ADVERSARIAL RADEMACHER COMPLEXITY OF DEEP NEURAL NETWORKS

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ABSTRACT

Deep neural networks are vulnerable to adversarial attacks. Adversarial training is one of the most effective algorithms to increase the model's robustness. However, the trained models cannot generalize well to the adversarial examples on the test set. In this paper, we study the generalization of adversarial training through the lens of adversarial Rademacher complexity. Current analysis of adversarial Rademacher complexity is up to two-layer neural networks. In adversarial settings, one major difficulty of generalizing these results to deep neural networks is that we cannot peel off the layer as the classical analysis for standard training. We provide a method to overcome this issue and provide upper bounds of adversarial Rademacher complexity of deep neural networks. Similar to the existing bounds of standard Rademacher complexity of neural nets, our bound also includes the product of weight norms. We provide experiments to show that the adversarially trained weight norms are larger than the standard trained weight norms, thus providing an explanation for the bad generalization performance of adversarial training.

1 INTRODUCTION

Deep neural networks (DNNs) (Krizhevsky et al. (2012); Hochreiter & Schmidhuber (1997)) have become successful in many machine learning tasks such as computer vision (CV) and natural language processing (NLP). But they are shown to be vulnerable to adversarial examples (Szegedy et al. (2013); Goodfellow et al. (2014)). A well-trained model can be easily attacked by adding a small perturbation to the original data. Adversarial training is one of the most effective algorithms to defend against adversarial attacks. However, generalization is one of the main issues of adversarial training. An adversarially trained model will over-fit the adversarial examples on the training dataset, and it cannot generalize well to the adversarial examples on the test set. For example, in the experiment of training ResNet (He et al. (2016)) on CIFAR-10 (Krizhevsky et al. (2009)), Projected gradient descent (PGD) adversarial training achieves 100% robust accuracy on the training set, but it only gets 45% robust accuracy on the test set (Madry et al. (2017)). Recent works (Gowal et al. (2020); Rebuffi et al. (2021)) mitigate the over-fitting issue, but it still has a 20% generalization gap between robust test accuracy (60%) and training accuracy (80%). On the other hand, a standard trained model can generalize well to the test set with a 5% generalization gap. To understand why the generalization of adversarial training behaves differently from standard training, we study the generalization issue of adversarial training through the lens of Rademacher complexity.

In classical machine learning theory, Rademacher complexity measures the generalization capacity of machine learning models. For depth-d neural networks, assuming that the weight matrices $W_1, W_2, \cdots, W_d$ in each of the d layers have Frobenius norms bounded by $M_1, \cdots, M_d$, and all the data $\boldsymbol{x}$ have ℓ_2-norm bounded by B, given m training samples, the generalization gap between population risk and empirical risk scales as $\mathcal{O}(B2^d \prod_{l=1}^{d} M_l/\sqrt{m})$ with high probability (Neyshabur et al. (2015)). Another works provide different norm-based complexity, such as $\|\cdot\|_{1,\infty}$-norm (Bartlett & Mendelson (2002)) and spectral norm (Bartlett et al. (2017)). The work of (Golowich et al. (2018)) reduces the dependence on depth-d from 2^d to $\sqrt{d}$. The proofs of the above bounds are based on the induction on layers, which is also called the 'peeling off' techniques. For more details, see section 3.

In adversarial training, adversarial Rademacher complexity was first introduced in (Yin et al. (2019); Khim & Loh (2018)) to measure the robust generalization gap. They prove that the robust generalization gap of linear function ($\boldsymbol{x} \to w^T \boldsymbol{x}$) scales as $\mathcal{O}((B+\epsilon)M/\sqrt{m})$, where M is the upper bound of norm of the weights w and ϵ is the perturbation intensity of adversarial attacks. Awasthi et al. (2020) provides an upper bound in two-layers neural network cases. For depth-2, width-h neural networks, with high probability, the generalization gap scales as $\mathcal{O}((B+\epsilon)\sqrt{hq}M_1 M_2 \sqrt{\log m/m})$, where q is the dimension of the data $\boldsymbol{x}$.

One might think it is straightforward to use the induction methods in (Neyshabur et al. (2015); Golowich et al. (2018)) to extend the adversarial Rademacher complexity in (Yin et al. (2019); Khim & Loh (2018)) to multi-layers cases. However, it seems challenging to apply their induction methods to adversarial cases. Let the adversarial loss be $\max_{\|x-x'\|\leq\epsilon} \ell(f(\boldsymbol{x}'), y)$ and f is a DNN. We cannot peel off the layer because of the max operation in the adversarial loss. The work of (Khim & Loh (2018)) and (Gao & Wang (2021)) also indicate the difficulty of analyzing adversarial Rademacher complexity of DNNs. They analyze other variants of adversarial Rademacher complexity, which are quite different from the original adversarial Rademacher complexity. See more detailed discussions of these works in section 3. To our knowledge, direct analysis of the original adversarial Rademacher complexity is largely missing.

In this paper, we analyze the adversarial Rademacher complexity of deep neural networks. Specifically, for depth-d, width-h fully connected neural networks, with high probability, the robust generalization gap scales as

$$\mathcal{O}\Big(\frac{(B+\epsilon)h\sqrt{d\log d}\prod_{l=1}^{d} M_l}{\sqrt{m}}\Big).$$

Similar to the existing bounds of standard Rademacher complexity of deep neural nets, the bound includes the product of weight norms $\prod_{l=1}^{d}\|W_l\|$, but they are trained by different algorithms. We empirically show that the adversarially trained weight norms are larger than the standard trained weight norms, which provide an explanation why adversarial training did not generalize well. Our contributions are listed as follow:

1. We provide a method and give upper bounds and lower bounds for adversarial Rademacher complexity of deep neural nets.
2. We provide experiments to analyze why adversarial training cannot generalize well.

2 Preliminaries

2.1 Generalization Gap and Rademacher Complexity

Generalization Gap. We start from the classical machine learning framework. Let $\mathcal{F}$ be the hypothesis class (e.g. Linear functions, Neural networks). The goal of the learning problem is to find $f \in \mathcal{F}$ to minimize the population risk $R(f) = \mathbb{E}_{(\boldsymbol{x},y)\sim\mathcal{D}}[\ell(f(\boldsymbol{x}), y)]$, where $\mathcal{D}$ is the true distribution, $\ell(\cdot)$ is the loss function. Since $\mathcal{D}$ is unknown, we minimize the empirical risk in practice. Given m i.i.d samples $S = \{(\boldsymbol{x}_1, y_1), \cdots, (\boldsymbol{x}_m, y_m)\}$, the empirical risk is $R_m(f) = \frac{1}{m}\sum_{i=1}^{m}[\ell(f(\boldsymbol{x}_i), y_i)]$. The generalization gap or generalization error is defined as follow:

$$\text{Generalization Gap} := R(f) - R_m(f).$$

Rademacher Complexity. A classical measure of the generalization error is Rademacher complexity (Bartlett & Mendelson (2002)). Given the hypothesis class $\mathcal{H}$, the (empirical) Rademacher complexity is defined as

$$\mathcal{R}_{\mathcal{S}}(\mathcal{H}) = \mathbb{E}_{\sigma}\frac{1}{m}\big[\sup_{h\in\mathcal{H}}\sum_{i=1}^{m}\sigma_i h(\boldsymbol{x}_i, y_i)\big],$$

where σ_i are i.i.d Rademacher random variables, i.e. σ_i equals to 1 or -1 with equal probability. Define the function class $\ell_{\mathcal{F}} = \{\ell(f(\boldsymbol{x}), y) | f \in \mathcal{F}\}$, we have the following generalization bound.

Proposition 1. *(Bartlett & Mendelson (2002)) Suppose that the range of the loss function $\ell(f(x), y)$ is $[0, 1]$. Then, for any $\delta \in (0, 1)$, with probability at least $1 - \delta$, the following holds for all $f \in \mathcal{F}$,*

$$R(f) \leq R_m(f) + 2\mathcal{R}_{\mathcal{S}}(\ell_{\mathcal{F}}) + 3\sqrt{\frac{\log \frac{2}{\delta}}{2m}}.$$

2.2 Robust Generalization Gap and Adversarial Rademacher Complexity

Robust Generalization Gap. Let $\tilde{\ell}(f(x), y) := \max_{\|x'-x\|_p \leq \epsilon} \ell(f(x'), y)$ be the adversarial loss. The adversarial population risk and the adversarial empirical risk are

$$\tilde{R}(f) = \mathbb{E}_{(x,y)\sim\mathcal{D}} \max_{\|x'-x\|_p \leq \epsilon} \ell(f(x'), y) \quad \textit{and} \quad \tilde{R}_m(f) = \frac{1}{m}\sum_{i=1}^{m} \max_{\|x'-x\|_p \leq \epsilon} \ell(f(x_i'), y_i),$$

respectively. In this paper we consider general ℓ_p attacks for $p \geq 1$. The robust generalization gap is defined as follow:

$$\text{Robust Generalization Gap} := \tilde{R}(f) - \tilde{R}_m(f).$$

Let the adversarial hypothesis class be $\tilde{\ell}_{\mathcal{F}} = \{\tilde{\ell}(f(x), y) | f \in \mathcal{F}\}$, according to Proposition 1, we have the following adversarial generalization bound.

Proposition 2. *(Khim & Loh (2018); Yin et al. (2019)) Suppose that the range of the loss function $\tilde{\ell}(f(x), y)$ is $[0, 1]$. Then, for any $\delta \in (0, 1)$, with probability at least $1 - \delta$, the following holds for all $f \in \mathcal{F}$,*

$$\tilde{R}(f) \leq \tilde{R}_m(f) + 2\mathcal{R}_{\mathcal{S}}(\tilde{\ell}_{\mathcal{F}}) + 3\sqrt{\frac{\log \frac{2}{\delta}}{2m}}.$$

Binary Classification. We first discuss the binary classification case, then we discuss the extension to the multi-class classification case in section 5. Following (Yin et al. (2019); Awasthi et al. (2020)), we assume that the loss function can be written as $\ell(f(\boldsymbol{x}), y) = \phi(yf(\boldsymbol{x}))$ where ϕ is a non-increasing function. Then

$$\max_{\boldsymbol{x}'} \ell(f(\boldsymbol{x}'), y) = \phi(\min_{\boldsymbol{x}'} yf(\boldsymbol{x}')).$$

Assume that the function ϕ is L_ϕ-Lipschitz, by Talagrand's Lemma (Ledoux & Talagrand (2013)), we have $\mathcal{R}_{\mathcal{S}}(\tilde{\ell}_{\mathcal{F}}) \leq L_\phi \mathcal{R}_{\mathcal{S}}(\tilde{\mathcal{F}})$, where we define the adversarial function class as

$$\tilde{\mathcal{F}} = \{\tilde{f} : (\boldsymbol{x}, y) \to \inf_{\|\boldsymbol{x}-\boldsymbol{x}'\|_p \leq \epsilon} yf(\boldsymbol{x}') | f \in \mathcal{F}\}. \tag{1}$$

Adversarial Rademacher Complexity. We define $\mathcal{R}_S(\tilde{\mathcal{F}})$ as adversarial Rademacher complexity. Our goal is to give upper bounds for adversarial Rademacher complexity. Then, it induces the guarantee of the robust generalization gap.

Hypothesis Class. We consider depth-d, width-h fully-connected neural networks,

$$\mathcal{F} = \{\boldsymbol{x} \to W_d\rho(W_{d-1}\rho(\cdots\rho(W_1\boldsymbol{x})\cdots)), \|W_l\| \leq M_l, l = 1\cdots, d\}, \tag{2}$$

where $\rho(\cdot)$ is an element-wise L_ρ-Lipschitz activation function, W_l are $h_l \times h_{l-1}$ matrices, for $l = 1, \cdots, d$. We have $h_d = 1$ and $h_0 = q$ is the dimension of the data $\boldsymbol{x}$. Let $h = \max\{h_0, \cdots, h_d\}$ be the width of the neural networks. Denote the (a, b)-group norm $\|W\|_{a,b}$ as the a-norm of the b-norm of the rows of W. We consider two cases, Frobenius norm and $\|\cdot\|_{1,\infty}$-norm in equation (2). Additionally, we assume that $\|\boldsymbol{X}\|_{p,\infty} = B$.

