ADVANTAGE OF DEEP NEURAL NETWORKS FOR ESTIMATING
FUNCTIONS WITH SINGULARITY ON CURVES

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ABSTRACT. We develop a theory to elucidate the reason that deep neural networks (DNNs) perform better than other methods. In terms of the nonparametric regression problem, it is well known that many standard methods attain the minimax optimal rate of estimation errors for smooth functions, and thus, it is not straightforward to identify the theoretical advantages of DNNs. This study fills this gap by considering the estimation for a class of non-smooth functions with singularities on smooth curves. Our findings are as follows: (i) We derive the generalization error of a DNN estimator and prove that its convergence rate is almost optimal. (ii) We reveal that a certain class of common models are sub-optimal, including linear estimators and other harmonic analysis methods such as wavelets and curvelets. This advantage of DNNs comes from a fact that a shape of singularity can be successfully handled by their multi-layered structure.

1. INTRODUCTION

Deep learning with deep neural networks (DNNs) has been applied extensively in various tasks owing to their remarkable performance. It has frequently been observed that DNNs empirically achieve substantially higher accuracy than many existing approaches [29, 23, 13, 22, 17]. To understand this empirical success, we investigate DNNs through the nonparametric regression problem.

Suppose that we have \( n \) independently and identically distributed pairs \((X_i, Y_i) \in [0, 1]^D \times \mathbb{R} \) for \( i = 1, \ldots, n \) generated from the model

\[
Y_i = f^*(X_i) + \xi_i, \quad i = 1, \ldots, n,
\]

where \( f^* : [0, 1]^D \to \mathbb{R} \) is an unknown function and \( (\xi_i) \) is an i.i.d. Gaussian noise that is independent of \( X_i \). The aim of this study is to investigate the generalization error of an estimator \( \hat{f}^{DL} \) by DNNs; that is

\[
\|f^{DL} - f^*\|_{L^2(P_X)}^2 := \mathbb{E}_{X \sim P_X} \left[ (\hat{f}^{DL}(X) - f^*(X))^2 \right].
\]

We prove that the estimator using DNNs achieves the minimax optimal convergence rate, and it is faster than the rates achieved by a certain class of existing methods when \( f^* \) has singularities on smooth curves in the domain.

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Figure 1. [Left] Example of piecewise smooth function $f(x_1, x_2)$ with two-dimensional input. The function is smooth within the pieces and singular on the boundaries of the pieces. [Right] Domain of example function, divided into three pieces. The bold red curve, which is a boundary of the pieces, is a curve for the singularity of $f$.

Understanding the relative advantages of DNNs remains challenging when analyzing deep learning with the nonparametric regression problem. This is because it is already well-known that several existing methods can achieve the minimax optimal rate with a smoothness assumption for the regression model (1). In particular, when $f^*$ is $\beta$-times (continuously) differentiable, numerous existing methods, such as the kernel method, the Fourier series method, and Gaussian process methods, provide an estimator $\hat{f}$, which satisfies

$$||\hat{f} - f^*||_2^2 \leq O_P\left(n^{-2\beta/(2\beta + D)}\right),$$

as standard knowledge in the nonparametric statistics (33 55). Since this convergence rate is known to be optimal in the minimax sense (31), it is almost impossible to present theoretical evidence for the empirical advantage of DNNs if we employ the smoothness assumption.

To overcome this limitation of the theoretical understanding, we consider the estimation of a piecewise smooth function, which is a natural class of non-smooth functions. More specifically, the functions are singular (non-differentiable or discontinuous) on a smooth curve in their multi-dimensional domain. Figure 1 presents an example of such a function, the domain of which is divided into three pieces with piecewise smooth boundaries. This class of functions is sufficiently flexible to express singularity, while being broader than the usual smooth functions. Similar function classes are suitable for the representation of edges in images, and have been studied in areas such as image analysis and harmonic analysis (19 6 5 20).

In this study, we make two contributions to statistical theory. The first contribution is to prove that the estimator by DNNs almost achieves the minimax optimal rate when estimating functions with singularities. Specifically, let $F_{\alpha, \beta, M}^{PS}$ be the set of piecewise smooth functions such that their domain is divided into $M$ pieces, they are $\beta$-times differentiable except on the boundaries of the
Following which the entire DNN model consists of a composite function of the two transforms. Owing to an important role: a first transform approximates $x$ indicator function methods under functions with singularity. These results indicate that DNNs certainly offer a theoretical advantage over the other methods: that is, we prove that \( \frac{q}{p} \) than that of the certain class of the other estimators sequences $t_n$ as $n \to \infty$ (Corollary 1). Here, $\tilde{O}_D$ denotes the Big O notation ignoring logarithmic factors. We further prove that this convergence rate in $n$ corresponds to the minimax optimal rate. The result indicates that DNNs can estimate a non-smooth function in the class without a loss of efficiency. Moreover, it is interesting to note that this result holds even if a DNN does not contain any singularities that are used in the field of image analysis, such as the wavelet ridge regression and Gaussian process regression. The other candidates are methods for resolving non-smooth elements, such as non-differentiable activation functions. That is, even smooth DNNs can estimate such a non-smooth function without being affected by singularity. We also evaluate the effect of the number of pieces in the domain.

The second contribution is to prove the advantages of DNNs compared to other methods. To make this claim, we consider the following candidates: One is a broad class of estimators known as linear estimators $\tilde{f}_{\text{lin}}$, which includes commonly used methods such as estimators by kernel ridge regression and Gaussian process regression. The other candidates are methods for resolving singularities that are used in the field of image analysis, such as the wavelet $\tilde{f}_{\text{wav}}$ and curvelet $\tilde{f}_{\text{curve}}$ methods. We investigate the minimax estimation errors and conclude that the above-mentioned methods do not achieve the optimal rate. That is, there exists a configuration of $\alpha, \beta, \text{and } D$ such that an estimator $\tilde{f} \in \{ \tilde{f}_{\text{lin}}, \tilde{f}_{\text{wav}}, \tilde{f}_{\text{curve}} \}$ by any of the other methods follows

$$
\inf_{\tilde{f}} \sup_{f* \in \mathcal{F}_{\alpha, \beta, M}} \mathbb{E}_{f*} \left[ \| \tilde{f} - f^* \|_{L^2}^2 \right] \gtrsim \max \left\{ n^{-2\beta/(2\beta+D)}, n^{-\alpha/(\alpha+D-1)} \right\}
$$

as $n \to \infty$ (Corollary 2). Here, we denote $a_n \sim b_n$ by $|a_n/b_n| \to \infty$ holds as $n \to \infty$ with the sequences $\{a_n\}_n$ and $\{b_n\}_n$. Consequently, the DNN estimator $\tilde{f}_{DL}$ can attain a faster minimax rate than that of the certain class of the other estimators $\tilde{f} \in \{ \tilde{f}_{\text{lin}}, \tilde{f}_{\text{wav}}, \tilde{f}_{\text{curve}} \}$ for piecewise smooth functions: that is, we prove that

$$
\sup_{f* \in \mathcal{F}_{\alpha, \beta, M}} \mathbb{E} \left[ \| \tilde{f} - f^* \|_{L^2}^2 \right] \gtrsim \sup_{f* \in \mathcal{F}_{\alpha, \beta, M}} \mathbb{E} \left[ \| \tilde{f}_{DL} - f^* \|_{L^2}^2 \right]
$$

holds. These results indicate that DNNs certainly offer a theoretical advantage over the other methods under functions with singularity.

As an intuitive reason for these results, we describe the following two roles of DNNs. First, a model by DNNs, which is a composition of several transforms, is suitable for decomposing non-smooth functions into simple elements. We begin with a simple example. Let us consider the indicator function $1_{S_{D-1}} : \mathbb{R}^D \to \mathbb{R}$ of the unit sphere $S_{D-1} \subset \mathbb{R}^D$; that is, $1_{S_{D-1}}(x) = 1$ when $x \in S_{D-1}$, and $1_{S_{D-1}}(x) = 0$ otherwise. Although $1_{S_{D-1}}(x)$ is discontinuous, DNNs can approximate $1_{S_{D-1}}(x)$ without a loss of efficiency from the discontinuity. Note that the function has the form $1_{S_{D-1}}(x) = 1_{\{x \geq 0\}} \circ h(x)$ with a certain smooth function $h(x)$ and a step function $1_{\{x \geq 0\}}$, such as $1_{\{x \geq 0\}}(x) = 1$ for $x \geq 0$ and $1_{\{x \geq 0\}}(x) = 0$ otherwise. The multi-transform structure of DNNs plays an important role: a first transform approximates $h(x)$, and a second transform approximates $1_{\{x \geq 0\}}$, following which the entire DNN model consists of a composite function of the two transforms. Owing to the composition, DNNs can approximate $1_{S_{D-1}}$ as if it were a smooth function. Second, the
activation function of DNNs plays a significant role in representing a step function. Several common activation functions, such as the sigmoid and rectified linear unit (ReLU) activations, can easily approximate a step function with an arbitrarily small error. The general conditions for achieving the approximation are explained in Assumption 1 below.

This paper is an extension of a previous conference proceeding [14]. There are three main updates in this paper compared to the preceding version. First, we develop a general class of activation functions for DNNs, whereas the previous study investigated DNNs with only the ReLU activation function. As the ReLU activation is a limited option among various activation functions, this study establishes a more general theory for DNNs. Further, in this study, all proofs have been rewritten to deal with the general activation function, since we cannot utilize the approximation theory for the ReLU activation. Second, we present a new definition of functions with discontinuity, which can represent a broader class of discontinuous functions. Third, this study additionally examines several methods that are adept at handling singularities, such as the wavelet and curvelet approaches, and subsequently demonstrates that they do not achieve optimality.

Related Studies: Several pioneering works have investigated deep learning according to the nonparametric regression problem. A recent study by Schmidt-Hieber [30] considered the case in which \( f^* \) is expressed as a composition of several smooth functions, and then derived the minimax optimal rate with this setting. Bauer & Kohler [4] also derived the convergence rate of errors when \( f^* \) had the form of a generalized hierarchical interaction model, and revealed that the obtained rate was dependent on the lower dimensionality of the model. These studies focused on the composition structure of \( f^* \), and they did not consider the non-smoothness and discontinuity of \( f^* \). Therefore, these works did not take into account singularity, which is the main focus of our study.

The works by Suzuki [32] and Hayakawa & Suzuki [12] also demonstrated the superiority of DNNs. The above works investigated the generalization error of DNNs when \( f^* \) belongs to the Besov space. Interestingly, the convergence rate of DNNs was faster than that of the linear estimator when the norm parameter of the Besov space was less than 1, following the theory of Donoho & Johnstone [7]. Although their motivation was similar to that of our study, the Besov space is not suitable for representing functions with singularities on a smooth curve. This is because the wavelet decomposition, which is used to define the Besov space, loses its efficiency for handling the curve for singularity, as explained in Section 5 of our paper. Moreover, note that the comparison of [32, 12] between DNNs and linear estimators was motivated by the preceding version of our study.

Our study was technically inspired by Peterson et al. [28], which investigated the approximation power of DNNs with discontinuity. The main difference between the above paper and our study is the focus on demonstrating the advantage of deep learning. Their study mainly investigated the approximation error of DNNs. Thus, a comparison with existing methods was not the main purpose of the study. Another major difference is that the mentioned study focused on the approximation power, whereas we investigate the generalization error, including the variance control of DNNs. A further difference is that our study investigates a broader class of discontinuous functions, as our definition directly controls curves in the domain, whereas [28] defined the discontinuity by a transform of the Heaviside function.
Organization of this paper: The remainder of this paper is organized as follows: Section 2 introduces a functional model by DNNs, following which an estimator for the regression problem with DNNs is defined. The notion of functions with singularities is explained in Section 3. Section 4 derives the convergence rate by the estimator by means of DNNs. Furthermore, the minimax optimality of the convergence rate is determined. Section 5 presents the non-optimal convergence rate obtained by a certain class of other estimators, and compares this rate with that of DNNs. Section 6 summarizes our work. Full proofs are deferred to the supplementary material.

1.1. Notation. Let $I := [0, 1]$ be the unit interval, $\mathbb{N}$ be natural numbers, and $\mathbb{N}_0 := \mathbb{N} \cup \{0\}$. For $z \in \mathbb{N}$, $\lfloor z \rfloor := \{1, 2, \ldots, z\}$ is the set of natural numbers that are no more than $z$. The $d$-th element of vector $b \in \mathbb{R}^D$ is denoted by $b_d$, and $b_{-d} = (b_1, \ldots, b_{d-1}, b_{d+1}, \ldots, b_D)$ for $d \in [D]$. $\|b\|_q := (\sum_d b_d^q)^{1/q}$ is the $q$-norm for $q \in (0, \infty)$, $\|b\|_\infty := \max_{j \in [J]} |b_j|$, and $\|b\|_0 := \sum_{j \in [J]} I_{(b_j \neq 0)}$. For a measure space $(A, \mathcal{B}, \mu)$ and a measurable function $f : A \to \mathbb{R}$, let $\|f\|_{L^2(\mu)} := (\int_A |f(x)|^2 \mu(x))^{1/2}$ denote the $L^2(\mu)$-norm if the integral is finite. When $\mu$ is the Lebesgue measure on a measurable set $A$ in $\mathbb{R}^D$, we omit $\mu$ and simply write $\|f\|_{L^2(A)}$. For a set $A \subset \mathbb{R}^D$, vol$(A)$ denotes the Lebesgue measure of $A$. The tensor product is denoted by $\otimes$. For a set $R \subset I^D$, let $1_R : I^D \to \{0, 1\}$ denote the indicator function of $R$; that is, $1_R(x) = 1$ if $x \in R$, and $1_R(x) = 0$ otherwise. For the sequences $(a_n)_n$ and $(b_n)_n$, $a_n \preceq b_n$ means that there exists $C > 0$ such that $a_n \leq C b_n$ holds for every $n \in \mathbb{N}$. $a_n \succeq b_n$ denotes the opposite of $a_n \preceq b_n$. Furthermore, $a_n \asymp b_n$ denotes both $a_n \succeq b_n$ and $a_n \preceq b_n$. $a_n \asymp b_n$ denotes $|a_n/b_n| \to 0$ as $n \to \infty$, and $a_n \asymp b_n$ is its opposite. For a set of parameters $\theta$, $C_\theta > 0$ denotes an existing finite constant depending on $\theta$. Let $O_P$ and $o_P$ be the Landau big O and small o in probability. $\tilde{O}$ ignores every polynomial of logarithmic factors.

2. Deep Neural Networks

A deep neural network (DNN) is a model of functions defined by a layered structure. Let $L \in \mathbb{N}$ be the number of layers in DNNs, and for $\ell \in [L + 1]$, let $D_\ell \in \mathbb{N}$ be the dimensionality of variables in the $\ell$-th layer. DNNs have a matrix parameter $A_\ell \in \mathbb{R}^{D_{\ell+1} \times D_\ell}$ and a vector parameter $b_\ell \in \mathbb{R}^{D_\ell}$ for $\ell \in [L]$ to represent weights and biases, respectively. We introduce an activation function $\eta : \mathbb{R} \to \mathbb{R}$, which will be specified later. For a vector input $z \in \mathbb{R}^d$, $\eta(z) = (\eta(z_1), \ldots, \eta(z_d))^\top$ denotes an element-wise operation. For $\ell \in [L - 1]$, with an input vector $z \in \mathbb{R}^{D_\ell}$, we define $g_\ell : \mathbb{R}^{D_\ell} \to \mathbb{R}^{D_{\ell+1}}$ as $g_\ell(z) = \eta(A_\ell z + b_\ell)$. We also define $g_L(z) = A_L z + b_L$ with $z \in \mathbb{R}^{D_L}$. Thereafter, we define a function $g : \mathbb{R}^{D_1} \to \mathbb{R}^{D_{L+1}}$ of DNNs with $(A_1, b_1), \ldots, (A_L, b_L)$ by

$$g(x) = g_L \circ g_{L-1} \circ \cdots \circ g_1(x).$$

Intuitively, $g(x)$ is constituted by compositions of $L$ mappings $\eta_{b_\ell} A_\ell(x)$.

For each $g$ with the form [3], we introduce several convenient operators to extract information of $g$. Let $L(g) = L$ be the number of layers, $S(g) := \sum_{\ell \in [L]} \|\text{vec}(A_\ell)\|_0 + \|b_\ell\|_0$ as a number of non-zero elements in $\Theta$, and $B(g) := \max_{\ell \in [L]} \|\text{vec}(A_\ell)\|_{\infty} \vee \max_{\ell \in [L]} \|b_\ell\|_{\infty}$ be the largest absolute value of the parameters. Here, $\text{vec}(\cdot)$ is a vectorization operator for matrices.

We define the set of functions of DNNs. With a tuple $(L', S', B') \in \mathbb{N}^3$, the set is written as

$$\mathcal{G}(L', S', B')$$
Figure 2. Common activation functions; Sigmoid: \( \eta(x) = 1/(1 + \exp(x)) \), ReLU: \( \eta(x) = \max\{x, 0\} \), LeakyReLU: \( \eta(x) = \max\{x, 0\} + 0.2 \min\{x, 0\} \), SoftPlus: \( \eta(x) = \log(1 + \exp(x)) \), and Swish: \( \eta(x) = x/(1 + \exp(x)) \).

\[
:= \left\{ g \in L^\infty(I^D) \mid g \text{ as } \boxed{\text{5}} : L(g) \leq L', S(g) \leq S', B(g) \leq B', \|g\|_{L^\infty(I^D)} \leq F \right\},
\]

where \( F > 0 \) is a threshold. Since the form of DNNs is flexible, we control the size and complexity of it through the layers and parameters through the tuple \((L', S', B')\). Here, the internal dimensionality \( D_\ell \) is implicitly regularized by the tuple.

The explicit form of \( \eta \) plays a critical role in DNNs, and numerous variations of activation functions have been suggested. We select several of the most representative activation functions in Figure 2. To investigate a wide class of activation functions, we introduce the following assumption.

Assumption 1. An activation function \( \eta : \mathbb{R} \to \mathbb{R} \) satisfies either of the following conditions:

(i) There exist parameters \( \gamma, q \geq 1 \) and \( k \in \{0, 1\} \) such that \( \partial^j \eta \) exists at every point and is bounded for \( j = 1, \ldots, N+1 \). Furthermore, there exists \( x' \in \mathbb{R} \) such that \( \min_{j=1,\ldots,N} |\partial^j \eta(x')| \geq c_\eta > 0 \) with a constant \( c_\eta > 0 \). Further, both of the following hold:

\[
|\eta(x) - \bar{c} x^k| = O(1/x^q), \quad (x \to \infty),
\]

and

\[
|\eta(x) - \underline{c}| = O(1/|x|^q), \quad (x \to -\infty),
\]

with some constants \( \bar{c} > \underline{c} \geq 0 \). There also exists \( C_K > 0 \) such that \( |\eta(x)| \leq C_K (1 + |x|^k) \) for any \( x \in \mathbb{R} \).

(ii) There exist constants \( c_1 > c_2 \geq 0 \) such that

\[
\eta(x) = \begin{cases} 
  c_1 x & \text{if } x \geq 0 \\
  c_2 x & \text{if } x < 0 
\end{cases}
\]

The condition (i) describes smooth activation functions such as the sigmoid function, the softplus function, and the Swish function with \( N = \infty \). The condition (ii) indicates a piecewise linear function such as the rectified linear unit (ReLU) function and the leaky ReLU function, which require another technique to investigate.

2.1. Regression Problem and Estimator by DNNs. We consider the least square estimator by DNNs for the regression problem \([1]\). Let the \( D \)-dimensional cube \( I^D \) \((D \geq 2)\) be a space for input variables \( X_i \). Suppose we have a set of observations \( (X_i, Y_i) \in I^D \times \mathbb{R} \) for \( i \in [n] \) which is
We also suppose that \( X \) is an unknown true function and \( \xi_i \) is Gaussian noise with mean 0 and variance \( \sigma^2 > 0 \) for \( i \in [n] \). We also suppose that \( X_i \) follows a marginal distribution \( P_X \) on \([0, 1]^D\) and it has a density function \( p_X \) which is bounded away from zero and infinity. Then, we define an estimator by empirical risk minimization with DNNs as

\[
\hat{f}^{DL} = \arg\min_{f \in \mathcal{G}(L,S,B)} \frac{1}{n} \sum_{i=1}^{n} (Y_i - f(X_i))^2.
\]

The minimizer always exists since \( \mathcal{G}(L,S,B) \) is a compact set in \( L^2(I^D) \) due to the parameter bound and continuity of \( \eta \). Note that we do not discuss the optimization issues from the non-convexity of the loss function, since we mainly focus on an estimation aspect.

3. Characterization of Functions with Singularity

In this section, we provide a rigorous formulation of functions with singularity on smooth curves. To describe the singularity of functions, we introduce a notion of piecewise smooth functions, which have its domain divided into several pieces and smooth only within each of the pieces. Furthermore, piecewise smooth functions are singular (non-differentiable or discontinuous) on the boundaries of the pieces.

