Robustness in deep learning: The width (good), the depth (bad), and the initialization (ugly)

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Abstract

We study the average robustness notion in deep neural networks in (selected) wide and narrow, deep and shallow, as well as lazy and non-lazy training settings. We prove that in the under-parameterized setting, width has a negative effect while it improves robustness in the over-parameterized setting. The effect of depth closely depends on the initialization and the training mode. In particular, when initialized with LeCun initialization, depth helps robustness with lazy training regime. In contrast, when initialized with Neural Tangent Kernel (NTK) and He-initialization, depth hurts the robustness. Moreover, under non-lazy training regime, we demonstrate how the width of a two-layer ReLU network benefits robustness. Our theoretical developments improve the results by Huang et al. [2021], Wu et al. [2021] and are consistent with Bubeck and Sellke [2021], Bubeck et al. [2021].

1 Introduction

It is now well-known that deep neural networks (DNNs) are susceptible to adversarially chosen, albeit imperceptible perturbations to their inputs [Goodfellow et al., 2015, Szegedy et al., 2014]. This lack of robustness is worrying as DNNs are now deployed in many real-world applications [Eykholt et al., 2018]. As a result, new algorithms are more and more being developed to defend against adversarial attacks to improve the DNN robustness. Among the current defense methods, the most commonly used and arguably the most successful method is adversarial training based minimax optimization [Athalye et al., 2018, Croce and Hein, 2020, Madry et al., 2018].

The literature focuses on several aspects of the robustness issue, from algorithms to their initialization as well as from width of neural networks to their depth (i.e., the architecture). On the practical side, Madry et al. [2018] advocate that adversarial training requires more parameters (e.g., width) for better performance in minimax optimization, which would fall into the so-called over-parameterized regime[1] [Zhang et al., 2021]. On the theory side, recent works suggest that over-parameterization may damage the adversarial robustness [Huang et al., 2021, Wu et al., 2021, Zhou and Schoellig, 2019]. In stark contrast, Bubeck and Sellke [2021], Bubeck et al. [2021] argue that the robustness of DNNs needs enough parameters to be guaranteed.

Our work is motivated to investigate this apparent contradiction in theory, and to close the gap as much as possible. We begin with a definition of *perturbation stability* of DNNs, which can be used to describe the robustness, following the spirit of Wu et al. [2021], Dohmatob and Bietti [2022]. Mathematically,

[1] Over-parameterized regime works in the setting that the number of parameters in DNN is (much) larger than the number of training data.

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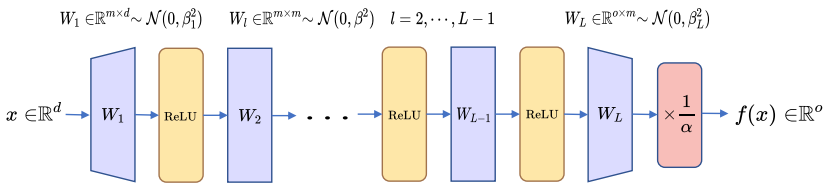


Figure 1: Schematic of our deep fully connected ReLU neural network.

Table 1: Comparison of the *perturbation stability* of a deep ReLU neural network (see Fig. 1) under three common Gaussian initializations with different variances. A formal definition of this neural network refers to Eq. (2).

Initialization name	Initialization form	Our bound for $\mathscr{P}(\boldsymbol{f}, \epsilon)/\epsilon$
LeCun et al. [2012]	$\beta = \beta_L = \sqrt{\frac{1}{m}}, \beta_1 = \sqrt{\frac{1}{d}}, \alpha = 1$	$\left(\sqrt{\frac{\pi L^3 m}{8d}} e^{-m/L^3} + 1\right)(\frac{\sqrt{2}}{2})^{L-2}$
He et al. [2015]	$\beta = \beta_L = \sqrt{\frac{2}{m}}, \beta_1 = \sqrt{\frac{2}{d}}, \alpha = 1$	$\sqrt{\frac{\pi L^3 m}{2d}} e^{-m/L^3} + 1$
Allen-Zhu et al. [2019a]	$\beta = \beta_1 = \sqrt{\frac{2}{m}}, \beta_L = \sqrt{\frac{1}{o}}, \alpha = 1$	$\sqrt{\frac{\pi L^3 m}{4o}} e^{-m/L^3} + 1$

Definition 1 (*perturbation stability*)**.** *The perturbation stability of the neural network $\boldsymbol{f}$ under data distrubution $\mathcal{D}_X$ and perturbation radius ϵ is defined as follows:*

$$\mathscr{P}(\boldsymbol{f}, \epsilon) = \mathbb{E}_{\boldsymbol{x}, \hat{\boldsymbol{x}}} \left\| \nabla_{\boldsymbol{x}} \boldsymbol{f}(\boldsymbol{x})^\top (\boldsymbol{x} - \hat{\boldsymbol{x}}) \right\|_2 , \quad \forall \boldsymbol{x} \sim \mathcal{D}_X, \ \ \hat{\boldsymbol{x}} \sim \mathit{Unif}(\mathbb{B}(\epsilon, \boldsymbol{x})) . \tag{1}$$

where $\hat{\boldsymbol{x}}$ is uniformly sampled from an ℓ_2 norm ball of $\boldsymbol{x}$ with radius ϵ, denoted as $\mathrm{Unif}(\mathbb{B}(\epsilon, \boldsymbol{x}))$. Since our definition of *perturbation stability* takes the expectation to clean and adversarial data points, it is natural to describe the *average robustness* of a neural network. It can be noticed that the larger value of *perturbation stability* means worse *average robustness*.

Based on *perturbation stability*, we study the *average robustness* of neural networks under different initializations in (selected) wide and narrow, deep and shallow, as well as lazy and non-lazy[2] training settings. Generally, non-lazy training makes the analysis of neural networks intractable as DNNs in this regime cannot be simplified as a time-independent model [Chizat and Bach, 2018], and accordingly, the analysis in this regime is mainly restricted to the two-layer setting [Mei et al., 2018, 2019].

Overall, our results suggest that the width (*good*) helps robustness in the over-parameterized regime but the depth (*bad*) can help only under certain initializations (*ugly*). To be specific, we make the following contributions and findings under the lazy/non-lazy training regimes, see Table 1.