2.3 Rademacher Complexity and Covering Number

Covering Number. Our solution for adversarial Rademacher complexity is based on the covering number. We first provide the definition of covering number.

Definition 1 (ε-cover)**.** *Let $\varepsilon > 0$ and $(V, d(\cdot,\cdot))$ be a metric space, where $d(\cdot,\cdot)$ is a (pseudo)-metric. $\mathcal{C} \subset V$ is an ε-cover of V, if for any $v \in V$, there exists $v' \in \mathcal{C}$ s.t. $d(v, v') \leq \varepsilon$. Define the smallest $|\mathcal{C}|$ as ε-covering number of V and denote as $\mathcal{N}(V, d(\cdot,\cdot), \varepsilon)$.*

Next, we define the ε-covering number of a function class $\mathcal{F}$. Given the sample dataset $S = \{(\boldsymbol{x}_1, y_1), \cdots, (\boldsymbol{x}_m, y_m)\}$ with $\boldsymbol{x}_i \in \mathbb{R}^d$, let $\|f\|_S^2 = \frac{1}{m}\sum_{i=1}^m f(\boldsymbol{x}_i, y_i)^2$ be a pseudometric of $\mathcal{F}$. Define the ε-covering number of $\mathcal{F}$ be $\mathcal{N}(\mathcal{F}, \|\cdot\|_S, \varepsilon)$. Let D be the diameter of $\mathcal{F}$ with $D = 2\max_{f\in\mathcal{F}} \|f\|_S$.

Proposition 3 (Dudley's integral)**.** *The Rademacher complexity $\mathcal{R}(\mathcal{F})$ satisfiy*

$$\mathcal{R}_S(\mathcal{F}) \leq \frac{12}{\sqrt{m}} \int_0^{D/2} \sqrt{\log \mathcal{N}(\mathcal{F}, \|\cdot\|_S, \varepsilon)} d\varepsilon.$$

The proof of Dudley's integral can be found in statistic textbooks (e.g. (Wainwright (2019))). Based on this, we can bound the covering number of the function class $\mathcal{F}$ to give an upper bound of the Rademacher complexity.

3 Discussion on Existing Methods for Rademacher Complexity

In this section, we discuss the related work, discuss the existing methods in calculating Rademacher complexity, and identify the difficulty of analyzing adversarial Rademacher complexity.

'Layer Peeling' Bounds. The main idea of calculating the Rademacher complexity of multi-layers neural networks is the 'peeling off' technique (Neyshabur et al. (2015)). We denote $g \circ \mathcal{F}$ as the function class $\{g \circ f | f \in \mathcal{F}\}$. By Talagrand's Lemma, we have $\mathcal{R}_{\mathcal{S}}(g \circ f) \leq L_g \mathcal{R}_{\mathcal{S}}(\mathcal{F})$. Based on this property, we can obtain $\mathcal{R}_{\mathcal{S}}(\mathcal{F}_l) \leq 2L_\rho M_l \mathcal{R}_{\mathcal{S}}(\mathcal{F}_{l-1})$, where $\mathcal{F}_l$ is the function class of l-layers neural networks. Since the Rdemacher complexity of linear function class is bounded by $\mathcal{O}(BM_1/\sqrt{m})$, we can get the upper bound $\mathcal{O}(B2^d L_\rho^{d-1} \prod_{l=1}^d M_l/\sqrt{m})$ by induction. We can remove the L_ρ by assuming that $L_\rho = 1$ (e.g. Relu activation function).

Golowich et al. (2018) improves the dependence on depth-d from d^2 to $\sqrt{d}$. The main idea is to rewrite the Rademacher complexity $\mathbb{E}_\sigma[\cdot]$ as $\mathbb{E}_\sigma \exp\ln[\cdot]$. Then, we can peel off the layer inside the $\ln(\cdot)$ function and the 2^d now appears inside the $\ln(\cdot)$.

Covering Number Bounds. Bartlett et al. (2017) uses a covering numbers argument to show that the generalization gap scale as

$$\tilde{\mathcal{O}}\Big(\frac{B\prod_{l=1}^d \|W_l\|}{\sqrt{m}} \Big(\sum_{l=1}^d \frac{\|W_l\|_{2,1}^{2/3}}{\|W_l\|^{2/3}}\Big)^{3/2}\Big),$$

where $\|\cdot\|$ is the spectral norm. The proof is based on the induction on layers. Let W_l be the weight matrix of the present layer and X_l be the output of X pass through the first to the $l-1$ layer. Then, one can compute the matrix covering number $\mathcal{N}(\{W_l X_l\}, \|\cdot\|_2, \epsilon)$ by induction.

Adversarial Generalization Bounds. Researchers have analyzed adversarial Rademacher complexity in linear and two-layers neural networks cases. In linear cases, the upper bounds can be directly derived by definition (Khim & Loh (2018); Yin et al. (2019)). In two-layers neural networks cases, an upper bound is derived using Massart's Lemma (Awasthi et al. (2020)). These proofs cannot be extended to multi-layers cases. Moreover, based on the definition of adversarial function class $\tilde{\mathcal{F}}$ in equation (1), the candidate functions are not composition functions, but with an $\inf$ operation in front of the neural networks. Then, the induction on layers seems not applicable in calculating adversarial Rademacher complexity for deep neural networks. The works of (Khim & Loh (2018)) and (Gao & Wang (2021)) indicate the difficulty of analyzing adversarial Rademacher complexity. They analyze other variants of adversarial Rademacher complexity of DNNs.

'Tree Transformation' Bound. Khim & Loh (2018) introduces a tree transformation T and shows that $\max_{\|x-x'\|\leq\epsilon} \ell(f(\boldsymbol{x}), y) \leq \ell(Tf(\boldsymbol{x}), y)$. Then, we have the following upper bound for the adversarial population risk. For $\delta \in (0, 1)$,

$$\tilde{R}(f) \leq R(Tf) \leq R_m(Tf) + 2L\mathcal{R}_S(T \circ \mathcal{F}) + 3\sqrt{\frac{\log\frac{2}{\delta}}{2m}}.$$

It gives an upper bound of the robust population risk by the empirical risk and the standard Rademacher complexity of $T \circ f$. $\mathcal{R}_S(T \circ \mathcal{F})$ can be viewed as an approximation of adversarial Rademacher complexity. However, the empirical risk $R_m(Tf)$ is not the objective in practice. This analysis does not provide a guarantee for robust generalization gaps.

The work of (Gao & Wang (2021)) tries to provide an upper bound for adversarial Rademacher complexity. To deal with the $\max$ operation in the adversarial loss, they consider FGSM adversarial examples. Then, the adversarial loss $\max_{\|\boldsymbol{x}'-\boldsymbol{x}\|\leq\epsilon} \ell(\boldsymbol{x}, y)$ becomes $\ell(f(\boldsymbol{x}_{FGSM}), y)$. By some assumptions on the gradient, they provide an upper bound for the Rademacher complexity of $\ell(f(\boldsymbol{x}_{FGSM}), y)$. However, the bound includes some parameters of the assumptions on the gradients, and FGSM underestimates the adversarial examples. It is hard to use this bound to analyze adversarial generalization. Therefore, the existing bounds give limited interpretations in understanding the generalization of adversarial training. Other related works are provided in Appendix B.

Current results do not provide an upper bound for adversarial Rademacher complexity in multi-layers cases. In the next section, we provide our solution of adversarial Rademacher complexity and analyze each factor in the upper bound.

4 Our Solution of Adversarial Rademacher Complexity

The following Theorem states an upper bound of adversarial Rademacher complexity in the Frobenius norm cases.

Theorem 1 (Frobenius Norm Bound)**.** *Given the function class $\mathcal{F}$ in equation (2) under Frobbenius Norm, and the corresponding adversarial function class $\tilde{\mathcal{F}}$ in equation (1). The adversarial Rademacher complexity of deep neural networks $\mathcal{R}_S(\tilde{\mathcal{F}})$ satisfies*

$$\mathcal{R}_S(\tilde{\mathcal{F}}) \leq \frac{24}{\sqrt{m}} \max\{1, q^{\frac{1}{2}-\frac{1}{p}}\}(\|\boldsymbol{X}\|_{p,\infty} + \epsilon) L_\rho^{d-1} \sqrt{\sum_{l=1}^{d} h_l h_{l-1} \log(3d)} \prod_{l=1}^{d} M_l. \tag{3}$$

By assuming that $L_\rho = 1$, $p \leq 2$, $\|\boldsymbol{X}\|_{p,\infty} = B$, and $h = \max\{h_0, \cdots, h_d\}$, we have

$$\mathcal{R}_S(\tilde{\mathcal{F}}) \leq \mathcal{O}\left(\frac{(B+\epsilon)h\sqrt{d\log(d)}\prod_{l=1}^{d} M_l}{\sqrt{m}}\right). \tag{4}$$

Because of the $\inf$ operation of the function in $\tilde{\mathcal{F}}$, we cannot peel off the layers or calculate the covering number by induction on layers. Our proof is based on calculating the covering number of $\tilde{\mathcal{F}}$ directly. Below we sketch the proof. The completed proof is provided in Appendix A.

Step 1: Diameter of $\tilde{\mathcal{F}}$. We first calculate the diameter of $\tilde{\mathcal{F}}$. We have

$$2\max_{\tilde{f}\in\tilde{\mathcal{F}}} \|\tilde{f}\|_S \leq 2L_\rho^{d-1} \max\{1, q^{\frac{1}{2}-\frac{1}{p}}\}(\|\boldsymbol{X}\|_{p,\infty} + \epsilon) \prod_{l=1}^{d} M_l \triangleq D.$$

Step 2: Distance to $\tilde{\mathcal{F}}^c$. Let $\mathcal{C}_l$ be δ_l-covers of $\{\|W_l\|_F \leq M_l\}$, $l = 1, 2, \cdots, d$. Let

$$\mathcal{F}^c = \{f^c : \boldsymbol{x} \to W_d^c \rho(W_{d-1}^c \rho(\cdots \rho(W_1^c \boldsymbol{x}) \cdots)), W_l^c \in \mathcal{C}_l, l = 1, 2 \cdots, d\}$$
$$\text{and } \tilde{\mathcal{F}}^c = \{\tilde{f} : (\boldsymbol{x}, y) \to \inf_{\|\boldsymbol{x}-\boldsymbol{x}'\|_p \leq \epsilon} y f(\boldsymbol{x}') | f \in \mathcal{F}^c\}.$$

For all $\tilde{f} \in \tilde{\mathcal{F}}$, we need to find the smallest distance to $\tilde{\mathcal{F}}^c$, i.e. we need to calculate the

$$\max_{\tilde{f}\in\tilde{\mathcal{F}}} \min_{\tilde{f}^c\in\tilde{\mathcal{F}}^c} \|\tilde{f} - \tilde{f}^c\|_S.$$

$\forall(\boldsymbol{x}, y) \in \mathcal{D}$, given f and f^c, let $\boldsymbol{x}^* = \arg\inf_{\|\boldsymbol{x}-\boldsymbol{x}'\|_p} y f(\boldsymbol{x}')$ and $\boldsymbol{x}^c = \arg\inf_{\|\boldsymbol{x}-\boldsymbol{x}'\|_p} y f^c(\boldsymbol{x}')$. Let $z = \begin{cases} \boldsymbol{x}^c & if \quad f(\boldsymbol{x}^*) \geq f^c(\boldsymbol{x}^c) \\ \boldsymbol{x} & if \quad f(\boldsymbol{x}^*) < f^c(\boldsymbol{x}^c) \end{cases}$ and $g_b^a(z) = W_b \rho(\cdots W_{a+1} \rho(W_a^c \cdots \rho(W_1^c z) \cdots)))$. Then

$$|f(z) - f^c(z)| = |g_d^0(z) - g_d^d(z)| \leq |g_d^0(z) - g_d^1(z)| + \cdots + |g_d^{d-1}(z) - g_d^d(z)| \leq \sum_{l=1}^{d} \frac{D\delta_l}{2M_l}.$$

Let $\delta_l = 2M_l\varepsilon/dD$, $l = 1, \cdots, d$, we have $\max_{\tilde{f}\in\tilde{\mathcal{F}}} \min_{\tilde{f}^c\in\tilde{\mathcal{F}}^c} \|\tilde{f} - \tilde{f}^c\|_S \leq \sum_{l=1}^{d} \frac{D\delta_l}{2M_l} \leq \varepsilon$.

