ADVERSARIAL RADEMACHER COMPLEXITY OF DEEP NEURAL NETWORKS

Anonymous authors
Paper under double-blind review

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 overfit the adversarial examples on the training dataset, and it cannot generalize well to the adversarial examples on the testset. 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

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

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 and lower bounds for the adversarial Rademacher complexity of deep neural nets. Compared to standard Rademacher complexity, the bound has a higher-order dependence on the depth and width and an additional factor ϵ.
2. We provide experiments to analyze the relationship between the generalization gap and the adversarial Rademacher complexity. We show that one of the reasons why adversarial training cannot generalize well is the large weight norms of an adversarially-trained model.

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 $[0, C]$. Then, for any $\delta \in (0, 1)$, with probability at least $1 - \delta$, the following holds for all $f \in \mathcal{F}$,*

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

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 $[0, C]$. Then, for any $\delta \in (0, 1)$, with probability at least $1 - \delta$, the following holds for all $f \in \mathcal{F}$,*

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

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. Convolution neural networks are also included in this hypothesis class because convolution layer can be viewed as a special form of fully-connected layer. 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 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 (Wu et al. (2020); 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); Zhai et al. (2019)) have shown that in some scenarios achieving adversarial generalization requires more data. The work of (Attias et al. (2021); 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 provides tighter generalization bounds (Bartlett (1998)). Neyshabur et al. (2017b) uses a pac-bayesian approach to provide a generalization bound for neural networks. Sinha et al. (2017) study the generalization of an adversarial training algorithm in terms of distributional robustness. The work of (Xing et al. (2021a;b); Javanmard et al. (2020)) study the generalization properties in the setting of linear regression. Gaussian mixture models are used to analyze adversarial generalization (Taheri et al. (2020); Javanmard et al. (2020); Dan et al. (2020)). The work of (Allen-Zhu & Li (2020)) explains adversarial generalization through the lens of feature purification.

Adversarial Rademacher Complexity. 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)). It seems that 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. The first one introduce tree transformation, but it overestimates the adversarial loss. The second one considers fast gradient sign methods (FGSM) adversarial examples, but it also requires additional assumption on the gradient.

In Appendix B, we provide the details of the above bounds and discuss why these methods seem not applicable in multi-layers cases. We also provide a comparison of adversarial generalization in Rademacher complexity framework and other frameworks. In the next section, we provide our solution of adversarial Rademacher complexity based on covering number 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). Exist sample dataset S, s.t. 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 $f \in \mathcal{F}$,*

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

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 $\phi_\gamma(\cdot)$, $\mathcal{R}_S(\tilde{\ell}_{\mathcal{F}^k}) \leq \frac{1}{\gamma}\mathcal{R}_S(\mathcal{F}^k)$. 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

$$\mathcal{R}_S(\ell_{\mathcal{F}}) \leq \mathcal{O}\left(\frac{B\sqrt{d}\prod_{l=1}^{d} M_l}{\gamma\sqrt{m}}\right) \text{ and } \mathcal{R}_S(\tilde{\ell}_{\mathcal{F}}) \leq \mathcal{O}\left(\frac{(B+\epsilon)h\sqrt{d\log d}\prod_{l=1}^{d} M_l}{\gamma\sqrt{m}}\right), \tag{10}$$

where we use the upper bound of $\mathcal{R}_S(\mathcal{F})$ in (Golowich et al. (2018)). We first discuss the algorithm-independent factors.

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, the ϵ has a small 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.

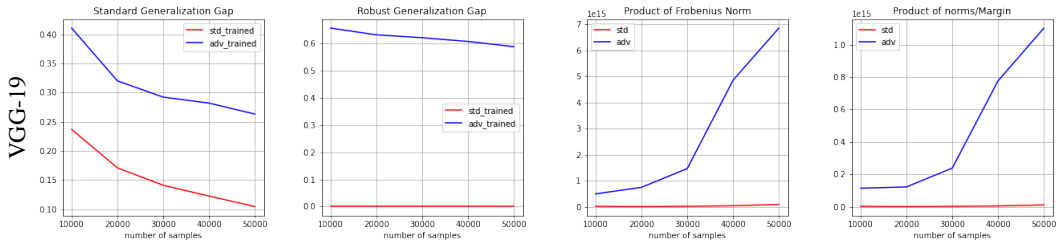
Ever though the optimal dependence on depth and width is unclear (which is not in the lower bound), the ϵ is unavoidable. The adversarial one in Equation (10) is always larger given the same M_l and γ. Therefore, the robust generalization guarantee is always weaker than the standard generalization guarantee for a model trained by any algorithms. Next, we discuss the algorithm-dependent factors.

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 are algorithm-dependent factors controlling the generalization gap. We provide experiments comparing the difference between these terms in standard and adversarial settings. To simplify the notations, we define $W_{std} := \prod_{l=1}^{d} \|W_l\|/\gamma$ if the training algorithm is standard training. Correspondingly, let $W_{adv} := \prod_{l=1}^{d} \|W_l\|/\gamma$ if the training algorithm is adversarial training. 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)). We use the experiments on VGG-19 to illustrate the results. Other experiments are provided in Appendix C.



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

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. (a): Standard Generalization gap. (b): Robust Generalization Gap. (c): $\prod_{l=1}^{d} \|W_l\|_F$ of the neural networks. (d): $\prod_{l=1}^{d} \|W_l\|_F/\gamma$ 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 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.

Standard and Robust Generalization Gap. In Figure 3 (a) and (b), we plot the standard and robust generalization gap of both standard-trained and adversarially-trained models. We use the results using 50000 training samples to discuss the experiments. Firstly, in Figure 3 (a), we can see that the generalization gap of a standard-trained model is small (about 10%). If we use a more complex model other than VGG, the generalization gap can be 0%. On the other hand, an adversarial-trained model has a larger standard generalization gap (26%). It is a widely observed phenomenon that adversarial training hurts standard generalization. One reason is that adversarial training overfits the adversarial examples and performs worse on the original examples. Secondly, in Figure 3 (b), the robust generalization gap of a standard-trained model is very small. It is because the standard-trained model can easily be attacked on both the training set and test set. Then, the robust training accuracy and test accuracy are closed to 0%. Therefore, the robust generalization gap is also 0. On the contrary, the robust generalization gap is of an adversarial-trained model is large (about 60%). This is also observed in the previous studies, and we aim to discuss the reason.

6.1 COMPARISON OF STANDARD AND ADVERSARIALLY-TRAINED MODEL

Adversarially-trained Models Have Larger Weight Norms, i.e. $W_{adv} > W_{std}$. In Figure 3 (c), 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), 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), W_{adv} is larger than W_{std}. Neural networks need more capacity to fit the adversarial examples.