In the **lazy training** regime, we derive upper-bounds, suggesting that

- along with the increase in width, the robustness first becomes worse in the under-parameterized setting and then gets better, and finally tends to be a constant in highly over-parameterized regions, which implies the existence of phase transition.
- the depth has more complex tendency on robustness , which largely depends on the initialization and the training mode. It can be grouped into two main classes (*cf.*, Table 1): depth helps robustness in an exponential order under LeCun initialization [LeCun et al., 2012], whereas it hurts robustness in a polynomial order under He-initialization [He et al., 2015] and under Neural Tangent Kernel (NTK) initialization [Allen-Zhu et al., 2019a].

Surprisingly, standard tools on training dynamics of neural networks [Allen-Zhu et al., 2019a, Du et al., 2018a] are sufficient to obtain our bounds, which explain the relationship between robustness and the structural/architectural parameters of neural network. Our theoretical developments improve the results by Huang et al. [2021], Wu et al. [2021], and are supported by empirical evidence.

[2]Here the lazy/non-lazy training regime indicates that neural network parameters change little/much during training. These two phases are determined by different initializations [Woodworth et al., 2020, Luo et al., 2021].

In the **non-lazy** training regime, we derive upper-bounds for two-layer networks, suggesting that

- the width improves robustness under different initializations.

We also derive a sufficient condition to identify when DNNs enter in this regime, as an initial but first attempt on understanding DNNs in this regime. Our technical contribution lies in connecting robustness to changes of neural network parameters during the early stages of training, which could expand the application scope of deep learning theory beyond *lazy training* analysis [Jacot et al., 2018, Allen-Zhu et al., 2019b].

Notations:

We use the shorthand $[n] := \{1, 2, \ldots, n\}$ for some positive integer n. We denote by $a(n) \lesssim b(n)$: there exists a positive constant c independent of n such that $a(n) \leqslant cb(n)$. The standard Gaussian distribution is $\mathcal{N}(\mathbf{0}, 1)$ with the zero-mean and the identity variance. Uniform distribution inside the sphere is $\text{Unif}(\mathbb{B}(\epsilon, \boldsymbol{x}))$ with the center $\boldsymbol{x}$ and radius ϵ. We follow the standard Bachmann–Landau notation in complexity theory e.g., $\mathcal{O}$, o, Ω, and Θ for order notation.

2 Related work

DNNs are demonstrated to be fragile, sensitive to adversarially chosen but undetectable noise both empiricallySzegedy et al. [2014] and theoretically Huang et al. [2021], Bubeck and Sellke [2021]. Adversarial training [Athalye et al., 2018, Croce and Hein, 2020, Zhang et al., 2020b] is a reliable way to obtain adversarially robust neural network. Nevertheless, improving the overall robustness of neural networks is still an unsolved problem in machine learning, especially when coupling with initializations and parameters.

Over-parameterized neural networks under lazy/non-lazy training regimes: Modern DNNs in practice [He et al., 2016] work under the setting where the number of parameters is (much) larger than the number of training data. Analysis of DNNs in terms of optimization [Safran et al., 2021, Zhou et al., 2021] and generalization [Cao and Gu, 2019] has received great attention in deep learning theory [Zhang et al., 2021], and further brings in new insights, e.g., double descent [Hassani and Javanmard, 2022], implicit bias [You et al., 2020].

In deep learning theory, neural tangent kernel (NTK) Jacot et al. [2018] and mean field analysis are two powerful tools for neural network analysis. To be specific, NTK builds an equivalence between training dynamics by gradient-based algorithms of DNNs and kernel regression under a specific initialization, and thus allows for deep networks analysis [Allen-Zhu et al., 2019a, Du et al., 2019, Chen et al., 2020]. However, this way actually requires neural networks falling in a *lazy training* regime [Chizat et al., 2019], where neural networks are able to achieve zero training loss but the parameters change little, or even remain unchanged during training. In contrast, mean-field theory establishes global convergence by casting network weights during training as an evolution in the space of probability distributions under some certain initialization to results [Mei et al., 2018, Chizat and Bach, 2018]. This strategy goes beyond lazy training regime, which allows for neural networks parameters changing in a constant order after training.

If neural networks parameters changes a lot after training, or even tend to infinity, then neural networks work in *non-lazy* training regime. Analysis of DNNs under this setting appears intractable and challenging, so current work mainly focus on two-layer neural networks [Maennel et al., 2018, Luo et al., 2021].

Robustness and over-parameterization Goodfellow et al. [2015] demonstrate that adversarial learning helps robustness and reduces overfitting, and in the following, many works focus on the trace the origin and influencing factors of adversarial examples and robustness for neural network [Schmidt et al., 2018b, Zhang et al., 2020a, Allen-Zhu and Li, 2022]. The relation between model capacity and robustness is empirically investigated by Madry et al. [2017], i.e., neural network with insufficient capacity can seriously hurt the robustness. Bubeck et al. [2021] theoretically study the inherent trade-off between the size of neural networks and their robustness, and they claim that over-parameterization is necessary for the robustness of two-layer neural networks.

However, some recent works propose the opposite view. Under the lazy training regime, Huang et al. [2021] demonstrate that when over-parameterized neural networks get wider, the robustness will be hurted in a polynomial order. At the same time, the depth hurts the robustness in an exponential order. Wu et al. [2021] affirm the view of Huang et al. [2021] on the width. However for depth, they

derive a stronger bound that the robustness gets worse in a polynomial decay as depth increases. In addition, Gao et al. [2019] also make a similar view: more model capacity (i.e., wider width and deeper depth) leads to the robustness of neural networks worse. These contradict the previous results in theoretical and experimental. In this work, we adopt a complementary view to these vast literature. We provide an in-depth theoretical analysis to investigate this apparent contradiction in theory, and to close the gap as much as possible.

3 Problem setting

Let $X \subseteq \mathbb{R}^d$ and $Y \subseteq \mathbb{R}^o$ be compact metric spaces. We assume that the training set $\mathcal{D}_{tr} = \{(\boldsymbol{x}_i, \boldsymbol{y}_i)\}_{i=1}^n$ with data dimension $\boldsymbol{x} \in \mathbb{R}^d$ and label dimension $\boldsymbol{y} \in \mathbb{R}^o$ is drawn from a probability measure $\mathcal{D}$ on $X \times Y$. Its marginal data distribution is denoted by $\mathcal{D}_X$. The goal of the classification task is to find a neural network $\boldsymbol{f} : X \to Y$ such that $\boldsymbol{f}(\boldsymbol{x}; \boldsymbol{W})$ parameterized by $\boldsymbol{W}$ is a good approximation of the label $\boldsymbol{y} \in Y$ corresponding to a new sample $\boldsymbol{x} \in X$. In this paper, we use the empirical risk $L(\boldsymbol{W}) = \frac{1}{2n}\sum_{i=1}^n \|\boldsymbol{f}(\boldsymbol{x}_i; \boldsymbol{W}) - \boldsymbol{y}_i\|_2^2$. Then we make the following assumptions.

