Generalization in Deep Learning

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Abstract

This paper provides non-vacuous and numerically-tight generalization guarantees for deep learning, as well as theoretical insights into why and how deep learning can generalize well, despite its large capacity, complexity, possible algorithmic instability, nonrobustness, and sharp minima, responding to an open question in the literature. We also propose new open problems and discuss the limitations of our results.

1. Introduction

Deep learning has seen significant practical success and has had a profound impact on the conceptual bases of machine learning and artificial intelligence. Along with its practical success, the theoretical properties of deep learning have been a subject of active investigation. For *expressivity* of neural networks, there are classical results regarding their universality (Leshno et al., 1993) and exponential advantages over hand-crafted features (Barron, 1993). Another series of theoretical studies have considered how *trainable* (or optimizable) deep hypothesis spaces are, revealing structural properties that may enable non-convex optimization (Choromanska et al., 2015; Kawaguchi, 2016a). However, merely having an *expressive* and *trainable* hypothesis space does not guarantee good performance in predicting the values of future inputs, because of possible over-fitting to training data. This leads to the study of *generalization*, which is the focus of this paper.

Some classical theory work attributes generalization ability to the use of a low-capacity class of hypotheses (Vapnik, 1998; Mohri et al., 2012). From the viewpoint of compact representation, which is related to small capacity, it has been shown that deep hypothesis spaces have an exponential advantage over shallow hypothesis spaces for representing some classes of natural target functions (Pascanu et al., 2014; Montufar et al., 2014; Livni et al., 2014; Telgarsky, 2016; Poggio et al., 2017). In other words, when some assumptions implicit in the hypothesis space (e.g., deep composition of piecewise linear transformations) are approximately satisfied by the target function, one can achieve very good generalization, compared to methods that do not rely on that assumption. However, a recent paper (Zhang et al., 2017) has empirically shown that successful deep hypothesis spaces have sufficient capacity to memorize random labels. This observation has been called an "apparent paradox" and has led to active discussion by many researchers (Arpit et al., 2017; Krueger et al., 2017; Hoffer et al., 2017; Wu et al., 2017; Dziugaite and Roy, 2017; Dinh et al., 2017). Zhang et al. (2017) concluded with an open problem stating that understanding such observations require rethinking generalization, while Dinh et al. (2017) stated that explaining why deep learning models can generalize well, despite their overwhelming capacity, is an open area of research.

We begin, in Section 3, by illustrating that, even in the case of linear models, hypothesis spaces with overwhelming capacity can result in arbitrarily small test errors and expected risks. Here, *test error* is the error of a learned hypothesis on data that it was not trained on, but which is often drawn

from the same distribution. Test error is a measure of how well the hypothesis generalizes to new data. We closely examine this phenomenon, extending the original open problem from previous papers (Zhang et al., 2017; Dinh et al., 2017) into a new open problem that strictly includes the original. We reconcile the possible apparent paradox by checking theoretical consistency and identifying a difference in the underlying assumptions. Considering a difference in the focuses of theory and practice, we outline possible practical roles that generalization theory can play.

Towards addressing these issues, Section 4 presents generalization bounds based on validation datasets, which can provide non-vacuous and numerically-tight generalization guarantees for deep learning in general. Section 5 analyzes generalization errors based on training datasets, focusing on a specific case of feed-forward neural networks with ReLU units and max-pooling. Under these conditions, the developed theory provides quantitatively tight theoretical insights into the generalization behavior of neural networks.

2. Background

Let $x \in \mathcal{X}$ be an input and $y \in \mathcal{Y}$ be a target. Let $\mathcal{L}$ be a loss function. Let $\mathcal{R}[f]$ be the expected risk of a function f, $\mathcal{R}[f] = \mathbb{E}_{x,y \sim \mathbb{P}_{(X,Y)}}[\mathcal{L}(f(x), y)]$, where $\mathbb{P}_{(X,Y)}$ is the true distribution. Let $f_{\mathcal{A}(S)} : \mathcal{X} \to \mathcal{Y}$ be a model learned by a learning algorithm $\mathcal{A}$ (including random seeds for simplicity) using a training dataset $S := S_m := \{(x_1, y_1), \ldots, (x_m, y_m)\}$ of size m. Let $\mathcal{R}_S[f]$ be the empirical risk of f as $\mathcal{R}_S[f] = \frac{1}{m} \sum_{i=1}^{m} \mathcal{L}(f(x_i), y_i)$ with $\{(x_i, y_i)\}_{i=1}^{m} = S$. Let $\mathcal{F}$ be a set of functions endowed with some structure or equivalently a *hypothesis space*. Let $\mathcal{L}_{\mathcal{F}}$ be a family of loss functions associated with $\mathcal{F}$, defined by $\mathcal{L}_{\mathcal{F}} = \{g : f \in \mathcal{F}, g(x, y) = \mathcal{L}(f(x), y)\}$. All vectors are *column* vectors in this paper. For any given variable v, let d_v be the dimensionality of the variable v.