Relating Standard generalization Gap and Standard Rademacher Complexity. In the upper bound of standard Rademacher complexity in Eq. (10), we can see that $\mathcal{O}(B\sqrt{d}W_{adv}/\sqrt{m}) > \mathcal{O}(B\sqrt{d}W_{std}/\sqrt{m})$, which means that adversarial training has a weaker standard generalization guarantee. It is consist with the generalization gap in Figure 3 (a) (26% versus 10%). The weight norms W_{adv} in the standard Rademacher complexity provides a different understanding why adversarial training hurts standard generalization.

Relating Robust generalization Gap and Adversarial Rademacher Complexity. Similarly, we have $\mathcal{O}((B+\epsilon)h\sqrt{d\log d}W_{adv}/\sqrt{m}) > \mathcal{O}((B+\epsilon)h\sqrt{d\log d}W_{std}/\sqrt{m})$, which means that adversarial training has a weaker robust generalization guarantee. It is consist with the robust generalization gap in Figure 3 (b) (60% versus 0%). We can see that a model with larger W_{adv} has larger robust generalization gap. Therefore, $\prod_{l=1}^{d} \|W_l\|_F/\gamma$ is a meaningful complexity measure of robust generalization gap.

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. We can see that W_{adv} grows faster than W_{std} in this regime (10000 to 50000 examples). This phenomenon also shows the difficulty of robust generalization.

6.2 Comparison of Algorithm-Independent Factors in the Two Bounds

To compare the effect of algorithm-independent factors in standard and adversarial Rademacher complexity, we fix the training algorithms and compare the difference of standard and robust generalization gap.

Comparing Two Generalization Gap in Standard Training. In Figure 3 (a) and (b), the standard and robust generalization gap of a standard-trained model (the two red lines) are both small, with generalization bounds scales as $\mathcal{O}(B\sqrt{d}W_{std}/\sqrt{m})$ and $\mathcal{O}((B+\epsilon)h\sqrt{d\log d}W_{std}/\sqrt{m})$. In this case, W_{std} is small and yields small generalization gaps. It is hard to identify the effects of $(B+\epsilon)h\sqrt{d\log d}$. We discuss the effects in adversarial cases.

Comparing Two Generalization Gap in Adversarial Training. The standard and robust generalization gap of an adversarially-trained model (the two blue lines) are about 30% and 60%, which corresponds to the generalization bounds $\mathcal{O}(B\sqrt{d}W_{adv}/\sqrt{m}) < \mathcal{O}((B+\epsilon)h\sqrt{d\log d}W_{adv}/\sqrt{m})$. The 30% gap may be positively related to the gap between $B\sqrt{d}$ and $(B+\epsilon)h\sqrt{d\log d}$. Since the optimal dependence of depth-d and width-h is unknown, it is difficult to decompose further the effects on the perturbation intensity ϵ, the depth-d, and the width-h. Since a deeper and wider model usually has better robustness, we think the effect comes from the perturbation intensity.

Ablation Studies. We provide other ablation studies in Appendix C. First, we consider different VGG architecture and give the experiments on VGG-11, 13, and 16. Secondly, We consider different percentile of the margins of the training dataset. Thirdly, we provide the experiments on $\|\cdot\|_{1,\infty}$-norm. We can see that the $\|\cdot\|_{1,\infty}$-norm bound has a larger magnitude than the Frobenius norm bound. Then, we provide the experiments on CIFAR-100. Finally, the large weight norms suggest adding a regularization term on the weights during training. We provide experiments with and without weight decay and see that the one with weight decay has a smaller generalization gap and a smaller $\prod_{l=1}^{d} \|W_l\|_F/\gamma$. These experiments suggest the strong relationship between robust generalization gap and the product of weight norms.

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.

REFERENCES

Zeyuan Allen-Zhu and Yuanzhi Li. Feature purification: How adversarial training performs robust deep learning. *arXiv preprint arXiv:2005.10190*, 2020.

Anish Athalye, Nicholas Carlini, and David Wagner. Obfuscated gradients give a false sense of security: Circumventing defenses to adversarial examples. *arXiv preprint arXiv:1802.00420*, 2018.

Idan Attias, Aryeh Kontorovich, and Yishay Mansour. Improved generalization bounds for adversarially robust learning. 2021.

Pranjal Awasthi, Natalie Frank, and Mehryar Mohri. Adversarial learning guarantees for linear hypotheses and neural networks. In *International Conference on Machine Learning*, pp. 431–441. PMLR, 2020.

Peter Bartlett, Dylan J Foster, and Matus Telgarsky. Spectrally-normalized margin bounds for neural networks. *arXiv preprint arXiv:1706.08498*, 2017.

Peter L Bartlett. The sample complexity of pattern classification with neural networks: the size of the weights is more important than the size of the network. *IEEE transactions on Information Theory*, 44(2):525–536, 1998.

Peter L Bartlett and Shahar Mendelson. Rademacher and gaussian complexities: Risk bounds and structural results. *Journal of Machine Learning Research*, 3(Nov):463–482, 2002.

Nicholas Carlini and David Wagner. Towards evaluating the robustness of neural networks. In *2017 ieee symposium on security and privacy (sp)*, pp. 39–57. IEEE, 2017.

Pin-Yu Chen, Huan Zhang, Yash Sharma, Jinfeng Yi, and Cho-Jui Hsieh. Zoo: Zeroth order optimization based black-box attacks to deep neural networks without training substitute models. In *Proceedings of the 10th ACM Workshop on Artificial Intelligence and Security*, pp. 15–26, 2017.

Jeremy Cohen, Elan Rosenfeld, and Zico Kolter. Certified adversarial robustness via randomized smoothing. In *International Conference on Machine Learning*, pp. 1310–1320. PMLR, 2019.

Daniel Cullina, Arjun Nitin Bhagoji, and Prateek Mittal. Pac-learning in the presence of evasion adversaries. *arXiv preprint arXiv:1806.01471*, 2018.

Chen Dan, Yuting Wei, and Pradeep Ravikumar. Sharp statistical guaratees for adversarially robust gaussian classification. In *International Conference on Machine Learning*, pp. 2345–2355. PMLR, 2020.

Qingyi Gao and Xiao Wang. Theoretical investigation of generalization bounds for adversarial learning of deep neural networks. *Journal of Statistical Theory and Practice*, 15(2):1–28, 2021.

Justin Gilmer, Luke Metz, Fartash Faghri, Samuel S Schoenholz, Maithra Raghu, Martin Wattenberg, and Ian Goodfellow. Adversarial spheres. *arXiv preprint arXiv:1801.02774*, 2018.

