|^{2} \omega_{m}^{2}(\mathbf{x}) d\mathbf{x}} \\ &= L_{f} \sqrt{\sum_{m=1}^{b_{U}} |\mathbf{z}_{m} - \bar{\mathbf{z}}_{m}|^{2} \int_{\Omega_{U}} \omega_{m}^{2}(\mathbf{x}) d\mathbf{x}} \\ &= L_{f} \|\mathbf{z} - \bar{\mathbf{z}}\|_{2}. \end{split}$$

By Theorem 5, for $\varepsilon > 0$, set $H = C\sqrt{b_U}\varepsilon^{-b_U}$ for some C depending on $b_U, d_1, \gamma_1, \beta_U$ and L_f . There exists a network architecture $\mathcal{F}_{NN}(n_x, 1, L, p, K, \kappa, R)$ and $\{\widetilde{q}_k\}_{k=1}^H$ with $\widetilde{q}_k \in \mathcal{F}_{NN}(n_x, 1, L, p, K, \kappa, R)$, for k = 1, ..., H such that

$$\sup_{u \in U} \left| g(A\mathbf{u}) - \sum_{k=1}^{H} a_k \widetilde{q}_k(\mathbf{u}) \right| \le \varepsilon,$$
(63)

where a_k are constants depending on f with $|a_k| \leq R_f$. Such an architecture has

$$L = O(\log(\varepsilon^{-1})), \ p = O(1), \ K = O(\log(\varepsilon^{-1}) + n_x), \ \kappa = O(\varepsilon^{-b_U - 1}), \ R = 1.$$

Note that κ depends on C_A as defined in Assumption 4 as the network weights are scaled up by A. We have for any $u \in U$,

$$\sup_{u \in U} \left| f(u) - \sum_{k=1}^{H} a_k \widetilde{q}_k(\mathbf{u}) \right| = \sup_{u \in U} \left| g(A\mathbf{u}) - \sum_{k=1}^{H} a_k \widetilde{q}_k(\mathbf{u}) \right| = \varepsilon.$$

B.4 Proof of Corollary 2

Proof of Corollary 2. Ω_U is bounded and closed; hence it is compact. Let $\{\mathcal{B}_{\delta}(\mathbf{c}_m)\}_{m=1}^{c_U}$ be a finite cover of Ω_U by c_U Euclidean balls, with centers $\{\mathbf{c}_m\}_{m=1}^{c_U}$ and radius δ . By Lemma 2, we have,

$$c_U \le C_2 \delta^{-d_1} = C_2 \left(\frac{2(2\gamma_1)^{d_1/2} L_f L_U}{\varepsilon} \right)^{d_1} \tag{64}$$

for some C_2 depending on γ_1 and d_1 . Then Corollary 2 is a direct result of Theorem 6.

B.5 Proof of Lemma 2

Proof of Lemma 2. By Conway and Sloane (2013, Chapter 2), we have,

$$c \le \left\lceil \frac{2\gamma}{\delta} \right\rceil^d + 7d\log d \le C\delta^{-d} \tag{65}$$

for some C depending on γ and d.

B.6 Proof of Lemma 3

Proof of Lemma 3. We derive an upper bound of the second term in (32) using the covering number of \mathcal{G}_{NN} . Denote $\|G_{NN}\|_n^2 = \frac{1}{n} \sum_{i=1}^n \frac{1}{n_y} \sum_{j=1}^{n_y} |G_{NN}(\mathbf{u}_i)(\mathbf{y}_{i,j})|^2$. Let $\mathcal{G}^* = \{G_k^*\}_{k=1}^{\mathcal{N}(\theta, \mathcal{G}_{NN}, \|\cdot\|_{\infty,\infty})}$ be a θ cover of \mathcal{G}_{NN} , where $\mathcal{N}(\theta, \mathcal{G}_{NN}, \|\cdot\|_{\infty,\infty})$ is the covering number. Specifically, for any $G_{NN} \in \mathcal{G}_{NN}$, there exists $G_{NN}^* \in \mathcal{G}^*$ satisfying $\|G_{NN}^* - \widehat{G}\|_{\infty,\infty} \leq \theta$. We have

$$\mathbb{E}_{\mathcal{S}}\left[\frac{1}{n}\sum_{i=1}^{n}\frac{1}{n_{y}}\sum_{j=1}^{n_{y}}\widehat{G}(\mathbf{u}_{i})(\mathbf{y}_{i,j})\xi_{i,j}\right] \\ = \mathbb{E}_{\mathcal{S}}\left[\frac{1}{n}\sum_{i=1}^{n}\frac{1}{n_{y}}\sum_{j=1}^{n_{y}}\left(\widehat{G}(\mathbf{u}_{i})(\mathbf{y}_{i,j}) - G_{\mathrm{NN}}^{*}(\mathbf{u}_{i})(\mathbf{y}_{i,j}) + G_{\mathrm{NN}}^{*}(\mathbf{u}_{i})(\mathbf{y}_{i,j}) - G(u_{i})(\mathbf{y}_{i,j})\right)\xi_{i,j}\right] \\ = \mathbb{E}_{\mathcal{S}}\left[\frac{1}{n}\sum_{i=1}^{n}\frac{1}{n_{y}}\sum_{j=1}^{n_{y}}\left(\widehat{G}(\mathbf{u}_{i})(\mathbf{y}_{i,j}) - G_{\mathrm{NN}}^{*}(\mathbf{u}_{i})(\mathbf{y}_{i,j})\right)\xi_{i,j}\right] \\ + \mathbb{E}_{\mathcal{S}}\left[\frac{1}{n}\sum_{i=1}^{n}\frac{1}{n_{y}}\sum_{j=1}^{n_{y}}\left(G_{\mathrm{NN}}^{*}(\mathbf{u}_{i})(\mathbf{y}_{i,j}) - G(u_{i})(\mathbf{y}_{i,j})\right)\xi_{i,j}\right] \\$$

$$\leq \sigma\theta + \mathbb{E}_{\mathcal{S}}\left[\frac{\|G_{NN}^{*} - G\|_{n}}{\sqrt{nn_{y}}} \frac{\sum_{i=1}^{n} \sum_{j=1}^{n_{y}} \left(G_{NN}^{*}(\mathbf{u}_{i})(\mathbf{y}_{i,j}) - G(u_{i})(\mathbf{y}_{i,j})\right) \xi_{i,j}}{\sqrt{nn_{y}}} \right].$$
(66)