**Smooth Functions (Hölder space):** Let \( \Omega \) be a closed subset of \( \mathbb{R}^D \) and \( \beta, F > 0 \) be parameters. For a multi-index \( a \in \mathbb{N}_0^D \), \( \partial^a = \partial^{a_1} \cdots \partial^{a_D} \) denotes a partial derivative operator. The Hölder space \( H^\beta(\Omega) \) is defined as a set of functions \( f : \Omega \to \mathbb{R} \) such as

\[
H^\beta(\Omega) := \left\{ f \left| \max_{|a| \leq \beta} \| \partial^a f \|_{L^\infty(\Omega)} + \max_{|a| = |\beta|} \sup_{x,x',x \neq x'} \frac{\| \partial^a f(x) - \partial^a f(x') \|}{|x - x'|^{\beta - |\beta|}} < \infty \right\},
\]

where \( a \in \mathbb{Z}^D \) be a non-negative multi-index and \( |a| = \sum_{i=1}^{D} a_i \). Also, let \( H^\beta_F(\Omega) \) be a ball in \( H^\beta(\Omega) \) with its radius \( F > 0 \) in terms of the norm \( \| \cdot \|_{L^\infty} \).

**Pieces in the Domain:** We describe pieces as subsets of the domain \( I^D \) by dividing \( I^D \) with several curves. For \( j = 1, \ldots, J \), let \( h_j \in H^\beta_F(I^{D-1}) \) be a function with input \( x_{-d_j} \in I^{D-1} \) for some \( d_j \in [D] \). We define a family of \( M \) pieces which are an intersection of one side of \( J \) curves. Let \( I^+_j := \{ x \in I^D \mid x_{d_j} \geq h_j(x_{-d_j}) \} \) and \( I^-_j := \{ x \in I^D \mid x_{d_j} \leq h_j(x_{-d_j}) \} \). For a \( J \)-tuple \( t = (t_j^i)_{j=1}^{J} \in \{+, -\}^{[J]} \), a unit piece of \( I^D \) is defined by \( I_t := \bigcap_{j \in [J]} I_j^{t_j} \). Let \( \mathcal{T} \) be a subset of \( \{+, -\}^{[J]} \), and define piece \( R_\mathcal{T} \) by

\[
R_\mathcal{T} := \bigcup_{t \in \mathcal{T}} I_t.
\]

Let \( \{\mathcal{T}_1, \ldots, \mathcal{T}_M\} \) be a partition of \( \{+, -\}^{[J]} \). Then, it is easy to see \( \bigcup_{m \in [M]} R_{T_m} = I^D \) and \( R_{T_m} \cap R_{T_{m'}} \) is of Lebesgue measure zero. The family of pieces that is of size \( M \) is given by

\[
\mathcal{R}_{\alpha,M} := \left\{ \{R_{T_m}\}_{m \in [M]} \mid \{T_m\}_{m \in [M]} \text{ is a partition of } \{+, -\}^{[J]} \right\}.
\]

Intuitively, \( \{R_{T_m}\}_{m \in [M]} \in \mathcal{R}_{\alpha,M} \) is a partition of \( I^D \), allowing overlap on the piecewise \( \alpha \)-smooth boundaries. Figure \ref{fig:partition} presents an example. In the following, when the partition \( \{T_m\}_{m \in [M]} \) is fixed, we can also write \( R_{\bar{m}} := R_{T_m} \) by slightly changing the notation.
Piecewise Smooth Functions: By using $H^\beta_F(I^D)$ and $\mathcal{R}_{\alpha,M}$, we introduce a space of piecewise smooth functions as

$$
\mathcal{F}_{\alpha,\beta,M}^{PS} := \left\{ \sum_{m \in [M]} f_m \otimes I_{R_m} : f_m \in H^\beta_F(I^D), \{R_m\}_{m \in [M]} \in \mathcal{R}_{\alpha,M} \right\}.
$$

Since $f_m(x)$ realizes only when $x \in R_m$, the notion of $\mathcal{F}_{\alpha,\beta,M}^{PS}$ can express a combination of smooth functions on each piece $R_m$. Hence, functions in $\mathcal{F}_{\alpha,\beta,M}^{PS}$ are non-smooth (and even discontinuous) on boundaries of $R_m$. Obviously, $H^\beta(I^D) \subset \mathcal{F}_{\alpha,\beta,M}^{PS}$ holds for any $M$ and $\alpha$, since $f_1 = f_2 = \cdots = f_M$ makes the function globally smooth.

Remark 1 (Other definitions). Several studies [28, 14] also define a class of piecewise smooth functions. There are mainly two differences of our definition in this study. First, our definition can describe a wider class of pieces. The definition utilizes a direct definition of a smooth curve function $h$, while the other definition defines pieces by a transformation of the Heaviside function which is slightly restrictive. Second, our definition is less redundant. We do not allow the pieces to overlap with one another, whereas some of the other definitions allow pieces to overlap. When overlap exists, it may make approximation and estimation errors worse, which is a problem that our definition can avoid.

4. Generalization Error of Deep Neural Networks

We provide theoretical results regarding DNN performances for estimating piecewise smooth functions. To begin with, we decompose the estimator error into an approximation error and a complexity error, analogously to the bias-variance decomposition. By a simple calculation on (4), we obtain the following inequality:

$$
\|\hat{f}^{DL} - f^*\|_2^2 \leq \inf_{f \in \mathcal{G}(L,S,B)} \|f - f^*\|_B^2 + \frac{2}{n} \sum_{i=1}^{n} \xi_i (\hat{f}^{DL}(X_i) - f(X_i)),
$$

where $\|f\|_n := n^{-1} \sum_{i \in [n]} f(X_i)^2$ is an empirical (pseudo) norm. We note that $\xi_i$ is the Gaussian noise displayed in (1). The term $\mathcal{B}$ in the right hand side is the approximation error, and the term $\mathcal{V}$ is the complexity error. In the following section, we bound $\mathcal{B}$ and subsequently combine it with the bound for $\mathcal{V}$.

4.1. Approximation Result. We evaluate the approximation error with piecewise smooth functions according to the following three preparatory steps: approximating (i) smooth functions, (ii) step functions, and (iii) indicator functions on the pieces. Thereafter, we provide a theorem for the approximation of piecewise smooth functions.

As the first step, we state the approximation power of DNNs for smooth functions in the Hölder space. Although this topic has been studied extensively [26, 37], we provide a formal statement because a condition on activation functions is slightly different.

Lemma 1 (Smooth function approximation). Let $\beta > 0$ be a constant. Suppose Assumption [1] holds with $N > \beta$. Then, there exist constants $C_{\beta,D,F}, C_{\beta,D,F,q} > 0$ such that a tuple $(L, S, B)$ such as
that satisfies
\[
L \geq C_{\beta,D,F}([\beta] + \log_2(1/\varepsilon) + 1)
\]
\[
S \geq C_{\beta,D,F} \varepsilon^{-D/\beta} (\log_2(1/\varepsilon))^2
\]
\[
B \geq C_{\beta,D,F,q} \varepsilon^{-\alpha},
\]
satisfies
\[
\inf_{g \in \mathbb{G}(L,S,B)} \sup_{f \in H^\alpha_B(I^D)} \|g - f\|_{L^2(R)} \leq \text{vol}(R) \varepsilon,
\]
for any non-empty measurable set \( R \subset I^D \) and \( \varepsilon > 0 \).

As we reform the result, the approximation error is written as \( O(\text{vol}(R) S^{-\beta/D}) \) up to logarithmic factors, with \( L \) and \( B \) satisfying the conditions.

As the second step, we investigate an approximation for a step function \( I_{\{\geq 0\}} \), which will play an important role in handling singularities of functions.

**Lemma 2** (Step function approximation). Suppose \( \eta \) satisfies Assumption 1 Then, for any \( \varepsilon \in (0,1) \) and \( T > 0 \), we obtain
\[
\inf_{g \in \mathbb{G}(2,6,C_{T,q}e^{-s})} \|g - I_{\{\geq 0\}}\|_{L^2([-T,T])} \leq \varepsilon.
\]

The result states that any activation functions satisfying Assumption 1 can approximate indicator functions. Importantly, DNNs can achieve an arbitrary error \( \varepsilon \) with \( O(1) \) parameters. The approximation with this constant number of parameters is very important in obtaining the desired rate, since the generalization error of DNNs is significantly influenced by the number of parameters.

As the third step, we investigate the approximation error for the indicator function of a piece. For approximation by DNNs, we reform the indicator function into a composition of a step function and a smooth function:
\[
I_{\{x_d \leq h_j(x_{-d})\}} = I_{\{\geq 0\}} \circ (x \mapsto \hat{\pm}(x_d - h_j(x_{-d}))), \quad x \in I^D.
\]
Using this formulation, we obtain the following result:

**Lemma 3** (Indicator functions for \( R_{\alpha,J} \)). Suppose that Assumption 1 holds with \( N > \alpha \). Then, there exist constants \( C_{\alpha,D,F,J} \), \( C_{F,J,q} > 0 \) such that for any \( \{R_m\}_{m\in[M]} \in R_{\alpha,M} \) and \( \varepsilon > 0 \) we can find a function \( f = (f_1, \ldots, f_M)^T \in \mathbb{G}(L,S,B) \) with
- \( L \geq C_{\alpha,D,F,J} ([\alpha] + \log_2(1/\varepsilon)) \),
- \( S \geq C_{\alpha,D,F,J} (J \varepsilon^{-2(D-1)}/\alpha (\log_2(1/\varepsilon))^2 + M (\log_2(1/\varepsilon))^2) \),
- \( B \geq C_{F,J,q} \varepsilon^{-\alpha} \)
that satisfies
\[
\|I_{R_m} - f_m\|_{L^2(I)} \leq \varepsilon, \quad \forall m \in [M].
\]

Since the model of DNNs has a composition structure, DNNs can implicitly decompose the indicator function into a step function and a smooth function, which derives the convergence rate. Importantly, even though the function \( I_{\{x_d \leq h_j(x_{-d})\}} \) with \( h_j \in H^\alpha_F(I^{D-1}) \) has singularity on a set \( \{x \in I^D \mid x_d = h_j(x_{-d})\} \), DNNs can achieve a fast approximation rate as if the boundary is a smooth function in \( H^\alpha_F(I^{D-1}) \).
Based on the above steps, we derive an approximation rate of DNNs for a piecewise smooth function $f \in \mathcal{F}_{\alpha,\beta,M}^{PS}$

**Theorem 1 (Approximation Error).** Suppose Assumption [1] holds with $N > \alpha \lor \beta$. Then, there exist constants $C_{\alpha,\beta,D,F}, C_{\alpha,\beta,D,F,I}, C_{F,M,q} > 0$ such that there exists a tuple $(L, S, B)$ such as

- $L \geq C_{\alpha,\beta,D,F}(1 + |\alpha| + |\beta| + \log_2(n/M))$,
- $S \geq C_{\alpha,\beta,D,F,I}(n^{(\beta/2) + (\beta/2)} + n^{(\beta/2 + \beta)/(\alpha + \beta)}) \log n$,
- $B \geq C_{F,M,q}(\alpha \land \beta)^{-16} - C_{\alpha,\beta}$,

which satisfies

$$\inf_{f \in \mathcal{G}(L,S,B)} \sup_{f^* \in \mathcal{F}_{\alpha,\beta,M}^{PS}} \|f - f^*\|_{L^2(I^D)} \leq \varepsilon_1 + \varepsilon_2,$$

for any $\varepsilon_1, \varepsilon_2 \in (0, 1)$.

The result states that the approximation error contains two main terms. A simple calculation yields that the error is reformulated as $O(S^{-\beta/D} + S^{-\alpha/(D-1)})$ up to logarithmic factors, with $L$ and $B$ satisfying the conditions. The first rate $O(S^{-\beta/D})$ describes approximation for $f_m \in H_{\alpha,D}^\beta(I^D)$, and the second rate $O(S^{-\alpha/(D-1)})$ describes the approximation for $1_{R_m}$.

4.2. **Generalization Result.** We evaluate a generalization error of DNNs, based on the decomposition [5], associated with the bound on $B$. To evaluate the remained term $\mathcal{V}$, we utilize the celebrated theory of the local Rademacher complexity [3, 18]. Then, we obtain one of our main results as follows. $\mathbb{E}_{f^*}[]$ denotes the expectation with respect to the true distribution of $(X, Y)$.

**Theorem 2 (Generalization Error).** Suppose $f^* \in \mathcal{F}_{\alpha,\beta,M}^{PS}$ and Assumption [1] holds with $N > \alpha \lor \beta$. Then, there exists a tuple $(S, B, L)$ satisfying

1. $L \geq C_{\alpha,\beta,D,F}(1 + |\alpha| + |\beta| + \log_2(n/M))$,
2. $S = C_{\alpha,\beta,D,F,I}(n^{D/2} + n^{D-1}) \log n$,
3. $B \geq C_{F,M,q} n^{C_{\alpha,\beta,D}}$,

such that there exist $C = C_{\alpha,\beta,D,F,I,M} > 0$ and $c_1 > 0$ which satisfy

$$\mathbb{E}_{f^*} \left[ \|\hat{f}^{DL} - f^*\|_{L^2(P_X)}^2 \right] \leq CM(n^{-2\beta/(2\beta + D)} + n^{-\alpha/(\alpha + D - 1)}) \log^2 n + \frac{C_{\alpha,F} \log n}{n}.$$

The dominant term appears in the first term in the right hand, thus it mainly describes the bound for $\hat{f}^{DL}$. We note that the main term of the squared error increases linearly in the number of pieces $M$. To simplify the order of the bound, we provide the following corollary:

**Corollary 1.** With the settings in Theorem [2] we obtain

$$\mathbb{E}_{f^*} \left[ \|\hat{f}^{DL} - f^*\|_{L^2(P_X)}^2 \right] = \tilde{O} \left( \max\{n^{-2\beta/(2\beta + D)}, n^{-\alpha/(\alpha + D - 1)}\} \right).$$

The order is interpreted as follows. The first term $n^{-2\beta/(2\beta + D)}$ describes an effect of estimating $f_m \in H_{\alpha,D}^\beta(I^D)$ for $m \in [M]$. The rate corresponds to the minimax optimal convergence rate of generalization errors for estimating smooth functions in $H_{\alpha,D}^\beta(I^D)$ (for a summary, see [13]). The second term $n^{-\alpha/(\alpha + D - 1)}$ reveals an effect from estimation of $1_{R_m}$ for $m \in [M]$ through estimating the boundaries of $R_m \in \mathcal{R}_{\alpha,\beta}$. The same rate of convergence appears in a problem for estimating
sets with smooth boundaries [24]. Based on the result, we state that DNNs can divide a piecewise smooth function into its various smooth functions and indicators, and estimate them by parts. Thus, the overall convergence rate is the sum of the rates of the parts.

**Remark 2 (Smoothness of \( \eta \)).** It is worth noting that the rate in Theorem 2 holds regardless of smoothness of the activation function \( \eta \), because Assumption 1 allows both smooth and non-smooth activation functions. That is, even when \( \hat{f}^{DL} \) by DNNs is a smooth function with smooth activation, we can obtain the convergence rate in Corollary 1 with non-smooth \( f^* \).

We can consider the error from optimization independently from the statistical generalization. The following proposition provides the statement.

**Proposition 1 (Effect of Optimization).** If a learning algorithm outputs \( \hat{f}^{\text{Algo}} \in G(L, S, B) \) such as
\[
\frac{1}{n} \sum_{i=1}^{n} (Y_i - \hat{f}^{\text{Algo}}(X_i))^2 \leq \min_{f \in G(L, S, B)} \frac{1}{n} \sum_{i=1}^{n} (Y_i - f(X_i))^2 \leq \Delta,
\]
with an existing constant \( \Delta > 0 \), then the following holds:
\[
\mathbb{E}_{f^*} \left[ \| \hat{f}^{\text{Algo}} - f^* \|_{L^2(D)}^2 \right] \leq \tilde{O} \left( \max \{ n^{-2\beta/(2\beta + D)}, n^{-\alpha/(\alpha + D - 1)} \} \right) + \Delta.
\]

We can evaluate the generalization error, including the optimization effect, by combining several results on the magnitude of \( \Delta \) (for example, [16, 11, 15]).

4.3. **Minimax Lower Bound of Generalization Error.** We investigate the efficiency of the convergence rate in Corollary 1. To this end, we consider the minimax generalization error for a functional class \( \mathcal{F} \) such as
\[
\mathcal{R}(\mathcal{F}) := \min_{\tilde{f}} \max_{f^* \in \mathcal{F}} \mathbb{E}_{f^*} \left[ \| \tilde{f} - f^* \|_{L^2(D)}^2 \right],
\]
where \( \tilde{f} = \tilde{f}(X_1, ..., X_n, Y_1, ..., Y_n) \) is taken from all possible estimators depending on the observations. In this section, we derive a lower bound of the generalization error of DNNs, and then prove that it corresponds to the rate Theorem 2 up to logarithmic factors. By the result, we can claim that the estimation by DNNs is (almost) optimal in the minimax sense.

We introduce several new notations. For set \( A \) equipped with a norm \( \| \cdot \| \), let \( \mathcal{N}(\varepsilon, A, \| \cdot \|) \) be the covering number of \( A \) in terms of \( \| \cdot \| \), and \( \mathcal{M}(\varepsilon, A, \| \cdot \|) \) be the packing number of \( A \), respectively. For sequences \( \{a_n\}_n \) and \( \{b_n\}_n \), we write \( a_n = \Omega(b_n) \) for \( \limsup_{n \to \infty} |a_n/b_n| > 0 \). Also, \( a_n = \Theta(b_n) \) means that both of \( a_n = O(b_n) \) and \( a_n = \Omega(b_n) \) hold.

To derive the lower bound, we apply the following celebrated information theoretic result by [36]:

**Theorem 3 (Theorem 6 in [36]).** Let \( \mathcal{F} \) be a set of functions, and \( \varepsilon_n \) be a sequence such that \( \varepsilon_n^2 = \mathcal{M}(\varepsilon_n, \mathcal{F}, \| \cdot \|_{L^2})/n \) holds. Then, we obtain
\[
\mathcal{R}(\mathcal{F}) = \Theta(\varepsilon_n^2).
\]

Since the minimax rate for \( \mathcal{F}_{\alpha, \beta, M}^{PS} \) is bounded below by that of its subset, we will find a suitable subset of \( \mathcal{F}_{\alpha, \beta, M}^{PS} \) and measure its packing number. In the rest of this section, we will take the following two steps. First, we define a subset of \( \mathcal{F}_{\alpha, \beta, M}^{PS} \) by introducing a notion of basic pieces. Second, we measure a packing number of the subset of \( \mathcal{F}_{\alpha, \beta, M}^{PS} \).
As the first step, we define a basic piece indicator, which is a set of piecewise functions whose piece is an embedding of \( D \)-dimensional balls, and then define a certain subset of \( F_{\alpha,\beta,M}^{PS} \). As a preparation, let \( S^{D-1} := \{ x \in \mathbb{R}^D : \| x \|_2 = 1 \} \) be the \( D - 1 \) dimensional sphere, and let \((V_j, F_j)_{j=1}^k \) be its coordinate system as a \( C^{\infty} \)-differentiable manifold such that \( F_j : V_j \rightarrow B^{D-1} := \{ x \in \mathbb{R}^{D-1} : \| x \| < 1 \} \) is a diffeomorphism. A function \( f : S^{D-1} \rightarrow \mathbb{R} \) is said to be in the Hölder class \( H^\alpha(S^{D-1}) \) with \( \alpha > 0 \) if \( f \circ F_j^{-1} \) is in \( H^\alpha(B) \).

**Basic Piece Indicator:** A subset \( R \subset I^D \) is called an \( \alpha \)-basic piece, if it satisfies two conditions: (i) there is a continuous embedding \( g : \{ x \in \mathbb{R}^D : \| x \| \leq 1 \} \rightarrow \mathbb{R}^D \) such that its restriction to the boundary \( S^{D-1} \) is in \( H^\alpha(S^{D-1}) \) and \( R = I^D \cap \text{Image}(g) \), (ii) there exist \( d \in [D] \) and \( h \in H_1^\alpha(I^D) \) such that the indicator function of \( R \) is given by the graph

\[
I_R(x) = \Psi_d(x_1, \ldots, x_{d-1}, x_d + h(x_{-d}), x_{d+1}, \ldots, x_D), x \in I^D,
\]

where \( \Psi_d(x) := 1_{\{x_d \geq 0\}} \) is the Heaviside function. Then, the set of basic piece indicators is defined as

\[
\mathcal{I}_\alpha := \{ I_R | R \text{ is an } \alpha \text{-basic piece} \}.
\]

The condition (i) tells that a basic piece belongs to the boundary fragment class which is developed by [8] and [25]. The condition (ii) means \( R \) is a set defined by a horizon function discussed in [28].

In the following, we consider a functional class

\[
H^\beta(I^D) \otimes \mathcal{I}_\alpha := \left\{ f \otimes I_R | f \in H^\beta(I^D), I_R \in \mathcal{I}_\alpha \right\},
\]

and use this set as a key subset for the minimax lower bound. Obviously, \( H^\beta(I^D) \otimes \mathcal{I}_\alpha \subset F_{\alpha,\beta,M}^{PS} \) holds for any \( M \in \mathbb{N} \).

At the second step of this section, we measure a packing number of \( H^\beta(I^D) \otimes \mathcal{I}_\alpha \).