Noah Golowich, Alexander Rakhlin, and Ohad Shamir. Size-independent sample complexity of neural networks. In *Conference On Learning Theory*, pp. 297–299. PMLR, 2018.

Ian J Goodfellow, Jonathon Shlens, and Christian Szegedy. Explaining and harnessing adversarial examples. *arXiv preprint arXiv:1412.6572*, 2014.

Sven Gowal, Chongli Qin, Jonathan Uesato, Timothy Mann, and Pushmeet Kohli. Uncovering the limits of adversarial training against norm-bounded adversarial examples. *arXiv preprint arXiv:2010.03593*, 2020.

Kaiming He, Xiangyu Zhang, Shaoqing Ren, and Jian Sun. Deep residual learning for image recognition. In *Proceedings of the IEEE conference on computer vision and pattern recognition*, pp. 770–778, 2016.

Sepp Hochreiter and Jürgen Schmidhuber. Long short-term memory. *Neural computation*, 9(8): 1735–1780, 1997.

Adel Javanmard, Mahdi Soltanolkotabi, and Hamed Hassani. Precise tradeoffs in adversarial training for linear regression. In *Conference on Learning Theory*, pp. 2034–2078. PMLR, 2020.

Justin Khim and Po-Ling Loh. Adversarial risk bounds via function transformation. *arXiv preprint arXiv:1810.09519*, 2018.

Marc Khoury and Dylan Hadfield-Menell. On the geometry of adversarial examples. *arXiv preprint arXiv:1811.00525*, 2018.

Alex Krizhevsky, Geoffrey Hinton, et al. Learning multiple layers of features from tiny images. 2009.

Alex Krizhevsky, Ilya Sutskever, and Geoffrey E Hinton. Imagenet classification with deep convolutional neural networks. In *Advances in neural information processing systems*, pp. 1097–1105, 2012.

Mathias Lecuyer, Vaggelis Atlidakis, Roxana Geambasu, Daniel Hsu, and Suman Jana. Certified robustness to adversarial examples with differential privacy. In *2019 IEEE Symposium on Security and Privacy (SP)*, pp. 656–672. IEEE, 2019.

Michel Ledoux and Michel Talagrand. *Probability in Banach Spaces: isoperimetry and processes*. Springer Science & Business Media, 2013.

Xingjun Ma, Bo Li, Yisen Wang, Sarah M Erfani, Sudanthi Wijewickrema, Grant Schoenebeck, Dawn Song, Michael E Houle, and James Bailey. Characterizing adversarial subspaces using local intrinsic dimensionality. *arXiv preprint arXiv:1801.02613*, 2018.

Aleksander Madry, Aleksandar Makelov, Ludwig Schmidt, Dimitris Tsipras, and Adrian Vladu. Towards deep learning models resistant to adversarial attacks. *arXiv preprint arXiv:1706.06083*, 2017.

Mehryar Mohri, Afshin Rostamizadeh, and Ameet Talwalkar. *Foundations of machine learning*. 2018.

Omar Montasser, Steve Hanneke, and Nathan Srebro. Vc classes are adversarially robustly learnable, but only improperly. In *Conference on Learning Theory*, pp. 2512–2530. PMLR, 2019.

Behnam Neyshabur, Ryota Tomioka, and Nathan Srebro. Norm-based capacity control in neural networks. In *Conference on Learning Theory*, pp. 1376–1401. PMLR, 2015.

Behnam Neyshabur, Srinadh Bhojanapalli, David McAllester, and Nathan Srebro. Exploring generalization in deep learning. *arXiv preprint arXiv:1706.08947*, 2017a.

Behnam Neyshabur, Srinadh Bhojanapalli, and Nathan Srebro. A pac-bayesian approach to spectrally-normalized margin bounds for neural networks. *arXiv preprint arXiv:1707.09564*, 2017b.

Aditi Raghunathan, Sang Michael Xie, Fanny Yang, John C Duchi, and Percy Liang. Adversarial training can hurt generalization. *arXiv preprint arXiv:1906.06032*, 2019.

Sylvestre-Alvise Rebuffi, Sven Gowal, Dan A Calian, Florian Stimberg, Olivia Wiles, and Timothy Mann. Fixing data augmentation to improve adversarial robustness. *arXiv preprint arXiv:2103.01946*, 2021.

Ludwig Schmidt, Shibani Santurkar, Dimitris Tsipras, Kunal Talwar, and Aleksander Madry. Adversarially robust generalization requires more data. In *Advances in Neural Information Processing Systems*, pp. 5014–5026, 2018.

Karen Simonyan and Andrew Zisserman. Very deep convolutional networks for large-scale image recognition. *arXiv preprint arXiv:1409.1556*, 2014.

Aman Sinha, Hongseok Namkoong, and John Duchi. Certifiable distributional robustness with principled adversarial training. *arXiv preprint arXiv:1710.10571*, 2, 2017.

Yang Song, Taesup Kim, Sebastian Nowozin, Stefano Ermon, and Nate Kushman. Pixeldefend: Leveraging generative models to understand and defend against adversarial examples. *arXiv preprint arXiv:1710.10766*, 2017.

Christian Szegedy, Wojciech Zaremba, Ilya Sutskever, Joan Bruna, Dumitru Erhan, Ian Goodfellow, and Rob Fergus. Intriguing properties of neural networks. *arXiv preprint arXiv:1312.6199*, 2013.

Hossein Taheri, Ramtin Pedarsani, and Christos Thrampoulidis. Asymptotic behavior of adversarial training in binary classification. *arXiv preprint arXiv:2010.13275*, 2020.

Florian Tramer, Nicholas Carlini, Wieland Brendel, and Aleksander Madry. On adaptive attacks to adversarial example defenses. *arXiv preprint arXiv:2002.08347*, 2020.

Martin J Wainwright. *High-dimensional statistics: A non-asymptotic viewpoint*, volume 48. Cambridge University Press, 2019.

Dongxian Wu, Shu-Tao Xia, and Yisen Wang. Adversarial weight perturbation helps robust generalization. *arXiv preprint arXiv:2004.05884*, 2020.

Yue Xing, Qifan Song, and Guang Cheng. On the generalization properties of adversarial training. In *International Conference on Artificial Intelligence and Statistics*, pp. 505–513. PMLR, 2021a.

Yue Xing, Ruizhi Zhang, and Guang Cheng. Adversarially robust estimate and risk analysis in linear regression. In *International Conference on Artificial Intelligence and Statistics*, pp. 514–522. PMLR, 2021b.

Dong Yin, Ramchandran Kannan, and Peter Bartlett. Rademacher complexity for adversarially robust generalization. In *International Conference on Machine Learning*, pp. 7085–7094. PMLR, 2019.