Assumption 1. *We assume that the data satisfy* $\|\boldsymbol{x}\|_2 = 1$.

Remark: This is a standard assumption in theory on over-parameterized neural networks and it is also commonly used in practice. [Du et al., 2018b, 2019, Allen-Zhu et al., 2019a, Oymak and Soltanolkotabi, 2020, Malach et al., 2020].

3.1 Network

We focus on the typical depth-L fully-connected ReLU neural networks with the width of the l-th hidden layer m_l, $\forall l \in [L]$ (*cf.*, Fig. 1):

$$\boldsymbol{h}_{i,0} = \boldsymbol{x}_i; \quad \boldsymbol{h}_{i,l} = \phi(\boldsymbol{W}_l \boldsymbol{h}_{i,l-1}); \quad \boldsymbol{f}(\boldsymbol{x}_i; \boldsymbol{W}) = \boldsymbol{f}_i = \frac{1}{\alpha}\boldsymbol{W}_L \boldsymbol{h}_{i,L-1}; \quad \forall l \in [L-1]\, i \in [n]\,, \quad (2)$$

where the $\boldsymbol{x} \in \mathbb{R}^d$, $\boldsymbol{f}(\boldsymbol{x}) \in \mathbb{R}^o$, α is the scaling factor, weights $\boldsymbol{W} := \{\boldsymbol{W}_i\}_{i=1}^L \in \{\mathbb{R}^{m\times d} \times (\mathbb{R}^{m\times m})^{L-2} \times \mathbb{R}^{o\times m}\}$ represent the tuple of weight matrices and $\phi = \max(0, x)$ is ReLU activation function. According to the property $\phi(x) = x\phi'(x)$ of ReLU, we have $\boldsymbol{h}_{i,l} = \boldsymbol{D}_{i,l}\boldsymbol{W}_l \boldsymbol{h}_{i,l-1}$, where $\boldsymbol{D}_{i,l}$ is a diagonal matrix under the ReLU activation function defined as below.

Definition 2 (Diagonal sign matrix)**.** *For each $i \in [n]$, $l \in [L-1]$ and $k \in [m]$, the diagonal sign matrix $\boldsymbol{D}_{i,l}$ is defined as:* $(\boldsymbol{D}_{i,l})_{k,k} = 1\{(\boldsymbol{W}_l \boldsymbol{h}_{i,l-1})_k \geq 0\}$.

Initialization: Let $m_0 = d$, $m_L = o$ and $m_2 = \cdots = m_{L-1} = m$, we make the standard random initialization $[\boldsymbol{W}_l]_{i,j} \sim \mathcal{N}(0, \beta_l^2)$ for every $(i,j) \in [m_l] \times [m_{l-1}]$ and $l \in [L]$. This work holds for three commonly used Gaussian initializations, i.e., LeCun initialization [LeCun et al., 2012], He-initialization [He et al., 2015] and Neural Tangent Kernel (NTK) initialization [Allen-Zhu et al., 2019a]. The formulation of these intilization refer to Table 1.

3.2 Discussion on various robustness metrics

In Section 1, we have proposed the our robustness metric: perturbation stability (*cf.*, Definition 1). This metric can be viewed as an expectation of inner product of first-order approximation of adversarial risk [Madry et al., 2017] and the perturbations with uniform distribution, which measures the *average robustness* of the neural network. As we mentioned before, under the same perturbation radius ϵ, smaller value of $\mathcal{P}(\boldsymbol{f}, \epsilon)$ implies better *perturbation stability*, that is better *average robustness*. Previous works [Hein and Andriushchenko, 2017, Weng et al., 2018, Wu et al., 2021, Bubeck and Sellke, 2021] use Lipschitzness to describe the robustness of the network, suggesting that smaller Lipschitzness leads to robust models. However, Lipschitzness is only a worst-case measure, and cannot reasonably describe the average changes of the entire dataset. Instead, we follow the measure of Wu et al. [2021], Dohmatob and Bietti [2022], that aims to comprehensively considers the overall distribution of the data, not only the extreme case. Compared with the definition of robustness in Schmidt et al. [2018a] relies on the misclassified error of an adversarial data point, our perturbation stability measures the function value changes at the clean data point via Taylor expansion which can exclude the influence of the learning capacity of the network.

4 Main results

In this section, we state the main theoretical results. Firstly, in Section 4.1 we provide the upper bound of *perturbation stability* in lazy training regime for deep neural networks defined by Eq. (2).

The sufficient condition that the neural network Eq. (2) is under non-lazy training regime is given in Section 4.2. Finally, in Section 4.3, we provide the upper bound on *perturbation stability* during early training of two-layer network under non-lazy training regime. The proofs of our theoretical results are deferred to Appendix B, C, and D, respectively.

4.1 Upper bound of perturbation stability of DNNs under the lazy training regime

We are now ready to state the main results under the lazy training regime. The following theorem provides the upper bound of *perturbation stability* and connects to depth and width of network and dimension of data for a deep fully-connected neural network under standard Gaussian initialization.

Theorem 1. *Given an L-layer neural network $\boldsymbol{f}$ defined by Eq. (2) trained by $\{(\boldsymbol{x}_i, \boldsymbol{y}_i)\}_{i=1}^n$ satisfying Assumption 1, for the convenience of analysis, we set $\alpha = 1$ and $\beta := \beta_2 = \cdots = \beta_{L-1}$, define a constant $\gamma := \beta/\sqrt{\frac{2}{m}}$, then under a small perturbation ϵ , we have the following:*

$$\frac{\mathscr{P}(\boldsymbol{f}, \epsilon)}{\epsilon} \lesssim \left(\sqrt{\frac{\pi L^3 m^2 \beta_1^2 \beta_L^2}{8}} e^{-m/L^3} + 1\right) \gamma^{L-2} . \tag{3}$$

Remark: Our results cover the effect of the width and depth of neural network on robustness under various common initializations depending on $\gamma \gtreqless 1$.