A goal in machine learning is typically framed as the minimization of the expected risk $\mathcal{R}[f_{\mathcal{A}(S)}]$. We typically aim to minimize the non-computable expected risk $\mathcal{R}[f_{\mathcal{A}(S)}]$ by minimizing the computable empirical risk $\mathcal{R}_S[f_{\mathcal{A}(S)}]$ (i.e., empirical risk minimization). One goal of generalization theory is to explain and justify when and how minimizing $\mathcal{R}_S[f_{\mathcal{A}(S)}]$ is a sensible approach to minimizing $\mathcal{R}[f_{\mathcal{A}(S)}]$ by analyzing

$$\text{the generalization gap} := \mathcal{R}[f_{\mathcal{A}(S)}] - \mathcal{R}_S[f_{\mathcal{A}(S)}].$$

In this section only, we use the typical assumption that S is generated by independent and identically distributed (i.i.d.) draws according to the true distribution $\mathbb{P}_{(X,Y)}$; the following sections of this paper do not utilize this assumption. Under this assumption, a primary challenge of analyzing the generalization gap stems from the *dependence* of $f_{\mathcal{A}(S)}$ on the same dataset S used in the definition of $\mathcal{R}_S$. Several approaches in *statistical learning theory* have been developed to handle this dependence.

The *hypothesis-space complexity* approach handles this dependence by decoupling $f_{\mathcal{A}(S)}$ from the particular S by considering the worst-case gap for functions in the hypothesis space as

$$\mathcal{R}[f_{\mathcal{A}(S)}] - \mathcal{R}_S[f_{\mathcal{A}(S)}] \leq \sup_{f \in \mathcal{F}} \mathcal{R}[f] - \mathcal{R}_S[f],$$

and by carefully analyzing the right-hand side. Because the cardinality of $\mathcal{F}$ is typically (uncountably) infinite, a direct use of the union bound over all elements in $\mathcal{F}$ yields a vacuous bound, leading to the need to consider different quantities to characterize $\mathcal{F}$; e.g., Rademacher complexity and the Vapnik–Chervonenkis (VC) dimension. For example, if the codomain of $\mathcal{L}$ is in $[0, 1]$, we have

(Mohri et al., 2012, Theorem 3.1) that for any $\delta > 0$, with probability at least $1 - \delta$,

$$\sup_{f \in \mathcal{F}} \mathcal{R}[f] - \mathcal{R}_S[f] \leq 2\mathfrak{R}_m(\mathcal{L}_{\mathcal{F}}) + \sqrt{\frac{\ln \frac{1}{\delta}}{2m}},$$

where $\mathfrak{R}_m(\mathcal{L}_{\mathcal{F}})$ is the Rademacher complexity of $\mathcal{L}_{\mathcal{F}}$, which then can be bounded by the Rademacher complexity of $\mathcal{F}$, $\mathfrak{R}_m(\mathcal{F})$. For the deep-learning hypothesis spaces $\mathcal{F}$, there are several well-known bounds on $\mathfrak{R}_m(\mathcal{F})$ including those with explicit exponential dependence on depth (Sun et al., 2016; Neyshabur et al., 2015b; Xie et al., 2015) and explicit linear dependence on the number of trainable parameters (Shalev-Shwartz and Ben-David, 2014). There has been significant work on improving the bounds in this approach, but all existing solutions with this approach still depend on the complexity of a hypothesis space or a sequence of hypothesis spaces.