Runtian Zhai, Tianle Cai, Di He, Chen Dan, Kun He, John Hopcroft, and Liwei Wang. Adversarially robust generalization just requires more unlabeled data. *arXiv preprint arXiv:1906.00555*, 2019.

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

$$
\begin{aligned}
&|f(z_i) - f^c(z_i)| \\
=&|g_d^0(z_i) - g_d^d(z_i)| \\
=&|g_d^0(z_i) - g_d^1(z_i) + \cdots + g_d^{d-1}(z_i) - g_d^d(z_i)| \\
\leq&|g_d^0(z_i) - g_d^1(z_i)| + \cdots + |g_d^{d-1}(z_i) - g_d^d(z_i)|.
\end{aligned} \tag{11}
$$

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

$$
\begin{aligned}
&|g_d^{l-1}(z_i) - g_d^l(z_i)| \\
\leq&L_\rho^{d-l}\prod_{j=l+1}^{d} M_j\|W_l\rho(g_{l-1}^{l-1}(z_i)) - W_l^c\rho(g_{l-1}^{l-1}(z_i))\|_2 \\
=&L_\rho^{d-l}\prod_{j=l+1}^{d} M_j\|(W_l - W_l^c)\rho(g_{l-1}^{l-1}(z_i)))\|_2 \\
\overset{(i)}{\leq}&L_\rho^{d-l}\prod_{j=l+1}^{d} M_j\|W_l - W_l^c\|_F\|\rho(g_{l-1}^{l-1}(z_i)))\|_2 \\
\overset{(ii)}{\leq}&L_\rho^{d-l}\prod_{j=l+1}^{d} M_j\delta_l\|\rho(g_{l-1}^{l-1}(z_i)))\|_2,
\end{aligned} \tag{12}
$$

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

$$\begin{aligned}
&\|\rho(g_{l-1}^{l-1}(z_i)))\|_2 \\
=&\rho(g_{l-1}^{l-1}(z_i))) - \rho(0)\|_2 \\
\leq& L_\rho \|g_{l-1}^{l-1}(z_i))\|_2 \\
=& L_\rho \|W_{l-1}^c \rho(g_{l-2}^{l-2}(z_i)))\|_2 \\
\leq& L_\rho \|W_{l-1}^c\|_F \|\rho(g_{l-2}^{l-2}(z_i)))\|_2 \\
\leq& L_\rho M_{l-1} \|\rho(g_{l-2}^{l-2}(z_i)))\|_2 \\
\leq& \cdots \\
\leq& L_\rho^{l-1} \prod_{j=1}^{l-1} M_j \max\{1, q^{\frac{1}{2}-\frac{1}{p}}\}(\|\boldsymbol{X}\|_{p,\infty} + \epsilon).
\end{aligned} \tag{13}$$

combining inequalities (12) and (13), we have

$$\begin{aligned}
&|g_d^{l-1}(z_i) - g_d^l(z_i)| \\
\leq& L_\rho^{d-1} \frac{\prod_{j=1}^d M_j}{M_l} \delta_l \max\{1, q^{\frac{1}{2}-\frac{1}{p}}\}(\|\boldsymbol{X}\|_{p,\infty} + \epsilon) \\
=& \frac{D\delta_l}{2M_l}.
\end{aligned} \tag{14}$$

Therefore, combining inequalities (15) and (14), we have

$$\begin{aligned}
&|f(z_i) - f^c(z_i)| \\
\leq& |g_d^0(z_i) - g_d^1(z_i)| + \cdots + |g_d^{d-1}(z_i) - g_d^d(z_i)| \\
\leq& \sum_{l=1}^d \frac{D\delta_l}{2M_l}.
\end{aligned} \tag{15}$$

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

$$\begin{aligned}
\mathcal{R}_S(\tilde{\mathcal{F}}) &\leq \frac{12}{\sqrt{m}} \int_0^{D/2} \sqrt{\log \mathcal{N}(\tilde{\mathcal{F}}, \|\cdot\|_S, \varepsilon)} d\varepsilon \\
&\leq \frac{12}{\sqrt{m}} \int_0^{D/2} \sqrt{(\sum_{l=1}^d h_l h_{l-1}) \log(3dD/2\varepsilon)} d\varepsilon \\
&= \frac{12D\sqrt{\sum_{l=1}^d h_l h_{l-1}}}{\sqrt{m}} \int_0^{1/2} \sqrt{\log(3d/2\varepsilon)} d\varepsilon.
\end{aligned} \tag{16}$$

Integration by part, we have

$$
\begin{aligned}
&\int_0^{1/2} \sqrt{\log(3d/2\varepsilon)} d\varepsilon \\
=&\frac{1}{2}\left(3\sqrt{\pi}\text{erfc}(\sqrt{\log 3d}) + \sqrt{\log 3d}\right) \\
\leq&\frac{1}{2}\left(3\sqrt{\pi}\exp(-\sqrt{\log 3d}^2) + \sqrt{\log 3d}\right) \\
=&\frac{1}{2}\left(\frac{\sqrt{\pi}}{d} + \sqrt{\log 3d}\right) \\
\leq&\frac{1}{2}\left(2\sqrt{\log 3d}\right) \\
=&\sqrt{\log 3d}.
\end{aligned} \tag{17}
$$

Plug equation (17) to equation (16), 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). Exist sample dataset S, s.t. 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, if $\mathcal{H}'$ is a subset of $\mathcal{H}$, we have

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

Therefore, it is enough to lower bound the complexity of $\tilde{\mathcal{F}}'$ in a particular distribution $\mathcal{D}$, where $\tilde{\mathcal{F}}'$ is a subset of $\tilde{\mathcal{F}}$. Let

$$\tilde{\mathcal{F}}' = \{\boldsymbol{x} \to \inf_{\|\boldsymbol{x}'-\boldsymbol{x}\|_p \leq \epsilon} y M_d \cdot M_2 w^T \boldsymbol{x} | w \in \mathbb{R}^q, \|w\|_2 \leq M_1\}.$$

We first prove that $\tilde{\mathcal{F}}'$ is a subset of $\tilde{\mathcal{F}}$. In $\tilde{\mathcal{F}}$, we let the activation function $\rho(\cdot)$ be a identity mapping. Let

$$W_1 = \begin{bmatrix} w \\ 0 \\ \vdots \\ 0 \end{bmatrix} \in \mathbb{R}^{h_1 \times h_0}, \quad W_l = \begin{bmatrix} M_l & 0 & \cdots & 0 \\ 0 & 0 & \cdots & 0 \\ \vdots & \vdots & & \vdots \\ 0 & 0 & \cdots & 0 \end{bmatrix} \in \mathbb{R}^{h_l \times h_{l-1}}, \quad l = 2, \cdots, d. \tag{18}$$

Then, we have $\|W_l\| \leq M_l$ and $\tilde{\mathcal{F}}$ with additional constraint in equation (18) reduce to $\tilde{\mathcal{F}}'$. In other words, $\tilde{\mathcal{F}}'$ is a subset of $\tilde{\mathcal{F}}$.