For the initializations used in practice, our theoretical results can be mainly divided into two classes. 1) Depth helps robustness in an exponential order under LeCun initialization: our Theorem 1 implies $\left(\sqrt{\frac{\pi L^3 m}{8d}} e^{-m/L^3} + 1\right)(\frac{\sqrt{2}}{2})^{L-2}$; 2) Depth hurts robustness in a polynomial order under He-initialization $\left(\sqrt{\frac{\pi L^3 m}{2d}} e^{-m/L^3} + 1\right)$ and under NTK initialization $\left(\sqrt{\frac{\pi L^3 m}{4o}} e^{-m/L^3} + 1\right)$ derived by Theorem 1. When employing other initializations, robustness could be hurted in a exponential order. Below, we elaborate on these three initalizations:

- LeCun initialization ($\gamma = \frac{\sqrt{2}}{2}$): The order has three main parts $\sqrt{\frac{\pi L^3 m}{8d}}$, e^{-m/L^3} and $(\frac{\sqrt{2}}{2})^{L-2}$. The first two parts implies a phase transition phenomenon between *perturbation stability* and over-parameterization for the width m. Concretely, $\sqrt{\frac{\pi L^3 m}{8d}}$ is an increasing function with respect to m and e^{-m/L^3} is a decreasing function with respect to m. In the under-parameterized region (m is small), $\sqrt{\frac{L^3 m}{d}}$ plays a major role, so the stability will increase as m increases . After a critical point, e^{-m/L^3} plays a major role, so the stability will decrease as m increases . When m tends to infinity, the first term of bound tends to 0. Hence the *perturbation stability* tends to be a constant and independent with width m as the width m tends to infinity. However, for depth L, it holds that $\gamma = \frac{\sqrt{2}}{2}$. So the third part has the faster increase/decrease speed than the first and second part and play a major role in the tendency. The *perturbation stability* of the neural network exponentially decreases with respect to the depth. That means that for LeCun initialization, the deeper the network, the better robustness . Nevertheless, the energy of LeCun initialization decreases with the increase of network depth, which means that training deep network with LeCun initialization is very difficult. Hence we need a trade off between robustness and training difficulty regarding network depth in practice for LeCun initialization.
- He initialization and NTK initialization ($\gamma = 1$): here the bounds only have the first two parts. From this, it is easy to see that for the network width m, the two initializations have similar phase transition phenomena with LeCun initialization. Regarding to the depth, when L is large, the first part $\sqrt{L^3}$ plays a major role in the *perturbation stability*. So these two initializations hurt the robustness of the neural network polynomially.
- In addition, if the initialization admits $\gamma \geq 1$, then the depth L of network will exponentially hurt robustness of the neural network.

Comparison with previous work: Theorem 1 provides a new relationship between the robustness with width and depth of DNNs. We compare our result with [Wu et al., 2021, Huang et al., 2021]

using a basic NTK initialization Allen-Zhu et al. [2019a] (suppose that $m \gg o$ and $m \gg d$). For better comparison, we derive their results under our robustness metric *perturbation stability*, reported by Table 2.

Table 2: Comparison of the orders of the proposed bound with other two recent works. Our results are general to cover both under- and over-parameterized regimes, which expands the application scope of previous results [Wu et al., 2021, Huang et al., 2021]. (The original result of [Wu et al., 2021] contains the condition $\frac{m}{(\log m)^6} \geq L^{12}$, then the result is reduced to $\sqrt{mL}$).

Metrics	Our result	Wu et al. [2021]	Huang et al. [2021]
$\mathscr{P}(\boldsymbol{f}, \epsilon)/\epsilon$	$\sqrt{\frac{\pi L^3 m}{4o}} e^{-m/L^3} + 1$	$L^2 m^{1/3} \sqrt{\log m} + \sqrt{mL}$	$2^{\frac{3L-5}{2}} \sqrt{m}$

Our results indicate a behavior transition on the width. For the over-parameterized regime, the robustness of neural network only depends on the perturbation energy, and it is almost independent of the width m. The results on width are significantly better than the previous results increasing as the square root of m. For depth L, our results provide a tighter and more precise estimate as compared to Wu et al. [2021] in a two-degree polynomial increasing order and Huang et al. [2021] in an exponential increasing order.

4.2 Sufficient condition for neural network under non-lazy training regime

Beyond the lazy training regime, we turn our attention to non-lazy training regime and present results about the sufficient condition for (well-chosen) initialization of neural networks when entering into the non-lazy training regime. This is a first attempt to understanding training dynamics of DNNs in this regime.

Our result requires a further assumption on the data and the empirical risk as follows.

Assumption 2. *For a single-output network defined in Eq.* (2)*, we assume that* $\max_{i\in[n]} y_i \geq C_1 \geq 0$. *We also assume that the neural network can be well-trained such that the empirical risk is* $\mathcal{O}(\frac{1}{n})$.

Remark: This is a common assumption in the field of optimization [Song et al., 2021] in the under- and over-parameterized regime, and we can even assume zero risk. Here we follow the specific assumption of Luo et al. [2021].

Now we are ready to present our result, a sufficient condition to identify when deep ReLU neural networks fall into non-lazy training regime, as a promising extension of Luo et al. [2021] on two-layer neural networks. To avoid cluttering the analysis, we consider a single-output i.e., $o = 1$.

Theorem 2. *Given an L-layer neural network* $\boldsymbol{f}$ *defined by Eq.* (2) *with one-dimensional output, trained by* $\{(\boldsymbol{x}_i, \boldsymbol{y}_i)\}_{i=1}^n$ *satisfy Assumptions 1 and 2. Suppose that* $\alpha \gg (m^{3/2} \sum_{i=1}^L \beta_i)^L$ *and* $m \gg d$ *in Eq.* (2)*, then for sufficiently large* m*, with probability at least* $1 - (L-2)\exp(-\Theta(m^2)) - \exp(-\Theta(md)) - \exp(-\Theta(m))$ *over the initialization, we have:*

$$\sup_{t\in[0,+\infty)} \frac{\|\boldsymbol{W}_l(t) - \boldsymbol{W}_l(0)\|_{\mathrm{F}}}{\|\boldsymbol{W}_l(0)\|_{\mathrm{F}}} \gg 1\,.$$

Remark: The condition $\alpha \gg (m^{3/2} \sum_{i=1}^L \beta_i)^L$ implies that, a neural network falls in a non-lazy training regime when the variance of the Gaussian initialization is very small. A typical case is, taking $m \gg L^2$, choosing $\alpha = 1$ and $\forall l \in [L];\ \beta_l = \frac{1}{m^2}$. Commonly used initializations such as NTK initialization, LeCun initialization, He's initialization lead to lazy training.