Note that

$$\|G_{NN}^{*} - G\|_{n}$$

$$= \sqrt{\frac{1}{n} \sum_{i=1}^{n} \frac{1}{n_{y}} \sum_{j=1}^{n_{y}} |G_{NN}^{*}(\mathbf{u}_{i})(\mathbf{y}_{i,j}) - \widehat{G}(\mathbf{u}_{i})(\mathbf{y}_{i,j}) + \widehat{G}(\mathbf{u}_{i})(\mathbf{y}_{i,j}) - G(u_{i})(\mathbf{y}_{i,j})|^{2}}$$

$$\leq \sqrt{\frac{2}{n} \sum_{i=1}^{n} \frac{1}{n_{y}} \sum_{j=1}^{n_{y}} \left(|G_{NN}^{*}(\mathbf{u}_{i})(\mathbf{y}_{i,j}) - \widehat{G}(\mathbf{u}_{i})(\mathbf{y}_{i,j})|^{2} + |\widehat{G}(\mathbf{u}_{i})(\mathbf{y}_{i,j}) - G(u_{i})(\mathbf{y}_{i,j})|^{2} \right)}$$

$$\leq \sqrt{\frac{2}{n} \sum_{i=1}^{n} \frac{1}{n_{y}} \sum_{j=1}^{n_{y}} \left(\theta^{2} + |\widehat{G}(\mathbf{u}_{i})(\mathbf{y}_{i,j}) - G(u_{i})(\mathbf{y}_{i,j})|^{2} \right)}$$

$$= \sqrt{2} (\|\widehat{G} - G\|_{n} + \theta). \tag{67}$$

Substituting (67) into (66) gives rise to

$$\mathbb{E}_{\mathcal{S}}\left[\frac{1}{n}\sum_{i=1}^{n}\frac{1}{n_{y}}\sum_{j=1}^{n_{y}}\widehat{G}(\mathbf{u}_{i})(\mathbf{y}_{i,j})\xi_{i,j}\right]$$

$$\leq \sqrt{2}\mathbb{E}_{\mathcal{S}}\left[\frac{\|\widehat{G}-G\|_{n}+\theta}{\sqrt{nn_{y}}}\left|\frac{\sum_{i=1}^{n}\sum_{j=1}^{n_{y}}\left(G_{\mathrm{NN}}^{*}(\mathbf{u}_{i})(\mathbf{y}_{i,j})-G(u_{i})(\mathbf{y}_{i,j})\right)\xi_{i,j}}{\sqrt{nn_{y}}\|G_{\mathrm{NN}}^{*}-G\|_{n}}\right|\right]+\sigma\theta.$$
(68)

Recall that $\{G_k^*\}_{k=1}^{\mathcal{N}(\theta,\mathcal{G}_{NN},\|\cdot\|_{\infty,\infty})}$ is a θ cover of \mathcal{G}_{NN} , and denote

$$z_k = \frac{\sum_{i=1}^n \sum_{j=1}^{n_y} \left(G_k^*(\mathbf{u}_i)(\mathbf{y}_{i,j}) - G(u_i)(\mathbf{y}_{i,j}) \right) \xi_{i,j}}{\sqrt{nn_y} \|G_{NN}^* - G\|_n}.$$

We have

$$\mathbb{E}_{\mathcal{S}}\left[\frac{\|\widehat{G}-G\|_{n}+\theta}{\sqrt{nn_{y}}}\left|\frac{\sum_{i=1}^{n}\sum_{j=1}^{n_{y}}\left(G_{NN}^{*}(\mathbf{u}_{i})(\mathbf{y}_{i,j})-G(u_{i})(\mathbf{y}_{i,j})\right)\xi_{i,j}}{\sqrt{nn_{y}}}\right\|\right]$$

$$\leq \mathbb{E}_{\mathcal{S}}\left[\frac{\|\widehat{G}-G\|_{n}+\theta}{\sqrt{nn_{y}}}\max_{k}|z_{k}|\right]$$

$$\leq \sqrt{\mathbb{E}_{\mathcal{S}}\left[\left(\|\widehat{G}-G\|_{n}+\theta\right)^{2}\right]\mathbb{E}_{\mathcal{S}}\left[\frac{1}{nn_{y}}\max_{k}|z_{k}|^{2}\right]}$$

$$\leq \sqrt{2\mathbb{E}_{\mathcal{S}}\left[\|\widehat{G}-G\|_{n}^{2}+\theta^{2}\right]}\sqrt{\frac{1}{nn_{y}}\mathbb{E}_{\mathcal{S}}\left[\max_{k}|z_{k}|^{2}\right]}$$

$$\leq \sqrt{2}\left(\sqrt{\mathbb{E}_{\mathcal{S}}\left[\|\widehat{G}-G\|_{n}^{2}\right]}+\theta\right)\sqrt{\frac{1}{nn_{y}}\mathbb{E}_{\mathcal{S}}\left[\max_{k}|z_{k}|^{2}\right]}, \qquad (69)$$

where Cauchy-Schwarz inequality is used in the second inequality, and the last inequality uses the relation $\sqrt{a+b^2} \leq \sqrt{a}+b$ for $a, b \geq 0$.

We next derive an upper bound of $\mathbb{E}_{\mathcal{S}}\left[\max_{k}|z_{k}|^{2}\right]$. Since each $\xi_{i,j}$ is a sub-Gaussian variable with variance proxy σ , for given $\left\{u_{i}, \left\{\mathbf{y}_{i,j}\right\}_{j=1}^{n_{y}}\right\}_{i=1}^{n}$, each z_{k} is a sub-Gaussian variable with variance proxy σ^{2} . Let t be a positive number depending on σ and will be made clear later, we deduce,