Step 3: Covering Number of $\tilde{\mathcal{F}}$. Then, We can calculate the ε-covering number $\mathcal{N}(\tilde{\mathcal{F}}, \|\cdot\|_S, \varepsilon)$. Because $\tilde{\mathcal{F}}^c$ is a ε-cover of $\tilde{\mathcal{F}}$. The cardinality of $\tilde{\mathcal{F}}^c$ is

$$\mathcal{N}(\tilde{\mathcal{F}}, \|\cdot\|_S, \varepsilon) = |\tilde{\mathcal{F}}^c| \leq (\frac{3dD}{2\varepsilon})^{\sum_{l=1}^{d} h_l h_{l-1}}. \tag{5}$$

Step 4, Integration. By Dudley's integral, we obtain the bound in Theorem 1. □

Remark: Step 2 is the critical step in the proof. In words, if we calculate the covering number of the class of d-layers neural nets directly, we only need to define the optimal adversarial example one time. Then we can calculate the other things using this adversarial example. In contrast, if we want to do it layer by layer, the optimal adversarial example will be changed when we add or peel off a layer. This is why the induction methods fail in adversarial settings.

Theorem 2 ($\|\cdot\|_{1,\infty}$-Norm Bound)**.** *Given the function class $\mathcal{F}$ in equation (2) under $\|\cdot\|_{1,\infty}$-norm, and the corresponding adversarial function class $\tilde{\mathcal{F}}$ in equation (1). The adversarial Rademacher complexity of deep neural networks $\mathcal{R}_S(\tilde{\mathcal{F}})$ satisfies*

$$\mathcal{R}_S(\tilde{\mathcal{F}}) \leq \frac{24}{\sqrt{m}}(\|\boldsymbol{X}\|_{p,\infty} + \epsilon) L_\rho^{d-1} \sqrt{\sum_{l=1}^{d} h_l h_{l-1} \log(3d)} \prod_{l=1}^{d} M_l. \tag{6}$$

In the case of $\|\cdot\|_{1,\infty}$-norm, the bound is similar to the bound in the Frobenius norm case except the term $\max\{1, q^{1/2-1/p}\}$. Therefore, for all $p \geq 1$, the $\|\cdot\|_{1,\infty}$-norm bound have the same order in equation (4).

Theorem 3 (Lower Bound)**.** *Given the function class of DNNs $\mathcal{F}$ in equation (2), and the corresponding adversarial function class $\tilde{\mathcal{F}}$ in equation (1). The adversarial Rademacher complexity of deep neural networks $\mathcal{R}_S(\tilde{\mathcal{F}})$ satisfies*

$$\mathcal{R}_S(\tilde{\mathcal{F}}) \geq \Omega\left(\frac{(B+\epsilon)\prod_{l=1}^{d} M_l}{\sqrt{m}}\right). \tag{7}$$

The proof of the above Theorem is based on constructing a scalar network and is provided in Appendix A. The gap between the upper bound and the lower bound is the dependence on depth-d and width-h, $h\sqrt{d \log d}$. In the next section, we extend the adversarial Rademacher complexity to the Multi-class classification cases.

5 Margin Bounds for Multi-Class Classification

5.1 Setting for Multi-Class Classification

The setting for multi-class classification follows (Bartlett & Mendelson (2002)). In a K-class classification problem, let $\mathcal{Y} = \{1, 2, \cdots, K\}$. The functions in the hypothesis class $\mathcal{F}$ map $\mathcal{X}$ to $\mathbb{R}^K$, the k-th output of f is the score of $f(\boldsymbol{x})$ assigned to the k-th class.

Define the margin operator $M(f(\boldsymbol{x}), y) = [f(\boldsymbol{x})]_y - \max_{y' \neq y}[f(\boldsymbol{x})]_{y'}$. The function makes a correct prediction if and only if $M(f(\boldsymbol{x}), y) > 0$. We consider a particular loss function $\ell(f(\boldsymbol{x}), y) = \phi_\gamma(M(f(\boldsymbol{x}), y))$, where $\gamma > 0$ and $\phi_\gamma : \mathbb{R} \to [0, 1]$ is the ramp loss:

$$\phi_\gamma(t) = \begin{cases} 1 & t \leq 0 \\ 1 - \frac{t}{\gamma} & 0 < t < \gamma \\ 0 & t \geq \gamma. \end{cases}$$

The loss function $\ell(f(\boldsymbol{x}), y)$ satisfies:

$$\mathbb{1}(y \neq \arg\max_{y' \in [K]} [f(\boldsymbol{x})]_{y'}) \leq \ell(f(\boldsymbol{x}), y) \leq \mathbb{1}([f(\boldsymbol{x})]_y \leq \gamma + \max_{y' \neq y} [f(\boldsymbol{x})]_{y'}). \tag{8}$$

Define the function class $\ell_{\mathcal{F}} := \{(\boldsymbol{x}, y) \mapsto \phi_\gamma(M(f(\boldsymbol{x}), y)) : f \in \mathcal{F}\}$. Since $\phi_\gamma(t) \in [0, 1]$ and $\phi_\gamma(\cdot)$ is $1/\gamma$-Lipschitz, by combining (8) with Theorem 1, we can obtain the following direct corollary as the generalization bound in the multi-class classification.

Corollary 1 (Bartlett & Mendelson (2002)). *Consider the above multi-class classification setting. For any fixed $\gamma > 0$, we have with probability at least $1-\delta$, for all $f \in \mathcal{F}$,*

$$\mathbb{P}_{(\boldsymbol{x},y)\sim\mathcal{D}}\left\{y \neq \arg\max_{y'\in[K]}[f(\boldsymbol{x})]_{y'}\right\}$$
$$\leq \frac{1}{m}\sum_{i=1}^{m}\mathbb{1}([f(\boldsymbol{x}_i)]_{y_i} \leq \gamma + \max_{y'\neq y}[f(\boldsymbol{x}_i)]_{y'}) + 2\mathcal{R}_S(\ell_{\mathcal{F}}) + 3\sqrt{\frac{\log\frac{2}{\delta}}{2m}}.$$

In adversarial training, let $\mathbb{B}^p_{\boldsymbol{x}}(\epsilon) = \{x' : \|\boldsymbol{x}' - \boldsymbol{x}\|_p \leq \epsilon\}$ and we define the adversarial function class $\tilde{\ell}_{\mathcal{F}} := \{(\boldsymbol{x}, y) \mapsto \max_{x'\in\mathbb{B}^p_{\boldsymbol{x}}(\epsilon)} \ell(f(\boldsymbol{x}'), y) : f \in \mathcal{F}\}$. We have

Corollary 2 (Yin et al. (2019)). *Consider the above adversarial multi-class classification setting. For any fixed $\gamma > 0$, we have with probability at least $1-\delta$, for all $f \in \mathcal{F}$,*

$$\mathbb{P}_{(\boldsymbol{x},y)\sim\mathcal{D}}\left\{\exists\, \boldsymbol{x}' \in \mathbb{B}^p_{\boldsymbol{x}}(\epsilon) \text{ s.t. } y \neq \arg\max_{y'\in[K]}[f(\boldsymbol{x}')]_{y'}\right\}$$
$$\leq \frac{1}{m}\sum_{i=1}^{m}\mathbb{1}(\exists\, \boldsymbol{x}'_i \in \mathbb{B}^p_{\boldsymbol{x}_i}(\epsilon) \text{ s.t. } [f(\boldsymbol{x}'_i)]_{y_i} \leq \gamma + \max_{y'\neq y}[f(\boldsymbol{x}'_i)]_{y'}) + 2\mathcal{R}_S(\tilde{\ell}_{\mathcal{F}}) + 3\sqrt{\frac{\log\frac{2}{\delta}}{2m}}.$$

5.2 Adversarial Rademacher Complexity

Under the multi-class setting, we have the following bound for adversarial Rademacher complexity.

Theorem 4. *Given the function class $\mathcal{F}$ in equation (2) under Frobbenius Norm, and the corresponding adversarial function class $\tilde{\mathcal{F}}$ in equation (1). The adversarial Rademacher complexity of deep neural networks $\mathcal{R}_S(\tilde{\ell}_{\mathcal{F}})$ satisfies*

$$\mathcal{R}_S(\tilde{\ell}_{\mathcal{F}}) \leq \frac{48K}{\gamma\sqrt{m}}\max\{1, q^{\frac{1}{2}-\frac{1}{p}}\}(\|\boldsymbol{X}\|_{p,\infty} + \epsilon)L_\rho^{d-1}\sqrt{\sum_{l=1}^{d} h_l h_{l-1}\log(3d)}\prod_{l=1}^{d} M_l. \tag{9}$$

The $\|\cdot\|_{1,\infty}$-norm bound is similar, except the term $\max\{1, q^{\frac{1}{2}-\frac{1}{p}}\}$. Below we sketch the proof. Step 1: Let $\tilde{\mathcal{F}}^k = \{(\boldsymbol{x}, y) \to \inf_{\|\boldsymbol{x}'-\boldsymbol{x}\|\leq\epsilon}([f(\boldsymbol{x}')]_y - [f(\boldsymbol{x}')]_k), f \in \mathcal{F}\}$, then $\mathcal{R}_S(\tilde{\ell}_{\mathcal{F}}) \leq K\mathcal{R}_S(\tilde{\ell}_{\mathcal{F}^k})$. Step 2: By the Lipschitz property of $\phi_\gamma(\cdot)$, $\mathcal{R}_S(\tilde{\ell}_{\mathcal{F}^k}) \leq \mathcal{R}_S(\mathcal{F}^k)$. Step 3: The calculation of $\mathcal{R}_S(\tilde{\mathcal{F}}^k)$ follows the binary case.

5.3 Comparison of the Bounds

Now we compare the difference between the bounds for (standard) Rademacher complexity and adversarial Rademacher complexity. We have shown that

$$\mathcal{R}_S(\ell_{\mathcal{F}}) \leq \mathcal{O}\left(\frac{B\sqrt{d}\prod_{l=1}^{d} M_l}{\gamma\sqrt{m}}\right) \text{ and } \mathcal{R}_S(\tilde{\ell}_{\mathcal{F}}) \leq \mathcal{O}\left(\frac{(B+\epsilon)h\sqrt{d\log d}\prod_{l=1}^{d} M_l}{\gamma\sqrt{m}}\right),$$

where we use the upper bound of $\mathcal{R}_S(\mathcal{F})$ in (Golowich et al. (2018)).

Number of Samples. The sample complexities are both $\mathcal{O}(1/\sqrt{m})$.

Sample Size. In the two bounds, the dependence on the sample size are B and $B+\epsilon$, respectively. Firstly, ϵ is small comparing to B. Secondly, B and $B+\epsilon$ are small comparing to the other terms in the upper bounds. Therefore, sample size has a minor effect on the difference of generalization properties in standard training and adversarial training.

Depth and Width. The difference of the dependence on the depth-d between these two bounds is $\sqrt{\log d}$, which is not critical. In terms of the dependence on the width-h, it appears in the upper bound of adversarial Rademacher complexity but not in the standard Rademacher complexity. As we can see in the proof, h is unavoidable because of the calculation of the covering number, but it is not in the lower bound. Therefore, the width of neural networks is possibly an important factor for the

generalization of adversarial training. However, it is hard to distinguish from the technical issues in calculating the bounds.

Margin. The margin γ exists in the divider in both of the two bounds. Based on the different definitions of γ in standard and adversarial training, the margin of the trained model may affect the generalization of standard and adversarial training.