4.3 Upper bound of perturbation stability for two-layer networks in non-lazy training

Unlike lazy training, weights of non-lazy training concentrate on few directions determined by the input data in the early stages of training. The following theorem describes the neural network *perturbation stability* in the early training stage as a function of network width in the non-lazy training regime. For ease of description, here we consider a special initialization scheme under the non-lazy regime, more cases under this theorem and proof are deferred to the Appendix D.

Theorem 3. *Given a two-layer neural network $\boldsymbol{f}$ defined by Eq.* (2) *and trained by* $\{(\boldsymbol{x}_i, y_i)\}_{i=1}^n$ *satisfying Assumption 1, using gradient descent under the squared loss, consider the following initialization in Eq.* (2) *:* $L = 2$, $\alpha \sim 1$, $\beta_1 \sim \beta_2 \sim \beta \sim \frac{1}{m^c}$ *with* $c \geq 1.5$, $m \gg n^2$ *and* $t \leq t^\star(n, m, \alpha)$, *then for a small range of perturbation* ϵ, *with probability at least* $1 - n\exp(-\frac{n}{2}) - \frac{3}{n}$ *over initialization, we have the following:*

$$\frac{\mathscr{P}(\boldsymbol{f}_t, \epsilon)}{\epsilon} \leq \Theta\left(\frac{\sqrt{n\log m} + n}{m^{c-1}}\left(\frac{1}{\sqrt{n^3 m}} + \frac{1}{m^{c-0.5}}\right)\right). \tag{4}$$

Remark: Under this setting of non-lazy training regime, the robustness and width of the neural network are positively correlated in the early stages of training. That is, as the width m increases in the over-parameterized regime, a Gaussian initialization with smaller variance results in the robustness increasing in a faster decay. Our result holds for other initialization schemes in the non-lazy training regime, e.g., $c = 2$ leads to $\mathscr{P}(\boldsymbol{f}_t, \epsilon)/\epsilon \leq \Theta\left(\frac{\sqrt{n\log m}+n}{m^{2.5}}\right)$; and $c = 3$ leads to $\mathscr{P}(\boldsymbol{f}_t, \epsilon)/\epsilon \leq \Theta\left(\frac{\sqrt{n\log m}+n}{m^{4.5}}\right)$.

5 Numerical evidence

We validate our theoretical results with a series of experiments. In Section 5.2 we first verify that our initialization settings belong in the lazy and the non-lazy training regimes. In Section 5.3, we then explore the effect of varying widths from under-parameterized to over-parameterized regions on the *perturbation stability* of neural networks. In Section 5.4, we finally compare the effect of two different initializations and the network depth on the *perturbation stability*. Additional experimental results can be found in Appendix E.

5.1 Experimental settings

Here we present our experimental setting including models, hyper-parameters, the choice of width and depth, and initialization schemes. We use the popular datasets of MNIST [Lecun et al., 1998] and CIFAR-10 [Krizhevsky et al., 2014] for experimental validation.

Models: We report results using the following models: fully connected ReLU neural network named "FCN" in main paper and convolutional ReLU neural network named "CNN" in Appendix E.

Hyper-parameters: Unless mentioned otherwise, all models are trained for 50 epochs with a batch size of 64. The initial value of the learning rate is 0.001. After the first 25 epochs, the learning rate is multiplied by a factor of 0.1 every 10 epochs. The SGD is used to optimize all the models, while the cross-entropy loss is used.

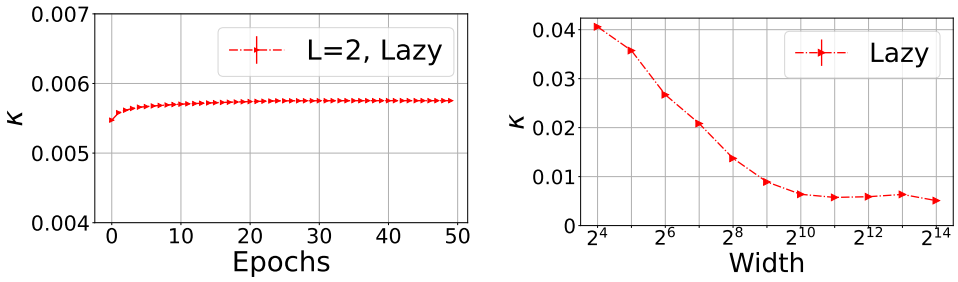
Width and depth: In order to verify our theoretical results, we conduct a series of experiments with different depths and widths of the same type neural network. Specifically, our experiments include 11 different widths from 2^4 to 2^{14}, and four different choices of depths, i.e., $2, 4, 6, 8, 10$.

Initialization: We report results using the following initializations: 1) He initialization where $W_{ij} \sim \mathcal{N}(0, \frac{2}{m_{in}})$, 2) LeCun initialization where $W_{ij} \sim \mathcal{N}(0, \frac{1}{m_{in}})$ and 3) An initialization allows for non-lazy training regime on two-layer networks, i.e., $\beta_1 = \beta_2 = 1/m^2$ and $\alpha = 1$.

5.2 Validation for lazy and non-lazy training regimes

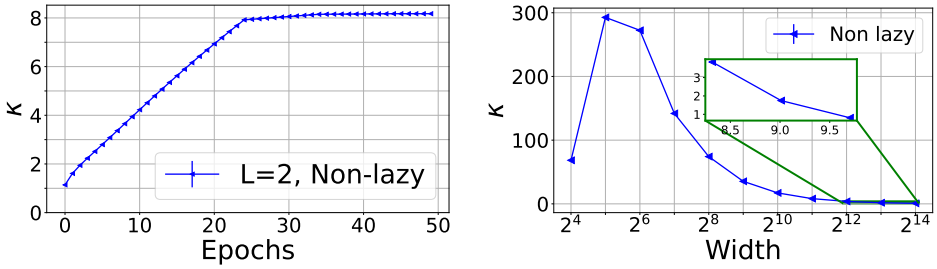
Before verifying our results, we need identify the lazy and non-lazy training regime under different initializations. To this end, we define a measure *lazy training ratio*, i.e., $\kappa = \frac{\sum_{l=1}^{L}\|\boldsymbol{W}_l(t) - \boldsymbol{W}_l(0)\|_{\mathrm{F}}}{\sum_{l=1}^{L}\|\boldsymbol{W}_l(0)\|_{\mathrm{F}}}$ to measure whether the neural network is under the lazy training regime. A smaller κ implies that the neural network is more close to lazy training.