It turns out that we need to lower bound the adversarial Rademacher complexity of linear hypothesis. The results are given by the work of (Yin et al. (2019); Awasthi et al. (2020)). Below we state the result.

Proposition 4. *Given the function class $\mathcal{G} = \{\boldsymbol{x} \to y w^T \boldsymbol{x} | w \in \mathbb{R}^q, \|w\|_r \leq W\}$ and $\tilde{\mathcal{G}} = \{\boldsymbol{x} \to \inf_{\|\boldsymbol{x}'-\boldsymbol{x}\|_r \leq \epsilon} y w^T \boldsymbol{x} | w \in \mathbb{R}^q, \|w\|_r \leq W\}$, the adversarial Rademacher complexity $\mathcal{R}_S(\tilde{\mathcal{G}})$ satisfies*

$$\mathcal{R}_S(\tilde{\mathcal{G}}) \geq \max\left\{\mathcal{R}_S(\mathcal{G}), \frac{\epsilon \max\{1, q^{1-\frac{1}{r}-\frac{1}{p}}\} W}{2\sqrt{m}}\right\}.$$

Since the standard Rademacher complexity

$$\mathcal{R}_S(\mathcal{G}) = \frac{W}{m}\mathbb{E}_\sigma \|\sum_{i=1}^{m} \sigma_i \boldsymbol{x}_i\|_{r*},$$

let $\|\boldsymbol{x}_i\| = B$ with equal entries for $i = 1, \cdots, m$, by Lemma 2 we have

$$\mathcal{R}_S(\mathcal{G}) = \frac{W}{m}\mathbb{E}_\sigma |\sum_{i=1}^{m} \sigma_i| \max\{1, q^{1-\frac{1}{r}-\frac{1}{p}}\} B.$$

By Khintchine's inequality, we know that there exists a universal constant $c > 0$ such that

$$\mathbb{E}_\sigma |\sum_{i=1}^m \sigma_i| \geq c\sqrt{m}.$$

Then, we have

$$\mathcal{R}_S(\mathcal{G}) = \frac{cW}{\sqrt{m}} \max\{1, q^{1-\frac{1}{r}-\frac{1}{p}}\} B.$$

Therefore,

$$\begin{aligned}
\mathcal{R}_S(\tilde{\mathcal{G}}) &\geq \max\left\{\mathcal{R}_S(\mathcal{F}), \frac{\epsilon \max\{1, q^{1-\frac{1}{r}-\frac{1}{p}}\} W}{2\sqrt{m}}\right\} \\
&\geq \frac{1}{1+2c}\mathcal{R}_S(\mathcal{F}) + \frac{2c}{1+2c} \times \frac{\epsilon \max\{1, q^{1-\frac{1}{r}-\frac{1}{p}}\} W}{2\sqrt{m}} \\
&\geq \frac{c}{1+2c}\left(\frac{(B+\epsilon)\max\{1, q^{1-\frac{1}{r}-\frac{1}{p}}\} W}{\sqrt{m}}\right).
\end{aligned}$$

Let $W = \prod_{l=1}^d M_l$, we have

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

where $r = 2$ for frobenius norm bound and $r = 1$ for $\|\cdot\|_{1,\infty}$-norm bound. □

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

$$\mathcal{R}(\tilde{\ell}_{\mathcal{F}}) \overset{(i)}{\leq} K\mathcal{R}(\phi_\gamma\circ\mathcal{H}^k) \overset{(ii)}{\leq} \frac{K}{\gamma}\mathcal{R}(\mathcal{H}^k), \tag{19}$$

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

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

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

$$\mathcal{R}(\mathcal{F}^k) \leq \frac{48}{\sqrt{m}}\max\{1, q^{\frac{1}{2}-\frac{1}{p}}\}(\|\boldsymbol{X}\|_{p,\infty}+\epsilon)L_\rho^{d-1}\sqrt{\sum_{l=1}^d h_l h_{l-1}\log(3d)}\prod_{l=1}^d M_l. \tag{20}$$

Combining inequalities (20) and (19), 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 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.

B.1 EXISTING METHODS

'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 2^d 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.

FGSM Attack Bound. 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.

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.

B.2 Why Layer Peeling is not Applicable in Adversarial Setting?

We first take a look at the layer peeling technique.

$$
\begin{aligned}
\mathcal{R}_{\mathcal{S}}(\mathcal{H}) &= \mathbb{E}_\sigma \frac{1}{m}\big[\sup_{h\in\mathcal{H}} \sum_{i=1}^m \sigma_i h(\boldsymbol{x}_i)\big] \\
&= \mathbb{E}_\sigma \frac{1}{m}\big[\sup_{h'\in\mathcal{H}_{d-1}, \|W_d\|\le M_d} \sum_{i=1}^m \sigma_i W_d \rho(h'(\boldsymbol{x}_i))\big] \\
&\le M_d \mathbb{E}_\sigma \frac{1}{m}\Big[\sup_{h'\in\mathcal{H}_{d-1}} \Big\|\sum_{i=1}^m \sigma_i \rho(h'(\boldsymbol{x}_i))\Big\|\Big] \\
&\le 2M_d L_\rho \mathbb{E}_\sigma \frac{1}{m}\Big[\sup_{h'\in\mathcal{H}_{d-1}} \sum_{i=1}^m \sigma_i h'(\boldsymbol{x}_i)\Big] \\
&= 2M_d L_\rho \mathcal{R}_{\mathcal{S}}(\mathcal{H}_{d-1}),
\end{aligned}
$$