$$\begin{split} & \mathbb{E}_{\mathcal{S}}\left[\max_{k}|z_{k}|^{2}\left|\left\{u_{i},\left\{\mathbf{y}_{i,j}\right\}_{j=1}^{n_{y}}\right\}_{i=1}^{n}\right]\right] \\ &=\frac{1}{t}\log\exp\left(\mathbb{E}_{\mathcal{S}}\left[t\max_{k}|z_{k}|^{2}\left|\left\{u_{i},\left\{\mathbf{y}_{i,j}\right\}_{j=1}^{n_{y}}\right\}_{i=1}^{n}\right]\right)\right] \\ &\leq\frac{1}{t}\log\mathbb{E}_{\mathcal{S}}\left[\exp\left(t\max_{k}|z_{k}|^{2}\right|\left\{u_{i},\left\{\mathbf{y}_{i,j}\right\}_{j=1}^{n_{y}}\right\}_{i=1}^{n}\right)\right] \\ &\leq\frac{1}{t}\log\mathbb{E}_{\mathcal{S}}\left[\sum_{k}\exp\left(t\left|z_{k}\right|^{2}\right|\left\{u_{i},\left\{\mathbf{y}_{i,j}\right\}_{j=1}^{n_{y}}\right\}_{i=1}^{n}\right)\right] \\ &=\frac{1}{t}\log\left(\mathcal{N}(\theta,\mathcal{G}_{NN},\|\cdot\|_{\infty,\infty})\mathbb{E}_{\mathcal{S}}\left[\exp\left(t\left|z_{k}\right|^{2}\right|\left\{u_{i},\left\{\mathbf{y}_{i,j}\right\}_{j=1}^{n_{y}}\right\}_{i=1}^{n}\right)\right]\right) \\ &\leq\frac{1}{t}\log\mathcal{N}(\theta,\mathcal{G}_{NN},\|\cdot\|_{\infty,\infty})+\frac{1}{t}\log\mathbb{E}_{\mathcal{S}}\left[\exp\left(t\left|z_{1}\right|^{2}\right|\left\{u_{i},\left\{\mathbf{y}_{i,j}\right\}_{j=1}^{n_{y}}\right\}_{i=1}^{n}\right)\right], \end{split}$$

where we use Jensen's inequality in the first inequality. Due to the i.i.d. assumption of $\left\{u_i, \{\mathbf{y}_{i,j}\}_{j=1}^{n_y}\right\}_{i=1}^n$, we have

$$\mathbb{E}_{\mathcal{S}}\left[\exp\left(t\,|z_{1}|^{2}\,\Big|\,\left\{u_{i},\left\{\mathbf{y}_{i,j}\right\}_{j=1}^{n_{y}}\right\}_{i=1}^{n}\right)\right] = 1 + \sum_{\ell=1}^{\infty}\frac{t^{\ell}\mathbb{E}_{\mathcal{S}}\left[z_{1}^{2\ell}\,\Big|\,\left\{u_{i},\left\{\mathbf{y}_{i,j}\right\}_{j=1}^{n_{y}}\right\}_{i=1}^{n}\right]}{\ell!}.$$

Since z_1 is sub-Gaussian with variance proxy σ^2 , it follows that

$$\begin{split} 1 + \sum_{\ell=1}^{\infty} \frac{t^{\ell} \mathbb{E}_{\mathcal{S}} \left[z_{1}^{2\ell} \middle| \left\{ u_{i}, \{\mathbf{y}_{i,j}\}_{j=1}^{n_{y}} \right\}_{i=1}^{n} \right]}{\ell!} \\ = 1 + \sum_{\ell=1}^{\infty} \frac{t^{\ell}}{\ell!} \int_{0}^{\infty} \mathbb{P} \left(|z_{1}| \ge \tau^{\frac{1}{2\ell}} \middle| \left\{ u_{i}, \{\mathbf{y}_{i,j}\}_{j=1}^{n_{y}} \right\}_{i=1}^{n} \right) d\tau \\ \le 1 + 2 \sum_{\ell=1}^{\infty} \frac{t^{\ell}}{\ell!} \int_{0}^{\infty} \exp\left(-\frac{\tau^{1/\ell}}{2\sigma^{2}} \right) d\tau \\ = 1 + \sum_{\ell=1}^{\infty} \frac{2\ell(2t\sigma^{2})^{\ell}}{\ell!} \Gamma_{G}(\ell) \\ = 1 + 2 \sum_{\ell=1}^{\infty} (2t\sigma^{2})^{\ell}, \end{split}$$

where Γ_G denotes the Gamma function. Setting $t = (4\sigma^2)^{-1}$, we have

$$\mathbb{E}_{\mathcal{S}}\left[\max_{k}|z_{k}|^{2}\left|\left\{u_{i},\left\{\mathbf{y}_{i,j}\right\}_{j=1}^{n_{y}}\right\}_{i=1}^{n}\right]\leq 4\sigma^{2}\log\mathcal{N}(\theta,\mathcal{G}_{\mathrm{NN}},\|\cdot\|_{\infty,\infty})+4\sigma^{2}\log3$$
$$\leq 4\sigma^{2}\log\mathcal{N}(\theta,\mathcal{G}_{\mathrm{NN}},\|\cdot\|_{\infty,\infty})+6\sigma^{2}.$$
(70)

Substituting (70) and (69) into (68) gives rise to

$$\mathbb{E}_{\mathcal{S}}\left[\frac{1}{n}\sum_{i=1}^{n}\frac{1}{n_{y}}\sum_{j=1}^{n_{y}}\widehat{G}(\mathbf{u}_{i})(\mathbf{y}_{i,j})\xi_{i,j}\right] \leq 2\sigma\left(\sqrt{\mathbb{E}_{\mathcal{S}}\left[\|\widehat{G}-G\|_{n}^{2}\right]}+\theta\right)\sqrt{\frac{4\log\mathcal{N}(\theta,\mathcal{G}_{\mathrm{NN}},\|\cdot\|_{\infty,\infty})+6}{nn_{y}}}+\sigma\theta.$$
(71)

B.7 Proof of Lemma 4

Proof of Lemma 4. Denote $\widehat{g}(\mathbf{u})(\mathbf{y}) = \left(\widehat{G}(\mathbf{u})(\mathbf{y}) - G(u)(\mathbf{y})\right)^2$. Due to the clipping by β_V , $\|\widehat{g}\|_{\infty,\infty} \leq 4\beta_V^2$. Then