According to the theory, we employ He initialization and non lazy training initialization we state in Section 5.1 then conduct the experiment under two-layer neural networks to verify that their lazy training ratio matches the theoretical results of lazy training and non-lazy training (i.e. the experiment is under the correct regime). Fig. 2(a) and Fig. 2(b) show the tendency of ratio with respect to time (training epochs) and relationship between width and lazy training ratio of neural networks under lazy training regime, respectively. We can find that the ratio of lazy traing regime is almost a constant



(a) (b)

Figure 2: (a) Tendency with respect to time (training epochs) and (b) relationship between width and lazy training ratio of neural networks. Fig. 2(a) shows that ratio κ is small and almost unchanged, recognized as *lazy training*. In Fig. 2(b), we can see that the κ decreases with the increasing width.



(a) (b)

Figure 3: (a) Tendency with respect to time (training epochs) and relationship with width of non-lazy training ratio of neural networks. Fig. 3(a) shows that ratio κ is changed a lot (increasing and then remains unchanged), recognized as *non-lazy training*. The tendency of κ for non-lazy training is increasing with the width and then decreasing, i.e., a phase transition in Fig. 3(b).

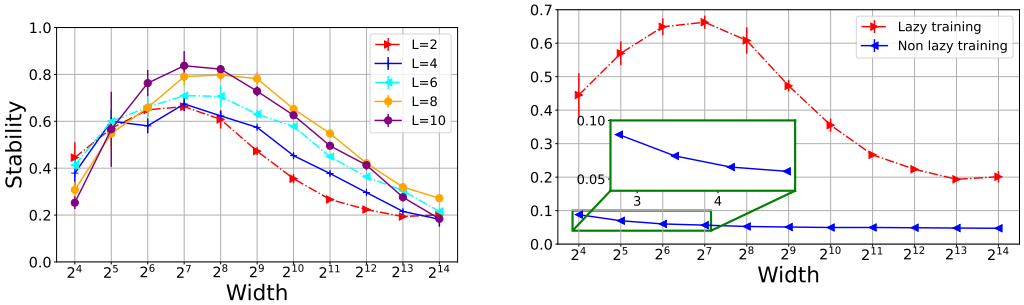
that does not change with time, and this constant decreases with the width of network increases. This is in line with what we know about lazy training [Chizat et al., 2019].

Likewise, Fig. 3 shows the ratio tendency with time and width under non-lazy training regime. The ratio increases almost linearly over time in Fig. 3(a). In epoch 25 we decrease the learning rate, which results in the increase rate of κ changes. At the same time Fig. 3(b) shows the similar tendency between width and lazy training ratio as lazy training. However, the value of κ is much higher than that of lazy training regime. Combining the results about tendency with time, the ratio will be expected to increase as time at a slow decay and tend to infinity under highly wide width setting.

5.3 Validation for width

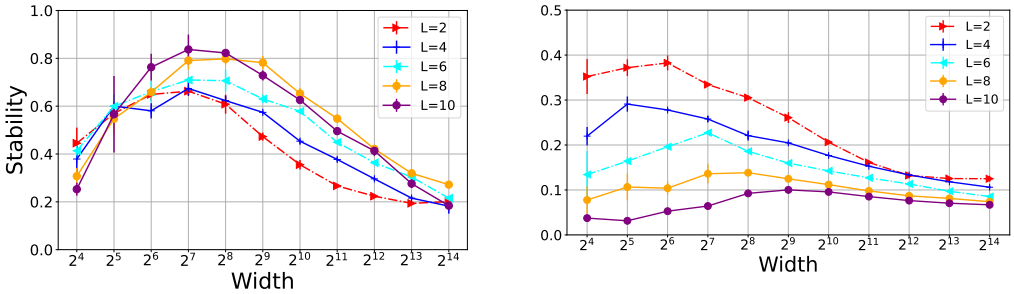
We verify the relationship between the *perturbation stability* and the width of network as illustrated by Eqs. (3) and (4). We conduct a series of experiments on MNIST dataset using FCN with different widths. Fig. 4 shows the relationship between *perturbation stability* and width of FCN with different depths and training regimes. Here for lazy training and non-lazy training we use the same initialization as Section 5.2.

Fig. 4(a) exhibits the relationship between the *perturbation stability* and the width for neural networks with different depths of $L = 2, 4, 6, 8$, and 10. All of the five curves show the phase transition with width, and the *perturbation stability* first increases and then decreases with width, which match our theoretical results. Fig. 4(b) shows the difference of the effect of width on the *perturbation stability* of lazy and non-lazy training for two-layer neural networks. First, the *perturbation stability* of non-lazy training is significantly smaller than that of lazy training, which means non-lazy training regime is more robust. Besides, the *perturbation stability* of non-lazy training decrease with the width of the neural network increases, which coincides with our theoretical result, i.e., no phase transition phenomenon.



(a) Lazy training with different widths and depths (b) Lazy and non-lazy training under different widths

Figure 4: Influence of width of neural network on *perturbation stability*. (a) phase transition of *perturbation stability vs.* width with five different depths under lazy training. (b) the difference between lazy training and non-lazy training regimes for two layer neural networks.



(a) (b)

Figure 5: Relationship between *perturbation stability* and depth of FCN under He initialization (a) and LeCun initialization (b) different depths of $L = 2, 4, 6, 8$ and 10.

5.4 Validation for depth and initialization

Here we explore the effect of depth on *perturbation stability* under lazy training regime with different initializations in Fig. 5(a) and Fig. 5(b). Our results show the tendency of *perturbation stability* for FCN with different widths and depths under He initialization and LeCun initialization, respectively. We observe a similar phase transition phenomenon, and find that, the *perturbation stability* under He initialization increases with depth, while the LeCun initialization shows the opposite tendency, which verified our theory.