**Proposition 2** (Packing Bound). For any \( D \geq 2 \) and \( \alpha, \beta \geq 2 \), we have

\[
\log \mathcal{M}(\varepsilon, H^\beta(I^D) \otimes \mathcal{I}_\alpha, \| \cdot \|_{L^2(I^D)}) = \Theta \left( \varepsilon^{-\beta/D} + \varepsilon^{-2\alpha/(D-1)} \right), \ (\varepsilon \to 0).
\]

With the bound, we apply Theorem 3 and thus obtain the minimax lower bound of the estimation with \( H^\beta(I^D) \otimes \mathcal{I}_\alpha \). By using the relation \( \mathcal{R}(F_{\alpha,\beta,M}^{PS}) \geq \mathcal{R}(H^\beta(I^D) \otimes \mathcal{I}_\alpha) \), we obtain the following theorem.

**Theorem 4** (Minimax Rate for \( F_{\alpha,\beta,M}^{PS} \)). For any \( \alpha, \beta \geq 1 \) and \( M \in \mathbb{N} \) we obtain

\[
\mathcal{R}(F_{\alpha,\beta,M}^{PS}) = \Omega \left( \max \left\{ n^{-2\beta/(2\beta + D)}, n^{-\alpha/(\alpha + D - 1)} \right\} \right), \ (n \to \infty).
\]

This result indicates that the convergence rate by \( \hat{f}^{DL} \) is almost optimal in the minimax sense, since the rates in Theorem 2 correspond to the lower bound of Theorem 3 up to a log factor. In other words, for estimating \( f^* \in F_{\alpha,\beta,M}^{PS} \), no other methods could achieve a better rate than the estimators by DNNs.
4.4. Singularity Control by Deep Neural Network. In this section, we present an intuition for the optimality of DNNs for the functions with singularities. In the following, we will present that the approximation error of a non-smooth function by DNNs is as if the function to be approximated is smooth.

Consider a simple example with $D = 2$ and $M = 2$. We use a function $f^S \in F^PS_{\alpha,\beta,2}$ defined by

$$f^S(x_1, x_2) = 1_{R}(x_1, x_2), \quad R = \{(x_1, x_2) \in I^2 \mid x_2 \geq h(x_1)\},$$

with a function $h \in H^\alpha(I)$. The function $f^S$ is singular on the set $\{(x_1, x_2) \in I^2 \mid x_2 = h(x_1)\}$. Moreover, the function $f^S$ is rewritten as

$$f^S(x_1, x_2) = 1_{\{\geq 0\}} \circ \{(x_1, x_2) \mapsto (x_2 - h(x_1))\},$$

where $1_{\{\geq 0\}}$ is the step function and $f^H \in H^\alpha(I^2)$ is a smooth function induced by $h$. We can rewrite the function $f^S$ with the singularities as a composition of the step function and the smooth function $f^H$.

To approximate and estimate $f^S$, we consider an explicit function $g_E$ by DNNs as

$$g_E(x_1, x_2) = g_s \circ g_H(x_1, x_2),$$

where $g_s$ is a DNN approximator for the step function by a DNN, and $g_H$ is a DNN approximator for $f^H$. Subsequently, we can measure its approximation as

$$\|f^E - g_E\|_{L^2(I^2)} \leq \|1_{\{\geq 0\}} - g_s\|_{L^2(I)} + \|f^H - g_H\|_{L^2(I^2)}.$$ 

For the right hand side, Lemma 2 indicates that the first term $\|1_{\{\geq 0\}} - g_s\|_{L^2(I)}$ is negligible, because it is arbitrary small with a constant number of parameters. Hence, a dominant error appears in the second term $\|f^H - g_H\|_{L^2(I^2)}$, which is an approximation error of a smooth function $f^H \in H^\beta(I^2)$.

In summary, DNNs can approximate and estimate non-smooth $f^E$, as if $f^E$ is a smooth function in $H^\beta(I^2)$. This is because DNNs can represent a composition of functions, which can eliminate the singularity of $f^E$.

5. Advantages of DNNs with Singularity

In this section, we compare the result of DNNs with a convergence rate of several other methods.

5.1. Sub-optimality of Linear Estimators. We discuss sub-optimality of some of other standard methods in estimating piecewise smooth functions. To this end, we consider a class of linear estimators.

**Definition 1** (Linear Estimator). The class contains any estimators with the following formulation:

$$\hat{f}^{\text{lin}}(x) = \sum_{i \in [n]} \Upsilon_i(x; X_1, ..., X_n)Y_i, \quad (6)$$

where $\Upsilon_i$ is an arbitrary measurable function which depends on $X_1, ..., X_n$. 

Linear estimators include various popular estimators such as kernel ridge regression, sieve regression, spline regression, and Gaussian process regression. If a regression model is a linear sum of (not necessarily orthogonal) basis functions and its parameter is a minimizer of the sum of square losses, the model is a linear estimator. Linear estimators have been studied extensively (e.g. [7,19]), particularly Section 6 in [19], and the results can be adapted to our setting, thereby providing the following results.

In the following, we prove the sub-optimality of linear estimators:

**Proposition 3 (Sub-Optimality of Linear Estimators).** For any $\alpha, \beta \geq 1$ and $D \in \mathbb{N}$, we obtain

$$
\sup_{f^{*} \in \mathcal{F}_{\alpha,\beta,M}} \mathbb{E}_{f^{*}} \left[ \| \hat{f}^{\text{fin}} - f^{*} \|_{L^2(P_x)}^2 \right] = \Omega \left( n^{-\alpha/(2\alpha+D-1)} \right).
$$

This rate is slower than the minimax optimal rate $O \left( (n^{-2\beta/(2\beta+D)} \vee n^{-\alpha/(\alpha+D-1)}) \right)$ in Theorem 4 with the parameter configuration $\alpha < 2\beta(D-1)/D$. This result implies that linear estimators perform worse than DNNs when it is relatively difficult to estimate a curve with singularity.

**Remark 3 (Linear Estimators with Cross-Validation).** We discuss a sub-optimality of a certain class of nonlinear estimators associated with cross-validation (CV). If we select the hyperparameters of a linear estimator by CV, the estimator is no longer a linear estimator. Typically, a bandwidth parameter of kernel methods and a number of basis functions for sieve estimators are examples of hyperparameters. Despite this fact, the generalization error of a CV-supported estimator is bounded below by that of the estimators with optimal hyperparameters, which are sometimes referred to as oracle estimators. Because oracle estimators are linear estimators in most cases, we can still claim that the CV-supported estimators are sub-optimal according to Proposition 3.

### 5.2. Sub-Optimality of Wavelet Estimator

We investigate the generalization error of a wavelet series estimator for $f^{*} \in \mathcal{F}_{\alpha,\beta,M}$. The estimator by wavelets is one of the most common estimators for the nonparametric regression problem, and can attain the optimal rate in many settings (for a summary, see [10]). Moreover, wavelets can handle discontinuous functions. In this section, we will prove the sub-optimality of the wavelet for the class of piecewise smooth functions. Since these methods are well known for dealing with singularities, their investigation can provide a better understanding of why linear estimators lose their optimality.

Intuitively, wavelets resolve singularity by fitting the support of their basis functions to the singularity’s shape. That is, their approximation error decreases, when the supports fit the shape and fewer basis functions overlap the singularity curve. As illustrated in the left panel of Figure 3, the wavelet divides $I^D$ into cubes, with each basis is concentrated on each cube.

To this end, we consider an orthogonal wavelet basis for $L^2(I)$. We define a set of indexes $\mathcal{H} := \{(j,k) : j \in \{-1,0\} \cup \mathbb{N}, k \in K_j\}$ be the index set with a set $K_j = \{0\} \cup [2^j - 1]$ and consider the wavelet basis $\{\phi_k\}_{k \in \mathcal{H}}$ of $L^2(\mathbb{R})$ with setting $\phi_{-1,k}$ be a shifted scaling function. Then, we restrict its domain to $I$ and obtain the wavelet basis for $L^2(I)$.

For a wavelet analysis for multivariate functions, we consider a tensor product of the basis $\{\phi_k\}_{k \in \mathcal{H}}$. Namely, let us define $\Phi_{\kappa_1,\ldots,\kappa_D}(x) := \prod_{d \in [D]} \phi_{\kappa_d}(x_d)$ with $x \in \mathbb{R}^D$. Then, consider a orthonormal basis $\{\Phi_{\kappa_1,\ldots,\kappa_D}\}_{(\kappa_1,\ldots,\kappa_D) \in \mathcal{H}^D}$ for $L^2(\mathbb{R}^D)$, then restrict it to $L^2(I^D)$. $\mathcal{H}^D$ is a $D$-times direct
Figure 3. [Left] Curve with singularity (black curve) in $l^2$ and cubes in which wavelet basis functions are concentrated. [Middle] Curve with singularity (black curve) in $l^2$ and ellipses in which curvelet basis functions are concentrated. [Right] Domain on the frequency of the curvelet basis. Each basis function is concentrated on a colored shape.

The product of $H$. Then, a decomposition of a restricted function $f \in L^2(I^D)$ is formulated as

$$f = \sum_{(\kappa_1, \ldots, \kappa_D) \in \mathcal{H} \times D} w_{\kappa_1, \ldots, \kappa_D}(f) \Phi_{\kappa_1, \ldots, \kappa_D},$$

where $w_{\kappa_1, \ldots, \kappa_D}(f) = \langle f, \Phi_{\kappa_1, \ldots, \kappa_D} \rangle$.

We define an estimator of $f^*$ by the wavelet decomposition. For simplicity, let $P_X$ be the uniform distribution on $I^D$. Using a truncation parameter $\tau \in \mathbb{N}$, we set $\mathcal{H}_\tau := \{(j, k) : j \in \{-1, 0\} \cup \{\tau\}, k \in K_j \} \subset \mathcal{H}$ be a subset of indexes. Since the decomposition is a linear sum of orthogonal basis, an wavelet estimator $\hat{f}^{\text{wav}}$ which minimizes an empirical squared loss has the following form

$$\hat{f}^{\text{wav}} = \sum_{(\kappa_1, \ldots, \kappa_D) \in \mathcal{H}_\tau} \hat{w}_{\kappa_1, \ldots, \kappa_D} \Phi_{\kappa_1, \ldots, \kappa_D},$$

Moreover, $\hat{w}_{\kappa_1, \ldots, \kappa_D}$ is an empirical analogue version of the inner product as

$$\hat{w}_{\kappa_1, \ldots, \kappa_D} = \frac{1}{n} \sum_{i \in [n]} Y_i \Phi_{\kappa_1, \ldots, \kappa_D}(X_i).$$

The truncation parameter $\tau$ is selected to minimize a generalization error.

With the wavelet estimator, we obtain the following result:

**Proposition 4** (Sub-Optimality of Wavelet Estimators). For any $\alpha, \beta \geq 1$ and $D \geq 2$, we obtain

$$\sup_{f^* \in \mathcal{F}^{PS}_{\alpha, \beta, M}} \mathbb{E}_{f^*} \left[ \left\| \hat{f}^{\text{wav}} - f^* \right\|_{L^2(P_X)}^2 \right] = \Omega \left( n^{-1/2} \right).$$

When comparing the derived rate with Theorem 4, we can find that the wavelet estimator cannot attain the minimax rate when both $\beta > D/2$ and $\alpha > (D - 1)$ hold. This result describes that wavelets are unable to adapt a higher smoothness of $f^*$ and the boundary of pieces.
5.3. Sub-optimality of Harmonic Based Estimator. We investigate another estimator from the harmonic analysis and its optimality. The harmonic analysis provides several methods for non-smooth structures, such as curvelets [5, 6] and shearlets [21]. The methods are designed to approximate piecewise smooth functions on pieces with $C^2$ boundaries. As illustrated in Figure 3, each base of the curvelet is concentrated on an ellipse with different scales, locations, and angles in $I^2$. The ellipses covering the curve resolve the singularity. Each basis has a fan-shaped support with a different radius and angle in the frequency domain (see [6] for details).

We focus on curvelets as one of the most common methods. For brevity, we study the case with $D = 2$, which is of primary concern for curvelets. Curvelets can be extended to higher dimensions $D \geq 3$, and we can study the case in a similar manner.

As preparation, we define curvelets. In this analysis, we consider the domain of $f^*$ is $[-1,1]^D$ for technical simplification. Furthermore, we set $P_X$ as the uniform distribution on $[-1,1]^D$, as similar to the wavelet case. Let $\mu := (j, \ell, k)$ be a tuple of scale index $j = 0, 1, 2, \ldots$, rotation index $\ell = 0, 1, 2, \ldots, 2^j$, and location parameter $k \in \mathbb{Z}^2$. For each $\mu$, we define the parabolic scaling matrix

$$ D_j = \begin{pmatrix} 2^{2j} & 0 \\ 0 & 2^j \end{pmatrix}, $$

the rotation angle $\theta_{j,\ell} = 2\pi 2^{-j} \ell$, and a location $k = k_\delta = (k_1 \delta_1, k_2 \delta_2)$ with hyper-parameters $\delta_1$ and $\delta_2$, where $\delta_1, \delta_2 > 0$. Thereafter, we consider a curvelet $\gamma_\mu : \mathbb{R}^2 \rightarrow \mathbb{R}$ as

$$ \gamma_\mu(x) = 2^{j/2} \gamma(D_j R_{\theta_{j,\ell}} x - k_\delta). $$

In this case, $\gamma$ is defined by an inverse Fourier transform of a localized function in the Fourier domain. Figure 3 provides an illustration of its support and its rigorous definition is deferred to the appendix. According to [6], it is shown that $\{\gamma_\mu\}_{\mu \in \mathcal{L}}$ is a tight frame in $L^2(\mathbb{R}^2)$, where $\mathcal{L}$ is a set of $\mu$. Hence, we obtain the following formulation $f(x) = \sum_{\mu \in \mathcal{L}} w_\mu(f) \gamma_\mu(x)$, where $w_\mu(f) = \langle f, \gamma_\mu \rangle$. For estimation, we consider the truncation parameter $\tau \in \mathbb{N}$ and define an index subset as $\mathcal{L}_\tau := \{\mu \mid j \in [\tau]\} \subset \mathcal{L}$. Thereafter, similar to the wavelet case, a curvelet estimator which minimizing an empirical squared loss is written as

$$ \hat{f}^{\text{curve}}(x) = \sum_{\mu \in \mathcal{L}_\tau} \hat{w}_\mu \gamma_\mu(x), \text{ where } \hat{w}_\mu = \frac{1}{n} \sum_{i=1}^{n} Y_i \gamma_\mu(X_i). $$

In this case, $\tau$ is selected to minimize the generalization error of the curvelet estimator. We then obtain the following statement.

**Proposition 5** (Sub-Optimality of Curvelet Estimators). For $D = 2$ and any $\alpha, \beta \geq 2$, we obtain

$$ \sup_{f^* \in F_{\alpha,\beta,M}} \mathbb{E}_{f^*} \left[ \| \hat{f}^{\text{curve}} - f^* \|^2_{L^2(P_X)} \right] = \Omega \left( n^{-1/3} \right). $$

The result implies the sub-optimality of the curvelet; that is, the rate is slower than the minimax rate when $\beta > D/4 = 1/2$ and $\alpha > (D - 1)/2 = 1/2$. Similar to the wavelet estimator, the curvelet estimator does not adapt to the higher smoothness in the nonparametric regression setting.
5.4. Advantage of DNNs against the Other Methods. We summarize the sub-optimality of the other methods and compare them with DNNs. To this end, we provide a formal statement for comparing the estimator $\hat{f}^{DL}$ by DNNs and the other estimators, namely, $\hat{f}^{\text{lin}}, \hat{f}^{\text{wac}},$ and $\hat{f}^{\text{curve}}$. The following corollary is the second main result of this study:

**Corollary 2** (Advantage of DNNs). Fix $M \geq 2$. If $\alpha < 2\beta(D-1)/D$ holds with $\alpha, \beta \geq 1$ and $D \geq 2$, the estimator $\tilde{f} = \hat{f}^{\text{lin}}$ satisfies

$$\sup_{f^* \in \mathcal{F}_{\alpha,\beta,M}^\text{PS}} \mathbb{E}_{f^*} \left[ \| \tilde{f} - f^* \|_{L^2(P_X)}^2 \right] \gtrsim \sup_{f^* \in \mathcal{F}_{\alpha,\beta,M}^\text{PS}} \mathbb{E}_{f^*} \left[ \| \hat{f}^{DL} - f^* \|_{L^2(P_X)}^2 \right].$$

(7)

If $\beta > D/2$ and $\alpha > D - 1$ hold, (7) holds with $\tilde{f} = \hat{f}^{\text{wac}}$. If $\beta > D/4$ and $\alpha > (D-1)/2$ hold with $D = 2$, (7) holds with $\tilde{f} = \hat{f}^{\text{curve}}$.

These results are naturally derived from the discussion of the minimax optimal rate of DNN (Corollary 1 and Theorem 4), and the sub-optimality of the other methods (Propositions 3, 4, and 5). We can conclude that DNNs offer a theoretical advantage over the other methods in terms of estimation for functions with singularity; that is, with the parameter configurations in Corollary 2, there exist $f^* \in \mathcal{F}_{\alpha,\beta,M}^\text{PS}$, such that

$$\mathbb{E}_{f^*} \left[ \| \hat{f}^{DL} - f^* \|_{L^2(P_X)}^2 \right] < \mathbb{E}_{f^*} \left[ \| \tilde{f} - f^* \|_{L^2(P_X)}^2 \right]$$

holds for a sufficiently large $n$.

The parameter configurations introduced in Corollary 2 are classified into two cases, as illustrated in Figure 4. First, the configuration for the sub-optimality of the linear estimators appears when $\alpha$ is relatively smaller than $\beta$. With a small $\alpha$, the rate $O(n^{\alpha/(\alpha+D-1)})$ in the minimax optimal rate dominates the generalization error, because it is more difficult to estimate the boundary of pieces than to estimate the function within the pieces. In this case, the linear estimators lose optimality, because their generalization error is sensitive to $\alpha$. The second case is that in which both $\alpha$ and $\beta$ are above certain thresholds. It is thought that the approximation of the singularity by the orthogonal bases has not been adapted to the higher smoothness of $f^*$.

We add a further explanation for the limitations of the other estimators by describing the difficulty of shape fitting to the curve of singularities. The other estimators take the form of sums of (not necessarily orthogonal) basis functions, and each base has a (nearly) compact support. When the other methods approximate a function with the curve of singularities, they approximate the curve by fitting its support. For example, consider the curvelet of which the basis function has an ellipsoid-shaped (nearly) compact support. The ellipsoid is fitted to the curve of the singularity with rotation, as illustrated in Figure 5. The number of bases determines the magnitude of the error. However, when the curve has higher-order smoothness, the fitting in the domain cannot adapt to the curve with optimality.

DNNs do not use shape fitting to the curve for singularity, but represent the curve using a composition of functions, as mentioned in Section 4.4. Therefore, even if the curve has larger smoothness, DNNs can handle this without losing efficiency.
Figure 4. Parameter spaces of $(\alpha, \beta)$. The gray region [Left] The red dashed line is $\alpha = 2\beta(D-1)/D$. The red region presents $\{ (\alpha, \beta) \mid \alpha < 2\beta(D-1)/D \}$, which a set of parameter configurations such that (7) holds with $\bar{f} = \bar{f}^{\text{lin}}$. [Right] The blue region presents $\{ (\alpha, \beta) \mid \alpha > D-1, \beta > D/2 \}$, which a set of parameter configurations such that (7) holds with $\bar{f} = \bar{f}^{\text{wav}}$. The blue dashed line is its boundary.

Figure 5. [Left] An example of piecewise smooth functions $f^C$ such as the indicator function of a disk. [Right] The singularities of $f^C$ (black circle), and an illustration of approximation for the circle by a curvelet basis. The curvelet basis concentrates in the gray ellipses, that cannot have sufficient approximation ability when the curves are too smooth.

6. Conclusion

In this study, we have derived theoretical results that explain why DNNs outperform other methods. We considered the regression setting in the situation whereby the true function is singular on a smooth curve in its domain. We derived the convergence rates of the estimator obtained by DNNs and proved that the rates were almost optimal in the minimax sense. We explained that the optimality of DNNs originates from their composition structure, which can resolve singularity.
Furthermore, to analyze the advantage of DNNs, we investigated the sub-optimality of several other estimators, such as linear, wavelet, and curvelet estimators. We proved the sub-optimality of each estimator with certain parameter configurations. This advantage of DNNs comes from the fact that the shape of smooth curves for the singularity can be handled by DNNs, while the other methods fail to capture the shape efficiently. Theoretically, this is a vital step for analyzing the mechanism of DNNs.