The *stability* approach deals with the dependence of $f_{\mathcal{A}(S)}$ on the dataset S by considering the *stability* of algorithm $\mathcal{A}$ with respect to different datasets. The considered stability is a measure of how much changing a data point in S can change $f_{\mathcal{A}(S)}$. For example, if the algorithm $\mathcal{A}$ has uniform stability β (w.r.t. $\mathcal{L}$) and if the codomain of $\mathcal{L}$ is in $[0, M]$, we have (Bousquet and Elisseeff, 2002) that for any $\delta > 0$, with probability at least $1 - \delta$,

$$\mathcal{R}[f_{\mathcal{A}(S)}] - \mathcal{R}_S[f_{\mathcal{A}(S)}] \leq 2\beta + (4m\beta + M)\sqrt{\frac{\ln \frac{1}{\delta}}{2m}}.$$

Based on previous work on stability (e.g., Hardt et al. 2015; Kuzborskij and Lampert 2017; Gonen and Shalev-Shwartz 2017), one may conjecture some reason for generalization in deep learning.

The *robustness* approach avoids dealing with certain details of the dependence of $f_{\mathcal{A}(S)}$ on S by considering the robustness of algorithm $\mathcal{A}$ for all possible datasets. In contrast to stability, robustness is the measure of how much the loss value can vary w.r.t. *the input space* of (x, y). For example, if algorithm $\mathcal{A}$ is $(\Omega, \zeta(\cdot))$-robust and the codomain of $\mathcal{L}$ is upper-bounded by M, given a dataset S, we have (Xu and Mannor, 2012) that for any $\delta > 0$, with probability at least $1 - \delta$,

$$|\mathcal{R}[f_{\mathcal{A}(S)}] - \mathcal{R}_S[f_{\mathcal{A}(S)}]| \leq \zeta(S) + M\sqrt{\frac{2\Omega \ln 2 + 2\ln \frac{1}{\delta}}{m}}.$$

The robustness approach requires an *a priori known and fixed* partition of the input space such that the number of sets in the partition is Ω and the change of loss values in each set of the partition is bounded by $\zeta(S)$ *for all S* (Definition 2 and the proof of Theorem 1 in Xu and Mannor 2012). In classification, if the *margin* is ensured to be large, we can fix the partition with balls of radius corresponding to the large *margin*, filling the input space. Recently, this idea was applied to deep learning (Sokolic et al., 2017a,b), producing insightful and effective generalization bounds, while still suffering from the curse of the dimensionality of the priori-known fixed input manifold.

With regard to the above approaches, *flat minima* can be viewed as the concept of low variation in the *parameter space*; i.e., a small perturbation in the parameter space around a solution results in a small change in the loss surface. Several studies have provided arguments for generalization in deep learning based on flat minima (Keskar et al., 2017). However, Dinh et al. (2017) showed that flat minima in practical deep learning hypothesis spaces can be turned into sharp minima via re-parameterization without affecting the generalization gap, indicating that it requires further investigation.

3. Rethinking generalization

Zhang et al. (2017) empirically demonstrated that several deep hypothesis spaces can memorize random labels, while having the ability to produce zero training error and small test errors for particular natural datasets (e.g., CIFAR-10). They also empirically observed that regularization on the norm of weights seemed to be unnecessary to obtain small test errors, in contradiction to conventional wisdom. These observations suggest the following open problem:

Open Problem 1. Tightly characterize the expected risk $\mathcal{R}[f]$ or the generalization gap $\mathcal{R}[f] - \mathcal{R}_S[f]$ with a sufficiently complex deep-learning hypothesis space $\mathcal{F} \ni f$, producing theoretical insights and distinguishing the case of "natural" problem instances $(\mathbb{P}_{(X,Y)}, S)$ (e.g., images with natural labels) from the case of other problem instances $(\mathbb{P}'_{(X,Y)}, S')$ (e.g., images with random labels).

Supporting and extending the empirical observations by Zhang et al. (2017), we provide a theorem (Theorem 1) stating that the hypothesis space of over-parameterized linear models can memorize any training data *and* decrease the training and test errors arbitrarily close to zero (including to zero) *with* the norm of parameters being arbitrarily large, *even when* the parameters are arbitrarily far from the ground-truth parameters. Furthermore, Corollary 2 shows that conventional wisdom regarding the norm of the parameters w can fail to explain generalization, even in linear models that might seem not to be over-parameterized. All proofs for this paper are presented in the appendix.