Matrix Norm. The product of the matrix norms $\prod_{l=1}^{d} \|W_l\|$ appears in both of the two bounds, but the weights are trained by different algorithms. The difference in $\prod_{l=1}^{d} \|W_l\|$ may be important in understanding the robust generalization of adversarial training.

6 EXPERIMENT

As we discuss in the previous section, the product of weight norm $\prod_{l=1}^{d} \|W_l\|$ and the margin γ maybe important factors controlling the generalization gap. We provide experiments comparing the difference between these terms in standard and adversarial settings. We also consider the trends of $\prod_{l=1}^{d} \|W_l\|/\gamma$ when we increase the number of training samples m. Since the bounds also hold for convolution neural networks, we consider the experiments of training VGG networks (Simonyan & Zisserman (2014)) on CIFAR-10 (Krizhevsky et al. (2009)). Experiments on CIFAR-100 are provided in Appendix C.

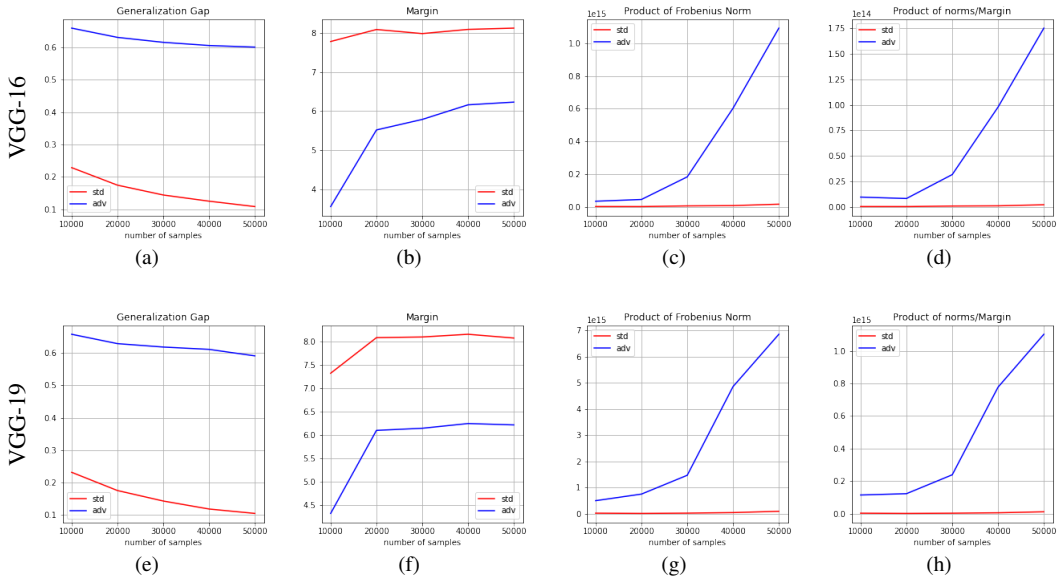
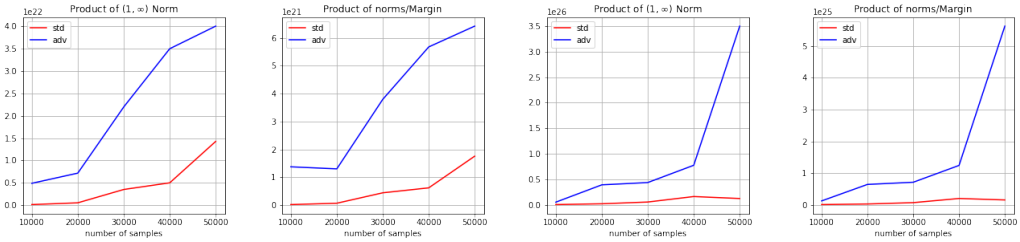


Figure 1: Product of the Frobenius norm in the experiments on CIFAR-10. The red lines are the results of standard training. The blue lines are the results of adversarial training. The first row is the experiments on VGG-16. The second row is the experiments on VGG-19. (a) and (e): Generalization gap. (b) and (f): Margins γ over training set. (c) and (g): $\prod_{l=1}^{d} \|W_l\|_F$ of the neural networks. (d) and (h): $\prod_{l=1}^{d} \|W_l\|_F/\gamma$ of the neural networks.

Training Settings. For both standard and adversarial training, we use the stochastic gradient descent (SGD) optimizer, along with a learning rate schedule, which is 0.1 over the first 100 epochs, down to 0.01 over the following 50 epochs, and finally be 0.001 in the last 50 epochs. For adversarial settings, we adopt the ℓ_∞ PGD adversarial training (Madry et al. (2017)). The perturbation intensity is set to be $8/255$. We set the number of steps as 20 and further increase it to 40 in the testing phase. For the stepsize in the inner maximization, we set it as 2/255. In Corollary 2, we need to use the optimal adversarial examples to calculate the margin and the robust generalization gap, but it is unknown in practice. We use the PGD adversarial examples as substitutes.

Calculation of Margins. We adopt the setting in (Neyshabur et al. (2017a)). In standard training, we set the margin over training set to be 5th-percentile of the margins of the data points in S. i.e. $\text{Prc}_5\{f(\boldsymbol{x}_i)[y_i] - \max_{y \neq y_i} f(\boldsymbol{x})[y] | (\boldsymbol{x}_i, y_i) \in S\}$. In adversarial settings, we set the margin over



(a) (b) (c) (d)

Figure 2: Product of the $\|\cdot\|_{1,\infty}$-Norm in the experiments on CIFAR-10. The red lines are the results of standard training. The blue lines are the results of adversarial training. (a) $\prod_{l=1}^{d}\|W_l\|_{1,\infty}$ of VGG-16 networks. (b) $\prod_{l=1}^{d}\|W_l\|_{1,\infty}/\gamma$ of VGG-16 networks. (c) $\prod_{l=1}^{d}\|W_l\|_{1,\infty}$ of VGG-19 networks. (d) $\prod_{l=1}^{d}\|W_l\|_{1,\infty}/\gamma$ of VGG-19 networks.

training set to be 5th-percentile of the margins of the PGD-adversarial examples of S. The choice of 5th-percentile is because the training accuracy is 100% in all the experiments. We provide ablation studies about the percentile in the Appendix C.

6.1 Comparison of Standard and Adversarial Training

In Figure 1, we provide the experiments of Frobenius norm bounds in standard and adversarial training on VGG-16 and 19 networks. We also give the experiments on VGG-11 and 13 networks in Appendix C. We train the networks using 10000 to 50000 samples. In Figure 1 (a) and (e), we can see that the robust generalization gaps (about 60%) are much larger than the standard generalization gaps (about 5%-10%).

Margins. In Figure 1 (b) and (f), we show the margins of the training set. In standard training, the margins are about 7 to 8. In adversarial settings, the margins are about 4 to 6, smaller than the margin in standard training. Therefore, the margins have some minor effects on the bad generalization of adversarial training.

Frobenius Norm Bounds. In Figure 1 (c) and (g), we can see that the $\prod_{l=1}^{d}\|W_l\|_F$ of adversarial training is much larger than the $\prod_{l=1}^{d}\|W_l\|_F$ of standard training. In (d) and (h), the $\prod_{l=1}^{d}\|W_l\|_F$ is divided by γ, we can see that the Figures is similar to the Figures in (c) and (g). There is a large gap between the two lines. The Product of weight norms has larger effects comparing to the margin. Therefore, the experiments show that one of the reasons why adversarial training cannot generalize well is that the adversarial training models have a much larger product of weight norms.

The Trends of $\prod_{l=1}^{d}\|W_l\|_F/\gamma$. To guarantee the generalization, we expect the $\prod_{l=1}^{d}\|W_l\|_F/\gamma$ grows slower than $\mathcal{O}(\sqrt{m})$, thus the generalization gap will be zero as the number of samples goes to infinity. In standard training, $\prod_{l=1}^{d}\|W_l\|_F/\gamma$ grows slowly as we increase the number of training samples. While in adversarial training, we see that the $\prod_{l=1}^{d}\|W_l\|_F/\gamma$ grows faster than $\mathcal{O}(\sqrt{m})$ in this regime. This phenomenon also shows the difficulty of robust generalization but more training data are needed to study the trends as m goes to $+\infty$.

$\|\cdot\|_{1,\infty}$-Norm Bounds. The $\|\cdot\|_{1,\infty}$-norm bounds are shown in Figure 2. Similar the the Frobenius norm bounds,The gap of $\prod_{l=1}^{d}\|W_l\|_{1,\infty}$ between adversarial training and standard training are large. But the magnitude of $\prod_{l=1}^{d}\|W_l\|_{1,\infty}$ is larger than the magnitude of $\prod_{l=1}^{d}\|W_l\|_F$.

7 Conclusion

In this paper, we first provide upper bounds for the adversarial Rademacher complexity of deep neural networks. Then, we experimentally investigate these bounds and show that the product of weight norms is a key factor explaining why adversarial training cannot generalize well. We think our results will motivate more theoretical research to understand adversarial training and empirical research to improve the generalization of adversarial training.

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A PROOF OF THE THEOREMS

A.1 PROOF OF THEOREM 1

Theorem 1 (Frobenius Norm Bound)**.** *Given the function class $\mathcal{F}$ in equation (2) under Frobbenius Norm, and the corresponding adversarial function class $\tilde{\mathcal{F}}$ in equation (1). The adversarial Rademacher complexity of deep neural networks $\mathcal{R}_S(\tilde{\mathcal{F}})$ satisfies*

$$\mathcal{R}_S(\tilde{\mathcal{F}}) \leq \frac{24}{\sqrt{m}} \max\{1, q^{\frac{1}{2}-\frac{1}{p}}\}(\|\boldsymbol{X}\|_{p,\infty} + \epsilon) L_\rho^{d-1} \sqrt{\sum_{l=1}^{d} h_l h_{l-1} \log(3d)} \prod_{l=1}^{d} M_l.$$

By assuming that $L_\rho = 1$, $p \leq 2$, $\|\boldsymbol{X}\|_{p,\infty} \leq B$, and $h = \max\{h_0, \cdots, h_d\}$, we have

$$\mathcal{R}_S(\tilde{\mathcal{F}}) \leq \mathcal{O}\left(\frac{(B+\epsilon) h \sqrt{d \log(d)} \prod_{l=1}^{d} M_l}{\sqrt{m}} \right).$$

Because of the $\inf$ operation of the function in $\tilde{\mathcal{F}}$, we cannot peel off the layers or calculate the covering number by induction on layers. Our proof is based on calculating the covering number of $\tilde{\mathcal{F}}$ directly. Before we provide the proof, we first introduce the following lemma.