Appendix A. Proof of Theorem 2

We start with the basic inequality \( \{5\} \). As preparation, we introduce additional notation. Given an empirical measure, the empirical (pseudo) norm of a random variable is defined by \( \|Y\|_n := (n^{-1} \sum_{i \in [n]} Y_i^2)^{1/2} \) and \( \|\xi\|_n := (n^{-1} \sum_{i \in [n]} \xi_i^2)^{1/2} \). By the definition of \( \hat{f}^{DL} \) in \( \{4\} \), we obtain the following inequality

\[
\|Y - \hat{f}^{DL}\|_n^2 \leq \|Y - f\|_n^2
\]

for all \( f \in \mathcal{G}(L, S, B) \). It follows from \( Y_i = f^*(X_i) + \xi_i \) that

\[
\|f^* + \xi - \hat{f}^{DL}\|_n^2 \leq \|f^* + \xi - f\|_n^2,
\]

then, simple calculation yields

\[
\|\hat{f}^{DL} - f^*\|_n^2 \leq \inf_{f \in \mathcal{G}(L, S, B)} \|f - f\|_n^2 + \frac{2}{n} \sum_{i \in [n]} \xi_i(\hat{f}^{DL}(X_i) - f(X_i)) =: \mathcal{B} + \mathcal{V}.
\]

In the first subsection, we bound \( \mathcal{B} \) by investigating an approximation power of DNNs. In the second subsection, we evaluate \( \mathcal{V} \) by evaluating a variance of the estimator. Afterward, we combine the results and derive an overall rate.

A.1. Approximate piecewise smooth functions by DNNs. In this subsection, we provide proof of Theorem 1. The result follows the following proposition:

**Proposition 6** (General Version of Theorem 1). Suppose Assumption 3 holds. Then, for any \( \varepsilon_1 \in (0, 1) \) and \( \varepsilon_2 \in (0, 1) \), there exists a tuple \( (L, S, B) \) such as

- \( L = C_{a, \beta, D, F}(\alpha + [\beta] + \log_2(1/\varepsilon_1) + \log_2(M/\varepsilon_2) + 1) \),
- \( S = C_{a, \beta, D, F}(M^{\varepsilon_1^{-D/\beta}}(\log_2(1/\varepsilon_1))^2 + (\varepsilon_2/M)^{-2(D-1)/\alpha}\log_2(M/\varepsilon_2)^2 + M(\log_2(M/\varepsilon_2))^2) \),
- \( B = C_{F, M, q}(\varepsilon_1 \wedge \varepsilon_2)^{-16} \wedge C_{a, \beta} \),

which satisfy

\[
\inf_{f \in \mathcal{G}(L, S, B)} \sup_{f^* \in \mathcal{F}^{PS}_{a, \beta, M}} \|f - f^*\|_{L^2} \leq \varepsilon_1 + \varepsilon_2.
\]

**Proof of Proposition 6** Fix \( f^* \in \mathcal{F}^{PS}_{a, \beta, M} \) such that \( f^* = \sum_{m \in [M]} f_m^* \otimes 1_{R_m} \) with \( f_m^* \in H_F^D(I^D) \) and \( \{R_m\}_{m \in [M]} \in \mathcal{R}_{a, M} \) for \( m \in [M] \). By Lemma 9, for any \( \delta_1 \in (0, 1) \), there exist a constant \( c_1 > 0 \) and functions \( g_{f, 1}, ..., g_{f, M} \in \mathcal{G}(C_{a, \beta, D, F}([\beta] + (\log_2(1/\delta_1) + 1), C_{a, \beta, D, F} \delta_1^{-D/\beta} (\log_2(1/\delta_1))^2, C_{F, q, \delta_1^{-16} \wedge C_{a, \beta}}) \) such that \( \|g_{f, m} - f_m^*\|_{L^2(R_m)} \leq \vol(R_m)\delta_1 \) for \( m \in [M] \). Similarly, by Lemma 10, we can find \( g_R \in \mathcal{G}(C_{a, \beta, D, F}([\alpha] + \log_2(1/\delta_2) + 1), C_{a, \beta, D, F} \delta_2^{-2(D-1)/\alpha} \log_2(1/\delta_2)^2 + 1 + M(\log_2(1/\delta_2))^2, C_{F, q, \delta_2^{-16} \wedge C_{a}}) \)
such that \( \|g_{R,m} - 1_{R_m^*}\|_{L^2} \leq \delta_2 \) for \( \delta_2 \in (0, 1) \). For approximation, we follow \([24]\) in the proof of Lemma \([6]\) as \( g_c \in \mathcal{G}(\log_2(1/\delta_1), C((\log_2(1/\delta_1))^2 + 1), C) \) which approximates a multiplication \( \|(x, x') \mapsto xx') - g_c(x, x')\|_{L^\infty([-F,F]^2)} \leq F^2 \delta_1 \).

With these components, we construct a function \( \hat{g} \in \mathcal{G}(C_{\alpha,\beta,D,F}([\alpha] + [\beta] + \log_2(1/\delta_1) + \log_2(1/\delta_1)^2 + 1), C_{F,q}(\delta_1^{-16} C_{\alpha} \wedge \delta_2^{-16} C_{\beta})) \) as

\[
\hat{g}(x) = \sum_{m \in [M]} g_c(g_{f,m}(x), g_{R,m}(x)), \tag{9}
\]

by setting between \( f^* \) and the combined DNN:

\[
\|f^* - \hat{g}\|_{L^2(I^D)}
\]

\[
= \left\| \sum_{m \in [M]} f^*_m 1_{R_m^*} - \sum_{m \in [M]} g_c(g_{f,m}(\cdot), g_{R,m}(\cdot)) \right\|_{L^2(I^D)}
\]

\[
\leq \sum_{m \in [M]} \|f^*_m \otimes 1_{R_m^*} - g_{f,m} \otimes g_{R,m}\|_{L^2(I^D)}
\]

\[
+ \sum_{m \in [M]} \|g_{f,m} \otimes g_{R,m} - g_c(g_{f,m}(\cdot), g_{R,m}(\cdot))\|_{L^2(I^D)}
\]

\[
\leq \sum_{m \in [M]} \|(f^*_m - g_{f,m}) \otimes 1_{R_m^*}\|_{L^2(I^D)} + \sum_{m \in [M]} \|g_{f,m} \otimes (1_{R_m^*} - g_{R,m})\|_{L^2(I^D)}
\]

\[
+ \sum_{m \in [M]} \|g_{f,m} \otimes g_{R,m} - g_c(g_{f,m}(\cdot), g_{R,m}(\cdot))\|_{L^2(I^D)}
\]

\[
=: \sum_{m \in [M]} B_{1,m} + \sum_{m \in [M]} B_{2,m} + \sum_{m \in [M]} B_{3,m}. \tag{10}
\]

We will bound \( B_{1,m}, B_{2,m} \) and \( B_{3,m} \) for \( m \in [M] \). About \( B_{1,m} \), the choice of \( g_{f,m} \) gives

\[
B_{1,m} = \|(f^*_m - g_{f,m}) \otimes 1_{R_m^*}\|_{L^2(I^D)} = \|f^*_m - g_{f,m}\|_{L^2(R_m^*)} \leq \text{vol}(R_m^*) \delta_1.
\]

About \( B_{2,m} \), similarly, the Hölder inequality yields

\[
B_{2,m} = \|g_{f,m} \otimes (1_{R_m^*} - g_{R,m})\|_{L^2(I^D)}
\]

\[
\leq \|g_{f,m}\|_{L^\infty(I^D)} \|1_{R_m^*} - g_{R,m}\|_{L^2(I^D)}
\]

\[
\leq (1 + \delta_2) \delta_2.
\]

About \( B_{3,m} \), since \( g_{f,m} \) and \( g_{R,m} \) is a bounded function by \( F \), we obtain

\[
B_{3,m} \leq \|(x, x') \mapsto xx') - g_c\|_{L^\infty([-F,F]^2)} \leq F^2 \delta_2.
\]

We combine the results about \( B_{1,m}, B_{2,m} \) and \( B_{3,m} \). Substituting the bounds for \([10]\) yields

\[
\|f^* - \hat{g}\|_{L^2(I^D)} \leq \sum_{m \in [M]} \{ \text{vol}(R_m^*) \delta_1 + \delta_2 + \delta_2^2 + F^2 \delta_2 \}
\]

\[
\leq \delta_1 + M \delta_2 + M \delta_2^2 + MF^2 \delta_2,
\]

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where the second inequality follows \( \sum_{m \in [M]} \text{vol}(R^*_m) = \text{vol}(I^D) = 1 \). Set \( \delta_1 = \varepsilon_1 \) and \( \delta_2 = C_F \varepsilon_2 / M \). Then we obtain
\[
\| f^* - \hat{g} \|_{L^2(I^D)} \leq \varepsilon_1 + \varepsilon_2 / 2 + \varepsilon_2^2 / 2 \leq \varepsilon_1 + \varepsilon_2.
\]
Adjusting the coefficients, we obtain the statement.

We are now ready to prove Theorem 1.

Proof of Theorem 1. We note that \( \mathcal{G}(L, S, B) \) has an inclusion property, namely, for \( L' \geq L, S' \geq S \) and \( B' \geq B \), we obtain
\[
\mathcal{G}(L', S', B') \supseteq \mathcal{G}(L, S, B).
\]
Applying Proposition 3 and adjusting the coefficients yield the statement.

A.2. Combining the Variance Bound. Here, we evaluate \( \mathcal{V} \) in (8) by the empirical process and its applications [18, 10, 30]. We then combine the result with Theorem 1, obtaining Theorem 2. Recall that \( F \) denotes an upper bound of \( g \in \mathcal{G}(L, S, B) \) by its definition.

Proof of Theorem 2. The proof starts with the basis inequality (8) and follows the following two steps: (i) apply the covering number bound for \( \mathcal{V} \) in (8), and (ii) combine the results with the approximation result (Theorem 1) on \( B \).

Step (i). Covering bound for the cross term. We substitute \( \hat{g} \) from (9) into \( f \) in \( \mathcal{V} \) and bound the expected term \( \mathbb{E}[\mathcal{V}] = \mathbb{E}[\frac{2}{n} \sum_{i \in [n]} \xi_i (\hat{f}^{DL}(X_i) - \hat{g}(X_i))] \) by the covering number of \( \mathcal{G}(L, S, B) \). We fix \( \delta \in (0, 1) \) and consider a covering set \( \{g_j\}_{j=1}^N \subset \mathcal{G}(L, S, B) \) for \( N = N(\delta, \mathcal{G}(L, S, B), \| \cdot \|_{L^\infty}) \), that is, for any \( g \in \mathcal{G}(L, S, B) \), there exists \( g_j \) with \( j \in [N] \) such that \( \| g - g_j \|_{L^\infty} \leq \delta \). For \( \hat{f}^{DL} \), let \( \hat{j} \in [N] \) be such that \( \| \hat{f}^{DL} - g_{\hat{j}} \|_{L^\infty} \leq \delta \) holds. Then, we bound the expected term as
\[
\mathbb{E} \left[ \frac{2}{n} \sum_{i \in [n]} \xi_i (\hat{f}^{DL}(X_i) - \hat{g}(X_i)) \right] \leq \mathbb{E} \left[ \frac{2}{n} \sum_{i \in [n]} \xi_i (\hat{f}^{DL}(X_i) - g_j(X_i)) \right] + \mathbb{E} \left[ \frac{2}{n} \sum_{i \in [n]} \xi_i (g_j(X_i) - \hat{g}(X_i)) \right] \leq 2\delta \mathbb{E} \left[ \frac{1}{n} \sum_{i \in [n]} |\xi_i| \right] + \mathbb{E} \left[ \frac{\| \hat{f}^{DL} - \hat{g} \|_n + \delta}{\| g_j - \hat{g} \|_n} \right] \frac{2}{n} \sum_{i \in [n]} \xi_i (g_j(X_i) - \hat{g}(X_i)) \leq 2\delta + \mathbb{E} \left[ \frac{\| \hat{f}^{DL} - \hat{g} \|_n + \delta}{\| g_j - \hat{g} \|_n} \right] \frac{2}{n} \sum_{i \in [n]} \xi_i (g_j(X_i) - \hat{g}(X_i)) \leq 2\delta + 2\mathbb{E} \left[ \frac{\| \hat{f}^{DL} - \hat{g} \|_n + \delta}{\sqrt{n}} \right] \frac{\sum_{i \in [n]} \xi_i (g_j(X_i) - \hat{g}(X_i))}{\sqrt{n} \| g_j - \hat{g} \|_n} \leq 2\delta + \frac{2(\mathbb{E}[\| \hat{f}^{DL} - \hat{g} \|_n^2]^{1/2} + \delta)}{\sqrt{n}} \mathbb{E}[\eta_{\hat{j}}^2]^{1/2},
\]
where the second inequality follows \( \|g_j - \hat{g}\|_n \leq \|\hat{f}_{DL} - \hat{g}\|_n + \delta \), and the last inequality follows the Cauchy-Schwartz inequality. With conditional on the observed covariates \( X_1, \ldots, X_n \), \( \eta_j \) follows a centered Gaussian distribution with its variance \( \sigma^2 \), hence \( \mathbb{E}[\eta_j^2] \leq \sigma^2 \mathbb{E}[\max_{j \in [N]} \eta_j^2] \leq 3 \log N + 1 \) by Lemma C.1 in [30]. Then, we have

\[
\mathbb{E}[|\mathcal{V}|] \leq 2\delta + \frac{2\sigma^2(\mathbb{E}[\|\hat{f}_{DL} - \hat{g}\|_n^2]^{1/2})}{\sqrt{n}}(3\log N(\delta, \mathcal{G}(L, S, B), \|\cdot\|_{L^x}) + 1)^{1/2}
\leq c_N \delta + \frac{2\sigma^2\mathbb{E}[\|\hat{f}_{DL} - \hat{g}\|_n^2]^{1/2}}{\sqrt{n}}(3\log N(\delta, \mathcal{G}(L, S, B), \|\cdot\|_{L^x}) + 1)^{1/2},
\]  

(11)

where \( c_N > 0 \) is a constant. The last inequality with \( c_N \) follows \( \mathcal{N}(\delta, \mathcal{G}(L, S, B), \|\cdot\|_{L^x})/\sqrt{n} = O(1) \).

**Step (ii). Combine the results.** We combine the results the bound for \( \mathcal{B} \) by Theorem [1] and \( |\mathbb{E}[\mathcal{V}]| \) in the Step (i), then evaluate \( \mathbb{E}[\|\hat{f}_{DL} - f^*\|_{L^2(P_X)}] \). Combining the bound (11) with (8) yields that

\[
\mathbb{E}[\|\hat{f}_{DL} - f^*\|_n^2] \leq \mathbb{E}[\mathcal{B}] + c_N \delta + \frac{2\sigma^2\mathbb{E}[\|\hat{f}_{DL} - \hat{g}\|_n^2]^{1/2}}{\sqrt{n}}(3\log N(\delta, \mathcal{G}(L, S, B), \|\cdot\|_{L^x}) + 1)^{1/2}.
\]

(12)

For any \( a, b, c \in \mathbb{R} \), \( a \leq b + c\sqrt{a} \) implies \( a^2 \leq c^2 + 2b \). Hence, we obtain

\[
\mathbb{E}[\|\hat{f}_{DL} - f^*\|_n^2] \leq 2\mathbb{E}[\mathcal{B}] + 2c_N \delta + \frac{12\sigma^2 \log N(\delta, \mathcal{G}(L, S, B), \|\cdot\|_{L^x}) + 4}{n}
\leq 2\mathbb{E}[\|\hat{g} - f^*\|_n^2] + 2c_N \delta + \frac{12\sigma^2 \log N(\delta, \mathcal{G}(L, S, B), \|\cdot\|_{L^x}) + 4}{n},
\]

(12)

by following \( \mathcal{B} \leq \|\hat{g} - f^*\|_n^2 \). Here, we apply the inequality (1) in the proof of Lemma 4 of [30] with \( \varepsilon = 1 \) and apply (12) as

\[
\mathbb{E}[\|\hat{f}_{DL} - f^*\|_{L^2(P_X)}^2] \leq 2 \left\{ \mathbb{E}[\|\hat{f}_{DL} - f^*\|_n^2] + \frac{2F^2}{n}(12\log N(\delta, \mathcal{G}(L, S, B), \|\cdot\|_{L^x}) + 70) + 26\delta F \right\}
\leq 4\mathbb{E}[\|\hat{g} - f^*\|_n^2] + (52F + 4c_N)\delta
\]

\[
+ \frac{24(\sigma^2 + 2F^2) \log N(\delta, \mathcal{G}(L, S, B), \|\cdot\|_{L^x}) + 8 + 280F^2}{n}.
\]

Substituting the covering bound in Lemma 4 yields

\[
\mathbb{E}[\|\hat{f}_{DL} - f^*\|_{L^2(P_X)}^2] \leq 4B_F\|\hat{g} - f^*\|_{L^2(P_D)}^2 + \frac{24(\sigma^2 + 2F^2)S}{n} \left\{ \left( \log(nLB^L(S + 1)^L) \vee 1 \right)^2 + 8 + 2c_N + 26F + 280F^2 \right\},
\]

(13)
by setting $\delta = 1/(2n)$. Here, $p_X$ is a density of $P_X$ and $\sup_{x \in D} p_X(x) \leq B_P$ is finite by the assumption. About the last inequality, we apply the following
\[
\mathbb{E} \left[ \| \tilde{g} - f^* \|_n^2 \right] = \int_{\mathcal{D}} (\tilde{g} - f^*)^2 d\lambda dP_X \leq \| \tilde{g} - f^* \|_{L_2(D)}^2 \sup_{x \in D} p_X(x)
\] (14)
by the Hölder’s inequality.

At last, we substitute the result of Theorem 1 and then adjust the coefficients. For $\varepsilon$ in the statement of Theorem 1 we set
\[
\varepsilon_1 = n^{-\beta/(2\beta+D)}, \quad \text{and} \quad \varepsilon_2 = M n^{-\alpha/(\alpha+D-1)},
\]
then, we rewrite the condition of Theorem 1 as
\[
L \geq C_{\alpha,\beta,D,F}(1 + [\alpha] + [\beta] + \log_2 n),
\]
\[
S \geq C_{\alpha,\beta,D,F,J}(M n^{D/(2\beta+D)} + n^{(D-1)/(\alpha+D-1)}) \log^2 n,
\]
and $B \geq C_{F,M,q} n^{C_{\alpha,\beta,D}}$. Then, substitute them into (13) and obtain
\[
\mathbb{E} \left[ \| \hat{f} - f^* \|_{L_2(\mathcal{D})}^2 \right] \leq 4B_P(n^{-\beta/(2\beta+D)} + n^{-\alpha/(\alpha+D-1)})
\]
\[
+ \frac{C_{\alpha,\beta,D,F,J}(\sigma^2 + \epsilon^2)}{n} (M n^{D/(2\beta+D)} + M n^{(D-1)/(\alpha+D-1)}) C_{\alpha,\beta,D,F} \log^2 n + \frac{C_F}{n}
\]
\[
\leq C_{\alpha,\beta,D,F,J} n \log^2(n) + \frac{C_F}{n}.
\]
Then, we adjust the coefficients and obtain the statement.

We provide a lemma which provides an upper bound for a covering number of $\mathcal{G}(L, S, B)$. Although similar results are well studied in several studies [2, 30], we cite the following result in [27], which is more suitable for our result.

**Lemma 4** (Covering Bound for $\mathcal{G}(L, S, B)$: Lemma 22 in [27]). For any $\varepsilon > 0$, we have
\[
\log N(\varepsilon, \mathcal{G}(L, S, B), \| \cdot \|_{L_2(D)}) \leq S \log \left( \frac{2 LB^L(S+1)^L}{\varepsilon} \right).
\]

**APPENDIX B. PROOF OF THEOREM 4**

We first provide a proof of Proposition 2 and then prove Theorem 4 by applying Theorem 3.

**Proof of Proposition 2.** We give an upper bound and lower bound separately.

(i) **Upper bound:** First, we bound the packing number by a covering number as
\[
\log \mathcal{M}(\varepsilon, H^\beta(I^D) \otimes \mathcal{I}_D, \| \cdot \|_{L_2(I^D)}) \leq \log N(\varepsilon/2, H^\beta(I^D) \otimes \mathcal{I}_D, \| \cdot \|_{L_2(I^D)}),
\]
by Section 2.2 in [34].