$$T_{2} = \mathbb{E}_{\mathcal{S}} \left\{ \mathbb{E}_{\{\mathbf{y}_{j}\}_{j=1}^{n_{y}} \sim \rho_{y}} \mathbb{E}_{u \sim \rho_{u}} \left[\frac{1}{n_{y}} \sum_{j=1}^{n_{y}} \widehat{g}(\mathbf{u})(\mathbf{y}_{j}) \right] - \frac{2}{n} \sum_{i=1}^{n} \frac{1}{n_{y}} \sum_{j=1}^{n_{y}} \widehat{g}(\mathbf{u})(\mathbf{y}_{i,j}) \right\}$$
$$= 2\mathbb{E}_{\mathcal{S}} \left\{ \frac{1}{2} \mathbb{E}_{\{\mathbf{y}_{j}\}_{j=1}^{n_{y}} \sim \rho_{y}} \mathbb{E}_{u \sim \rho_{u}} \left[\frac{1}{n_{y}} \sum_{j=1}^{n_{y}} \widehat{g}(\mathbf{u})(\mathbf{y}_{j}) \right] - \frac{1}{n} \sum_{i=1}^{n} \frac{1}{n_{y}} \sum_{j=1}^{n_{y}} \widehat{g}(\mathbf{u})(\mathbf{y}_{i,j}) \right\}$$
$$= 2\mathbb{E}_{\mathcal{S}} \left\{ \mathbb{E}_{\{\mathbf{y}_{j}\}_{j=1}^{n_{y}} \sim \rho_{y}} \mathbb{E}_{u \sim \rho_{u}} \left[\frac{1}{n_{y}} \sum_{j=1}^{n_{y}} \widehat{g}(\mathbf{u})(\mathbf{y}_{j}) \right] - \frac{1}{n} \sum_{i=1}^{n} \frac{1}{n_{y}} \sum_{j=1}^{n_{y}} \widehat{g}(\mathbf{u})(\mathbf{y}_{i,j}) \right\}$$
$$- \frac{1}{2} \mathbb{E}_{\{\mathbf{y}_{j}\}_{j=1}^{n_{y}} \sim \rho_{y}} \mathbb{E}_{u \sim \rho_{u}} \left[\frac{1}{n_{y}} \sum_{j=1}^{n_{y}} \widehat{g}(\mathbf{u})(\mathbf{y}_{j}) \right] \right\}.$$
(72)

A lower bound of $\mathbb{E}_{\{\mathbf{y}_j\}_{j=1}^{n_y} \sim \rho_y} \mathbb{E}_{u \sim \rho_u} \left[\frac{1}{n_y} \sum_{j=1}^{n_y} \widehat{g}(\mathbf{u})(\mathbf{y}_j) \right]$ is given as

$$\mathbb{E}_{\{\mathbf{y}_j\}_{j=1}^{n_y} \sim \rho_y} \mathbb{E}_{u \sim \rho_u} \left[\frac{1}{n_y} \sum_{j=1}^{n_y} \widehat{g}(\mathbf{u})(\mathbf{y}_j) \right] = \mathbb{E}_{\{\mathbf{y}_j\}_{j=1}^{n_y} \sim \rho_y} \mathbb{E}_{u \sim \rho_u} \left[\frac{1}{n_y} \sum_{j=1}^{n_y} \frac{4\beta_V^2}{4\beta_V^2} \widehat{g}(\mathbf{u})(\mathbf{y}_j) \right]$$
$$\geq \mathbb{E}_{\{\mathbf{y}_j\}_{j=1}^{n_y} \sim \rho_y} \mathbb{E}_{u \sim \rho_u} \left[\frac{1}{n_y} \sum_{j=1}^{n_y} \frac{1}{4\beta_V^2} \widehat{g}^2(\mathbf{u})(\mathbf{y}_j) \right].$$
(73)

Substituting (73) into (72) implies

$$T_{2} \leq 2\mathbb{E}_{\mathcal{S}} \left\{ \mathbb{E}_{\{\mathbf{y}_{j}\}_{j=1}^{n_{y}} \sim \rho_{y}} \mathbb{E}_{u \sim \rho_{u}} \left[\frac{1}{n_{y}} \sum_{j=1}^{n_{y}} \widehat{g}(\mathbf{u})(\mathbf{y}_{j}) \right] - \frac{1}{n} \sum_{i=1}^{n} \frac{1}{n_{y}} \sum_{j=1}^{n_{y}} \widehat{g}(\mathbf{u})(\mathbf{y}_{j}) - \frac{1}{8\beta_{V}^{2}} \mathbb{E}_{\{\mathbf{y}_{j}\}_{j=1}^{n_{y}} \sim \rho_{y}} \mathbb{E}_{u \sim \rho_{u}} \left[\frac{1}{n_{y}} \sum_{j=1}^{n_{y}} \widehat{g}^{2}(\mathbf{u})(\mathbf{y}_{j}) \right] \right\}.$$

$$(74)$$

Denote $\mathcal{S}' = \left\{ u'_i, \{\mathbf{y}'_{i,j}\}_{j=1}^{n_y} \right\}_{i=1}^n$ as an independent copy of \mathcal{S} . Define the set $\mathcal{R} = \{g(\mathbf{u})(\mathbf{y}) = (G_{NN}(\mathbf{u})(\mathbf{y}) - G(u)(\mathbf{y}))^2 \text{ for } G_{NN} \in \mathcal{G}_{NN}, u \in U, \mathbf{y} \in \Omega_V \}.$ (75) We have

$$T_{2} \leq 2\mathbb{E}_{\mathcal{S}} \left\{ \sup_{g \in \mathcal{R}} \left(\mathbb{E}_{\mathcal{S}'} \left[\frac{1}{n} \sum_{i=1}^{n} \frac{1}{n_{y}} \sum_{j=1}^{n_{y}} g(\mathbf{u}'_{i})(\mathbf{y}'_{i,j}) \right] - \frac{1}{n} \sum_{i=1}^{n} \frac{1}{n_{y}} \sum_{j=1}^{n_{y}} g(\mathbf{u}_{i})(\mathbf{y}_{i,j}) \right] \right) \right\}$$
$$- \frac{1}{8\beta_{V}^{2}} \mathbb{E}_{\mathcal{S}'} \left[\frac{1}{n} \sum_{i=1}^{n} \frac{1}{n_{y}} \sum_{j=1}^{n_{y}} g^{2}(\mathbf{u}'_{i})(\mathbf{y}'_{i,j}) \right] \right) \right\}$$
$$= 2\mathbb{E}_{\mathcal{S}} \left\{ \sup_{g \in \mathcal{R}} \left(\mathbb{E}_{\mathcal{S}'} \left[\frac{1}{n} \sum_{i=1}^{n} \frac{1}{n_{y}} \sum_{j=1}^{n_{y}} \left(g(\mathbf{u}'_{i})(\mathbf{y}'_{i,j}) - g(\mathbf{u}_{i})(\mathbf{y}_{i,j}) \right) \right] \right) \right\}$$
$$- \frac{1}{16\beta_{V}^{2}} \mathbb{E}_{\mathcal{S},\mathcal{S}'} \left[\frac{1}{n} \sum_{i=1}^{n} \frac{1}{n_{y}} \sum_{j=1}^{n_{y}} \left(g^{2}(\mathbf{u}'_{i})(\mathbf{y}'_{i,j}) + g^{2}(\mathbf{u}_{i})(\mathbf{y}_{i,j}) \right) \right] \right) \right\}$$
$$\leq 2\mathbb{E}_{\mathcal{S},\mathcal{S}'} \left\{ \sup_{g \in \mathcal{R}} \left(\frac{1}{n} \sum_{i=1}^{n} \frac{1}{n_{y}} \sum_{j=1}^{n_{y}} \left(g(\mathbf{u}'_{i})(\mathbf{y}'_{i,j}) - g(\mathbf{u}_{i})(\mathbf{y}_{i,j}) \right) - \frac{1}{16\beta_{V}^{2}} \mathbb{E}_{\mathcal{S},\mathcal{S}'} \left[(g^{2}(\mathbf{u}'_{i})(\mathbf{y}'_{i,j}) + g^{2}(\mathbf{u}_{i})(\mathbf{y}_{i,j}) \right] \right) \right\}$$
(76)