Lemma 1 (Covering number of norm-balls)**.** *Let $\mathcal{B}$ be a ℓ_p norm ball with radius W. Let $d(\boldsymbol{x}_1, \boldsymbol{x}_2) = \|\boldsymbol{x}_1 - \boldsymbol{x}_2\|_p$. Define the ε-covering number of B as $\mathcal{N}(\mathcal{B}, d(\cdot,\cdot), \varepsilon)$, we have*

$$\mathcal{N}(\mathcal{B}, d(\cdot,\cdot), \varepsilon) \leq (1 + 2W/\varepsilon)^q.$$

In the case of Frobenius norm ball of $m \times n$ matrices, we have the dimension $q = m \times n$ and

$$\mathcal{N}(\mathcal{B}, \|\cdot\|_F, \varepsilon) \leq (1 + 2W/\varepsilon)^{m \times n} \leq (3W/\varepsilon)^{m \times n}.$$

Lemma 2. *if $\boldsymbol{x}_i^* \in \{\boldsymbol{x}_i' | \|\boldsymbol{x}_i - \boldsymbol{x}_i'\|_p \leq \epsilon\}$, we have*

$$\|\boldsymbol{x}_i^*\|_{r^*} \leq \max\{1, q^{1-\frac{1}{r}-\frac{1}{p}}\}(\|\boldsymbol{X}\|_{p,\infty} + \epsilon).$$

Proof: If $p \geq r^*$, by Holder's inequality with $1/r^* = 1/p + 1/s$,

$$\|\boldsymbol{x}_i^*\|_{r^*} \leq \sup \|\mathbf{1}\|_s \|\boldsymbol{x}_i^*\|_p = \|\mathbf{1}\|_s \|\boldsymbol{x}_i^*\|_p = q^{\frac{1}{s}} \|\boldsymbol{x}_i^*\|_p = q^{1-\frac{1}{r}-\frac{1}{p}} \|\boldsymbol{x}_i^*\|_p.$$

Equality holds when all the entries are equal. If $p < r^*$, we have

$$\|\boldsymbol{x}_i^*\|_{r^*} \leq \|\boldsymbol{x}_i^*\|_p.$$

Equality holds when one of the entries of θ equals to one and the others equal to zero. Then

$$\begin{aligned}
\|\boldsymbol{x}_i^*\|_{r^*} &\leq \max\{1, q^{1-\frac{1}{r}-\frac{1}{p}}\} \|\boldsymbol{x}_i^*\|_p \\
&\leq \max\{1, q^{1-\frac{1}{r}-\frac{1}{p}}\}(\|\boldsymbol{x}_i\|_p + \|\boldsymbol{x}_i - \boldsymbol{x}_i^*\|_p) \\
&\leq \max\{1, q^{1-\frac{1}{r}-\frac{1}{p}}\}(\|\boldsymbol{X}\|_{p,\infty} + \epsilon).
\end{aligned}$$

□

Lemma 3. *Let A be a $m \times n$ matrix and b be a n-dimension vector, we have*

$$\|A \cdot b\|_2 \leq \|A\|_F \|b\|_2.$$

Proof: let A_i be the rows of A, $i = 1 \cdots m$, we have

$$\|A \cdot b\|_2 = \sqrt{\sum_{i=1}^{m} (A_i b)^2} \leq \sqrt{\sum_{i=1}^{m} \|A_i\|_2^2 \|b\|_2^2} = \sqrt{\sum_{i=1}^{m} \|A_i\|_2^2} \sqrt{\|b\|_2^2} = \|A\|_F \|b\|_2.$$

□

Step 1: Diameter of $\tilde{\mathcal{F}}$. We first calculate the diameter of $\tilde{\mathcal{F}}$. $\forall f \in \mathcal{F}$, given $(\boldsymbol{x}_i, y_i)$, let $\boldsymbol{x}_i^* = \inf_{\|\boldsymbol{x}_i - \boldsymbol{x}_i'\|_p \le \epsilon_p} y f(\boldsymbol{x}_i')$, and we let $\boldsymbol{x}_i^l$ be the output of $\boldsymbol{x}_i^*$ pass through the first to the $l-1$ layer, we have

$$
\begin{aligned}
|\tilde{f}(\boldsymbol{x}_i, y_i)| &= |\inf_{\|\boldsymbol{x}_i - \boldsymbol{x}_i'\|_p \le \epsilon_p} y f(\boldsymbol{x}_i')| \\
&= |W_d \rho(W_{d-1} \boldsymbol{x}_i^{d-1})| \\
&\overset{(i)}{\le} \|W_d\|_F \cdot \|\rho(W_{d-1}\boldsymbol{x}_i^{d-1})\|_2 \\
&= \|W_d\|_F \cdot \|\rho(W_{d-1}\boldsymbol{x}_i^{d-1}) - \rho(0)\|_2 \\
&\overset{(ii)}{\le} L_\rho M_d \|W_{d-1}(\boldsymbol{x}_i^{d-1})\|_2 \\
&\le \cdots \\
&\le L_\rho^{d-1} \prod_{l=2}^{d} M_l \|W_1 \boldsymbol{x}_i^*\|_2 \\
&\le L_\rho^{d-1} \prod_{l=1}^{d} M_l \cdot \|\boldsymbol{x}_i^*\|_2 \\
&\overset{(iii)}{\le} L_\rho^{d-1} \prod_{l=1}^{d} M_l \max\{1, q^{\frac{1}{2}-\frac{1}{p}}\}(\|\boldsymbol{X}\|_{p,\infty} + \epsilon),
\end{aligned}
$$

where inequality (i) is because of Lemma 3, inequality (ii) is because of the Lipschitz propertiy of activation function $\rho(\cdot)$, inequality (iii) is because of Lemma 2. Therefore, we have

$$
2\max_{\tilde{f} \in \tilde{\mathcal{F}}} \|\tilde{f}\|_S = 2\left(\frac{1}{m}\sum_{i=1}^{m} |\tilde{f}(\boldsymbol{x}_i, y_i)|^2\right)^{\frac{1}{2}} \le 2L_\rho^{d-1} \max\{1, q^{\frac{1}{2}-\frac{1}{p}}\}(\|\boldsymbol{X}\|_{p,\infty} + \epsilon) \prod_{l=1}^{d} M_l \triangleq D.
$$

Step 2: Distance to $\tilde{\mathcal{F}}^c$. Let $\mathcal{C}_l$ be δ_l-covers of $\{\|W_l\|_F \le M_l\}$, $l = 1, 2, \cdots, d$. Let

$$
\mathcal{F}^c = \{f^c : \boldsymbol{x} \to W_d^c \rho(W_{d-1}^c \rho(\cdots \rho(W_1^c \boldsymbol{x}) \cdots)), W_l^c \in \mathcal{C}_l, l = 1, 2 \cdots, d\}
$$

$$
\text{and } \tilde{\mathcal{F}}^c = \{\tilde{f} : (\boldsymbol{x}, y) \to \inf_{\|\boldsymbol{x} - \boldsymbol{x}'\|_p \le \epsilon} y f(\boldsymbol{x}') | f \in \mathcal{F}^c\}.
$$

For all $\tilde{f} \in \tilde{\mathcal{F}}$, we need to find the smallest distance to $\tilde{\mathcal{F}}^c$, i.e. we need to calculate the

$$
\max_{\tilde{f} \in \tilde{\mathcal{F}}} \min_{\tilde{f}^c \in \tilde{\mathcal{F}}^c} \|\tilde{f} - \tilde{f}^c\|_S.
$$

$\forall (\boldsymbol{x}_i, y_i), i = 1, \cdots, n$, given $\tilde{f}$ and $\tilde{f}^c$ with $\|W_l - W_l^c\|_F \le \delta_l$, $l = 1, \cdots, d$, consider

$$
\begin{aligned}
&|\tilde{f}(\boldsymbol{x}_i, y_i) - \tilde{f}^c(\boldsymbol{x}_i, y_i)| \\
=&|\inf_{\|\boldsymbol{x}_i - \boldsymbol{x}_i'\|_p} y_i f(\boldsymbol{x}_i') - \inf_{\|\boldsymbol{x}_i - \boldsymbol{x}_i'\|_p} y_i f^c(\boldsymbol{x}_i')|
\end{aligned}
$$

Let

$$
x_i^* = \arg\inf_{\|\boldsymbol{x}_i - \boldsymbol{x}_i'\|_p} y_i f(\boldsymbol{x}_i'), \quad \text{and} \quad x_i^c = \arg\inf_{\|\boldsymbol{x}_i - \boldsymbol{x}_i'\|_p} y_i f^c(\boldsymbol{x}_i'),
$$

we have

$$
\begin{aligned}
&|\tilde{f}(\boldsymbol{x}_i, y_i) - \tilde{f}^c(\boldsymbol{x}_i, y_i)| \\
=&|y_i f(\boldsymbol{x}_i^*) - y_i f^c(\boldsymbol{x}_i^c)| \\
=&|f(\boldsymbol{x}_i^*) - f^c(\boldsymbol{x}_i^c)|.
\end{aligned}
$$

Let

$$
z_i = \begin{cases} \boldsymbol{x}_i^c & if \quad f(\boldsymbol{x}_i^*) \ge f^c(\boldsymbol{x}_i^c) \\ \boldsymbol{x}_i & if \quad f(\boldsymbol{x}_i^*) < f^c(\boldsymbol{x}_i^c) \end{cases}
$$

Then,

$$
\begin{aligned}
&|\tilde{f}(\boldsymbol{x}_i, y_i) - \tilde{f}_c(\boldsymbol{x}_i, y_i)| \\
=&|f(\boldsymbol{x}_i^*) - f^c(\boldsymbol{x}_i^c)| \\
\leq&|f(z_i) - f^c(z_i)|.
\end{aligned}
$$

Define $g_b^a(\cdot)$ as

$$
g_b^a(z) = W_b \rho(W_{b-1}\rho(\cdots W_{a+1}\rho(W_a^c \cdots \rho(W_1^c z)\cdots))).
$$

In words, for the layers $b \geq l > a$ in $g_b^a(\cdot)$, the weight is W_l, for the layers $a \geq l \geq 1$ in $g_b^a(\cdot)$, the weight is W_l^c. Then we have $f(z_i) = g_d^0(z_i)$, $f(z_i) = g_d^L(z_i)$. We can decompose

$$
\begin{aligned}
&|f(z_i) - f^c(z_i)| \\
=&|g_d^0(z_i) - g_d^d(z_i)| \\
=&|g_d^0(z_i) - g_d^1(z_i) + \cdots + g_d^{d-1}(z_i) - g_d^d(z_i)| \\
\leq&|g_d^0(z_i) - g_d^1(z_i)| + \cdots + |g_d^{d-1}(z_i) - g_d^d(z_i)|.
\end{aligned} \tag{10}
$$

To bound the gap $|f(z_i) - f^c(z_i)|$, we first calculate $|g_d^{l-1}(z_i) - g_d^l(z_i)|$ for $l = 1, \cdots, d$.

$$
\begin{aligned}
&|g_d^{l-1}(z_i) - g_d^l(z_i)| \\
=&|W_d\rho(g_{d-1}^{l-1}(z_i)) - W_d\rho(g_{d-1}^l(z_i))| \\
\overset{(i)}{\leq}&\|W_d\|_F\|\rho(g_{d-1}^{l-1}(z_i)) - \rho(g_{d-1}^l(z_i))\|_2 \\
\overset{(ii)}{\leq}&L_\rho M_d\|g_{d-1}^{l-1}(z_i) - g_{d-1}^l(z_i)\|_2 \\
\overset{(iii)}{=}&L_\rho M_d\|W_{d-1}\rho(g_{d-2}^{l-1}(z_i)) - W_{d-1}\rho(g_{d-2}^l(z_i))\|_2 \\
\leq&\cdots \\
\leq&L_\rho^{d-l}\prod_{j=l+1}^{d} M_j\|W_l\rho(g_{l-1}^{l-1}(z_i)) - W_l^c\rho(g_{l-1}^{l-1}(z_i))\|_2
\end{aligned}
$$

where (i) is due to Lemma 3, (ii) is due to the bound of $\|W_L\|$ and the Lipschitz of $\rho(\cdot)$, (iii) is because of the definition of $g_b^a(z)$. Then

$$
\begin{aligned}
&|g_d^{l-1}(z_i) - g_d^l(z_i)| \\
\leq&L_\rho^{d-l}\prod_{j=l+1}^{d} M_j\|W_l\rho(g_{l-1}^{l-1}(z_i)) - W_l^c\rho(g_{l-1}^{l-1}(z_i))\|_2 \\
=&L_\rho^{d-l}\prod_{j=l+1}^{d} M_j\|(W_l - W_l^c)\rho(g_{l-1}^{l-1}(z_i)))\|_2 \\
\overset{(i)}{\leq}&L_\rho^{d-l}\prod_{j=l+1}^{d} M_j\|W_l - W_l^c\|_F\|\rho(g_{l-1}^{l-1}(z_i)))\|_2 \\
\overset{(ii)}{\leq}&L_\rho^{d-l}\prod_{j=l+1}^{d} M_j\delta_l\|\rho(g_{l-1}^{l-1}(z_i)))\|_2,
\end{aligned} \tag{11}
$$

where inequality (i) is due to Lemma 3, inequality (ii) is due to Lemma 3 the assumption that $\|W_l - W_l^c\|_F \leq \delta_l$. It is lefted to bound $\|\rho(g_{l-1}^{l-1}(z_i)))\|_\infty$, we have

$$\begin{aligned}
&\|\rho(g_{l-1}^{l-1}(z_i)))\|_2 \\
=&\rho(g_{l-1}^{l-1}(z_i))) - \rho(0)\|_2 \\
\leq& L_\rho \|g_{l-1}^{l-1}(z_i))\|_2 \\
=& L_\rho \|W_{l-1}^c \rho(g_{l-2}^{l-2}(z_i)))\|_2 \\
\leq& L_\rho \|W_{l-1}^c\|_F \|\rho(g_{l-2}^{l-2}(z_i)))\|_2 \\
\leq& L_\rho M_{l-1} \|\rho(g_{l-2}^{l-2}(z_i)))\|_2 \\
\leq& \cdots \\
\leq& L_\rho^{l-1} \prod_{j=1}^{l-1} M_j \max\{1, q^{\frac{1}{2}-\frac{1}{p}}\}(\|\boldsymbol{X}\|_{p,\infty} + \epsilon).
\end{aligned} \tag{12}$$

combining inequalities (11) and (12), we have

$$\begin{aligned}
&|g_d^{l-1}(z_i) - g_d^l(z_i)| \\
\leq& L_\rho^{d-1} \frac{\prod_{j=1}^d M_j}{M_l} \delta_l \max\{1, q^{\frac{1}{2}-\frac{1}{p}}\}(\|\boldsymbol{X}\|_{p,\infty} + \epsilon) \\
=& \frac{D\delta_l}{2M_l}.
\end{aligned} \tag{13}$$