Further, we decompose the covering number of $H^\beta(I^D) \otimes \mathcal{I}_D$. Let $\{f_j\}_{j=1}^{N_1} \subset H^\beta(I^D)$ be a set of centers of covering points with $N_1 = N(\varepsilon/2, H^\beta(I^D), \| \cdot \|_{L_2(I^D)})$, and $\{t_{j}\}_{j=1}^{N_2} \subset \mathcal{I}_D$ be centers of $\mathcal{I}_D$ as $N_2 = N(\varepsilon/2, \mathcal{I}_D, \| \cdot \|_{L_2(I^D)})$. Then, we consider a set of points $\{f_j \otimes t_{j}\}_{j=1}^{N_1 N_2} \subset H^\beta(I^D) \otimes \mathcal{I}_D$ whose cardinality is $N_1 N_2$. Then, for any element $f \otimes 1_R \in H^\beta(I^D) \otimes \mathcal{I}_D$, there exists $f_j \in H^\alpha(I^D)$
and \( t_j \) such as \( \| f - f_j \|_{L^2(I^D)} \vee \| 1_R - t_j \|_{L^2(I^D)} \leq \varepsilon/2 \) due to the property of covering centers. Also, we can obtain
\[
\| f \otimes 1_R - f_j \otimes t_j' \|_{L^2(I^D)} \\
\leq \| f \otimes (1_R - t_j') \|_{L^2(I^D)} + \| (f - f_j) \otimes t_j' \|_{L^2(I^D)} \\
\leq \| f \|_{L^x(I^D)} \| 1_R - t_j' \|_{L^2(I^D)} + \| f - f_j \|_{L^2(I^D)} \| t_j' \|_{L^x(I^D)} \\
\leq \frac{(F + 1)\varepsilon}{2},
\]
where the second inequality follows the Hölder’s inequality. By this result, we find that the set \( \{ f_j \otimes t_j' \}_{j,j'=1}^{N_1,N_2} \) is a \((F + 1)\varepsilon/2\) covering set of \( H^\beta(I^D) \otimes I_\alpha \). Hence, we obtain
\[
\log \mathcal{M}(F + 1)\varepsilon/2, H^\beta(I^D) \otimes I_\alpha, \| \cdot \|_{L^2(I^D)} \\
\leq \log \mathcal{M}(\varepsilon/2, H^\beta(I^D), \| \cdot \|_{L^2(I^D)}) + \log \mathcal{M}(\varepsilon/2, I_\alpha, \| \cdot \|_{L^2(I^D)}).
\]

We will bound the two entropy terms for \( H^\beta(I^D) \) and \( I_\alpha \). For \( H^\beta(I^D) \), Theorem 8.4 in [9] provides
\[
\log \mathcal{N}(\varepsilon/2, H^\beta(I^D), \| \cdot \|_{L^2(I^D)}) \leq \log \mathcal{N}(\varepsilon/2, H^\beta(I^D), \| \cdot \|_{L^x(I^D)}) \\
= C_H(\varepsilon/2)^{-D/\beta},
\]
with a constant \( C_H > 0 \). About the covering number of \( I_\alpha \), we use the relation
\[
\| 1_R - 1_{R'} \|^2_{L^2} = \int_{I^D} (1_R(x) - 1_{R'}(x))^2dx = \int |1_R(x) - 1_{R'}(x)|dx \\
= \int_{I^D} (1_{R \cap R'}(x) - 1_{R \cap R'}(x))dx =: d_1(R, R'),
\]
for basic sets \( R, R' \subseteq I^D \), and \( d_1 \) is a difference distance with a Lebesgue measure for sets by [8]. Here, we consider a boundary fragment class \( \tilde{R}_\alpha \) defined by [8], which is a set of subset of \( I^D \) with \( \alpha \)-smooth boundaries. Since \( R \subseteq I^D \) such that \( 1_R \in I_\alpha \) is a basis piece, we can see \( R \in \tilde{R}_\alpha \). Hence, we obtain
\[
\log \mathcal{M}(\varepsilon/2, I_\alpha, \| \cdot \|_{L^2(I^D)}) \\
= \log \mathcal{N}(\varepsilon^2/16, \{ R \subseteq I^D \mid 1_R \in I_\alpha \}, d_1) \\
\leq \log \mathcal{N}(\varepsilon^2/16, \tilde{R}_\alpha, d_1) \\
= C_\lambda(\varepsilon/2)^{-2(D-1)/\alpha},
\]
with a constant \( C_\lambda > 0 \). Here, the last equality follows Theorem 3.1 in [8].

Combining (16) and (17) with (15), we obtain
\[
\log \mathcal{M}((F + 1)\varepsilon/2, H^\beta(I^D) \otimes I_\alpha, \| \cdot \|_{L^2(I^D)}) \\
\leq C_H(\varepsilon/2)^{-D/\beta} + C_\lambda(\varepsilon/2)^{-2(D-1)/\alpha}.
\]

Adjusting the coefficients yields the upper bound.

(ii) **Lower bound:** We provide the lower bound by evaluating the packing number \( \log \mathcal{M}(\varepsilon, H^\beta(I^D) \otimes I_\alpha, \| \cdot \|_{L^2(I^D)}) \) directory. Let \( 1(x) \) be a constant function \( 1(x) := 1, \forall x \in I^D \).
Here, we claim $\mathcal{I}_\alpha \subset H^\beta(I^D) \otimes \mathcal{I}_\alpha$, because $1 \in H^\beta(I^D)$ yields that $H^\beta(I^D) \otimes \mathcal{I}_\alpha \supset \{1\} \otimes \mathcal{I}_\alpha = \mathcal{I}_\alpha$. Hence, we have

$$\log \mathcal{M}(\varepsilon, H^\beta(I^D) \otimes \mathcal{I}_\alpha, \| \cdot \|_{L^2(I^D)}) \geq \log \mathcal{M}(\varepsilon, \mathcal{I}_\alpha, \| \cdot \|_{L^2(I^D)})$$

$$= C_\lambda \varepsilon^{-2(D-1)/\alpha}, \quad (18)$$

by Theorem 3.1 in [8]. Similarly, $1 = 1_{I^D} \in \mathcal{I}_\alpha$ yields $H^\beta(I^D) \subset H^\beta(I^D) \otimes \mathcal{I}_\alpha$. Hence, we achieve

$$\log \mathcal{M}(\varepsilon, H^\beta(I^D) \otimes \mathcal{I}_\alpha, \| \cdot \|_{L^2(I^D)}) \geq \log \mathcal{M}(\varepsilon, H^\beta(I^D), \| \cdot \|_{L^2(I^D)})$$

$$= C_H \varepsilon^{-D/\beta}, \quad (19)$$

by Theorem 8.4 in [9]. Combining (18) and (19), we obtain

$$\log \mathcal{M}(\varepsilon, H^\beta(I^D) \otimes \mathcal{I}_\alpha, \| \cdot \|_{L^2(I^D)}) \geq \max\{C_H \varepsilon^{-D/\beta}, C_\lambda \varepsilon^{-2(D-1)/\alpha}\}.$$

Adjusting the coefficients, we obtain the statement. \hfill \Box

Now, we are ready to prove Theorem 4.

**Proof of Theorem 4.** In this proof, we develop a lower bound of

$$\inf_{f} \sup_{f^* \in H^\beta(I^D) \otimes \mathcal{I}_\alpha} \mathbb{E}_{f^*} \left[ \| \tilde{f} - f^* \|_{L^2(P_X)}^2 \right],$$

where $\tilde{f}$ is any estimator. Then the statement is immediate because of the following inequality

$$\sup_{f^* \in F_{\alpha,\beta,M}^{PS}} \mathbb{E}_{f^*} \left[ \| \tilde{f} - f^* \|_{L^2(P_X)}^2 \right] \geq \sup_{f^* \in H^\beta(I^D) \otimes \mathcal{I}_\alpha} \mathbb{E}_{f^*} \left[ \| \tilde{f} - f^* \|_{L^2(P_X)}^2 \right] \quad (20)$$

due to $H^\beta(I^D) \otimes \mathcal{I}_\alpha \subset F_{\alpha,\beta,M}^{PS}$.

To develop the lower bound with $H^\beta(I^D) \otimes \mathcal{I}_\alpha$, we apply Theorem 3. Let $\varepsilon_n^*$ be a sequence for $n \in \mathbb{N}$ which satisfies

$$\left(\varepsilon_n^*\right)^2 = \log \mathcal{M}(\varepsilon_n^*, H^\beta(I^D) \otimes \mathcal{I}_\alpha, \| \cdot \|_{L^2(I^D)})/n.$$

From Proposition 2, we obtain

$$\left(\varepsilon_n^*\right)^2 = \Theta \left(\left(\varepsilon_n^*\right)^{-D/\beta} + \left(\varepsilon_n^*\right)^{-2(D-1)/\alpha}\right)/n.$$

Solving this equation gives

$$\left(\varepsilon_n^*\right)^2 = \Theta \left(n^{-2\beta/(2\beta+D)} + n^{-\alpha/(\alpha+D-1)}\right). \quad (21)$$

Application of Theorem 3 with (21) derives

$$\inf_{f} \sup_{f^* \in H^\beta(I^D) \otimes \mathcal{I}_\alpha} \mathbb{E}_{f^*} \left[ \| \tilde{f} - f^* \|_{L^2(P_X)}^2 \right] = \Theta \left(\varepsilon_n^2\right)$$

$$= \Theta \left(n^{-2\beta/(2\beta+D)} + n^{-\alpha/(\alpha+D-1)}\right),$$

which with (20) yields the claim. \hfill \Box
APPENDIX C. APPROXIMATION RESULTS OF DNNs WITH GENERAL ADMISSIBLE ACTIVATION

First, we show that the activation functions with Assumption 1 is suitable for DNNs to approximate polynomial functions, including an identity function.

Lemma 5. Suppose \( \eta \) satisfies the condition (i) in Assumption 2. Then, for \( \gamma \in \mathbb{N} \cup \{0\} \) with \( \gamma \leq N + 1 \), any \( \varepsilon > 0 \) and \( T > 0 \), there exists a tuple \((L, S, B)\) such that

- \( L = 2 \),
- \( S = 3(\gamma + 1) \),
- \( B = C_{\gamma, T} \varepsilon^{-C_{\gamma}} \),

and it satisfies

\[
\inf_{g \in G(L, S, B)} \| g - (x \mapsto x^{\gamma}) \|_{L^{\infty}([-T, T])} \leq \varepsilon.
\]

Proof of Lemma 5. Consider the following neural network with one layer:

\[
g_{sp}(x) := \sum_{j=1}^{\gamma+1} a_{2,j} \eta(a_{1,j}x + b_j). \tag{22}
\]

Since \( \eta \) is \( N \)-times continuously differentiable by the condition (i) in Assumption 2 we set \( b_j = x' \) for \( j = 1, \ldots, \gamma + 1 \) and consider the Taylor expansion of \( \eta \) around \( b_j = x' \). Then, for \( j = 1, \ldots, \gamma + 1 \), we obtain

\[
\eta(a_{1,j}x + b_j) = \sum_{k=0}^{\gamma+1} \frac{\partial^k \eta(x')a_{1,j}^k x^k}{k!} + \frac{\partial^{\gamma+1} \eta(x) a_{1,j}^{\gamma+1} x^{\gamma+1}}{(\gamma+1)!},
\]

with some \( \bar{x} \). We substitute it into (22) and obtain

\[
\sum_{j=1}^{\gamma+1} a_{2,j} \left( \sum_{k=0}^{\gamma} \frac{\partial^k \eta(x')a_{1,j}^k x^k}{k!} + \frac{\partial^{\gamma+1} \eta(x) a_{1,j}^{\gamma+1} x^{\gamma+1}}{(\gamma+1)!} \right)
\]

\[
= \sum_{k=0}^{\gamma} \frac{\partial^k \eta(x')x^k}{k!} \sum_{j=0}^{\gamma} a_{2,j+1}a_{1,j+1}^{k} + \sum_{j=1}^{\gamma+1} a_{2,j} \frac{\partial^{\gamma+1} \eta(x) a_{1,j}^{\gamma+1} x^{\gamma+1}}{(\gamma+1)!}. \tag{23}
\]

For each \( j' = 0, \ldots, \gamma \), we set \( a_{1,j'+1} = j'/\bar{a} \) with \( \bar{a} > 0 \) and \( a_{2,j'+1} = (-1)^{\gamma+j'} \bar{a} \gamma (j') / \partial^\gamma \eta(x') \). Note that \( \partial^\gamma \eta(x') > 0 \) holds by Assumption 1. Then, we obtain the following equality:

\[
\sum_{j'=0}^{\gamma} a_{2,j'+1}a_{1,j'+1}^{k} = \sum_{j'=0}^{\gamma} (-1)^{-\gamma+j'} \bar{a}^{\gamma-k} \left( \frac{j'}{j'} \right) \frac{j'^k}{\partial^\gamma \eta(x')}
\]

\[
= \frac{\bar{a}^{\gamma-k}}{(-1)^{\gamma} \partial^\gamma \eta(x')} \sum_{j'=0}^{\gamma} (-1)^{j'} \left( \frac{j'}{j'} \right) j'^k
\]

\[
= \begin{cases} 
\frac{\bar{a}^{\gamma-k}}{(-1)^{\gamma} \partial^\gamma \eta(x')} \gamma! (-1)^{\gamma}, & \text{if } k = \gamma \\
0 & \text{otherwise}, 
\end{cases}
\]

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where the last equality follows the Stirling number of the second kind (described in [11]). Substituting it for \(23\) yields
\[
\sum_{j=1}^{\gamma+1} a_{2,j} \eta(a_{1,j} x + b_j) = x^\gamma + \sum_{j=1}^{\gamma+1} \frac{(-1)^{-\gamma+j-1} \gamma+1 \eta(x)(j-1)^{\gamma+1} x^{\gamma+1}}{\gamma+1} (j-1) \frac{\gamma+1}{\gamma+1}
\]
\[
= x^\gamma + \frac{\gamma+1}{\gamma+1} \eta(x) \sum_{j=1}^{\gamma+1} (-1)^{-\gamma+j-1} (j-1)^{\gamma+1} (j-1) \frac{\gamma+1}{\gamma+1}.
\]

Regarding the second term, we obtain
\[
\left| \frac{\partial^{\gamma+1} \eta(x) x^{\gamma+1}}{\partial x^{\gamma+1}} \right| \sum_{j=1}^{\gamma+1} (-1)^{-\gamma+j-1} (j-1)^{\gamma+1} (j-1) \frac{\gamma+1}{\gamma+1} \leq \frac{T^{\gamma+1}}{\alpha c_n} \| \partial^{\gamma+1} \eta \|_{L^\infty([-B,B])} \| x^\gamma \|_{L^\infty((-T,T))} =: \frac{C_{T,\gamma,n}}{a}.
\]
As setting \(a = C_{T,\gamma,n}/\varepsilon\), we obtain the approximation with \(\varepsilon\)-error. From the result, we know that \(g_{s,p} \in \mathcal{G}(2,3(\gamma+1), C_{T,\gamma} \varepsilon^{-C_{\gamma}})\).

**Lemma 6.** Suppose \(\eta\) satisfies the condition (ii) in Assumption [1]. Then, for \(\gamma \in \mathbb{N} \cup \{0\}\) with \(\gamma \leq N + 1\), any \(\varepsilon > 0\) and \(T > 0\), there exists a tuple \((L, S, B)\) such that
- \(L = (\gamma+1)(\log_2(C_{T,\gamma}/\varepsilon)/2 + 1)\),
- \(S = C_{T,\gamma}((\log_2(1/\varepsilon))^2 + \log_2(1/\varepsilon))\),
- \(B = C_{T,\gamma} \varepsilon^{-C_{\gamma}}\),

and it satisfies
\[
\inf_{g \in \mathcal{G}(L,S,B)} \| g - (x \mapsto x^\gamma) \|_{L^\infty([-T,T])} \leq \varepsilon.
\]

**Proof of Lemma 6** As a preparation, we construct a saw-tooth function by [37] with our Assumption [1]. Let us define a teeth function \(g_w : [0, 1] \to [0, 1]\) by a difference of two \(\eta\) as
\[
g_w(x) := \frac{2c_2 + 2c_1}{c_2(c_2 - c_1)} \eta(x) - \frac{4}{c_2 - c_1} \eta(x - 1/2) - \frac{2\pi}{c_2 - c_1}
\]

\[
= \begin{cases} 
2x, & \text{if } x \in [0,1/2], \\
-2x + 2, & \text{if } x \in [1/2, 1].
\end{cases}
\]

Then, we consider the \(t\)-hold composition of \(g_w \in \mathcal{G}(2,6, c_w)\) with \(c_w > 0\) as \(g_t = g_w \circ \cdots \circ g_w \in \mathcal{G}(t+1, 3(t+1), c_w)\) which satisfies
\[
g_t(x) = \begin{cases} 
2^t(x - 2k 2^{-t}), & \text{if } x \in [2k2^{-t}, (2k+1)2^{-t}], k = 0, 1, \ldots, 2^{t-1} - 1 \\
-2^t(x - 2k 2^{-t}), & \text{if } x \in [(2k-1)2^{-t}, 2k 2^{-t}], k = 1, \ldots, 2^{t-1}.
\end{cases}
\]

Here, the domain \([0, 1]\) of \(g_t\) is divided into \(2^{t+1}\) sub-intervals.

Then, we approximate a quadratic function by a linear sum of \(g_t\). For \(m \in \mathbb{N}\), We define a function \(g_m : [0, 1] \to [0, 1]\) as
\[
g_m(x) := x - \sum_{t=1}^{m} \frac{g_t(x)}{2^t},
\]
and it satisfies \( \|g_m - (x \mapsto x^2)\|_{L^\infty([0,1])} \leq 2^{-2-2m} \) for \( g_m \in \mathcal{G}(m + 1, 3m^2/2 + 5m/2 + 1, c_m) \) with \( c_m > 0 \), by the similar way in Proposition 3 in [37].

Further, we approximate a multiplicative function by \( f_m \), intuitively, we represent a multiplication by a sum of a quadratic function as \( xx' = \{(x + x')^2 - |x|^2 - |x'|^2\}/2 \). To the aim, we define an absolute function \( g_a : [-1, 1] \to [0, 1] \) by DNNs as

\[
    g_a(x) := (\eta(x) - \eta(-x))/(c_2 + c_1) = |x|.
\]

Then, we define \( g_c : [-T, T] \times [-T, T] \to \mathbb{R} \) as

\[
    g_c(x, x') := \frac{T^2}{2} \left\{ g_m \circ g_a((x + x')/T) - g_m \circ g_a(x/T) - g_m \circ g_a(x'/T) \right\}.
\]

(24)

By the similar proof in Proposition 3 in [37], we obtain \( \|(x, x') \mapsto xx'\) \( - g_c(x, x')\|_{L^\infty([-T,T]^2)} \leq T^2 2^{-2m} \) with \( g_c \in \mathcal{G}(m + 1, (9m^2 + 15m)/2 + 10, c_c) \) with \( c_c > 0 \).

Finally, we approximate the polynomial function \( x^\gamma \) by an induction by \( g_c \). When \( \gamma = 1 \), we consider

\[
    g_{p,1}(x) := (c_2 + c_1)^{-1} (\eta(x) - \eta(-x)) = x,
\]

then obviously \( \|g_{p,1} - (x \mapsto x)\|_{L^\infty([−T,T])} = 0 \) holds with \( g_{p,1} \in \mathcal{G}(2, 3, c_{p,1}) \) with a constant \( c_{p,1} > 0 \).

Now, for the induction, assume that there exists a function by DNNs \( g_{p,\gamma-1} \in \mathcal{G}(\gamma(m + 1), c_{\gamma-1,T}, (9m^2 + 15m)/2 + 10, c_p) \) with constants \( c_p > 0 \) and \( C_{\gamma-1,T} \) depending \( \gamma - 1 \) and \( T \), and it satisfies \( \|g_{p,\gamma-1} - (x \mapsto x^{\gamma-1})\|_{L^\infty([-T,T])} \leq C_{\gamma-1,T} 2^{-2m} \) with \( C_{\gamma-1,T} > 0 \). Also, we set \( g_m \) as (24). Then, we consider the following approximation function by DNNs as

\[
    g_{p,\gamma}(x) := g_m(g_{p,\gamma-1}(x), g_{p,1}(x)).
\]

Then, we consider the following approximation error

\[
    \|g_{p,\gamma} - (x \mapsto x^{\gamma})\|_{L^\infty([-T,T])}
    = \|g_m(g_{p,\gamma-1}(\cdot), g_{p,1}(\cdot)) - (x \mapsto x^{\gamma-1}) \otimes (x \mapsto x)\|_{L^\infty([-T,T])}
    \leq \|g_m(g_{p,\gamma-1}(\cdot), g_{p,1}(\cdot)) - g_{p,\gamma-1} \otimes g_{p,1}\|_{L^\infty([-T,T]^2)}
    + \|g_{p,\gamma-1} \otimes g_{p,1} - (x \mapsto x^{\gamma-1}) \otimes g_{p,1}\|_{L^\infty([-T,T])}
    + \|(x \mapsto x^{\gamma-1}) \otimes (x \mapsto x)\|_{L^\infty([-T,T])}
    \leq 2T^2 2^{-2m} + 2T \|g_{p,\gamma-1} - (x \mapsto x^{\gamma-1})\|_{L^\infty([-T,T])} + 0
    \leq 2T^2 2^{-2m} + 2TC_{\gamma-1,T} 2^{-2m}
    = (2T^2 + 2TC_{\gamma-1,T}) 2^{-2m} =: C_{\gamma,T} 2^{-2m}.
\]

Then, we obtain the statement with the condition \( (ii) \) in Assumption [1].