By Lemma 7, let $\mathcal{R}^* = \{g_k^*\}_{k=1}^{\mathcal{N}(\theta,\mathcal{R},\|\cdot\|_{\infty,\infty})}$ be a θ -cover of \mathcal{R} . Then for any $g \in \mathcal{R}$, there exists $g^* \in \mathcal{R}^*$ satisfying $\|g - g^*\|_{\infty,\infty} \leq \theta$. We will derive an upper bound of (76) using g^* . For the first term in (76), we have

$$g(\mathbf{u}'_{i})(\mathbf{y}'_{i,j}) - g(\mathbf{u}_{i})(\mathbf{y}_{i,j}) = g(\mathbf{u}_{i})(\mathbf{y}_{i,j}) = (g(\mathbf{u}'_{i})(\mathbf{y}'_{i,j}) - g^{*}(\mathbf{u}'_{i})(\mathbf{y}'_{i,j}) - g^{*}(\mathbf{u}_{i})(\mathbf{y}_{i,j})) + (g^{*}(\mathbf{u}_{i})(\mathbf{y}_{i,j}) - g(\mathbf{u}_{i})(\mathbf{y}_{i,j})) \\ \leq (g^{*}(\mathbf{u}'_{i})(\mathbf{y}'_{i,j}) - g^{*}(\mathbf{u}_{i})(\mathbf{y}_{i,j})) + 2\theta.$$
(77)

For the second term in (76), we have

$$g^{2}(\mathbf{u}_{i}')(\mathbf{y}_{i,j}') + g^{2}(\mathbf{u}_{i})(\mathbf{y}_{i,j})$$

$$= \left(g^{2}(\mathbf{u}_{i}')(\mathbf{y}_{i,j}') - (g^{*})^{2}(\mathbf{u}_{i}')(\mathbf{y}_{i,j}')\right) + \left(g^{2}(\mathbf{u}_{i})(\mathbf{y}_{i,j}) - (g^{*})^{2}(\mathbf{u}_{i})(\mathbf{y}_{i,j})\right)$$

$$+ \left((g^{*})^{2}(\mathbf{u}_{i})(\mathbf{y}_{i,j}) + (g^{*})^{2}(\mathbf{u}_{i}')(\mathbf{y}_{i,j}')\right)$$

$$\geq (g^{*})^{2}(\mathbf{u}_{i})(\mathbf{y}_{i,j}) + (g^{*})^{2}(\mathbf{u}_{i}')(\mathbf{y}_{i,j}') - |g(\mathbf{u}_{i}')(\mathbf{y}_{i,j}') - g^{*}(\mathbf{u}_{i}')(\mathbf{y}_{i,j}')||g(\mathbf{u}_{i}')(\mathbf{y}_{i,j}') + g^{*}(\mathbf{u}_{i}')(\mathbf{y}_{i,j}')|$$

$$- |g(\mathbf{u}_{i})(\mathbf{y}_{i,j}) - g^{*}(\mathbf{u}_{i})(\mathbf{y}_{i,j})||g(\mathbf{u}_{i})(\mathbf{y}_{i,j}) + g^{*}(\mathbf{u}_{i})(\mathbf{y}_{i,j})||$$

$$\geq (g^{*})^{2}(\mathbf{u}_{i})(\mathbf{y}_{i,j}) + (g^{*})^{2}(\mathbf{u}_{i}')(\mathbf{y}_{i,j}') - 16\beta_{V}^{2}\theta.$$

$$(78)$$

Substituting (77) and (78) into (76) gives rise to

$$T_{2} \leq 2\mathbb{E}_{\mathcal{S},\mathcal{S}'} \left[\sup_{g^{*} \in \mathcal{R}^{*}} \left(\frac{1}{n} \sum_{i=1}^{n} \frac{1}{n_{y}} \sum_{j=1}^{n_{y}} \left(g^{*}(\mathbf{u}_{i}')(\mathbf{y}_{i,j}') - g^{*}(\mathbf{u}_{i})(\mathbf{y}_{i,j}) \right) - \frac{1}{16\beta_{V}^{2}} \mathbb{E}_{\mathcal{S},\mathcal{S}'} \left[\left((g^{*})^{2}(\mathbf{u}_{i})(\mathbf{y}_{i,j}) + (g^{*})^{2}(\mathbf{u}_{i}')(\mathbf{y}_{i,j}') \right) \right] \right) \right] + 6\theta$$
$$= 2\mathbb{E}_{\mathcal{S},\mathcal{S}'} \left[\max_{k} \left(\frac{1}{n} \sum_{i=1}^{n} \frac{1}{n_{y}} \sum_{j=1}^{n_{y}} \left(g^{*}_{k}(\mathbf{u}_{i}')(\mathbf{y}_{i,j}') - g^{*}_{k}(\mathbf{u}_{i})(\mathbf{y}_{i,j}) \right) \right] \right] \right]$$

$$-\frac{1}{16\beta_V^2}\mathbb{E}_{\mathcal{S},\mathcal{S}'}\left[(g_k^*)^2(\mathbf{u}_i)(\mathbf{y}_{i,j}) + (g_k^*)^2(\mathbf{u}'_i)(\mathbf{y}'_{i,j})\right]\right)\right] + 6\theta$$
(79)