Therefore, combining inequalities (14) and (13), we have

$$\begin{aligned}
&|f(z_i) - f^c(z_i)| \\
\leq& |g_d^0(z_i) - g_d^1(z_i)| + \cdots + |g_d^{d-1}(z_i) - g_d^d(z_i)| \\
\leq& \sum_{l=1}^d \frac{D\delta_l}{2M_l}.
\end{aligned} \tag{14}$$

Then

$$\max_{\tilde{f} \in \tilde{\mathcal{F}}} \min_{\tilde{f}^c \in \tilde{\mathcal{F}}^c} \|\tilde{f} - \tilde{f}^c\|_S \leq \sum_{l=1}^d \frac{D\delta_l}{2M_l}.$$

Let $\delta_l = 2M_l\varepsilon/dD$, $l = 1, \cdots, d$, we have

$$\max_{\tilde{f} \in \tilde{\mathcal{F}}} \min_{\tilde{f}^c \in \tilde{\mathcal{F}}^c} \|\tilde{f} - \tilde{f}^c\|_S \leq \sum_{l=1}^d \frac{D\delta_l}{2M_l} \leq \varepsilon.$$

Step 3: Covering Number of $\tilde{\mathcal{F}}$. We then calculate the ε-covering number $\mathcal{N}(\tilde{\mathcal{F}}, \|\cdot\|_S, \varepsilon)$. Because $\tilde{\mathcal{F}}^c$ is a ε-cover of $\tilde{\mathcal{F}}$. The cardinality of $\tilde{\mathcal{F}}^c$ is

$$\mathcal{N}(\tilde{\mathcal{F}}, \|\cdot\|_S, \varepsilon) = |\tilde{\mathcal{F}}^c| = \prod_{l=1}^d |\mathcal{C}_l| \overset{(i)}{\leq} \prod_{l=1}^d (\frac{3M_l}{\delta_l})^{h_l h_{l-1}} = (\frac{3dD}{2\varepsilon})^{\sum_{l=1}^d h_l h_{l-1}},$$

where inequality (i)) is due to Lemma 1.

Step 4, Integration. By Dudley's integral, we have

$$\begin{aligned}
\mathcal{R}_S(\tilde{\mathcal{F}}) &\leq \frac{12}{\sqrt{m}} \int_0^{D/2} \sqrt{\log \mathcal{N}(\tilde{\mathcal{F}}, \|\cdot\|_S, \varepsilon)} d\varepsilon \\
&\leq \frac{12}{\sqrt{m}} \int_0^{D/2} \sqrt{(\sum_{l=1}^d h_l h_{l-1}) \log(3dD/2\varepsilon)} d\varepsilon \\
&= \frac{12D\sqrt{\sum_{l=1}^d h_l h_{l-1}}}{\sqrt{m}} \int_0^{1/2} \sqrt{\log(3d/2\varepsilon)} d\varepsilon.
\end{aligned} \tag{15}$$

Integration by part, we have

$$
\begin{aligned}
&\int_0^{1/2} \sqrt{\log(3d/2\varepsilon)} d\varepsilon \\
=&\frac{1}{2}\left(3\sqrt{\pi}\text{erfc}(\sqrt{\log 3d}) + \sqrt{\log 3d}\right) \\
\leq&\frac{1}{2}\left(3\sqrt{\pi}\exp(-\sqrt{\log 3d}^2) + \sqrt{\log 3d}\right) \\
=&\frac{1}{2}\left(\frac{\sqrt{\pi}}{d} + \sqrt{\log 3d}\right) \\
\leq&\frac{1}{2}\left(2\sqrt{\log 3d}\right) \\
=&\sqrt{\log 3d}.
\end{aligned} \tag{16}
$$

Plug equation (16) to equation (15), we have

$$
\mathcal{R}_S(\tilde{\mathcal{F}}) \leq \frac{24}{\sqrt{m}} \max\{1, q^{\frac{1}{2}-\frac{1}{p}}\}(\|\boldsymbol{X}\|_{p,\infty} + \epsilon) L_\rho^{d-1} \sqrt{\sum_{l=1}^{d} h_l h_{l-1} \log(3d)} \prod_{l=1}^{d} M_l.
$$

□

A.2 Proof of Theorem 2

Theorem 2 (($\|\cdot\|_{1,\infty}$-Norm Bound)**.** *Given the function class $\mathcal{F}$ in equation (1) under $\|\cdot\|_{1,\infty}$-norm, and the corresponding adversarial function class $\tilde{\mathcal{F}}$ in equation (2). The adversarial Rademacher complexity of deep neural networks $\mathcal{R}_S(\tilde{\mathcal{F}})$ satisfies*

$$
\mathcal{R}_S(\tilde{\mathcal{F}}) \leq \frac{24}{\sqrt{m}} (\|\boldsymbol{X}\|_{p,\infty} + \epsilon) L_\rho^{d-1} \sqrt{\sum_{l=1}^{d} h_l h_{l-1} \log(3d)} \prod_{l=1}^{d} M_l.
$$

The proof is mimilar to the proof of the Frobenius norm bound. We first introduce the following inequality.

Lemma 4. *Let A be a $m \times n$ matrix and b be a n-dimension vector, we have*

$$
\|A \cdot b\|_\infty \leq \|A\|_{1,\infty} \|b\|_\infty.
$$

Proof: let A_i be the rows of A, $i = 1 \cdots m$, we have

$$
\|A \cdot b\|_\infty = \max |A_i b| \leq \max \|A_i\|_1 \|b\|_\infty = \|A\|_{1,\infty} \|b\|_\infty.
$$

□

Step 1: Diameter of $\tilde{\mathcal{F}}$. We first calculate the diameter of $\tilde{\mathcal{F}}$. $\forall f \in \mathcal{F}$, given $(\boldsymbol{x}_i, y_i)$, let $\boldsymbol{x}_i^* = \inf_{\|\boldsymbol{x}_i - \boldsymbol{x}_i'\|_p \leq \epsilon_p} y f(\boldsymbol{x}_i')$, and we let $\boldsymbol{x}_i^l$ be the output of $\boldsymbol{x}_i^*$ pass through the first to the $l-1$ layer, we have

$$
\begin{aligned}
|\tilde{f}(\boldsymbol{x}_i, y_i)| &= |\inf_{\|\boldsymbol{x}_i - \boldsymbol{x}_i'\|_p \le \epsilon_p} y f(\boldsymbol{x}_i')| \\
&= |W_d \rho(W_{d-1} \boldsymbol{x}_i^{d-1})| \\
&\overset{(i)}{\le} \|W_d\|_{1,\infty} \cdot \|\rho(W_{d-1} \boldsymbol{x}_i^{d-1})\|_\infty \\
&= \|W_d\|_F \cdot \|\rho(W_{d-1} \boldsymbol{x}_i^{d-1}) - \rho(0)\|_\infty \\
&\overset{(ii)}{\le} L_\rho M_d \|W_{d-1}(\boldsymbol{x}_i^{d-1})\|_\infty \\
&\le \cdots \\
&\le L_\rho^{d-1} \prod_{l=1}^{d} M_l \cdot \|\boldsymbol{x}_i^*\|_\infty \\
&\overset{(iii)}{\le} L_\rho^{d-1} \prod_{l=1}^{d} M_l (\|\boldsymbol{X}\|_{p,\infty} + \epsilon),
\end{aligned}
$$

where inequality (i) is because of Lemma 4, inequality (ii) is because of the Lipschitz propertiy of activation function $\rho(\cdot)$, inequality (iii) is because of Lemma 2. Therefore, we have

$$
2 \max_{\tilde{f} \in \tilde{\mathcal{F}}} \|\tilde{f}\|_S = 2 \left(\frac{1}{m} \sum_{i=1}^{m} |\tilde{f}(\boldsymbol{x}_i, y_i)|^2 \right)^{\frac{1}{2}} \le 2 L_\rho^{d-1} (\|\boldsymbol{X}\|_{p,\infty} + \epsilon) \prod_{l=1}^{d} M_l \triangleq D.
$$

Step 2: Distance to $\tilde{\mathcal{F}}^c$. Let $\mathcal{C}_l^i$ be δ_l-covers of $\{\|W_l^i\|_1 \le M_l\}$, $l = 1, 2, \cdots, d$, $i = 1, \cdots, h_l$, where W_l^i is the ith row of W_l^i. Let

$$
\mathcal{F}^c = \{f^c : \boldsymbol{x} \to W_d^c \rho(W_{d-1}^c \rho(\cdots \rho(W_1^c \boldsymbol{x}) \cdots)), W_l^{ci} \in \mathcal{C}_l^i, i = 1, \cdots, h_l, l = 1, 2 \cdots, d\}
$$

$$
\text{and } \tilde{\mathcal{F}}^c = \{\tilde{f} : (\boldsymbol{x}, y) \to \inf_{\|\boldsymbol{x} - \boldsymbol{x}'\|_p \le \epsilon} y f(\boldsymbol{x}') | f \in \mathcal{F}^c\}.
$$

For all $\tilde{f} \in \tilde{\mathcal{F}}$, we need to find the smallest distance to $\tilde{\mathcal{F}}^c$, i.e. we need to calculate the

$$
\max_{\tilde{f} \in \tilde{\mathcal{F}}} \min_{\tilde{f}^c \in \tilde{\mathcal{F}}^c} \|\tilde{f} - \tilde{f}^c\|_S.
$$

$\forall (\boldsymbol{x}_i, y_i), i = 1, \cdots, n$, given $\tilde{f}$ and $\tilde{f}^c$ with $|W_l^i - W_l^{ci}| \le \delta_l$, $i = 1, \cdots, h_l$, $l = 1, \cdots, d$, we have $\|W_l - W_l^c\|_{1,\infty} \le \delta_l$. By the same argument as the step 2 of the proof o Theorem 3, we have

$$
\max_{\tilde{f} \in \tilde{\mathcal{F}}} \min_{\tilde{f}^c \in \tilde{\mathcal{F}}^c} \|\tilde{f} - \tilde{f}^c\|_S \le \sum_{l=1}^{d} \frac{D \delta_l}{2 M_l}.
$$

Let $\delta_l = 2 M_l \varepsilon / dD$, $l = 1, \cdots, d$, we have

$$
\max_{\tilde{f} \in \tilde{\mathcal{F}}} \min_{\tilde{f}^c \in \tilde{\mathcal{F}}^c} \|\tilde{f} - \tilde{f}^c\|_S \le \sum_{l=1}^{d} \frac{D \delta_l}{2 M_l} \le \varepsilon.
$$

Step 3: Covering Number of $\tilde{\mathcal{F}}$. We then calculate the ε-covering number $\mathcal{N}(\tilde{\mathcal{F}}, \|\cdot\|_S, \varepsilon)$. Because $\tilde{\mathcal{F}}^c$ is a ε-cover of $\tilde{\mathcal{F}}$. The cardinality of $\tilde{\mathcal{F}}^c$ is

$$
\mathcal{N}(\tilde{\mathcal{F}}, \|\cdot\|_S, \varepsilon) = |\tilde{\mathcal{F}}^c| = \prod_{l=1}^{d} \prod_{i=1}^{h_l} |\mathcal{C}_l^i| \overset{(i)}{\le} \prod_{l=1}^{d} \left(\frac{3 M_l}{\delta_l}\right)^{h_l h_{l-1}} = \left(\frac{3dD}{2\varepsilon}\right)^{\sum_{l=1}^{d} h_l h_{l-1}},
$$

where inequality (i)) is due to Lemma 1.