We combine the result with the conditions \( (i) \) and \( (ii) \), and obtain the statement with \( \varepsilon = 2^{-2m} \).

\[
    \square
\]

\textbf{Lemma 7} (General version of Lemma [2]). \textit{Suppose \( \eta \) satisfies Assumption [4]. Then, for any \( \varepsilon \in (0, 1) \) and \( T > 0 \), we obtain}

\[
    \inf_{g \in \mathcal{G}(2, 6, C_{T,\eta})} \|g - I_{\{x \geq 0\}}\|_{L^2([-T,T])} \leq \varepsilon.
\]

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Proof of Lemma. First, we consider \( \eta \) that satisfies the condition (i) in Assumption 1. Without loss of generality, we set \( \bar{\sigma} = 1 \) and \( \xi = 0 \). We start with \( \eta \) with \( k = 0 \), where \( k \) is given in Assumption 1. Let us consider a shifted activation \( \eta(ax) \) with \( a > 0 \). Then, the difference between \( \eta(ax) \) and \( 1_{\{a \geq 0\}} \) is decomposed as

\[
|\eta(ax) - 1_{\{a \geq 0\}}| \leq \begin{cases} 
   c_\eta(a^{-q}x^{-q} \land 1), & \text{if } x > 0, \\
   c_\eta(a^{-q}|x|^{-q} \land 1), & \text{if } x < 0,
\end{cases}
\]

with an existing constant \( c_\eta > 0 \). The upper bound by 1 comes from the uniform bound by \( C_\eta \) in Assumption 1. Hence, the difference of them in terms of \( L^2(\mathbb{R}) \) norm is

\[
\|\eta(ax) - 1_{\{a \geq 0\}}\|_{L^2(\mathbb{R})} \leq \left( 2c_\eta \int_0^\infty (a^{-2q}x^{-2q} + 1)dx \right)^{1/2} \leq \left( \frac{2c_\eta}{a} + \frac{2c_\eta}{(2q - 1)a^{4q-1}} \right)^{1/2} .
\]

As we set \( a \geq (4c_\eta/\varepsilon^2) \vee (4c_\eta(2q - 1)/\varepsilon^2)q^{-1} \), we obtain the statement with \( G(2, 1, C_\eta \varepsilon^{-(2q-1)/2}) \).

We consider \( \eta \) with \( k = 1 \). With a scale parameters \( a \) and a shift parameters \( \delta/2 > 0 \), we consider a difference of two \( \eta \) with difference shift as \( g_s(x; a, \delta) = \eta(ax - \delta/2) - \eta(ax + \delta/2) \).

Let \( t \in (0, B) \) be a parameter for threshold. When \( x > t \), the property of \( \eta \) yields

\[
g_s(x; a, \delta) \in [\delta \pm 2c_\eta|ax - \delta/2|^{-q}].
\]

We set \( \delta = 1 \), hence we obtain

\[
|g_s(x; a, 1) - 1| \leq 2c_\eta|ax - 1/2|^{-q}, \quad (25)
\]

for \( x > t \). Similarly, when \( x < -t \), we have

\[
g_s(x; a, \delta) \in [0 \pm 2c_\eta|ax - \delta/2|^{-q}]. \quad (26)
\]

When \( x \in [-t, t] \), the bounded property of \( \eta \) yields

\[
g_s(x; a, \delta) \in [0 \pm C_\eta(2 + |ax - \delta/2| + |ax + \delta/2|)]. \quad (27)
\]

Combining the inequalities (25), (26) and (27) with \( \delta = 1 \), we bound the difference between \( \eta(ax - \delta/2) - \eta(ax + \delta/2) \) and \( 1_{\{a \geq 0\}} \) as

\[
\|
g_s(\cdot; a, 1) - 1_{\{a \geq 0\}}\|_{L^2([-B,B])}^2 \\
\leq \|
g_s(\cdot; a, 1)\|_{L^2([-B,-t])}^2 + \|
g_s(\cdot; a, 1) - 1_{\{a \geq 0\}}\|_{L^2([t,B])}^2 \\
+ \|
g_s(\cdot; a, 1) - 1_{\{a \geq 0\}}\|_{L^2([-t,0])}^2 \\
\leq 4c_\eta^2 \int_{[-B,-t]} |ax - 1/2|^{-2q}dx + 4c_\eta^2 \int_{[t,B]} |ax - 1/2|^{-2q}dx \\
+ C_\eta^2 \int_{[-t,0]} \{2 + |ax - 1/2| + |ax + 1/2|\}^2dx \\
=: T_{s,1} + T_{s,2} + T_{s,3}.
\]
About $T_{s,2}$, simple calculation yields

$$T_{s,2} \leq 4c_n^2(B-t)|at-1/2|^{-2q} \leq 4c_n^2B|at-1/2|^{-2q}.$$  

By the symmetric property, we can also obtain $T_{s,1} = 4c_n^2B(at-1/2)^{-2q}$. About $T_{s,3}$, the similar calculation yields

$$T_{s,3} \leq 8C_K^2t(1 + |at + 1/2|)^2 \leq 8C_K^2t(at + 3/2)^2.$$  

Combining the results of the terms, we bound the norm $\|g_\eta(\cdot; a, 1) - 1\{\cdot \leq 0\}\|_{L^2([-B,B])}^2$. Here, we set $t = a^{-3/4}$ and $a \geq 1/16$, then we obtain

$$\|g_\eta(\cdot; a, 1) - 1\{\cdot \geq 0\}\|_{L^2([-B,B])}^2 = 4c_n^2Ba^{-3q/4} + 8C_K^2a^{-3/4}(a^{1/4} + 3/2)^2$$

$$= 4c_n^2Ba^{-3q/4} + 8C_K^2(a^{-1/4} + 3a^{-1/2} + 9a^{-3/4}/4).$$

Then, we set $a = 16c_n^2B\varepsilon^{-8/3q} \vee 32C_K^2\varepsilon^{-8} \vee 96C_\beta^2\varepsilon^{-4} \vee 9\varepsilon^{-8/3} \vee 1/16$, then we obtain the statement, then we have $g_\eta \in G(2,6,C_B,q\varepsilon^{-1})$.

Second, we consider $\eta$ satisfies the condition (ii) in Assumption \[. We consider a sum of two $\eta(x) = c_1x + (c_2 - c_1)x_+$ with some scale change as

$$\eta(x) + \eta\left(-\frac{c_1}{c_2}x\right) = (c_1x + (c_2 - c_1)x_+) + \left(-c_1x + \left(c_1 - \frac{c_1^2}{c_2}\right)x_+\right)$$

$$= \left(c_2 - \frac{c_1^2}{c_2}\right)x_+ =: \eta_s(x : c_1, c_2).$$

Then, we consider a difference of two $\eta_s(x : c_1, c_2)$ with shift change by $\delta/2 > 0$ and scale change $a > 0$ as

$$\eta_d(x) = \eta_s(ax - \delta/2 : c_1, c_2) - \eta_s(ax + \delta/2 : c_1, c_2)$$

$$= \begin{cases} 
(c_2 - \frac{c_1^2}{c_2})\delta, & \text{if } x > \delta/2a, \\
(c_2 - \frac{c_1^2}{c_2})(ax - \delta/2), & \text{if } x \in [-\delta/2a, \delta/2a], \\
0, & \text{if } x < -\delta/2a.
\end{cases}$$

Here, we set $\delta = (c_2 - c_1^2/c_2)^{-1} < (c_2 - c_1)^{-1} < \infty$. Then, the $L^2([-B,B])$-distance between $g_d(x)$ and $1\{\cdot \geq 0\}$ is written as

$$\|g_d - 1\{\cdot \geq 0\}\|_{L^2([-B,B])} = \left(\int_{[-\delta/2a,\delta/2a]} \frac{|ax - \delta|}{\delta} dx \right)^{1/2} = \frac{\delta^{1/2}}{12^{1/2}a}.$$  

As we set $a = \delta^{1/2}/(12^{1/2}\varepsilon)$, we obtain the statement with $g_d \in G(2,6,C_B,q\varepsilon^{-1})$.

We combine the results with all the conditions and consider the largest functional set, and then we obtain the statement.  

\[ 

**Lemma 8** (General Version of Lemma \[). Suppose Assumption \[ holds with $N \geq \alpha \lor \beta$. For any non-empty measurable set $R \subset I^D$ and $\delta > 0$, a tuple $(L,S,B)$ such as

- $L = C_{\beta,D,F,J}(\beta) + \log_2(1/\delta) + 1$
- $S = C_{\beta,D,F,J}\delta^{-D/\beta}(\log(1/\delta))^2$
- $B = C_{\beta,D,F,J,q}\delta^{-16\alpha} - C_{\beta}$,
satisfies

$$\inf_{g \in G(L, S, B)} \sup_{f \in H^D_p(I^D)} \| g - f \|_{L^2(R)} \leq \text{vol}(R) \delta.$$

**Proof of Lemma** Before the central part of the proof, we provide some preparation. We divide the domain $I^D$ into several hypercubes. Let $\ell \in \mathbb{N}$ and consider a $D$-dimensional multi-index $\lambda \in \{1, 2, ..., \ell\}^D =: \Lambda$. For each $\lambda$, define a hypercube

$$I_\lambda := \prod_{d=1}^{D} \left[ \frac{\lambda_d - 1}{\ell}, \frac{\lambda_d}{\ell} \right]$$

By the definition, $I_\lambda$ is a $D$-dimensional hypercube whose side has a length $1/\ell$, and $\bigcup_{\lambda \in \Lambda} I_\lambda = I^D$. Also, the center of $I_\lambda$ is denoted by $x_\lambda$; i.e.,

$$x_\lambda := \left( \frac{\lambda_1 - 1/2}{\ell}, \frac{\lambda_2 - 1/2}{\ell}, ..., \frac{\lambda_D - 1/2}{\ell} \right) \in I^D$$

We provide a Taylor polynomial for a smooth function. Fix $\lambda \in \Lambda$ and $f \in H^D_p(I^D)$ arbitrary. Let $a \in \mathbb{N}^D$ be a multi-index. Then, we consider the Taylor expansion of $f$ in $I_\lambda$ as

$$f(x) = f(x_\lambda) + \sum_{a:|a|\leq|\beta|-1} \frac{\partial^a f(x_\lambda)}{a!} (x - x_\lambda)^a $$

$$+ \sum_{a:|a|=|\beta|} \frac{1}{a!} (x - x_\lambda)^a \int_0^1 (1 - t)^{|\beta|-1} \partial^a f(x_\lambda + t(x - x_\lambda)) dt $$

$$= f(x_\lambda) + \sum_{a:|a|\leq|\beta|-1} \frac{\partial^a f(x_\lambda)}{a!} (x - x_\lambda)^a $$

$$+ \sum_{a:|a|=|\beta|} \frac{1}{a!} (x - x_\lambda)^a \int_0^1 (1 - t)^{|\beta|-1} \partial^a f(x_\lambda) dt $$

$$+ \sum_{a:|a|=|\beta|} \frac{1}{a!} (x - x_\lambda)^a \int_0^1 (1 - t)^{|\beta|-1} \{ \partial^a f(x_\lambda + t(x - x_\lambda)) - \partial^a f(x_\lambda) \} dt $$

$$= f(x_\lambda) + \sum_{a:|a|\leq|\beta|} \frac{\partial^a f(x_\lambda)}{a!} (x - x_\lambda)^a $$

$$+ \sum_{a:|a|=|\beta|} \frac{1}{a!} (x - x_\lambda)^a \int_0^1 (1 - t)^{|\beta|-1} \{ \partial^a f(x_\lambda + t(x - x_\lambda)) - \partial^a f(x_\lambda) \} dt$$

where $a! = \prod_{d \in [D]} a_d!$, $f_{[\beta]-1}(x; x_\lambda)$ is the Taylor polynomial with an order $|\beta|$, and $R_\lambda(x)$ is the remainder. By the Hölder continuity and the bounded property of $\partial^a f(x)$, the remainder $R_\lambda(x)$ is bounded as

$$|R_\lambda(x)| \leq \sum_{a:|a|=|\beta|} \frac{F}{a!} |(x - x_\lambda)^a| \int_0^1 (1 - t)^{|\beta|-1} |t(x - x_\lambda)|^{|\beta|-|\beta|} dt$$
\[ \leq F \sum_{a:|a|=|\beta|} (a!)^{-1}|x - x_\lambda|^\beta \leq C_{D,\beta,F} \left( \frac{1}{\ell} \right)^\beta, \]

for \( x \in I_\lambda \). Here, \( C_{F,\beta} > 0 \) is a constant which depends on \( F \) and \( \beta \). The last inequality follows since \( \|x - x_\lambda\|_\infty \leq 1/\ell \) holds for any \( x \in I_\lambda \).

Now, we approximate the Taylor polynomial \( f_{[\beta]}(x; x_\lambda) \) by DNNs for each \( \lambda \in \Lambda \). By the binomial theorem, we can rewrite the Taylor polynomial with a multi-index \( b \in \mathbb{N}^D \) and \( x \in I_\lambda \) as

\[
f_{[\beta]}(x; x_\lambda) = \sum_{a:|a|\leq|\beta|} \frac{\partial^a f(x_\lambda)}{a!} \sum_{b\leq a} \binom{a}{b} (-x_\lambda)^{a-b}x^b.
\]

The last inequality follows from \( \|x_\lambda\|_\infty \leq 1 \) and \( \partial^a f(x_\lambda) \leq F \) by their definition, we obtain \( |c_b| \leq F \) for any \( b \). Then, for each \( d \in [D] \), we define a univariate function by DNNs \( g_{\lambda,d} \in \mathcal{G}(C_b, g_{\beta}(\log_2(2/\varepsilon) + 1), C_\beta(\log_2(1/\varepsilon))^2, C_b \varepsilon^{-C_b}) \) which satisfies \( \|(x \mapsto x^b) - g_{\lambda,d}\|_{L^\infty([-1/\varepsilon,1/\varepsilon])} \leq \varepsilon \) with any \( \varepsilon > 0 \) by following Lemma 3 or Lemma 6.

Also, we set \( g_{c,D} \in \mathcal{G}(C_{D,\beta}(\log_2(1/\varepsilon)), C_{D,\beta}(\log_2(1/\varepsilon))^2, C_c \) which approximate \( D \)-variate multiplication as Lemma 3 by substituting \( m = \log_2(1/\varepsilon)/2 \). With the functions, we consider the following difference

\[
\|(x \mapsto x^b) - g_{c,D}(g_{\lambda,1}(\cdot), \ldots, g_{\lambda,D}(\cdot))\|_{L^\infty([-1/\varepsilon,1/\varepsilon]^D)} \leq \ell^{-2}\varepsilon + C_{D,\beta}D\varepsilon^{-2}\varepsilon.
\]

We then define a function by DNNs as \( g_{\lambda}(x) := f(x_\lambda) + \sum_{b:|b|\leq|\beta|} c_b g_{c,D}(g_{\lambda,1}(x + x_\lambda,1), \ldots, g_{\lambda,D}(x + x_\lambda,D)) \in \mathcal{G}(C_{\beta,D}[\beta](\log_2(1/\varepsilon) + 1), C_{\beta,D}(\log_2(1/\varepsilon))^2, C_{\beta,D} \varepsilon^{-C_{\beta,D}}) \) with \( C_{\beta,D} > 0 \), which satisfies

\[
\|f - g_{\lambda}\|_{L^\infty(I_\lambda)} \leq \sum_{b:|b|\leq|\beta|} c_b \|(x \mapsto x^b) - g_{c,D}(g_{\lambda,1}(\cdot + x_\lambda,1), \ldots, g_{\lambda,D}(\cdot + x_\lambda,D))\|_{L^\infty(I_\lambda)} \\
+ \|R_{\lambda}\|_{L^\infty(I_\lambda)} \leq 2C_{\beta,D}\ell^{-2}\varepsilon + C_{D,\beta,F}\ell^{-\beta}, \tag{28}
\]

for any \( \lambda \in \Lambda \).

Finally, we approximate \( f \in H^\beta(I^D) \) on \( R \). For a preparation, we define an approximator for the indicator function \( \mathbf{1}_{I_\lambda} \) for \( \lambda \in \Lambda \). From Lemma 7, we define \( g_s \in \mathcal{G}(3, 11, C_{B,\beta} \varepsilon^{-8}) \) be an approximator for a step function \( \mathbf{1}_{\{\cdot \geq 0\}} \). Then, we define

\[
g_I(x) := (g_s(x + 1/2) + g_s(-x - 1/2) - 1),
\]

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which satisfies
\[
\|g_t - 1_{\{-1/2 \leq t \leq 1/2\}}\|_{L^2(\mathbb{R})} \\
\leq \|(g_t(\cdot + 1/2) + g_s(\cdot - 1/2) - 1) - (1_{\{\cdot \geq -1/2\}} + 1_{\{-1/2 \leq \cdot \leq 1/2\}} - 1)\|_{L^2(\mathbb{R})} \\
+ \|1_{\{-1/2 \leq \cdot \leq 1/2\}} - 1\|_{L^2(\mathbb{R})} \\
\leq \|g_s(\cdot + 1/2) - 1_{\{\cdot \geq -1/2\}}\|_{L^2(\mathbb{R})} + \|g_s(\cdot - 1/2) + 1_{\{-1/2 \leq \cdot \leq 1/2\}}\|_{L^2(\mathbb{R})} + 0 \\
\leq 2\varepsilon.
\]
Further, for \(\lambda \in \Lambda\) and \(x \in I^D\), we define \(g_{I,\lambda} \in \mathcal{G}(4 + (\log_2(1/\varepsilon)/2 + 1)(D - 1), 25D + (\log_2(1/\varepsilon)/2)^2 D, C_{B,\varepsilon}e^{-8})\) as
\[
g_{I,\lambda}(x) = g_{c,d}(g_t((x_1 - x_{\lambda,1})\ell), ..., g_t((x_D - x_{\lambda,D})\ell)),
\]
which is analogous to \(1_{I,\lambda}(x) = \Pi_{d \in [D]} 1_{\{x_{\lambda,d}-1/(2\ell) \leq x_d \leq x_{\lambda,d}+1/(2\ell)\}}(x)\). We bound the distance as
\[
\|1_{I,\lambda} - g_{I,\lambda}\|_{L^2(I^D)} \\
\leq \|\Pi_{d=1}^{D} 1_{\{x_{\lambda,d}-1/(2\ell) \leq x_d \leq x_{\lambda,d}+1/(2\ell)\}} - \Pi_{d=1}^{D} g_c((x_d - x_{\lambda,d})\ell)\|_{L^2(I^D)} \\
+ \|\Pi_{d=1}^{D} g_c((x_d - x_{\lambda,d})\ell) - g_s(g_c((x_1 - x_{\lambda,1})\ell), ..., g_c((x_D - x_{\lambda,D})\ell))\|_{L^2(I^D)} \\
\leq \sum_{d=1}^{D} \|1_{\{x_{\lambda,d}-1/(2\ell) \leq x_d \leq x_{\lambda,d}+1/(2\ell)\}} - g_c((x_d - x_{\lambda,d})\ell)\|_{L^2(I^D)} \\
\times \prod_{d' \neq d}^{D-1} 1_{\{x_{\lambda,d'}-1/(2\ell) \leq x_d \leq x_{\lambda,d'}+1/(2\ell)\}} \vee g_c((x_{d'} - x_{\lambda,d'})\ell))\|_{L^2(I^D)} + D\varepsilon \\
\leq \sum_{d=1}^{D} \|1_{\{x_{\lambda,d}-1/(2\ell) \leq x_d \leq x_{\lambda,d}+1/(2\ell)\}} - g_c((x_d - x_{\lambda,d})\ell)\|_{L^2(I^D)} + D\varepsilon \\
\leq D\varepsilon/\ell + D\varepsilon.
\] (29)
Here, the second last inequality follows a bounded property of the indicator functions and \(g_c\), and the Hölder’s inequality.

Finally, we unify the approximator on a set \(R \subset I^D\). Let us define \(\Lambda_R := \{\lambda : \text{vol}(R \cap I_\lambda) \neq 0\}\), and
\[
I_R := \bigcup_{\lambda \in \Lambda_R} I_\lambda.
\]
Now, we can find a constant \(C_\lambda\) such that we have
\[
|\text{vol}(R) - \text{vol}(I_R)| \leq \bigcup_{\lambda \in \Lambda \cap \partial R \cap I_\lambda \neq \emptyset} \text{vol}(I_\lambda) \leq C_{\lambda,f}\ell^{-1},
\] (30)
where \(\partial R\) is a boundary of \(R\). The second inequality holds since \(\partial R\) is a \((D - 1)\)-dimensional set in the sense of the box counting dimension. Then, we define an approximator \(g_f \in \mathcal{G}(C_{\beta,D}(\|\beta\| + \log_2(1/\varepsilon) + 1), C_{\beta,D}\ell^D((\log_2(1/\varepsilon))^2 + 1), C_{B,\varepsilon}e^{-8\lambda - C_{\beta}}\) as
\[
g_f(x) := \sum_{\lambda \in \Lambda_R} g_c(g_{\lambda}(x), g_{I,\lambda}(x)).
\]
Then, the error between \(g_f\) and \(f\) is decomposed as
\[
\|f - g_f\|_{L^2(\mathbb{R})} \\
\leq \|\sum_{\lambda \in \Lambda_R} 1_{I_\lambda} \otimes f - \sum_{\lambda \in \Lambda_R} g_s(g_{\lambda}(\cdot), g_{I,\lambda}(\cdot))\|_{L^2(I_R)}
\]
Then, we bound the difference as
\[
\|f - g\|_{L^2(R)} \leq \sum_{\lambda \in \Lambda} \|I_{I_\lambda} \otimes \mathbf{1} \mathbf{1} - g_{\lambda, \lambda} \|_{L^2(I^D)} + |\Lambda_R|2^\ell \varepsilon
\]
by the Hölder’s inequality and the result in (28), (29) and (30). We set \(\ell = \lceil \delta^{-1/\beta} \rceil\) and \(\varepsilon = \delta^2\) with \(\delta > 0\), hence we have
\[
\|f - g\|_{L^2(R)} \leq C_{\beta,D,F,J} \text{vol}(R)(\delta + \delta^{2+2/\beta} + \delta^{2+1/\beta}) + C_{D,F}(\delta^2 + \delta^{2+(D+1)/\beta}).
\]
Then, adjusting the coefficients as we can ignore the smaller order terms than \(\Theta(\delta^2)\) as \(\delta \to 0\), we obtain the statement.