Denote $r_k(\mathbf{u}'_i, \mathbf{y}'_{i,j}, \mathbf{u}_i, \mathbf{y}_{i,j}) = g_k^*(\mathbf{u}'_i)(\mathbf{y}'_{i,j}) - g_k^*(\mathbf{u}_i)(\mathbf{y}_{i,j})$. We have

$$\begin{split} \mathbb{E}_{\mathcal{S},\mathcal{S}'}[r_k(\mathbf{u}'_i,\mathbf{y}'_{i,j},\mathbf{u}_i,\mathbf{y}_{i,j})] =& 0,\\ \operatorname{Var}(r_k(\mathbf{u}'_i,\mathbf{y}'_{i,j},\mathbf{u}_i,\mathbf{y}_{i,j})) =& \mathbb{E}_{\mathcal{S},\mathcal{S}'}[r_k^2(\mathbf{u}'_i,\mathbf{y}'_{i,j},\mathbf{u}_i,\mathbf{y}_{i,j})]\\ =& \mathbb{E}_{\mathcal{S},\mathcal{S}'}[(g_k^*(\mathbf{u}'_i)(\mathbf{y}'_{i,j}) - g_k^*(\mathbf{u}_i)(\mathbf{y}_{i,j}))^2]\\ \leq& 2\mathbb{E}_{\mathcal{S},\mathcal{S}'}[(g_k^*(\mathbf{u}'_i)(\mathbf{y}'_{i,j}))^2 + (g_k^*(\mathbf{u}_i)(\mathbf{y}_{i,j}))^2] \end{split}$$

Next we define and estimate \widetilde{T}_2 ,

$$\widetilde{\mathbf{T}}_{2} \leq 2\mathbb{E}_{\mathcal{S},\mathcal{S}'}\left[\max_{k}\left(\frac{1}{n}\sum_{i=1}^{n}\frac{1}{n_{y}}\sum_{j=1}^{n_{y}}\left(r_{k}(\mathbf{u}_{i}',\mathbf{y}_{i,j}',\mathbf{u}_{i},\mathbf{y}_{i,j}) - \frac{1}{16\beta_{V}^{2}}\operatorname{Var}\left[r_{k}(\mathbf{u}_{i}',\mathbf{y}_{i,j}',\mathbf{u}_{i},\mathbf{y}_{i,j})\right]\right)\right)\right].$$
(80)

We estimate \widetilde{T}_2 using the moment generating function of r_k . Note that $||r_k||_{\infty,\infty} \leq 4\beta_V^2$. For $0 < t < 3/4\beta_V^2$, we have

$$\mathbb{E}_{\mathcal{S},\mathcal{S}'}[\exp(tr_{k}(\mathbf{u}'_{i},\mathbf{y}'_{i,j},\mathbf{u}_{i},\mathbf{y}_{i,j})]$$

$$=\mathbb{E}_{\mathcal{S},\mathcal{S}'}\left[1+tr_{k}(\mathbf{u}'_{i},\mathbf{y}'_{i,j},\mathbf{u}_{i},\mathbf{y}_{i,j})+\sum_{\ell=2}^{\infty}\frac{t^{\ell}r_{k}^{\ell}(\mathbf{u}'_{i},\mathbf{y}'_{i,j},\mathbf{u}_{i},\mathbf{y}_{i,j})}{\ell!}\right]$$

$$\leq\mathbb{E}_{\mathcal{S},\mathcal{S}'}\left[1+tr_{k}(\mathbf{u}'_{i},\mathbf{y}'_{i,j},\mathbf{u}_{i},\mathbf{y}_{i,j})+\sum_{\ell=2}^{\infty}\frac{(4\beta_{V}^{2})^{\ell-2}t^{\ell}r_{k}^{2}(\mathbf{u}'_{i},\mathbf{y}'_{i,j},\mathbf{u}_{i},\mathbf{y}_{i,j})}{2\times 3^{\ell-2}}\right]$$

$$=\mathbb{E}_{\mathcal{S},\mathcal{S}'}\left[1+tr_{k}(\mathbf{u}'_{i},\mathbf{y}'_{i,j},\mathbf{u}_{i},\mathbf{y}_{i,j})+\frac{\ell^{2}r_{k}^{2}(\mathbf{u}'_{i},\mathbf{y}'_{i,j},\mathbf{u}_{i},\mathbf{y}_{i,j})}{2}\sum_{\ell=2}^{\infty}\frac{(4\beta_{V}^{2})^{\ell-2}t^{\ell-2}}{3^{\ell-2}}\right]$$

$$=\mathbb{E}_{\mathcal{S},\mathcal{S}'}\left[1+tr_{k}(\mathbf{u}'_{i},\mathbf{y}'_{i,j},\mathbf{u}_{i},\mathbf{y}_{i,j})+\frac{\ell^{2}r_{k}^{2}(\mathbf{u}'_{i},\mathbf{y}'_{i,j},\mathbf{u}_{i},\mathbf{y}_{i,j})}{2}\frac{1}{1-4\beta_{V}^{2}t/3}\right]$$

$$=1+t^{2}\operatorname{Var}[r_{k}^{2}(\mathbf{u}'_{i},\mathbf{y}'_{i,j},\mathbf{u}_{i},\mathbf{y}_{i,j})]\frac{3t^{2}}{6-8\beta_{V}^{2}t}}, (81)$$

where the last inequality comes from the relation $1 + x \leq \exp(x)$ for $x \geq 0$.

For $0 < t/nn_y < 3/4\beta_V^2$, we have

$$\exp\left(\frac{t\widetilde{T}_{2}}{2}\right)$$

$$=\exp\left(t\mathbb{E}_{\mathcal{S},\mathcal{S}'}\left[\max_{k}\left(\frac{1}{n}\sum_{i=1}^{n}\frac{1}{n_{y}}\sum_{j=1}^{n_{y}}\left(r_{k}(\mathbf{u}'_{i},\mathbf{y}'_{i,j},\mathbf{u}_{i},\mathbf{y}_{i,j})-\frac{1}{16\beta_{V}^{2}}\operatorname{Var}\left[r_{k}(\mathbf{u}'_{i},\mathbf{y}'_{i,j},\mathbf{u}_{i},\mathbf{y}_{i,j})\right]\right)\right)\right]\right)$$

$$\leq \mathbb{E}_{\mathcal{S},\mathcal{S}'}\left[\exp\left(t\max_{k}\left(\frac{1}{n}\sum_{i=1}^{n}\frac{1}{n_{y}}\sum_{j=1}^{n_{y}}\left(r_{k}(\mathbf{u}'_{i},\mathbf{y}'_{i,j},\mathbf{u}_{i},\mathbf{y}_{i,j})-\frac{1}{16\beta_{V}^{2}}\operatorname{Var}\left[r_{k}(\mathbf{u}'_{i},\mathbf{y}'_{i,j},\mathbf{u}_{i},\mathbf{y}_{i,j})\right]\right)\right)\right)\right]$$