6 Conclusions

In this work, we explore the interplay of the width, the depth and the initialization of neural networks on their average robustness with new theoretical bounds in an effort to address the apparent contradiction in the literature. Our theoretical results hold in both under- and over-parameterized regimes. Intriguingly, we find a change of behavior in average robustness with respect to the depth, initially exacerbating robustness and then alleviating it. We suspect that this could help explain the contradictory messages in the literature. We also characterize the average robustness in the non-lazy training regime for two layer neural networks and find that width always help, coinciding the with the results [Bubeck and Sellke, 2021, Bubeck et al., 2021]. We also provide numerical evidence to support the theoretical developments.

References

Z. Allen-Zhu and Y. Li. Feature purification: How adversarial training performs robust deep learning. In *2021 IEEE 62nd Annual Symposium on Foundations of Computer Science (FOCS)*, pages 977–988. IEEE, 2022.

Z. Allen-Zhu, Y. Li, and Z. Song. A convergence theory for deep learning via over-parameterization. In *International Conference on Machine Learning*, pages 242–252. PMLR, 2019a.

Z. Allen-Zhu, Y. Li, and Z. Song. A convergence theory for deep learning via over-parameterization. In *International Conference on Machine Learning (ICML)*, 2019b.

A. Athalye, N. Carlini, and D. Wagner. Obfuscated gradients give a false sense of security: Circumventing defenses to adversarial examples, 2018.

A. Bietti and J. Mairal. On the inductive bias of neural tangent kernels. *Advances in neural information processing systems (NeurIPS)*, 2019.

S. Bubeck and M. Sellke. A universal law of robustness via isoperimetry. In *Advances in neural information processing systems (NeurIPS)*, 2021. URL `https://openreview.net/forum?id=z71OSKqTFh7`.

S. Bubeck, Y. Li, and D. M. Nagaraj. A law of robustness for two-layers neural networks. In *Conference on Learning Theory*, 2021.

Y. Cao and Q. Gu. Generalization bounds of stochastic gradient descent for wide and deep neural networks. *Advances in neural information processing systems (NeurIPS)*, 32, 2019.

L. Chen and S. Xu. Deep neural tangent kernel and laplace kernel have the same {rkhs}. In *International Conference on Learning Representations*, 2021.

Z. Chen, Y. Cao, D. Zou, and Q. Gu. How much over-parameterization is sufficient to learn deep ReLU networks? In *International Conference on Learning Representations (ICLR)*, 2020.

L. Chizat and F. Bach. On the global convergence of gradient descent for over-parameterized models using optimal transport. *Advances in neural information processing systems (NeurIPS)*, 31, 2018.

L. Chizat, E. Oyallon, and F. Bach. On lazy training in differentiable programming. *Advances in neural information processing systems (NeurIPS)*, 32, 2019.

F. Croce and M. Hein. Reliable evaluation of adversarial robustness with an ensemble of diverse parameter-free attacks. In *International Conference on Machine Learning (ICML)*, pages 2206–2216. PMLR, 2020.

E. Dohmatob and A. Bietti. On the (non-)robustness of two-layer neural networks in different learning regimes, 2022.

S. Du, J. Lee, H. Li, L. Wang, and X. Zhai. Gradient descent finds global minima of deep neural networks. In *International Conference on Machine Learning*, pages 1675–1685. PMLR, 2019.

S. S. Du, W. Hu, and J. D. Lee. Algorithmic regularization in learning deep homogeneous models: Layers are automatically balanced. In *Advances in neural information processing systems (NeurIPS)*, 2018a.

S. S. Du, X. Zhai, B. Poczos, and A. Singh. Gradient descent provably optimizes over-parameterized neural networks, 2018b.

K. Eykholt, I. Evtimov, E. Fernandes, B. Li, A. Rahmati, C. Xiao, A. Prakash, T. Kohno, and D. Song. Robust physical-world attacks on deep learning visual classification. In *Conference on Computer Vision and Pattern Recognition (CVPR)*, 2018.

R. Gao, T. Cai, H. Li, C.-J. Hsieh, L. Wang, and J. D. Lee. Convergence of adversarial training in overparametrized neural networks. *Advances in neural information processing systems (NeurIPS)*, 32, 2019.

A. Geifman, A. Yadav, Y. Kasten, M. Galun, D. Jacobs, and R. Basri. On the similarity between the laplace and neural tangent kernels. *Advances in neural information processing systems (NeurIPS)*, 2020.

I. J. Goodfellow, J. Shlens, and C. Szegedy. Explaining and harnessing adversarial examples. In *International Conference on Learning Representations (ICLR)*, 2015.

H. Hassani and A. Javanmard. The curse of overparametrization in adversarial training: Precise analysis of robust generalization for random features regression, 2022.

K. He, X. Zhang, S. Ren, and J. Sun. Delving deep into rectifiers: Surpassing human-level performance on imagenet classification. In *International Conference on Computer Vision (ICCV)*, pages 1026–1034, 2015.

K. He, X. Zhang, S. Ren, and J. Sun. Deep residual learning for image recognition. In *Conference on Computer Vision and Pattern Recognition (CVPR)*, pages 770–778, 2016.

M. Hein and M. Andriushchenko. Formal guarantees on the robustness of a classifier against adversarial manipulation. In *Advances in neural information processing systems (NeurIPS)*, volume 30, 2017.

H. Huang, Y. Wang, S. M. Erfani, Q. Gu, J. Bailey, and X. Ma. Exploring architectural ingredients of adversarially robust deep neural networks. In *Advances in neural information processing systems (NeurIPS)*, 2021.

A. Jacot, F. Gabriel, and C. Hongler. Neural tangent kernel: Convergence and generalization in neural networks, 2018.

A. Krizhevsky, V. Nair, and G. Hinton. The cifar-10 dataset. *online: http://www. cs. toronto. edu/kriz/cifar. html*, 55, 2014.

Y. Lecun, L. Bottou, Y. Bengio, and P. Haffner. Gradient-based learning applied to document recognition. *Proceedings of the IEEE*, 86(11):2278–2324, 1998. doi: 10.1109/5.726791.

Y. A. LeCun, L. Bottou, G. B. Orr, and K.-R. Müller. Efficient backprop. In *Neural networks: Tricks of the trade*, pages 9–48. Springer, 2012.

T. Luo, Z.-Q. J. Xu, Z. Ma, and Y. Zhang. Phase diagram for two-layer relu neural networks at infinite-width limit. *Journal of Machine Learning Research*, 2021.