**Lemma 9.** Suppose Assumption \(A\) holds. Then, for any \(m \in \mathbb{N}\), \(B > 0\), and \(D' \geq 2\), we obtain
\[
\inf_{g \in \mathcal{G}((m+1)(D'-1), h_c(m)(D'-1), c_m)} \|\mathbf{1} \mathbf{1} - g\|_{L^\infty([-B,B]^{D'})} \leq D'B^{2}2^{-2m},
\]
where \(h_c(m) := \frac{9m^2 + 15m}{2} + 10\).

**Proof of Lemma 9** Let \(g_c \in \mathcal{G}(m+1, h_c(m), c_c)\) from the proof of Lemma 6. We prove it by induction. When \(D' = 2\), the statement holds by the property of \(g_c\). Then, consider \(D' = D-1\) case with \(D\), and suppose that \(g_{c,D} \in \mathcal{G}((m+1)(D-2), h_c(m)(D-2), c_m)\) satisfies \(\|\mathbf{1} \mathbf{1} - g\|_{L^\infty([-B,B]^{D'})} \leq (D'-1)B^{2}2^{-2m}\). Then, we define \(g_{c,D+1} \in \mathcal{G}((m+1)(D+1), h_c(m)(D), c_m)\) such as
\[
g_{c,D} = g_{c,D-1}(x_1, ..., x_{D-1}, x_D).
\]
Then, we bound the difference as
\[
\|\mathbf{1} \mathbf{1} - g_{c,D}\|_{L^\infty([-B,B]^{D})} \leq B^{2}2^{-2m} + \|\mathbf{1} \mathbf{1} - g_{c,D-1}\|_{L^\infty([-B,B]^{D-1})} \leq B^{2}2^{-2m} + (D-1)B^{2}2^{-2m} = DB^{2}2^{-2m}.
\]
Then, by the induction, we obtain the statement for any \(D' \geq 2\).

**Lemma 10 (General Version of Lemma 3).** Suppose Assumption \(A\) holds with \(N > \alpha\). Then, for \(\{R_m\}_{m=1}^M \in \mathcal{R}_{\alpha,M}\) and any \(\varepsilon > 0\) and \(m' \in \mathbb{N}\), there exists \(f \in \mathcal{G}(C_{\alpha,D,F,J}(\alpha + \log_2(1/\varepsilon) + 1), C_{\alpha,D,F,J}(\varepsilon^{-2(\alpha-1)/\alpha}(\log_2(1/\varepsilon))^2 + M(\log_2(1/\varepsilon))^2 + 1), C_{F,J,0}(\varepsilon^{-10} - C\alpha)\) with a \(M\)-dimensional output \(f(x) = (f_1(x), ..., f_M(x))^T\) such that
\[
\|\mathbf{1} _{R_m} - f_m\|_{L^2(I)} \leq \varepsilon,
\]
and
\[ \|f_m\|_{L^\infty(I^D)} \leq 1 + \varepsilon, \]
for all \( m \in [M] \).

**Proof of Lemma 10.** We define a function by DNNs \( g_{h,j} \in \mathcal{G}((C_{\alpha,D,F}([\alpha] + \log_2(1/\delta) + 1), C_{\alpha,D,F}^{\delta-(D-1)/\alpha}(\log_2(1/\delta))^2, \mathbb{D}) \) such that \( \|h_j - g_{h,j}\|_{L^2(I^{D-1})} \leq \delta \) by Lemma 8 for \( \delta > 0 \). Also, we define \( g_{c,j} \in \mathcal{G}(\mathbb{D}) \) with \( m' \geq 1 \) as Lemma 9 and \( g_s \in \mathcal{G}(2,6, C_{F,q}^{\delta^-5}) \) such that \( \|g_s - 1_{\{1 > 0\}}\|_{L^2([-\delta, \delta])} \leq \delta \) as Lemma 7. Then, for \( m \in [M] \), we define a function \( g_{h,j} \in \mathcal{G}((C_{\alpha,D,F}([\alpha] + \log_2(1/\delta) + 1), C_{\alpha,D,F}^{\delta-(D-1)/\alpha}(\log_2(1/\delta))^2 + 1), C_{B,q}^{\delta^-16} \) to approximate \( 1_{\{x_j \leq h_j(x_j)\}} \) as
\[
g_{h,j}(x) = g_s(x_d - h_j(x_d)), \quad \text{and} \quad g_{h,j}(x) = g_s(x_d + h_j(x_d)).
\]
To approximate \( 1_{R_m}(x) = \prod_{j \in [J]} 1_{\{x_j \leq h_j(x_d)\}} \), we define \( g_{R,m} \in \mathcal{G}(\mathbb{D}) \) as \( g_{R,m} : [0,1]^D \to [0,1]^M \) as
\[
g_{R,m}(x) = g_{c,J}(g_{h,1}(x), \ldots, g_{h,J}(x)),
\]
and define \( g_R \in \mathcal{G}(\mathbb{D}) \) as \( g_R : [0,1]^D \to [0,1]^M \) as
\[
g_R(x) = (g_{R,1}(x), \ldots, g_{R,M}(x))\]
Then, its approximation error is bounded as
\[
\left\| 1_{R_m} - g_{R,m} \right\|_{L^2(I^D)} \\
\leq \left\| (x \mapsto \prod_{j \in [J]} 1_{\{x_j \leq h_j(x_d)\}}) - \prod_{j \in [J]} g_{h,j,\pm}(x) \right\|_{L^2(I^D)} + J\delta \\
\leq \sum_{j \in [J]} \left\| (x \mapsto 1_{\{x_j \leq h_j(x_d)\}} - g_{h,j,\pm}(x) \right\|_{L^2(I^D)} \\
\times \prod_{j \in [J]} \left\| (x \mapsto 1_{\{x_j \leq h_j(x_d)\}} - g_{h,j,\pm}(x) \right\|_{L^\infty(I^D)} \prod_{j \in [J]} \left\| g_{h,j,\pm} \right\|_{L^\infty(I^D)} + J\delta \\
\leq \sum_{j \in [J]} \left\| (x \mapsto 1_{\{x_j \leq h_j(x_d)\}} - g_{h,j,\pm}(x) \right\|_{L^2(I^D)} + J\delta \\
\leq \sum_{j \in [J]} \left\| (x \mapsto 1_{\{x_j \leq h_j(x_d)\}} - (x \mapsto 1_{\{x_j \leq g_{h,j}(x_d)\}}) \right\|_{L^2(I^D)} \\
+ \sum_{j \in [J]} \left\| (x \mapsto 1_{\{x_j \leq g_{h,j}(x_d)\}} - g_{h,j,\pm}(x) \right\|_{L^2(I^D)} + J\delta \\
=: \sum_{j \in [J]} T_{h,1,j} + \sum_{j \in [J]} T_{h,2,j} + J\delta,
\]
where \( \|g_{h,j,\pm}\|_{L^\infty(I^D)} \leq 1 \) is used in the last inequality.

We evaluate each of the two terms \( T_{h,1,j} \) and \( T_{h,2,j} \). As preparation, for sets \( \Omega, \Omega' \subset I^{D-1} \), we define \( \Omega \Delta \Omega' := (\Omega \cup \Omega') \setminus (\Omega \cap \Omega') \). For each \( j \in [J] \), we obtain
\[
T_{h,1,j} = \left\| (x \mapsto 1_{\{x_j \leq h_j(x_d)\}} - (x \mapsto 1_{\{x_j \leq g_{h,j}(x_d)\}}) \right\|_{L^2(I^D)}
\]

\[
= \lambda \left( \{ x \in I^D \mid x_{d_j} \leq h_j(x_{-d_j}) \} \Delta \{ x \in I^D \mid x_{d_j} \leq g_{h,j}(x_{-d_j}) \} \right)^{1/2}
\]
= \|h_j - g_{h,j}\|_{L^1(I^{D-1})}^{1/2} \leq \|h_j - g_{h,j}\|_{L^1(I^{D-1})} \leq \delta^{1/2},
\]
where the second last inequality follows the Cauchy-Schwartz inequality. About \( T_{h,2,j} \), we obtain
\[
T_{h,2,j} = \left\| (x \mapsto 1 \{ x_{d_j} \leq g_{h,j}(x_{-d_j}) \}) - g_{h,j},_+ \right\|_{L^2(I^D)}
\]
\[
\leq \left\| \mathbf{1}_{\{ > 0 \}} \circ (x \mapsto x_{d_j} - h_j(x_{-d_j})) - g_s \circ (x \mapsto x_{d_j} - g_{h,j}(x_{-d_j})) \right\|_{L^2(I^D)}
\]
\[
\leq CF \left\| \mathbf{1}_{\{ > 0 \}} - g_s \right\|_{L^1([-F,F])} \leq CF \left\| \mathbf{1}_{\{ > 0 \}} - g_s \right\|_{L^2([-F,F])} \leq CF \delta,
\]
by the setting of \( g_s \) and the second last inequality follows the Cauchy-Schwartz inequality.

Combining the results on \( T_{h,1,j} \) and \( T_{h,2,j} \), we obtain
\[
\left\| \mathbf{I}_{Rm} - g_{R,m} \right\|_{L^2(I^D)} \leq J(\delta^{1/2} + CF \delta + \delta).
\]
For the second inequality of the statement, we apply the following inequality:
\[
\left\| g_{R,m} \right\|_{L^\infty(I^D)} \leq \left\| g_{R,m} - (x \mapsto \Pi_{j \in J} \mathbf{1}_{\{ x_{d_j} \leq h_j(x_{-d_j}) \}}) \right\|_{L^\infty(I^D)}
\]
\[
+ \left\| (x \mapsto \Pi_{j \in J} \mathbf{1}_{\{ x_{d_j} \leq h_j(x_{-d_j}) \}}) \right\|_{L^\infty(I^D)}
\]
\[
\leq \left\| g_{\pi_{\cdot,J}} - (x \mapsto \Pi_{j \in J} x_j) \right\|_{L^\infty([0,1]^J)} + 1
\]
\[
\leq J \delta + 1,
\]
We set \( \varepsilon = CF J \delta^{1/2} \), we obtain the statement. \( \square \)

**APPENDIX D. PROOF OF PROPOSITION 3**

The sub-optimality is well studied by Section 6 in [19]. We slightly adapt the result to our setting, and obtain the following proof.

**Proof of Proposition 3** We divide this proof into the following five steps: (i) preparation, (ii) define a sub-class of functions, (iii) reparametrize a lower bound of errors, (iv) define a subset of parameters, and (v) combine all the results.

**Step (i). Preparation.** First, we decompose the distance \( \| f^* - \hat{f}_{\text{lin}} \|_{L^2(P_X)}^2 \). Let us define \( \Upsilon_i(\cdot) := \Upsilon_i(\cdot; X_1, \ldots, X_n) \). By the definition of linear estimators, we obtain
\[
\left\| f^* - \hat{f}_{\text{lin}} \right\|_{L^2(P_X)}^2 = \left\| f^* - \sum_{i=1}^n (f^*(X_i) + \xi_i) \Upsilon_i \right\|_{L^2(P_X)}^2
\]
\[
= \left\| f^* - \sum_{i=1}^n f^*(X_i) \Upsilon_i \right\|_{L^2(P_X)}^2 + \sum_{i=1}^n \xi_i \Upsilon_i \left\|_{L^2(P_X)}^2
\]
\[
+ 2 \left\langle f^* - \sum_{i=1}^n f^*(X_i) \Upsilon_i, \sum_{i=1}^n \xi_i \Upsilon_i \right\rangle_{L^2(P_X)}
\]
\[
=: T_1^{(L)} + T_2^{(L)} + T_3^{(L)},
\]
36
where $\langle f, f' \rangle_{L^2(P_X)} := \int f \otimes f' dP_X$ is an inner product with respect to $P_X$. Since $\xi_i$ is a noise variable which is independent to $m$ for following subset of $I$, we can simplify the expectations of the terms as

$$
E_{f^*}[T_3^{(L)}] = 2 \sum_{i=1}^{m} E_{f^*}[\xi_i] \left\langle f^* - \sum_{i=1}^{n} f^*(X_i) \mathcal{Y}_i, \mathcal{Y}_i \right\rangle_{L^2(P_X)} = 0,
$$

and

$$
E_{f^*}[T_2^{(L)}] = \sum_{i,i' = 1}^{n} E_{f^*}[\xi_i \xi_{i'}] \langle \mathcal{Y}_i, \mathcal{Y}_{i'} \rangle_{L^2(P_X)} = \sigma^2 \sum_{i=1}^{n} \| \mathcal{Y}_i \|^2_{L^2(P_X)}.
$$

Since $T_1^{(L)}$ is a deterministic term with fixed $X_1, \ldots, X_n$, we obtain

$$
E_{f^*} \left[ \left\| f^* - \hat{f}^{\text{lin}} \right\|^2_{L^2(P_X)} \right] = \left\| f^* - \sum_{i=1}^{n} f^*(X_i) \mathcal{Y}_i \right\|^2_{L^2(P_X)} + \sigma^2 \sum_{i=1}^{n} \| \mathcal{Y}_i \|^2_{L^2(P_X)}
\geq \left\| f^* - \sum_{i=1}^{n} f^*(X_i) \mathcal{Y}_i \right\|^2_{L^2(P_X)} + \sigma^2 \sum_{i=1}^{n} \| \mathcal{Y}_i \|^2_{L^2(P_X)}.
$$

(31)

Step (ii). Define a class of functions. We investigate a lower bound of the term $\sup_{f^* \in \mathcal{F}^{P \mathcal{S}}_{\alpha, \beta, M}} E_{f^*} \left[ \left\| f^* - \sum_{i=1}^{n} f^*(X_i) \mathcal{Y}_i \right\|^2 \right]$ by considering an explicit class of piecewise smooth functions by dividing the domain $I^D$. For $m = 1, \ldots, M - 1$, we will consider a smooth boundary function $B_m : I^{D - 1} \ni (x_1, \ldots, x_{D - 1}) \mapsto x_D \in I$, then define pieces

$$
R_m = \begin{cases} 
\{ x \in I^D \mid 0 \leq x_D < B_1(x_{-D}) \}, & \text{if } m = 1, \\
\{ x \in I^D \mid B_{m-1}(x_{-D}) \leq x_D < B_m(x_{-D}) \}, & \text{if } m = 2, \ldots, M - 1, \\
\{ x \in I^D \mid B_m(x_{-D}) \leq x_D \leq 1 \}, & \text{if } m = M.
\end{cases}
$$

An explicit form of $B_m$ is provided below. Let $N \in \mathbb{N}$ be a parameter, and consider a grid for $I^{D - 1}$ such that $q_j := ((j_d - 0.5)/N)_{d=1,\ldots,D-1}$ for $j \in \{1, \ldots, N\}^{D-1} =: J$. We also define another index set $J^+ := \{N + 1, \ldots, 2N\}^{D-1}$. Also, let $\phi \in H_1^0(\mathbb{R}^{D-1})$ be a function such that $\phi(x) = 0$ for $x \notin I^{D-1}$, and $\phi(x) = 1$ for $x \in [0.1, 0.9]^{D-1}$. Then, we define a boundary function for $j \in J \cup J^+$ as

$$
B_m(x_{-D}; j, r) = \begin{cases} 
\frac{m - 1}{M} + \frac{r}{MN^\alpha} \phi(N(x_{-D} - q_j)), & \text{if } j \in J, \\
\frac{m - 1}{M}, & \text{if } j \in J^+.
\end{cases}
$$

for $r \in \{ r' \in \mathbb{N} \mid 0 < r' < N^\alpha - 1 \} =: D_R$ and $m = 1, \ldots, M - 1$. Here, $\phi(N(x - q_j))$ is a smooth approximator for the indicator function of a hyper-cube with a center $q_j$, and $B_m$ is constructed by the approximated indicator functions. We also define a subset of $I^D$ by $B_m$ as Also, we define the following subset of $I^D$ as

$$
\hat{R}_{j,r,m} := \left\{ x \in I^D \mid \frac{m - 1}{M} \leq x_D < B_m(x_{-D}; j, r) \right\},
$$

for $m = 1, \ldots, M - 1$. Moreover, we define

$$
\hat{R}_m := \left\{ x \in I^D \mid \frac{m - 1}{M} \leq x_D < \frac{m}{M} \right\}.
$$

for $m = 1, \ldots, M$. Obviously, $\hat{R}_{j,r,m} \subset \hat{R}_m$ for any $j, r$, and $m$. Figure 6 provides its illustration.
Figure 6. Illustration of $I^D$ with $D = 2$ case. The red curve denotes $B_m(x_D; j_m, r)$. Also, $\tilde{R}_m$ (gray region) and $\tilde{R}_{j_m, r, m}$ (red region) are illustrated.

We provide a specific functional form characterized by $B_m(\cdot; j, r)$ with $r \in D_R$ and $j \in J \cup J^+$ for each $m = 1, \ldots, M - 1$. Let $j := (j_1, \ldots, j_{M-1}) \in (J \cup J^+)^{M-1}$, and $c_m$ be a fixed coefficient for $m = 1, \ldots, M - 1$ such that $c_{m+1} - c_m = c > 0$ holds. For $r \in D_R$ and $j \in (J \cup J^+)^{M-1}$, we define the following function

$$\tilde{f}(x; r, j) := \sum_{m=1}^{M-1} c_m I_{\tilde{R}_{j_m, r, m}}(x).$$

$\tilde{f} \in F_{a, \beta, M}^{PS}$ holds by its construction.

**Step (iii). Reparametrize a lower bound by the parameters of $B_m$.** We develop a lower bound of the minimax risk by parameters $r, j, m$ of the boundary function $B_m$, with fixed $c_1, \ldots, c_M$ and $N$. Now, we provide a lower bound of the minimax risk as

$$\sup_{f^* \in F_{a, \beta, M}} \mathbb{E}_{f^*} \left[ \left\| f^* - \tilde{f}^{\text{lin}} \right\|_{L^2(P_X)}^2 \right]$$

$$= \sup_{f^* \in F_{a, \beta, M}} \mathbb{E}_{f^*} \left[ \left\| f^* - \sum_{i=1}^{n} f^*(X_i) \Upsilon_i \right\|_{L^2(P_X)}^2 \right]$$

$$\geq \sup_{r \in D_R} \sup_{j \in (J \cup J^+)^{M-1}} \mathbb{E}_{\tilde{f}} \left[ \left\| \tilde{f} - \sum_{i=1}^{n} \tilde{f}(X_i; r, j) \Upsilon_i \right\|_{L^2(P_X)}^2 \right]$$

$$\geq \frac{1}{|D_R|(|J| + |J^+|)^{M-1}}$$

$$\times \sum_{r \in D_R} \sum_{j \in (J \cup J^+)^{M-1}} \mathbb{E}_{\tilde{f}} \left[ \left\| \tilde{f}(\cdot; r, j) - \sum_{i=1}^{n} \tilde{f}(X_i; r, j) \Upsilon_i \right\|_{L^2(\tilde{R}_{j, r, m})}^2 \right].$$

$$\geq \frac{1}{|D_R|(|J| + |J^+|)^{M-1}}$$

(32)
To derive the second inequality, we consider all possible configurations. The last inequality holds since \( P_X \) has a finite and positive density by its definition. Also, for any \( r \in D_R, \tilde{R}_{j,r,m} \cap \tilde{R}_{j',r,m} = \emptyset \) for \( j \neq j' \in \mathcal{J} \), and \( \cup_{j \in \mathcal{J}} \tilde{R}_{j,r,m} \subset \tilde{R}_m \) yield the last inequality.