$$\leq \mathbb{E}_{\mathcal{S},\mathcal{S}'} \left[\sum_{k} \exp\left(\sum_{i=1}^{n} \sum_{j=1}^{n_y} \left(\frac{t}{nn_y} r_k(\mathbf{u}'_i, \mathbf{y}'_{i,j}, \mathbf{u}_i, \mathbf{y}_{i,j}) - \frac{1}{nn_y} \frac{t}{16\beta_V^2} \operatorname{Var}\left[r_k(\mathbf{u}'_i, \mathbf{y}'_{i,j}, \mathbf{u}_i, \mathbf{y}_{i,j}) \right] \right) \right) \right]$$

$$\leq \sum_{k} \exp\left(\sum_{i=1}^{n} \sum_{j=1}^{n_y} \left(\operatorname{Var}[r_k^2(\mathbf{u}'_i, \mathbf{y}'_{i,j}, \mathbf{u}_i, \mathbf{y}_{i,j})] \frac{3(t/nn_y)^2}{6 - 8\beta_V^2 t/nn_y} - \frac{1}{nn_y} \frac{t}{16\beta_V^2} \operatorname{Var}\left[r_k(\mathbf{u}'_i, \mathbf{y}'_{i,j}, \mathbf{u}_i, \mathbf{y}_{i,j}) \right] \right) \right) \right]$$

$$= \sum_{k} \exp\left(\sum_{i=1}^{n} \sum_{j=1}^{n_y} \frac{t}{nn_y} \operatorname{Var}[r_k^2(\mathbf{u}'_i, \mathbf{y}'_{i,j}, \mathbf{u}_i, \mathbf{y}_{i,j})] \left(\frac{3t/nn_y}{6 - 8\beta_V^2 t/nn_y} - \frac{1}{16\beta_V^2} \right) \right)$$

$$(82)$$

where the first inequality follows from Jensen's inequality and the third inequality uses (81) by replacing t by t/nn_y . Setting

$$\frac{3t/nn_y}{6-8\beta_V^2 t/nn_y} - \frac{1}{16\beta_V^2} = 0,$$

we have $t = \frac{3nn_y}{28\beta_V^2}$ and $\frac{t}{nn_y} < \frac{3}{4\beta_V^2}$. Substituting the choice of t into (82) gives rise to

$$\frac{tT_2}{2} \le \log \sum_k \exp(0).$$

Thus

$$\widetilde{\mathbf{T}}_2 \leq \frac{2}{t} \log \mathcal{N}(\theta, \mathcal{R}, \|\cdot\|_{\infty, \infty}) = \frac{56\beta_V^2}{3nn_y} \log \mathcal{N}(\theta, \mathcal{R}, \|\cdot\|_{\infty, \infty})$$

and

$$T_{2} \leq \frac{56\beta_{V}^{2}}{3nn_{y}}\log \mathcal{N}(\theta, \mathcal{R}, \|\cdot\|_{\infty, \infty}) + 6\theta \leq \frac{19\beta_{V}^{2}}{nn_{y}}\log \mathcal{N}(\theta, \mathcal{R}, \|\cdot\|_{\infty, \infty}) + 6\theta.$$
(83)

The following lemma (see a proof in Section B.9) gives a relation between the covering number of \mathcal{R} and \mathcal{G}_{NN} :

Lemma 7. Let \mathcal{G}^* be a θ cover with the covering number $\mathcal{N}(\theta, \mathcal{G}_{NN}, \|\cdot\|_{\infty,\infty})$. There exists a finite θ cover \mathcal{R}^* of \mathcal{R} , and the covering number is bounded by,

$$\mathcal{N}(\theta, \mathcal{R}, \|\cdot\|_{\infty,\infty}) \leq \mathcal{N}\left(\frac{\theta}{4\beta_V}, \mathcal{G}_{\mathrm{NN}}, \|\cdot\|_{\infty,\infty}\right).$$

By Lemma 7, we have

$$T_{2} \leq \frac{19\beta_{V}^{2}}{nn_{y}} \log \mathcal{N}\left(\frac{\theta}{4\beta_{V}}, \mathcal{G}_{NN}, \|\cdot\|_{\infty,\infty}\right) + 6\theta.$$
(84)

B.8 Proof of Lemma 5

Proof of Lemma 5. For h > 0 and each k, let $\tilde{a}'_k \in \mathcal{F}_2$ be some network so that each nonzero parameter of \tilde{a}'_k is at most different from the corresponding one in \tilde{a}_k by h. Similarly, let $\tilde{q}'_k \in \mathcal{F}_1$ be some network so that each nonzero parameter of \tilde{q}'_k is at most different from the corresponding one in \tilde{q}_k by h.

According to Chen et al. (2022, Proof of Lemma 5.3), we have

$$\|\widetilde{a}_{k}' - \widetilde{a}_{k}\|_{\infty} \le hL_{2}(p_{2}\beta_{U} + 2)(\kappa_{2}p_{2})^{L_{2}-1}, \quad \|\widetilde{q}_{k}' - \widetilde{q}_{k}\|_{\infty} \le hL_{1}(p_{1}\gamma_{2} + 2)(\kappa_{1}p_{1})^{L_{1}-1}.$$