Step 4, Integration. By the same argument as the step 4 of the proof o Theorem 1, integration by part, we have

$$\mathcal{R}_S(\tilde{\mathcal{F}}) \leq \frac{24}{\sqrt{m}}(\|\boldsymbol{X}\|_{p,\infty}+\epsilon)L_\rho^{d-1}\sqrt{\sum_{l=1}^{d} h_l h_{l-1}\log(3d)}\prod_{l=1}^{d} M_l.$$

□

A.3 Proof of Theorem 3

Theorem 3 (Lower Bound)**.** *Given the function class $\mathcal{F}$ in equation (2), and the coressponding adversarial function class $\tilde{\mathcal{F}}$ in equation (1). The adversarial Rademacher complexity of deep neural networks $\mathcal{R}_S(\tilde{\mathcal{F}})$ satisfies*

$$\mathcal{R}_S(\tilde{\mathcal{F}}) \geq \Omega\left(\frac{(B+\epsilon)\prod_{l=1}^{d} M_l}{\sqrt{m}}\right).$$

The proof of the above Theorem is based on constructing a scalar network. By the definition of Rademacher complexity, it is enough to lower bound the complexity of $\tilde{\mathcal{F}}'$, where $\tilde{\mathcal{F}}'$ is a subset of $\tilde{\mathcal{F}}$. Let

$$\tilde{\mathcal{F}}' = \{\boldsymbol{x} \to \inf_{\|\boldsymbol{x}'-\boldsymbol{x}\|_p \leq \epsilon} yM_d \cdot M_2 w\boldsymbol{x} | w \in \mathbb{R}^q, \|w\|_2 \leq M_1\}.$$

By the results of the lower bounds of adversarial Rademacher complexity of linear hypothesis (Yin et al. (2019); Awasthi et al. (2020)), we obtain that

$$\mathcal{R}_S(\tilde{\mathcal{F}}) \geq \Omega\left(\frac{\max\{1, q^{\frac{1}{2}-\frac{1}{p}}\}(B+\epsilon)\prod_{l=1}^{d} M_l}{\sqrt{m}}\right).$$

similarly to the upper bound, we assume that $p \leq 2$ and we can get the bound in Theorem 3. □

A.4 Proof of Theorem 4

Theorem 4. *Given the function class $\mathcal{F}$ in equation (2) under Frobbenius Norm, and the corresponding adversarial function class $\tilde{\mathcal{F}}$ in equation (1). The adversarial Rademacher complexity of deep neural networks $\mathcal{R}_S(\tilde{\ell}_{\mathcal{F}})$ satisfies*

$$\mathcal{R}_S(\tilde{\ell}_{\mathcal{F}}) \leq \frac{48K}{\gamma\sqrt{m}}\max\{1, q^{\frac{1}{2}-\frac{1}{p}}\}(\|\boldsymbol{X}\|_{p,\infty}+\epsilon)L_\rho^{d-1}\sqrt{\sum_{l=1}^{d} h_l h_{l-1}\log(3d)}\prod_{l=1}^{d} M_l.$$

The $(1,\infty)$-norm bound is similar, except the term $\max\{1, q^{\frac{1}{2}-\frac{1}{p}}\}$.

Proof: Firstly, we have

$$\begin{aligned}
\tilde{\ell}(f(\boldsymbol{x}), y) =& \max_{\|\boldsymbol{x}-\boldsymbol{x}'\|\leq\epsilon} \phi_\gamma(M(f(\boldsymbol{x}), y)) \\
=& \phi_\gamma(\inf_{\|\boldsymbol{x}-\boldsymbol{x}'\|\leq\epsilon} M(f(\boldsymbol{x}), y)) \\
=& \phi_\gamma(\inf_{\|\boldsymbol{x}-\boldsymbol{x}'\|\leq\epsilon}([f(\boldsymbol{x})]_y - \max_{y'\neq y}[]f(\boldsymbol{x})]_{y'})) \\
=& \phi_\gamma(\inf_{\|\boldsymbol{x}-\boldsymbol{x}'\|\leq\epsilon}\inf_{y'\neq y}([f(\boldsymbol{x})]_y - [f(\boldsymbol{x})]_{y'})) \\
=& \phi_\gamma(\inf_{y'\neq y}\inf_{\|\boldsymbol{x}-\boldsymbol{x}'\|\leq\epsilon}([f(\boldsymbol{x})]_y - [f(\boldsymbol{x})]_{y'})). \\
=& \max_{y'\neq y}\phi_\gamma(\inf_{\|\boldsymbol{x}-\boldsymbol{x}'\|\leq\epsilon}([f(\boldsymbol{x})]_y - [f(\boldsymbol{x})]_{y'})).
\end{aligned}$$

Define

$$h^k(\boldsymbol{x}, y) = \inf_{\|\boldsymbol{x}-\boldsymbol{x}'\|\leq\epsilon}([f(\boldsymbol{x})]_y - [f(\boldsymbol{x})]_k) + \gamma\mathbb{1}(y=k),$$

we now prove that

$$\max_{y'\neq y}\phi_\gamma(\inf_{\|\boldsymbol{x}-\boldsymbol{x}'\|\leq\epsilon}([f(\boldsymbol{x})]_y-[f(\boldsymbol{x})]_{y'}))=\max_k\phi_\gamma(h^k(\boldsymbol{x},y)).$$

If

$$\inf_{y'\neq y}\inf_{\|\boldsymbol{x}-\boldsymbol{x}'\|\leq\epsilon}([f(\boldsymbol{x})]_y-[f(\boldsymbol{x})]_{y'})\leq\gamma,$$

we have

$$\inf_{y'\neq y}\inf_{\|\boldsymbol{x}-\boldsymbol{x}'\|\leq\epsilon}([f(\boldsymbol{x})]_y-f(\boldsymbol{x})]_{y'}))=\inf_k h^k(\boldsymbol{x},y).$$

If

$$\inf_{y'\neq y}\inf_{\|\boldsymbol{x}-\boldsymbol{x}'\|\leq\epsilon}([f(\boldsymbol{x})]_y-[f(\boldsymbol{x})]_{y'})>\gamma,$$

we have

$$\phi_\gamma(\inf_{y'\neq y}\inf_{\|\boldsymbol{x}-\boldsymbol{x}'\|\leq\epsilon}([f(\boldsymbol{x})]_y-[f(\boldsymbol{x})]_{y'}))=\phi_\gamma(\inf_k h^k(\boldsymbol{x},y))=0.$$

Therefore, we have

$$\tilde{\ell}(f(\boldsymbol{x}),y)=\phi_\gamma(\inf_k h^k(\boldsymbol{x},y))=\max_k\phi_\gamma(h^k(\boldsymbol{x},y)).$$

Define $\mathcal{H}^k=\{h^k(\boldsymbol{x},y)=\inf_{\|\boldsymbol{x}-\boldsymbol{x}'\|\leq\epsilon}([f(\boldsymbol{x})]_y-f(\boldsymbol{x})]_k)+\gamma\mathbb{1}(y=k)|f\in\mathcal{F}\}$, we have

$$\mathcal{R}(\tilde{\ell}_{\mathcal{F}})\overset{(i)}{\leq}K\mathcal{R}(\phi_\gamma\circ\mathcal{H}^k)\overset{(ii)}{\leq}\frac{K}{\gamma}\mathcal{R}(\mathcal{H}^k),\tag{17}$$

where inequality (i) is the Lemma 9.1 of (Mohri et al. (2018)), inequality (ii) is due to the Lipschitz property of $\phi_\gamma(\cdot)$. Now, define $f^k(\boldsymbol{x},y)=\inf_{\|\boldsymbol{x}-\boldsymbol{x}'\|\leq\epsilon}([f(\boldsymbol{x})]_y-f(\boldsymbol{x})]_k)$, we have $h^k(\boldsymbol{x},y)=f^k(\boldsymbol{x},y)+\gamma\mathbb{1}(y=k)$. Define the function class

$$\mathcal{F}^k=\{f^k(\boldsymbol{x},y)=\inf_{\|\boldsymbol{x}-\boldsymbol{x}'\|\leq\epsilon}([f(\boldsymbol{x})]_y-[f(\boldsymbol{x})]_k)|f\in\mathcal{F}\}.$$

We have

$$\begin{aligned}\mathcal{R}(\mathcal{H}^k)=&\frac{1}{m}\mathbb{E}_\sigma\sup_{h^k\in\mathcal{H}^k}\sum_{i=1}^m\sigma_i h^k(\boldsymbol{x}_i,y_i)\\=&\frac{1}{m}\mathbb{E}_\sigma\sup_{h^k\in\mathcal{H}^k}\sum_{i=1}^m\sigma_i\Big[f^k(\boldsymbol{x},y)+\gamma\mathbb{1}(y=k)\Big]\\=&\frac{1}{m}\mathbb{E}_\sigma\sup_{h^k\in\mathcal{H}^k}\sum_{i=1}^m\sigma_i f^k(\boldsymbol{x},y)+\frac{1}{m}\mathbb{E}_\sigma\sum_{i=1}^m\sigma_i\gamma\mathbb{1}(y=k)\\=&\frac{1}{m}\mathbb{E}_\sigma\sup_{f^k\in\mathcal{F}^k}\sum_{i=1}^m\sigma_i f^k(\boldsymbol{x},y)\\=&\mathcal{R}(\mathcal{F}^k)\end{aligned}$$

Finally, we need to bound the Rademacher complexity of $\mathcal{R}(\mathcal{F}^k)$. Notice that

$$[f(\boldsymbol{x})]_y-[f(\boldsymbol{x})]_k=(W_d^y-W_d^k)\rho(W_{d-1}(\rho(\cdots W_1(\boldsymbol{x})\cdots))),$$

and we have $\|W_d^y-W_d^k\|_F\leq 2M_l$. By Theorem 3 (the results in binary classification case), we have

$$\mathcal{R}(\mathcal{F}^k)\leq\frac{48}{\sqrt{m}}\max\{1,q^{\frac{1}{2}-\frac{1}{p}}\}(\|\boldsymbol{X}\|_{p,\infty}+\epsilon)L_\rho^{d-1}\sqrt{\sum_{l=1}^d h_l h_{l-1}\log(3d)}\prod_{l=1}^d M_l.\tag{18}$$

Combining inequalities (18) and (17), we obtain that

$$\mathcal{R}_S(\tilde{\ell}_{\mathcal{F}})\leq\frac{48K}{\gamma\sqrt{m}}\max\{1,q^{\frac{1}{2}-\frac{1}{p}}\}(\|\boldsymbol{X}\|_{p,\infty}+\epsilon)L_\rho^{d-1}\sqrt{\sum_{l=1}^d h_l h_{l-1}\log(3d)}\prod_{l=1}^d M_l.$$

□

B OTHER RELATED WORK

Adversarial Attacks and Defense. Starting from the work of (Szegedy et al. (2013)), it has now been well known that deep neural networks trained via standard gradient descent based algorithms are highly susceptible to imperceptible corruptions to the input data (Goodfellow et al. (2014); Chen et al. (2017); Carlini & Wagner (2017); Madry et al. (2017)). This has led to a series of work aimed at training neural networks robust to such perturbations (Gowal et al. (2020); Wu et al. (2020)) and works aimed at designing more sophisticated attacks to attack the classifiers (Athalye et al. (2018); Tramer et al. (2020); Chen et al. (2017)).