Afterwards, we provide a lower bound of \( \| \tilde{f}(\cdot; r, j) - \sum_{i=1}^{n} \tilde{f}(X_i; r, j) \mathcal{Y}_i \|_{L^2(\tilde{R}_{j,r,m})}^2 \). For \( m = 1, \ldots, M-1 \) and \( r \in D_R \), we can achieve

\[
\begin{align*}
&\sum_{j_m \in \mathcal{J} \cup \mathcal{J}^+} \left\| \tilde{f}(\cdot; r, j) - \sum_{i=1}^{n} \tilde{f}(X_i; r, j) \mathcal{Y}_i \right\|_{L^2(\tilde{R}_{j,r,m})}^2 \\
&= \sum_{j_m \in \mathcal{J}} \int_{\tilde{R}_{j,r,m}} \left( c_m + c_1 {1}_{x_D \geq B_m (x_{-j_m}, r)}(x) \right)^2 \\
&\quad - \sum_{i=1}^{n} \left( c_m + c_1 {1}_{x_D \geq B_m (x_{-j_m}, r)}(X_i) \right)^2 \\
&\quad + \left( c_m + c_1 {1}_{x_D \geq m+1}(x) - \sum_{i=1}^{n} (c_m + c_1 {1}_{x_D \geq m+1}(X_i)) \mathcal{Y}_i(x) \right)^2 dx \\
&\geq \sum_{j_m \in \mathcal{J}} \frac{c^2}{2} \int_{\tilde{R}_{j,r,m}} \left( \sum_{i: X_i \in \tilde{R}_{j_m, r, m}} \mathcal{Y}_i(x) - {1}_{\tilde{R}_{j_m, r, m}}(x) \right)^2 dx \\
&\geq |\mathcal{J}|c^2 \left\| \sum_{i: X_i \in \tilde{R}_{j, r, m}} \mathcal{Y}_i - 1 \right\|_{L^2(\tilde{R}_{j, r, m})}^2.
\end{align*}
\]

The second last inequality follows \( x^2 + y^2 \geq (x - y)^2/2 \). Substituting it into (32) yield

\[
\sup_{f^* \in \mathcal{F}_{\alpha, \beta, M}} \mathbb{E}_{f^*} \left[ \| f^* - \tilde{f}^{\text{lin}} \|_{L^2(P_X)}^2 \right] \geq \frac{c^2}{|D_R|2^{M-1}} \sum_{r \in D_R} \sum_{m=1}^{M-1} \sum_{j \in \mathcal{J}} \mathbb{E}_{f^*} \left[ \left\| \sum_{i: X_i \in \tilde{R}_{j, r, m}} \mathcal{Y}_i - 1 \right\|_{L^2(\tilde{R}_{j, r, m})}^2 \right].
\] (33)

**Step (iv). Define subsets of parameters.** Here, we will consider suitable subsets \( \tilde{D}_R \subset D_R \) and \( \tilde{\mathcal{J}} \subset \mathcal{J} \) for a tight lower bound. Let us define \( n_m := |\{ X_i \in \tilde{R}_m \}| \) and \( \tau_m^2 := \sum_{i: X_i \in \tilde{R}_m} \| \mathcal{Y}_i \|_{L^2(\tilde{R}_m)}^2 \) for each \( m \in [M] \). For \( m \in [M] \), let \( S_{m, r} := \{ x \in I^D \mid x_D \in [m/M + r/N^\alpha, m/M + (r + 1)/N^\alpha) \} \), for \( r = 0, \ldots, N^\alpha - 1 \). Then, let \( \tilde{D}_R \) be a set of integers which satisfies

\[
|\{ i : X_i \in S_{m, r} \}| \leq \frac{cn_m}{N^\alpha}, \quad \text{and} \quad \sum_{i: X_i \in S_{m, r}} \| \mathcal{Y}_i \|_{L^2(I^D)} \leq \frac{c' \tau_m^2}{N^\alpha},
\]

where \( c, c' > 2 \) are coefficients. We can claim that at least \( (1 - 1/c)N^\alpha \) and \( (1 - 1/c')N^\alpha \) integers from \( D_R \) satisfy each of the conditions, because the rest \( N^\alpha/c \) and \( N^\alpha/c' \) integers from \( D_R \) should
sum to \( N^\alpha \). Then, at least \((1 - 1/c)N^\alpha + (1 - 1/c')N^\alpha - N^\alpha = (1 - 1/c - 1/c')N^\alpha\) integers from \( D_R \) satisfies the both conditions simultaneously. We set \( \hat{D}_R \) as a set of such the integers, then \( |\hat{D}_R| \geq (1 - 1/c - 1/c')N^\alpha \geq N^\alpha \) holds since \( c, c' > 2 \).

Further, for each \( r \in \hat{D}_R \), we consider the subset \( \tilde{J} \subset J \). Similarly, we consider \( \tilde{J} \) is a set of indexes \( j \in J \) such as

\[
|\{i : X_i \in \hat{R}_{j,r,m}\}| \leq \frac{c''n_m}{N^\alpha N^{D-1}}, \quad \text{and} \quad \sum_{i : X_i \in \hat{R}_{j,r,m}} \|\gamma_i\|_{L^2(I_D)} \leq \frac{c'''r_m^2}{N^\alpha N^{D-1}},
\]

with coefficients \( c'', c''' > 2 \). Repeating the argument for \( \hat{D}_R \), we can claim that there exist at least \((1 - 1/c'' - 1/c''')N^\alpha N^{D-1}\) indexes which satisfy the both conditions simultaneously, then we have \( \tilde{J} \geq (1 - 1/c'' - 1/c''')N^\alpha N^{D-1} \geq N^{\alpha + D - 1} \) since \( c'', c''' > 2 \).

**Step (v). Combining all the results.** With the subsets \( \hat{D}_R \) and \( \tilde{J} \), we derive a lower bound of the norm \( \|\sum_{i : X_i \in \hat{R}_{j,r,m}} \gamma_i - 1\|_{L^2(\hat{R}_{j,r,m})} \). For \( m \in [M] \), \( r \in \hat{D}_R \), and \( j \in \tilde{J} \), we obtain

\[
\left\| \sum_{i : X_i \in \hat{R}_{j,r,m}} \gamma_i - 1 \right\|_{L^2(\hat{R}_{j,r,m})} \geq \left\| 1 \right\|_{L^2(\hat{R}_{j,r,m})} - \left\| \sum_{i : X_i \in \hat{R}_{j,r,m}} \gamma_i \right\|_{L^2(\hat{R}_{j,r,m})} = \text{vol}(\hat{R}_{j,r,m})^{1/2} - |\{i : X_i \in \hat{R}_{j,r,m}\}|^{1/2} \left( \int_{\hat{R}_{j,r,m}} \sum_{i : X_i \in \hat{R}_{j,r,m}} \gamma_i(x)^2 dx \right)^{1/2} \geq \left( \frac{1}{MN^{D-1}N^\alpha} \right)^{1/2} - \frac{n_m}{N^{D-1}N^\alpha}.
\]

Then, we substitute the result into (33). Here, note that \( n_m \leq n \). Also, by (31), we have \( \sum_{m \in [M]} \tau_m^2 \leq \sigma^{-2} \| f^* - \hat{f} \|_{L^2(X)}^2 \) and its integrable conditions, \( \sum_{m \in [M]} \tau_m^2 = O(1) \) with probability at least \( 1/2 \). Then, we continue the inequality as

\[
\sup_{f^* \in \mathcal{F}_{a,\beta,M}} \mathbb{E}_{f^*} \left[ \| f^* - \hat{f} \|_{L^2(X)}^2 \right] \geq \frac{c^2}{|D_R|2^{M-1}} \left( \sum_{m = 2}^{M} \sum_{r \in D_R} \sum_{j \in \tilde{J}} \sum_{i : X_i \in \hat{R}_{j,r,m}} \mathbb{E}_{f^*} \left[ \left\| \sum_{i : X_i \in \hat{R}_{j,r,m}} \gamma_i - 1 \right\|_{L^2(\hat{R}_{j,r,m})}^2 \right] \right) \geq \frac{N^{D-1}}{2} \sum_{m = 2}^{M} \left( \frac{1}{MN^{D-1}N^\alpha} \right)^{1/2} - \frac{n_m}{N^{D-1}N^\alpha} \geq \left( \frac{1}{MN^{D-1}N^\alpha} \right)^{1/2} - \frac{n_m}{N^{D-1}N^\alpha} \geq \left( \frac{1}{MN^{D-1}N^\alpha} \right)^{1/2} - \frac{n_m}{N^{D-1}N^\alpha}.
\]

We substitute \( N = [n^{1/(2\alpha + D - 1)}] \) and ignore negligible terms, then obtain the statement. \( \square \)
Appendix E. Sub-optimality of Wavelet Estimators

Proof of Proposition 4. As preparation, we derive a lower bound of the minimax risk. Note that $P_X$ is a uniform distribution on $I^D$, we have $\|f\|_{L^2(P_X)} = \|f\|_{L^2}$ for any measurable $f : I^D \to \mathbb{R}$. By the definition of $\hat{f}^\text{wav}$ and the Parseval’s equality, we obtain

$$\|f^* - \hat{f}^\text{wav}\|_{L^2(P_X)}^2 = \sum_{(\kappa_1, \ldots, \kappa_D) \in \mathcal{H}^D_\tau} (\hat{w}_{\kappa_1, \ldots, \kappa_D} - w_{\kappa_1, \ldots, \kappa_D}(f^*))^2 + \sum_{(\kappa_1, \ldots, \kappa_D) \in \mathcal{H}^D \setminus \mathcal{H}^D_\tau} w_{\kappa_1, \ldots, \kappa_D}(f^*)^2. \quad (34)$$

For the first term in the right hand side, we evaluate the expectation of $(\hat{w}_{\kappa_1, \ldots, \kappa_D} - w_{\kappa_1, \ldots, \kappa_D}(f^*))^2$. Since $\mathbb{E}_f[\hat{w}_{\kappa_1, \ldots, \kappa_D}] = \langle f^*, \Phi_{\kappa_1, \ldots, \kappa_D} \rangle = w_{\kappa_1, \ldots, \kappa_D}(f^*)$, we rewrite the expectation as

$$\mathbb{E}_f[\langle \hat{w}_{\kappa_1, \ldots, \kappa_D} - w_{\kappa_1, \ldots, \kappa_D}(f^*) \rangle^2] = \text{Var} \left( \frac{1}{n} \sum_{i \in [n]} Y_i \Phi_{\kappa_1, \ldots, \kappa_D}(X_i) \right) = \frac{1}{n} \text{Var}_{f^*}((f^*(X_i) + \xi_i)\Phi_{\kappa_1, \ldots, \kappa_D}(X_i)) = \frac{1}{n} \mathbb{E}_X[\text{Var}_\xi((f^*(X_i) + \xi_i)\Phi_{\kappa_1, \ldots, \kappa_D}(X_i) | X_i)] 
\geq \frac{\sigma^2}{n} \mathbb{E}_X[\Phi_{\kappa_1, \ldots, \kappa_D}(X_i)^2] = \frac{\sigma^2}{n},$$

where the third equality follows the iterated law of expectation, and the last equality follows $\Phi_{\kappa_1, \ldots, \kappa_D}$ is an orthonormal function. Substituting the result into (34) yields

$$\mathbb{E}_f[\|f^* - \hat{f}^\text{wav}\|_{L^2(P_X)}^2] \geq \frac{\sigma^2 |\mathcal{H}_\tau|^D}{n} + \sum_{(\kappa_1, \ldots, \kappa_D) \in \mathcal{H}^D \setminus \mathcal{H}^D_\tau} w_{\kappa_1, \ldots, \kappa_D}(f^*)^2. \quad (35)$$

We will prove the statement by providing a specific configuration of $f^*$. Let $\hat{R} \subset I^D$ be a hyper-rectangle as

$$\hat{R} := \left\{ x \in I^D \mid 0 \leq x_d \leq \frac{2}{3}, d \in [D] \right\}.$$ 

Then, we define $f^* \in \mathcal{F}_{\alpha, \beta, M}^{PS}$ as

$$f^* := \mathbf{1}_{\hat{R}}.$$ 

Since $\hat{R}$ is regarded as $\cap_{d \in [D]} \{ x \in I^D \mid x_d \leq 2/3 \}$, $\mathbf{1}_{\hat{R}}$ is a piecewise smooth function for any $M \geq 2, \alpha \geq 1$ and $\beta \geq 1$.

Then, we define the coefficient $w_{\kappa_1, \ldots, \kappa_D}(f^*)$. Fix $j_d \in \{-1, 0, 1, 2, \ldots\}$ for all $d \in [D]$. Since $\mathbf{1}_{\hat{R}}(x) = \prod_{d \in [D]} \mathbf{1}_{\{ \leq 2/3 \}}(x_d)$, we can decompose the coefficient as

$$\langle f^*, \Phi_{\kappa_1, \ldots, \kappa_D} \rangle = \int_{I^D} \prod_{d \in [D]} \mathbf{1}_{\{ \leq 2/3 \}}(x_d) \prod_{d \in [D]} \phi_{k_d}(x_d) d(x_1, \ldots, x_D).$$
where with $\xi$, we consider $f$. Let $c_d$ be a constant such that $2/3 \in [k_d, k_d + 2^{-j_d}]$. By the result of integration, we can rewrite $w_{\kappa_1, \ldots, \kappa_D}$ as

$$w_{\kappa_1, \ldots, \kappa_D} \geq \prod_{d \in [D]} c 2^{-j_d/2} 1_{[k_d, k_d + 2^{-j_d}]}.$$ 

Finally, we will select the truncation parameter $\tau$ for $H_\tau$ and update the inequality (35). By its definition, we obtain $|H_\tau| = \sum_{t=-1}^{T} 2^t = 2^{t+1}$. Also, about the second term of (35), we have

$$\sum_{(\kappa_1, \ldots, \kappa_D) \in H \times D \setminus H_\tau D} w_{\kappa_1, \ldots, \kappa_D} (f^\ast)^2 \geq \sum_{j_1 > \tau} \sum_{j_2 > \tau} \cdots \sum_{j_D > \tau} \prod_{d \in [D]} c^2 2^{-j_d} \geq c^{2D} \prod_{d \in [D]} \left( \sum_{j_d > \tau} 2^{-j_d} \right) = c^{2D} 2^{-\tau D}.$$ 

Substituting the results into (35), we obtain

$$\mathbb{E}_{f^\ast} \left[ \| f^\ast - \hat{f}^\text{wave} \|_{L^2(P_X)}^2 \right] \geq \frac{2\sigma^2 2^\tau D}{n} + c^{2D} 2^{-\tau D}. \quad (36)$$ 

By setting $\tau = [(2D)^{-1} \log_2 n]$ to minimize the right hand side of (36), we obtain the statement. \hfill \square

**APPENDIX F. SUB-OPTIMALITY OF OTHER HARMONIC ESTIMATORS**

*Proof of Proposition 5.* In this proof, we provide an explicit example of $f^\ast \in \mathcal{F}_{\alpha, \beta, M}^{PS}$, and then derive a lower bound of a risk of $\hat{f}^\text{curve}$. Note that $P_X$ is the uniform distribution on $[-1, 1]^2$. Also, we consider $f^\ast$ to be the following non-smooth function

$$f^\ast(x_1, x_2) = 1_{[x_1 \geq 0]} \cdot 1_{[x_2 \geq 0]}, \quad (37)$$

and restrict it to $[-1, 1]^2$.

For analysis of curvelets, we consider a Fourier transformed curvelets $\hat{\gamma}_\mu$. As shown in (2.9) in [6], with $\xi = (\xi_1, \xi_2)$, $\hat{\gamma}_\mu$ is written as

$$\hat{\gamma}_\mu(\xi) = 2\pi \cdot \chi_{j, \ell}(\xi) \cdot u_{j, k}(R^*_{\theta, j} \xi).$$

Here, $\chi_{j, \ell}$ is a polar symmetric window function

$$\chi_{j, \ell}(\xi) = \omega(2^{-2j} \| \xi \|_2) (\nu_{j, \ell}(\theta(\xi)) + \nu_{j, \ell}(\theta(\xi + \pi))),$$

where $\theta(\xi) = \arcsin(\xi_2/\xi_1)$. Here, $\omega : \mathbb{R} \rightarrow \mathbb{R}$ is a compactly supported function, such as the Meyer wavelet, and we introduce $\nu_{j, \ell}(z) = \nu(2^j z - \pi \ell)$ where $\nu : \mathbb{R} \rightarrow \mathbb{R}$ is a function with a
support $[-\pi, \pi]$ and satisfies $|\nu(\theta)|^2 + |\nu(\theta - \pi)|^2 = 1$ for $\theta \in [0, 2\pi)$. Without loss of generality, we assume that there exists a constant $c > 0$ such as $\text{vol}(\{z \mid \omega(z) \geq 0\})/2 \leq \text{vol}(\{z \mid \omega(z) \geq c\})$ and $\text{vol}(\{z \mid \nu(z) \geq 0\})/2 \leq \text{vol}(\{z \mid \nu(z) \geq c\})$, and the support of $\omega$ is $[1, 2]$. Also, $u_{j,k} : \mathbb{R}^2 \to \mathbb{R}$ is defined as

$$u_{j,k}(\xi) = \frac{2^{-3j/2}}{2\pi \sqrt{\delta_1\delta_2}} \exp(ik_1 + 1/2)2^{-2j}\xi_1/\delta_1) \exp(ik_22^{-j}\xi_2/\delta_2),$$

and $\{u_{j,k}\}_k$ is an orthonormal basis for an $L^2$-space on a rectangle which covers the support of $\chi_{j,\ell}$, with fixed $j$ and $\ell$.

Further, we provide a Fourier transform of $f^\ast$. Since a Fourier transform of $I_{\{x \geq 0\}}$ is $\frac{1}{i\xi}$ and $f^\ast$ a product of two step functions, its Fourier transform $\hat{f}^\ast$ is written as $\frac{-1}{\xi^2}$.

To obtain the statement of Proposition 5, we repeat the argument for (35), and obtain

$$E_{f^\ast} \left[ \|f^\ast - \hat{f}^\ast\|_{L^2(R^2)}^2 \right] \geq \frac{\sigma^2|\mathcal{L}_\tau|}{n} + \sum_{\mu \in \mathcal{L}_{\tau}} w_\gamma(f^\ast)^2. \quad (38)$$

Let us consider a partial sum of the coefficients $\{\gamma_\mu\}_\mu$. Here, fix $j$ and $\ell$, then consider a subset of indexes $\mathcal{L}_{j',\ell'} := \{\mu \mid j = j', \ell = \ell'\}$. Then, since $\{u_{j,k}\}_k$ is an orthonormal basis, we obtain

$$\sum_{\mu \in \mathcal{L}_{j,\ell}} |w_\mu(f^\ast)|^2 = \int |\hat{f}^\ast(\xi)|^2 |\chi_{j,\ell}(\xi)|^2 d\xi.$$ 

Then, we utilize the form of $\hat{f}^\ast$ and a compact support of $\chi_{j,\ell}$, hence obtain

$$\int |\hat{f}^\ast(\xi)|^2 |\chi_{j,\ell}(\xi)|^2 d\xi \geq \frac{c}{2} \text{vol}(\text{Supp}(\chi_{j,\ell})) \inf_{\xi \in \text{Supp}(\chi_{j,\ell})} \frac{1}{\xi^4}. \quad (39)$$

Since $\text{Supp}(\chi_{j,\ell})$ is a set

$$\{\xi \in \mathbb{R}^2 \mid 2^{2j} \leq \|\xi\|_2 \leq 2^{2j+1}, |\theta(\xi) - \pi \ell 2^{-j}| \leq \pi 2^{-j-1}\},$$

Hence, simply we obtain

$$\text{vol}(\text{Supp}(\chi_{j,\ell})) = \frac{3\pi}{4} 2^{4j+2} = 3\pi 2^{4j}. \quad (40)$$

Also, about the infimum term, we obtain

$$\inf_{\xi \in \text{Supp}(\chi_{j,\ell})} \frac{1}{\xi^4} \geq \inf_{\|\xi\|_2 \leq 2^{2j+1}} \frac{1}{\xi^4} = \frac{1}{(2^{2j+1}/\sqrt{2})^4} = 2^{-8j-2}. \quad (41)$$

Substituting (40) and (41) into (39), then we obtain

$$\sum_{\mu \in \mathcal{L}_{j,\ell}} |w_\mu(f^\ast)|^2 = \int |\hat{f}^\ast(\xi)|^2 |\chi_{j,\ell}(\xi)|^2 d\xi \geq 3\pi 2^{-4j-2}. \quad (42)$$

Now, we will establish a lower bound by specifying $\mathcal{L}_\tau$ and associate it with (38). Let us define $\mathcal{L}_{j'} := \{\mu \mid j = j'\}$. By the setting of $\ell$ and $k$, we can obtain $|\mathcal{L}_j| = 2^j(1 + 2/\sqrt{2}) = 2^j + 2^{3j}/2$. Also, with the truncation parameter $\tau$, we have $|\mathcal{L}_\tau| = c_\tau(2^\tau + 2^{3\tau/2} - 1)$ with a coefficient $c_\tau > 0$. 
For an approximation error, we consider

$$\sum_{\mu \in \mathcal{L} \setminus \mathcal{L}_{\tau}} w_{\mu}(f^*)^2 = \sum_{j \in \mathbb{N}_0 \setminus \{r\} \cup \{0\}} \sum_{\ell} \sum_{k} w_{(j,\ell,k)}(f^*)^2 \geq \sum_{j \in \mathbb{N}_0 \setminus \{r\} \cup \{0\}} \sum_{\ell} 3\pi 2^{-4j-2}$$

$$= \frac{3\pi}{4} \sum_{j \in \mathbb{N}_0 \setminus \{r\} \cup \{0\}} 2^{-3j}$$

$$= \frac{3\pi}{28} 2^{-3\tau}.$$ 

where the inequality follows (42) and the second equality follows $\ell = 0, 1, ..., 2^j - 1$.

Combining the results with (38) by setting $\mathcal{L}_{\tau} = \mathcal{L}_r$, we obtain

$$\mathbb{E}_{f^*} \left[ \|f^* - \hat{f}_{\text{curve}}\|^2_{L^2(P_X)} \right] \geq \frac{\sigma^2 c_{\mathcal{L}_r}(2^\tau + 2^{3\tau/2} - 1)}{n} + \frac{3\pi}{28} 2^{-3\tau}. \quad (43)$$

As we set $\tau$ as $2^{3\tau/2} = \Theta(n^{1/3})$, then obtain the statement. $\square$

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