We deduce

$$\begin{split} & \left\| \operatorname{CL}_{c} \left(\sum_{k=1}^{N} \widetilde{a}_{k}^{\prime}(\mathbf{u}) \widetilde{q}_{k}^{\prime}(\mathbf{y}) \right) - \operatorname{CL}_{c} \left(\sum_{k=1}^{N} \widetilde{a}_{k}(\mathbf{u}) \widetilde{q}_{k}(\mathbf{y}) \right) \right\|_{\infty,\infty} \\ & \leq \left\| \sum_{k=1}^{N} \widetilde{a}_{k}^{\prime}(\mathbf{u}) \widetilde{q}_{k}^{\prime}(\mathbf{y}) - \sum_{k=1}^{N} \widetilde{a}_{k}(\mathbf{u}) \widetilde{q}_{k}(\mathbf{y}) \right\|_{\infty,\infty} \\ & \leq \sum_{k=1}^{N} \left\| \widetilde{a}_{k}^{\prime}(\mathbf{u}) \widetilde{q}_{k}^{\prime}(\mathbf{y}) - \widetilde{a}_{k}(\mathbf{u}) \widetilde{q}_{k}(\mathbf{y}) \right\|_{\infty,\infty} \\ & \leq \sum_{k=1}^{N} \left(\left\| \widetilde{a}_{k}^{\prime}(\mathbf{u}) \widetilde{q}_{k}^{\prime}(\mathbf{y}) - \widetilde{a}_{k}^{\prime}(\mathbf{u}) \widetilde{q}_{k}(\mathbf{y}) \right\|_{\infty,\infty} + \left\| \widetilde{a}_{k}^{\prime}(\mathbf{u}) \widetilde{q}_{k}(\mathbf{y}) - \widetilde{a}_{k}(\mathbf{u}) \widetilde{q}_{k}(\mathbf{y}) \right\|_{\infty,\infty} \right) \\ & \leq \sum_{k=1}^{N} \left(\left\| \widetilde{a}_{k}^{\prime} \right\|_{\infty} \left\| \widetilde{q}_{k}^{\prime}(\mathbf{y}) - \widetilde{q}_{k}(\mathbf{y}) \right\|_{\infty} + \left\| \widetilde{q}_{k} \right\|_{\infty} \left\| \widetilde{a}_{k}^{\prime}(\mathbf{u}) - \widetilde{a}_{k}(\mathbf{u}) \right\|_{\infty} \right) \\ & \leq \sum_{k=1}^{N} \left(R_{1} h L_{1}(p_{1} \gamma_{2} + 2)(\kappa_{1} p_{1})^{L_{1} - 1} + R_{2} h L_{2}(p_{2} \beta_{U} + 2)(\kappa_{2} p_{2})^{L_{2} - 1} \right) \\ & = h N \left(R_{1} L_{1}(p_{1} \gamma_{2} + 2)(\kappa_{1} p_{1})^{L_{1} - 1} + R_{2} L_{2}(p_{2} \beta_{U} + 2)(\kappa_{2} p_{2})^{L_{2} - 1} \right). \end{split}$$

Set h so that $hN\left(R_1L_1(p_1\gamma_2+2)(\kappa_1p_1)^{L_1-1}+R_2L_2(p_2\beta_U+2)(\kappa_2p_2)^{L_2-1}\right)=\theta$ gives

$$h = \frac{\theta}{H} \text{ with } H = N \left(R_1 L_1 (p_1 \gamma_2 + 2) (\kappa_1 p_1)^{L_1 - 1} + R_2 L_2 (p_2 \beta_U + 2) (\kappa_2 p_2)^{L_2 - 1} \right).$$

We uniformly discretize the parameters of \mathcal{F}_1 and \mathcal{F}_2 by $2\kappa_1/h$ and $2\kappa_2/h$. The collection of all networks corresponding to those grid parameters forms a θ -cover of \mathcal{G} . The covering number is bounded by

$$\mathcal{N}(\theta, \mathcal{G}_{NN}, \|\cdot\|_{\infty,\infty}) \leq \binom{L_1 p_1^2}{K_1} \left(\frac{2\kappa_1}{h}\right)^{NK_1} \cdot \binom{L_2 p_2^2}{K_2} \left(\frac{2\kappa_2}{h}\right)^{NK_2}$$
$$\leq (L_1 p_1^2)^{NK_1} \left(\frac{2\kappa_1}{h}\right)^{NK_1} \cdot (L_2 p_2^2)^{K_2} \left(\frac{2\kappa_2}{h}\right)^{K_2}$$
$$\leq \left(\frac{2L_1 p_1^2 \kappa_1 H}{\theta}\right)^{NK_1} \left(\frac{2L_2 p_2^2 \kappa_2 H}{\theta}\right)^{NK_2}.$$

B.9 Proof of Lemma 7

Proof of Lemma 7. For any $g, \bar{g} \in \mathcal{R}$, we have

$$g(\mathbf{u})(\mathbf{y}) = (G_{\rm NN}(\mathbf{u})(\mathbf{y}) - G(u)(\mathbf{y}))^2, \quad \bar{g}(\mathbf{u})(\mathbf{y}) = (\bar{G}_{\rm NN}(\mathbf{u})(\mathbf{y}) - G(u)(\mathbf{y}))^2$$
(85)

for some $G_{NN}, \overline{G}_{NN} \in \mathcal{G}$. We have

$$\begin{split} \|g - \bar{g}\|_{\infty,\infty} &= \sup_{\boldsymbol{u} \in U} \sup_{\boldsymbol{y} \in \Omega_{V}} |(G_{\mathrm{NN}}(\boldsymbol{u})(\boldsymbol{y}) - G(\boldsymbol{u})(\boldsymbol{y}))^{2} - (\bar{G}_{\mathrm{NN}}(\boldsymbol{u})(\boldsymbol{y}) - G(\boldsymbol{u})(\boldsymbol{y}))^{2}| \\ &= \sup_{\boldsymbol{u} \in U} \sup_{\boldsymbol{y} \in \Omega_{V}} |(G_{\mathrm{NN}}(\boldsymbol{u})(\boldsymbol{y}) - \bar{G}_{\mathrm{NN}}(\boldsymbol{u})(\boldsymbol{y})) (G_{\mathrm{NN}}(\boldsymbol{u})(\boldsymbol{y}) + \bar{G}_{\mathrm{NN}}(\boldsymbol{u})(\boldsymbol{y}) - 2G(\boldsymbol{u})(\boldsymbol{y}))| \\ &\leq \sup_{\boldsymbol{u} \in U} \sup_{\boldsymbol{y} \in \Omega_{V}} |G_{\mathrm{NN}}(\boldsymbol{u})(\boldsymbol{y}) - \bar{G}_{\mathrm{NN}}(\boldsymbol{u})(\boldsymbol{y})| |G_{\mathrm{NN}}(\boldsymbol{u})(\boldsymbol{y}) + \bar{G}_{\mathrm{NN}}(\boldsymbol{u})(\boldsymbol{y}) - 2G(\boldsymbol{u})(\boldsymbol{y})| \\ &\leq 4\beta_{V} \|G_{\mathrm{NN}} - \bar{G}_{\mathrm{NN}}\|_{\infty,\infty}. \end{split}$$

We thus have

$$\mathcal{N}(heta, \mathcal{R}, \|\cdot\|_{\infty,\infty}) \leq \mathcal{N}\left(rac{ heta}{4eta_V}, \mathcal{G}_{NN}, \|\cdot\|_{\infty,\infty}
ight).$$