In adversarial settings, if we directly apply the layer peeling technique, we have

$$
\begin{aligned}
\mathcal{R}_{\mathcal{S}}(\tilde{\mathcal{H}}) &= \mathbb{E}_\sigma \frac{1}{m}\big[\sup_{h\in\mathcal{H}} \sum_{i=1}^m \sigma_i \max_{\|\boldsymbol{x}_i-\boldsymbol{x}_i'\|\le\epsilon} h(\boldsymbol{x}_i')\big] \\
&= \mathbb{E}_\sigma \frac{1}{m}\big[\sup_{h'\in\mathcal{H}_{d-1}, \|W_d\|\le M_d} \sum_{i=1}^m \sigma_i W_d \rho(h'(\boldsymbol{x}_i^*(h)))\big] \\
&\le M_d \mathbb{E}_\sigma \frac{1}{m}\Big[\sup_{h'\in\mathcal{H}_{d-1}} \Big\|\sum_{i=1}^m \sigma_i \rho(h'(\boldsymbol{x}_i^*(h)))\Big\|\Big] \\
&\le 2M_d L_\rho \mathbb{E}_\sigma \frac{1}{m}\Big[\sup_{h'\in\mathcal{H}_{d-1}} \sum_{i=1}^m \sigma_i h'(\boldsymbol{x}_i^*(h))\Big] \\
&\ne 2M_d L_\rho \mathbb{E}_\sigma \frac{1}{m}\Big[\sup_{h'\in\mathcal{H}_{d-1}} \sum_{i=1}^m \sigma_i h'(\boldsymbol{x}_i^*(h'))\Big] \\
&= 2M_d L_\rho \mathcal{R}_{\mathcal{S}}(\tilde{\mathcal{H}}_{d-1}),
\end{aligned}
$$

where $\boldsymbol{x}_i^*(h)$ is the optimal adversarial example given a d-layers neural networks, $\boldsymbol{x}_i^*(h')$ is the optimal adversarial example given a $d-1$-layers neural networks. $\boldsymbol{x}_i^*(h) \ne \boldsymbol{x}_i^*(h')$ is the main reason why layer peeling cannot be directly extended to the adversarial settings.

This is the main reason why the work we introduce above studied the variants of adversarial Rademacher complexity. Once they take off the $\max$ operation by some approximation (e.g., let $\max_{\|x-x'\|\le\epsilon} \ell(f(\boldsymbol{x}), y) \le \ell(Tf(\boldsymbol{x}), y)$), they don't have the issue $\boldsymbol{x}_i^*(h) \ne \boldsymbol{x}_i^*(h')$ and they can use the layer peeling technique to bound the variants of adversarial Rademacher complexity. The main drop back is that they change the definition of adversarial Rademacher complexity. These bounds cannot provide theoretical guarantee on the robust generalization gap.

B.3 Why covering number can help avoiding this issue?

In our opinion, it is hard to modify the procedure of layer peeling such that it is applicable in adversarial settings. Therefore, we try to bound the adversarial Rademacher complexity in a different

way, using the covering number. In the proof of Theorem 1, we can see that we can avoid the issue of $\boldsymbol{x}_i^*(h) \neq \boldsymbol{x}_i^*(h')$. Specifically, when we calculate the covering number of the whole function class $\tilde{\mathcal{F}}$ directly, we only need to define the optimal adversarial examples $\boldsymbol{x}_i^*$ for a d-layer neural networks. We don't need to consider the optimal adversarial examples of neural networks with fewer layers. This is the benefit of covering numbers.

B.4 Comparison of Different Adversarial Generalization Bounds

In this section, we compare the tightness of adversarial bounds in different frameworks. Most of the adversarial generalization bounds are introduced in section 3.

The work of (Xing et al. (2021a;b); Javanmard et al. (2020)) study the generalization properties in the setting of linear regression. Gaussian mixture models are used to analyze adversarial generalization (Taheri et al. (2020); Javanmard et al. (2020); Dan et al. (2020)). These works consider particular settings which are different from the problem of adversarial training in practice (e.g. adversarial attack and defense on CIFAR-10). Based on the very special assumptions, it is hard to compare the tightness between adversarial Rademacher complexity bounds and these bounds.

The work of (Attias et al. (2021)) provides an adversarial generalization bound in terms of VC-dimension. They assume that the perturbation set $|U| \leq k$. For each benign sample $\boldsymbol{x}$, there are at most k adversarial examples that can be chosen. To achieve ε adversarial generalization with high probability, we need the number of samples in

$$\mathcal{O}\left(\frac{1}{\varepsilon^2}(\sqrt{kVC(\mathcal{H})}\log(\frac{3}{2}+a)kVC(\mathcal{H}))+\log\frac{1}{\delta}\right),$$

for any $a > 0$. Since the different assumptions on the perturbation sets, it is hard to compare the bounds. But we can compare the Rademacher complexity and VC-dimension. We have shown that Rademacher complexity can be bounded by the weight norms of neural networks. The VC-dimension of the function class $\mathcal{H}$ can be bounded by the number of parameters of the neural networks in $\mathcal{H}$. In general, the weight norms are smaller, and Rademacher complexity provides a tighter bound.

The work of (Cullina et al. (2018)) define adversarial VC-dimension (AVC) and prove that robust generalization gap can be bounded in terms of AVC. The work of (Montasser et al. (2019)) consider whether the VC-class of the adversarial function class, denoted as $\mathcal{L}_{\mathcal{H}}^U$, is learnable. The VC-dimension of $\mathcal{L}_{\mathcal{H}}^U$ is not computable. Therefore, it is hard to compare the adversarial Rademacher complexity $\mathcal{R}_S(\tilde{\mathcal{H}})$ and the VC-dimension $VC(\mathcal{L}_{\mathcal{H}}^U)$.

C Additional Experiments

In this section, we provide additional experiments.

C.1 Experiments on VGG-11 and VGG-13

In Figure 2, we show the experiments on VGG-11 and VGG-13. As we can see, the results are the same as the results in Figure 3, the gap of product of Frobenius norm between standard and adversarial training is large, which yields bad generalization.

$\|\cdot\|_{1,\infty}$-Norm Bounds. The $\|\cdot\|_{1,\infty}$-norm bounds are shown in Figure 4. 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 $\prod_{l=1}^d \|W_l\|_F$.

C.2 Ablation Study of Margins

In Figure 5, 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.