A. Madry, A. Makelov, L. Schmidt, D. Tsipras, and A. Vladu. Towards deep learning models resistant to adversarial attacks, 2017.

A. Madry, A. Makelov, L. Schmidt, D. Tsipras, and A. Vladu. Towards deep learning models resistant to adversarial attacks. In *International Conference on Learning Representations (ICLR)*, 2018.

H. Maennel, O. Bousquet, and S. Gelly. Gradient descent quantizes relu network features, 2018.

E. Malach, G. Yehudai, S. Shalev-Schwartz, and O. Shamir. Proving the lottery ticket hypothesis: Pruning is all you need. In *International Conference on Machine Learning (ICML)*, 2020.

S. Mei, A. Montanari, and P.-M. Nguyen. A mean field view of the landscape of two-layers neural networks, 2018.

S. Mei, T. Misiakiewicz, and A. Montanari. Mean-field theory of two-layers neural networks: dimension-free bounds and kernel limit. In *Conference on Learning Theory*. PMLR, 2019.

Q. Nguyen, M. Mondelli, and G. F. Montufar. Tight bounds on the smallest eigenvalue of the neural tangent kernel for deep relu networks. In *International Conference on Machine Learning (ICML)*, 2021.

S. Oymak and M. Soltanolkotabi. Toward moderate overparameterization: Global convergence guarantees for training shallow neural networks. *IEEE Journal on Selected Areas in Information Theory*, 1(1):84–105, 2020.

I. M. Safran, G. Yehudai, and O. Shamir. The effects of mild over-parameterization on the optimization landscape of shallow relu neural networks. In *Conference on Learning Theory*, pages 3889–3934. PMLR, 2021.

L. Schmidt, S. Santurkar, D. Tsipras, K. Talwar, and A. Madry. Adversarially robust generalization requires more data. In *Advances in neural information processing systems (NeurIPS)*, 2018a.

L. Schmidt, S. Santurkar, D. Tsipras, K. Talwar, and A. Madry. Adversarially robust generalization requires more data. *Advances in neural information processing systems (NeurIPS)*, 31, 2018b.

C. Song, A. Ramezani-Kebrya, T. Pethick, A. Eftekhari, and V. Cevher. Subquadratic overparameterization for shallow neural networks. *Advances in neural information processing systems (NeurIPS)*, 34, 2021.

C. Szegedy, W. Zaremba, I. Sutskever, J. Bruna, D. Erhan, I. Goodfellow, and R. Fergus. Intriguing properties of neural networks. In *International Conference on Learning Representations (ICLR)*, 2014.

R. Vershynin. *High-Dimensional Probability: An Introduction with Applications in Data Science*. Cambridge University Press, 2018.

T.-W. Weng, H. Zhang, P.-Y. Chen, J. Yi, D. Su, Y. Gao, C.-J. Hsieh, and L. Daniel. Evaluating the robustness of neural networks: An extreme value theory approach. In *International Conference on Learning Representations (ICLR)*, 2018.

B. Woodworth, S. Gunasekar, J. D. Lee, E. Moroshko, P. Savarese, I. Golan, D. Soudry, and N. Srebro. Kernel and rich regimes in overparametrized models. In *Conference on Learning Theory*. PMLR, 2020.

B. Wu, J. Chen, D. Cai, X. He, and Q. Gu. Do wider neural networks really help adversarial robustness? In *Advances in neural information processing systems (NeurIPS)*, volume 34, 2021.

C. You, Z. Zhu, Q. Qu, and Y. Ma. Robust recovery via implicit bias of discrepant learning rates for double over-parameterization. *Advances in neural information processing systems (NeurIPS)*, 33: 17733–17744, 2020.

C. Zhang, S. Bengio, M. Hardt, B. Recht, and O. Vinyals. Understanding deep learning (still) requires rethinking generalization. *Communications of the ACM*, 64(3):107–115, 2021.

X. Zhang, J. Chen, Q. Gu, and D. Evans. Understanding the intrinsic robustness of image distributions using conditional generative models. In *International Conference on Artificial Intelligence and Statistics (AISTATS)*, pages 3883–3893. PMLR, 2020a.

Y. Zhang, O. Plevrakis, S. S. Du, X. Li, Z. Song, and S. Arora. Over-parameterized adversarial training: An analysis overcoming the curse of dimensionality. *Advances in neural information processing systems (NeurIPS)*, 33:679–688, 2020b.

M. Zhou, R. Ge, and C. Jin. A local convergence theory for mildly over-parameterized two-layer neural network. In *Conference on Learning Theory*, pages 4577–4632. PMLR, 2021.

S. Zhou and A. P. Schoellig. An analysis of the expressiveness of deep neural network architectures based on their lipschitz constants, 2019.

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1. For all authors...
   (a) Do the main claims made in the abstract and introduction accurately reflect the paper's contributions and scope? [Yes]
   (b) Did you describe the limitations of your work? [Yes] We clearly discuss the limitation of this work in the Appendix F.
   (c) Did you discuss any potential negative societal impacts of your work? [Yes] We clearly discuss the societal impact of this work in the Appendix G.
   (d) Have you read the ethics review guidelines and ensured that your paper conforms to them? [Yes]
2. If you are including theoretical results...
   (a) Did you state the full set of assumptions of all theoretical results? [Yes] We have detailed the rationale of the applied assumptions in this paper.
   (b) Did you include complete proofs of all theoretical results? [Yes] We include the complete proofs of our theoretical results.
3. If you ran experiments...
   (a) Did you include the code, data, and instructions needed to reproduce the main experimental results (either in the supplemental material or as a URL)? [No] The datasets we use in this work are all in the public domain and standard for image-related tasks. Thus, our setup can be reproduced by interested practitioners. The code will be open-sourced upon the acceptance of the paper.
   (b) Did you specify all the training details (e.g., data splits, hyperparameters, how they were chosen)? [Yes] Our experiments are mainly for validation our theory, all of the settings and hyper-parameters are mentioned in the main paper.
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4. If you are using existing assets (e.g., code, data, models) or curating/releasing new assets...
   (a) If your work uses existing assets, did you cite the creators? [Yes] We cite all the corresponding papers that provide the assets we use.
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   (d) Did you discuss whether and how consent was obtained from people whose data you're using/curating? [N/A] The datasets we utilize are publicly available and contain tens or hudrends of thousands of images. We refer to the authors original papers describing the datasets.
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