Adversarial Generalization. The work of (Schmidt et al. (2018); Raghunathan et al. (2019)) have shown that in some scenarios achieving adversarial generalization requires more data. The work of (Montasser et al. (2019)) explains generalization in adversarial settings using VC-dimension. Cullina et al. (2018) studies PAC-learning guarantees in the adversarial setting via VC-dimension. VC-dimension usually depends on the number of parameters in the model while Rademacher complexity usually depends on the weight matrices, Rademacher complexity usually provide tighter generalization bounds (Bartlett (1998)). Neyshabur et al. (2017b) uses a pac-bayesian approach to provide a generalization bound for neural networks. The work of (Zhang et al. (2021); Neyshabur et al. (2017a)) provide empirical analysis of the bounds of Rademacher complexity. Sinha et al. (2017) study the generalization of an adversarial training algorithm in terms of distributional robustness.

Certified robustness. A series of works study the certified robustness within the norm constraint around the original data. Cohen et al. (2019) privides an analysis on certified robustness via random smoothing. Lecuyer et al. (2019) studies certified robustness through the lens of differential privacy.

Other Theoretical Studies on Adversarial Examples. A series of works (Gilmer et al. (2018); Khoury & Hadfield-Menell (2018)) study the geometry of adversarial examples. The off-manifold assumption tells us that the adversarial examples leave the underlying data manifold (Szegedy et al. (2013)). Pixeldefends (Song et al. (2017)) uses a generative model to show that adversarial examples lie in a low probability region of the data distribution. The work of (Ma et al. (2018)) uses Local Intrinsic Dimensionality (LID) to argues that the adversarial subspaces are of low probability, and lie off the data submanifold.

C EXPERIMENT

In this section, we provide additional experiments.

C.1 EXPERIMENTS ON VGG-11 AND VGG-13

In Figure 3, we show the experiments on VGG-11 and VGG-13. As we can see, the results are the same as the results in Figure 1, the gap of product of Frobenius norm between standard and adversarial training is large, which yields bad generalization.

C.2 ABLATION STUDY OF MARGINS

In Figure 4, we show the results of the margins in 1th, 3th, and, 5th-percentile of the training dataset. Since the (robust) training accuracy is 100%, the choice of percentile will not affect the results. As we can see in the Figure, in all the cases, the margins of standard training are larger than the margins of adversarial training. Since the margins appear in the divider in the upper bound of Rademacher complexity, the margins of the training dataset have some small effects on the bad generalization of adversarial training.

C.3 EXPERIMENTS ON CIFAR-100

Perfomance. In Table 1, we show the performance of standard training and adversarial training on CIFAR-100 using VGG-16 and 19 networks. We can see that using smaller number of training samples is unable to train an acceptable VGG-networks on CIFAR-100. Therefore it is hard use only

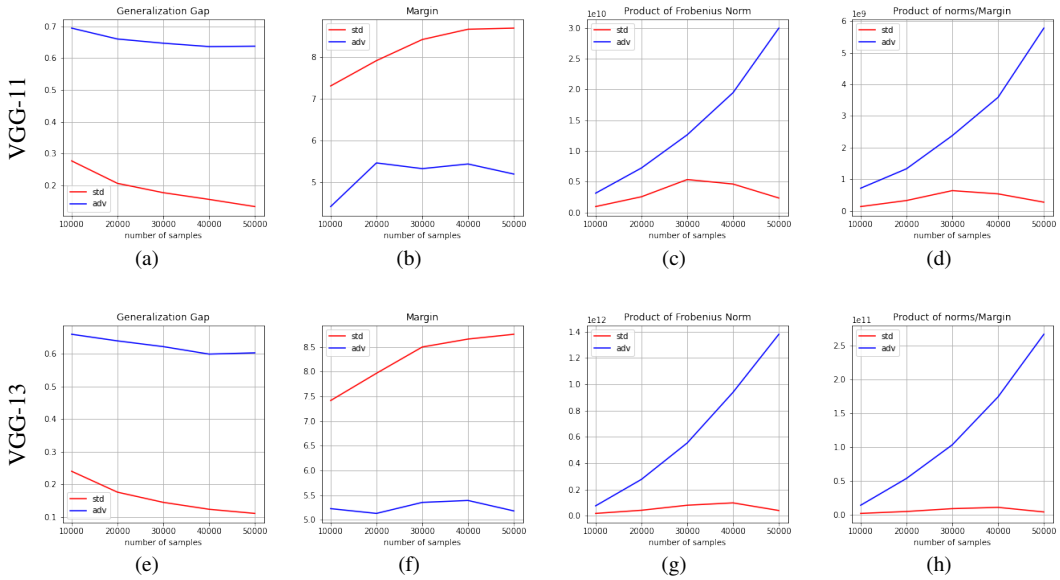

Figure 3: Product of the Frobenius norm in the experiments on VGG networks. The red lines are the results of standard training. The blue lines are the results of adversarial training. The first row are the experiments on VGG-11. The second row are the experiments on VGG-13. (a) and (e): Generalization gap. (b) and (f): Margin γ over training set. (c) and (g): $\prod_{l=1}^{d} \|W_l\|_F$ of the neural networks. (d) and (h): $\prod_{l=1}^{d} \|W_l\|_F/\gamma$ of the neural networks.

50000 training samples to study the trends of the weight norm using the experiments on CIFAR-100. We compare the product of weight norm between standard and adversarial training.

Product of Weight Norms. In Figure 5, we show the results of on training VGG-19-16 and VGG-19 on CIFAR-100. Similar to the experiments on CIFAR-10, we can see that the adversarially trained models have larger weight norm that that of the standard trained model.

Table 1: Accuracy of standard and adversarial training on CIFAR-100 using VGG-16 and 19 networks. For standard training model, we shows the clean accuracy. For adversarial training model, we show the robust accuracy against PGD attacks.

No. of Samples	10000	20000	30000	40000	50000
VGG-16-STD	0.26	0.44	0.54	0.60	0.63
VGG-16-ADV	0.12	0.15	0.17	0.18	0.19
VGG-19-STD	0.32	0.47	0.53	0.58	0.62
VGG-19-ADV	0.12	0.16	0.17	0.19	0.21

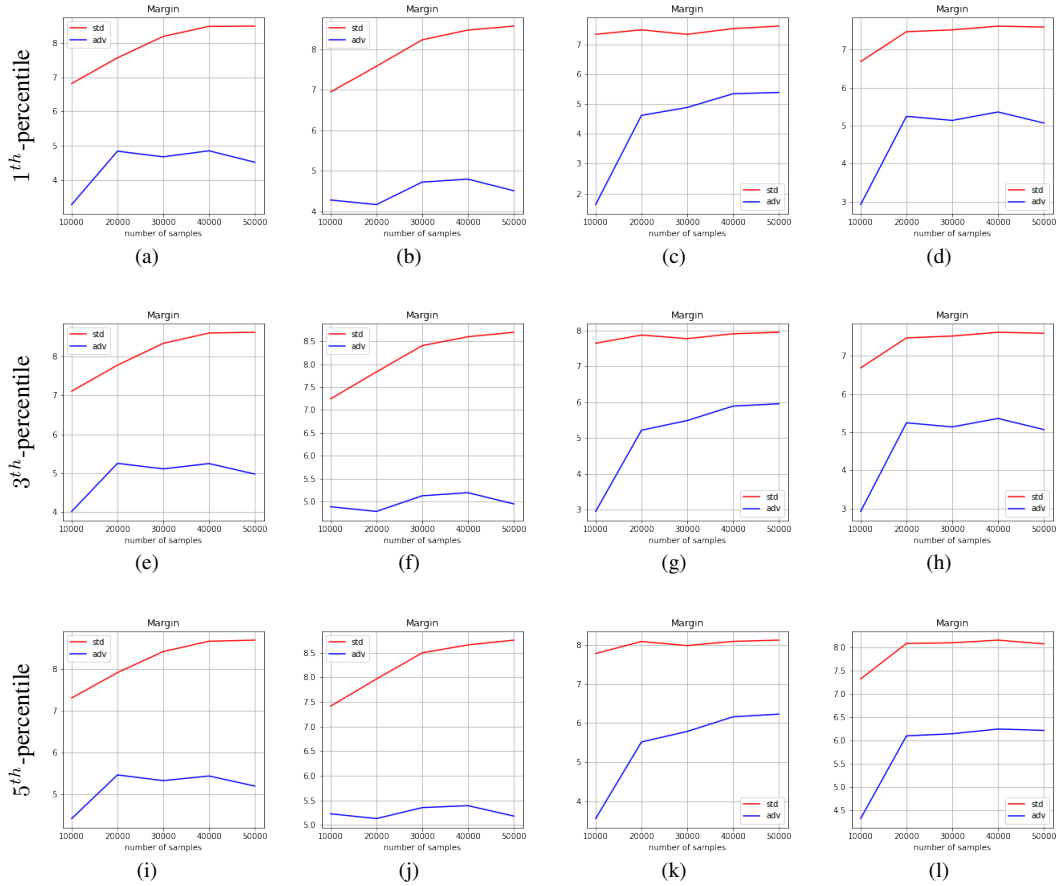

Figure 4: Ablation study of margins. The first to the 4th rows are the experiments on VGG-11, 13, 16, and 19, respectively.

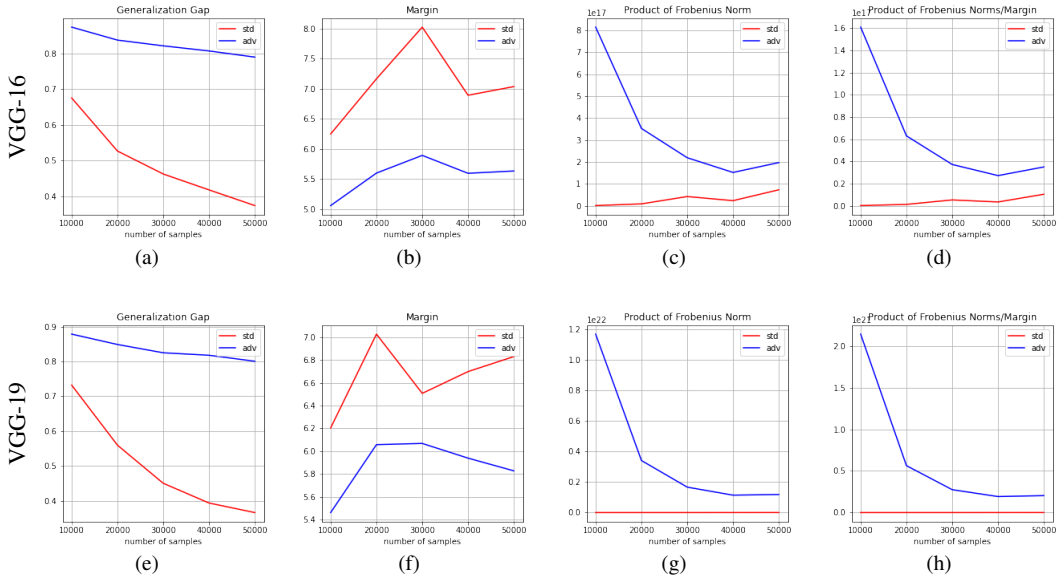

Figure 5: Product of the Frobenius norm in the experiments on VGG networks on CIFAR-100. The red lines are the results of standard training. The blue lines are the results of adversarial training. The first row are the experiments on VGG-16. The second row are the experiments on VGG-19. (a) and (e): Generalization gap. (b) and (f): Margin γ over training set. (c) and (g): $\prod_{l=1}^{d} \|W_l\|_F$ of the neural networks. (d) and (h): $\prod_{l=1}^{d} \|W_l\|_F/\gamma$ of the neural networks.