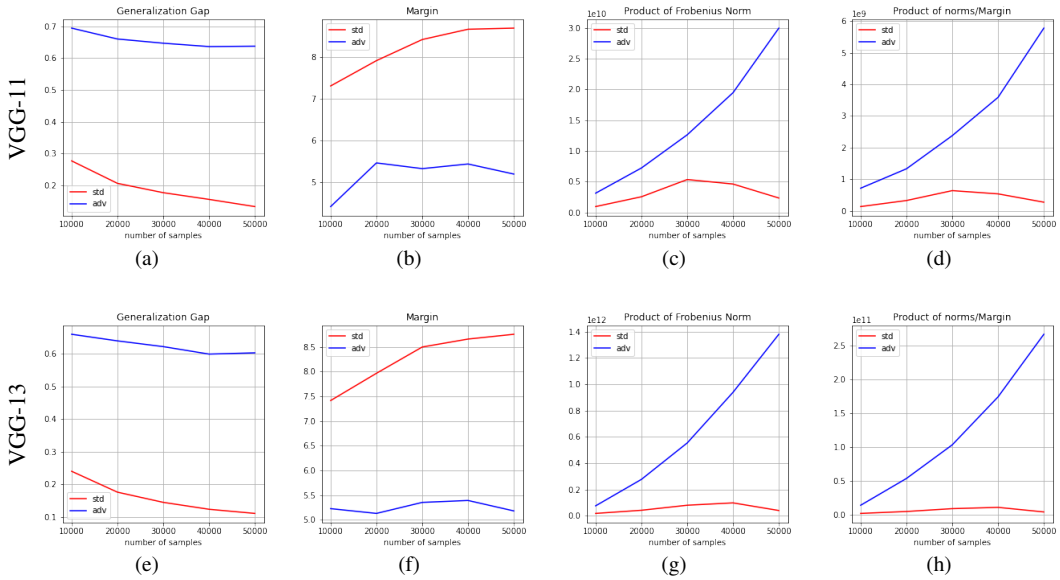


Figure 2: Product of the Frobenius norm in the experiments on VGG networks. The red lines are the results of standard training. The blue lines are the results of adversarial training. The first row are the experiments on VGG-11. The second row are the experiments on VGG-13. (a) and (e): Generalization 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.

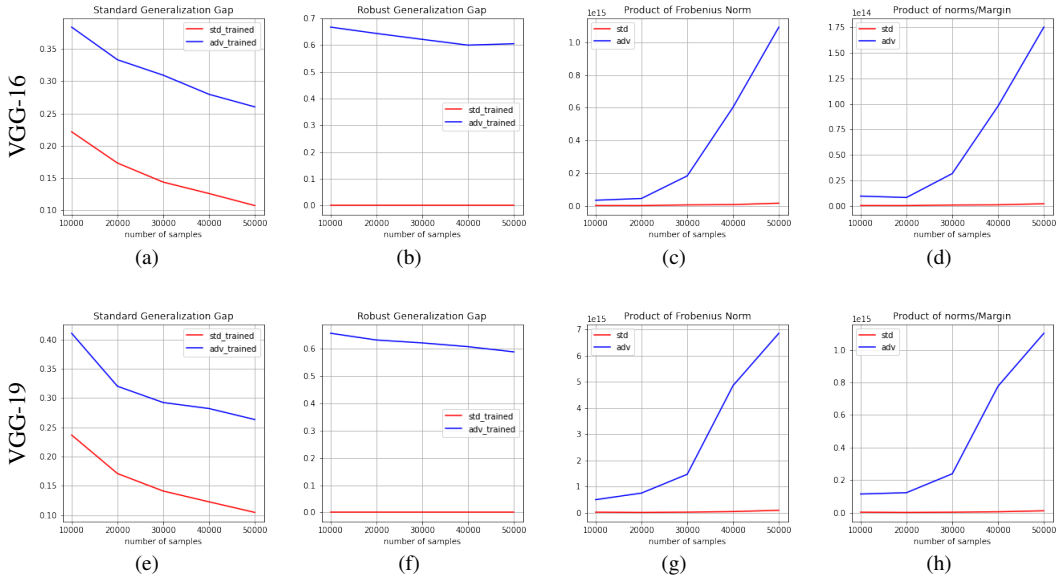
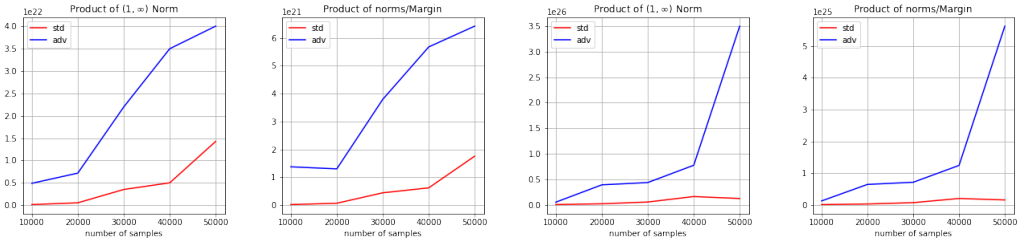


Figure 3: Product of the Frobenius norm in the experiments on CIFAR-10. The red lines are the results of standard training. The blue lines are the results of adversarial training. The first row is the experiments on VGG-16. The second row is the experiments on VGG-19. (a) and (e): Standard Generalization gap. (b) and (f): Robust Generalization Gap. (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.

C.3 Experiments on CIFAR-100

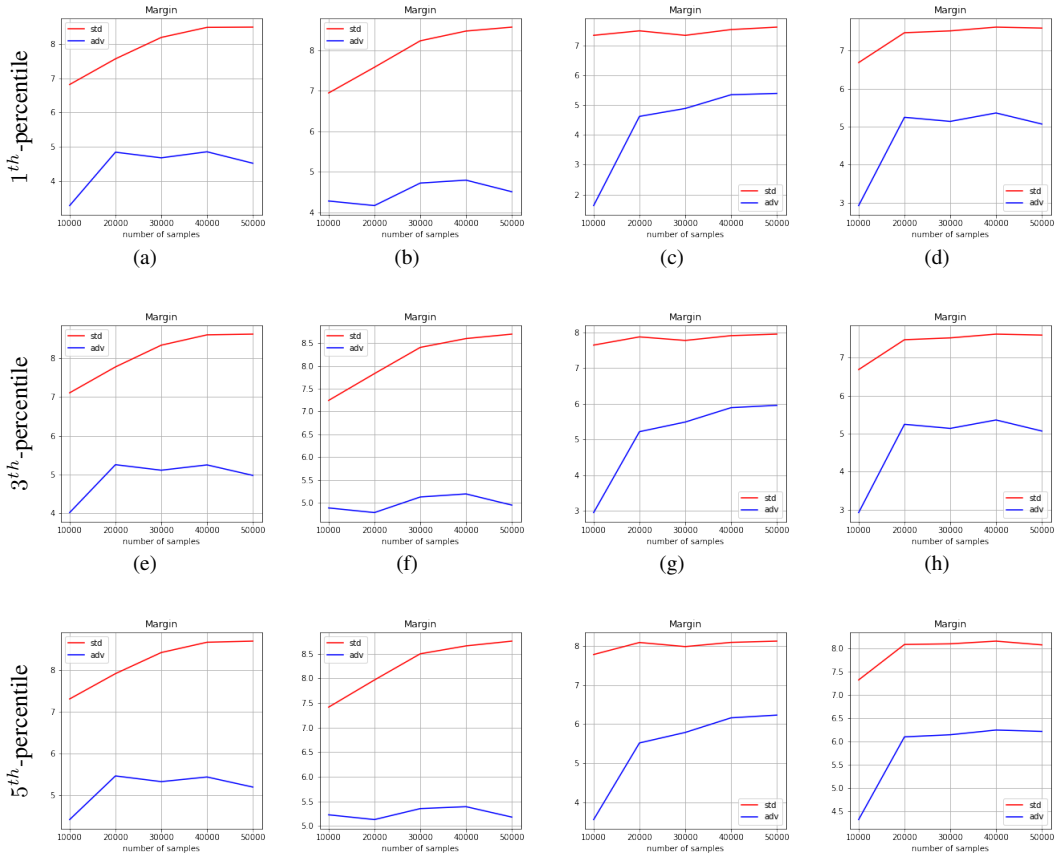
Perfomance. In Table 1, we show the performance of standard training and adversarial training on CIFAR-100 using VGG-16 and 19 networks. We can see that using smaller number of training samples is unable to train an acceptable VGG-networks on CIFAR-100. Therefore it is hard use only



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

Figure 4: 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.

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.



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

(e) (f) (g) (h)

(i) (j) (k) (l)

Figure 5: Ablation study of margins. The first to the 4th rows are the experiments on VGG-11, 13, 16, and 19, respectively.

Product of Weight Norms. In Figure 6, 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.

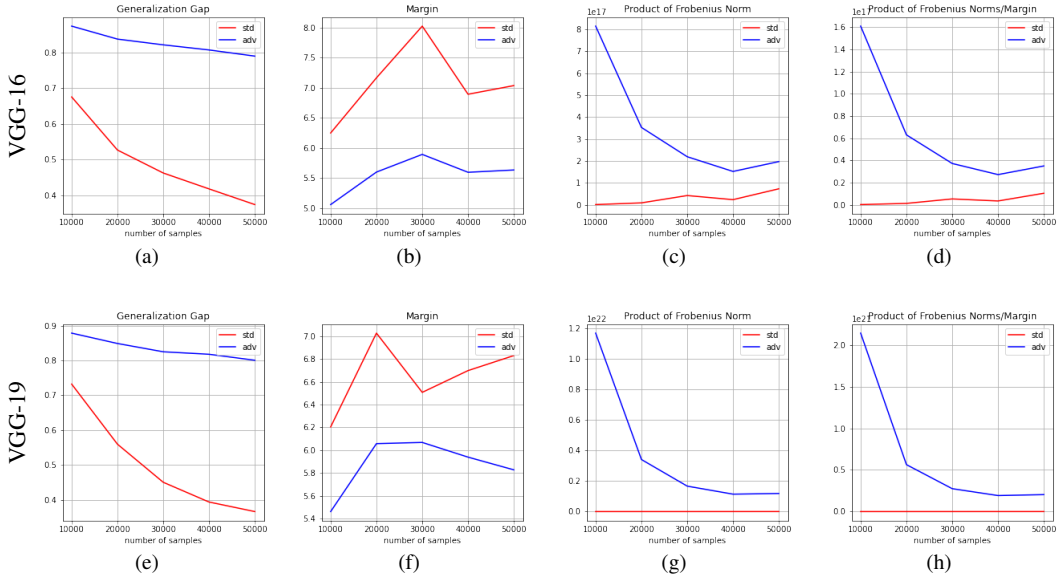


Figure 6: Product of the Frobenius norm in the experiments on VGG networks on CIFAR-100. The red lines are the results of standard training. The blue lines are the results of adversarial training. The first row are the experiments on VGG-16. The second row are the experiments on VGG-19. (a) and (e): 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.

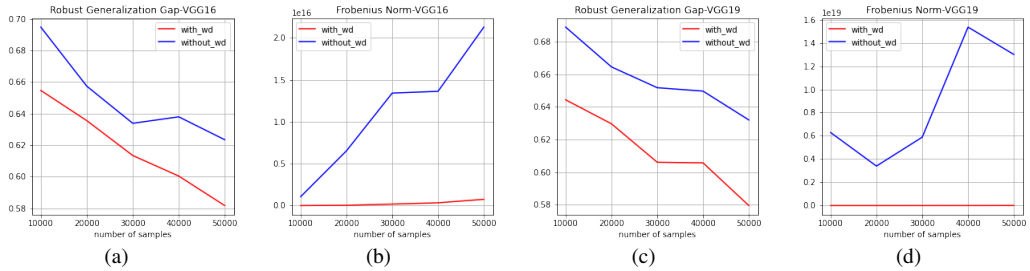


Figure 7: Experiments on the effects of weight decay. (a) Robust generalization gap with or without weight decay on VGG-16. (b) Frobenius norm with or without weight decay on VGG-16. (c) Robust generalization gap with or without weight decay on VGG-19. (d) Frobenius norm with or without weight decay on VGG-19.

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

C.4 Weight Decay

The upper bounds of adversarial Rademacher complexity suggest adding a regularization term on the weights to improve generalization, which is essentially weight decay. In Figure 7, we provide the experiments of adversarial training with and without weight decay. In Figure 7 (a) and (c), we can see that adversarial training with weight decay has a smaller robust generalization gap. In Figure 7 (b) and (d), adversarial training with weight decay have a smaller product of weight norms. These experiments show the relationship between the robust generalization gap and the product of weight norms.

D Open Problem

In this section, with list some open problems.

How to bridge the gap between the upper bound and the lower bound? These are two questions. 1, Can we obtain a depth/width-dependent lower bound? In the current analysis, we construct a class of scalar networks to provide the lower bound. Therefore, it reduced to the linear case, and we could have a closed-form expression of the adversarial examples. To obtain a depth/width-dependent lower bound, we need to construct a more general function class of neural networks. We should be able to calculate the optimal adversarial examples in this class of neural networks. 2, Can we reduce the dependence on depth/width in the upper bound? In the current analysis on the upper bound, we find that the dependence $h\sqrt{d \log d}$ is unavoidable because of the calculation of the covering number. In our opinion, we may need a new tool other than covering number (yields the dependence on depth/width) and layer peeling (seem not applicable in adversarial settings) to reduce the dependence.

Why adversarial training yields larger weight norms? In our opinion, we think it is because we require the additional capacity of the neural networks to fit the adversarial examples. As in the discussion of the work of (Neyshabur et al. (2017a)), we require more capacity of the model to fit random labels. A model with larger weight norms has a better ability to fit the training data. There might be other reasons, for example, the loss landscape of the minimax problem of adversarial training, the implicit bias of PGD attacks, or the implicit bias of adversarial training.

Is the widely used regularization techniques essentially reducing weight norms? In adversarial training, there are many training tricks to reduce overfitting and yield better generalization, for example, stochastic weight averaging, early stopping, adversarial weight perturbation, and cyclic learning. It is an open problem that whether these techniques are related to the weight norms.

How to design better algorithms to improve generalization? The most direct way to control the weight norms is weight decay, which is widely used. How to design implicit control on the weight norms is an open problem.