Theorem 1. *Consider a linear model with the training prediction $\hat{Y}(w) = \Phi w \in \mathbb{R}^{m \times d_y}$, where $\Phi \in \mathbb{R}^{m \times n}$ is a fixed feature matrix of the training inputs. Let $\hat{Y}_{\text{test}}(w) = \Phi_{\text{test}} w \in \mathbb{R}^{m_{\text{test}} \times d_y}$ be the test prediction, where $\Phi_{\text{test}} \in \mathbb{R}^{m_{\text{test}} \times n}$ is a fixed feature matrix of the test inputs. Let $M = [\Phi^\top, \Phi_{\text{test}}^\top]^\top$. Then, if $n > m$ and if $\operatorname{rank}(\Phi) = m$ and $\operatorname{rank}(M) < n$,*

- *(i) For any $Y \in \mathbb{R}^{m \times d_y}$, there exists a parameter w' such that $\hat{Y}(w') = Y$, and*

- *(ii) if there exists a ground truth w^* satisfying $Y = \Phi w^*$ and $Y_{\text{test}} = \Phi_{\text{test}} w^*$, then for any $\epsilon, \delta \geq 0$, there exists a parameter w such that*

  - *(a) $\hat{Y}(w) = Y + \epsilon A$ for some matrix A with $\|A\|_F \leq 1$, and*
  - *(b) $\hat{Y}_{\text{test}}(w) = Y_{\text{test}} + \epsilon B$ for some matrix B with $\|B\|_F \leq 1$, and*
  - *(c) $\|w\|_F \geq \delta$ and $\|w - w^*\|_F \geq \delta$.*

Corollary 2. *If $n \leq m$ and if $\operatorname{rank}(M) < n$, then statement (ii) in Theorem 1 holds.*

Whereas Theorem 1 and Corollary 2 concern test errors instead of expected risk (in order to be consistent with empirical studies), Remark 3 shows the existence of the same phenomena for expected risk for general machine learning models not limited to deep learning and linear hypothesis spaces; i.e., Remark 3 shows that none of small capacity, low complexity, stability, robustness, and flat minima is *necessary* for generalization in machine learning for each given problem instance $(\mathbb{P}_{(X,Y)}, S)$, although one of them can be *sufficient* for generalization. This statement does not contradict necessary conditions and no free lunch theorem from previous learning theory, as explained in the subsequent subsections.

Remark 3. Given a pair $(\mathbb{P}_{(X,Y)}, S)$ and a desired $\epsilon > \inf_{f \in \mathcal{Y}^{\mathcal{X}}} \mathcal{R}[f] - \mathcal{R}_S[f]$, let f_ϵ^* be a function such that $\epsilon \geq \mathcal{R}[f_\epsilon^*] - \mathcal{R}_S[f_\epsilon^*]$. Then,

(i) For any hypothesis space $\mathcal{F}$ whose hypothesis-space complexity is large enough to memorize any dataset and which includes f_ϵ^* possibly at an arbitrarily sharp minimum, there exist learning algorithms $\mathcal{A}$ such that the generalization gap of $f_{\mathcal{A}(S)}$ is at most ϵ, and

(ii) There exist arbitrarily unstable and arbitrarily non-robust algorithms $\mathcal{A}$ such that the generalization gap of $f_{\mathcal{A}(S)}$ is at most ϵ.

To see this, first consider statement (i). Given such a $\mathcal{F}$, consider any $\mathcal{A}$ such that $\mathcal{A}$ takes $\mathcal{F}$ and S as input and outputs f_ϵ^*. Clearly, there are many such algorithms $\mathcal{A}$. For example, given a S, fix $\mathcal{A}$ such that $\mathcal{A}$ takes $\mathcal{F}$ and S as input and outputs f_ϵ^* (which already proves the statement), or even $f_\epsilon^* + \delta$ where δ becomes zero by the right choice of hyper-parameters and of small variations of $\mathcal{F}$ (e.g., architecture search in deep learning) such that $\mathcal{F}$ still satisfy the condition in the statement. This establishes statement (i).

Consider statement (ii). Given any dataset S', consider a look-up algorithm $\mathcal{A}'$ that always outputs f_ϵ^* if $S = S'$, and outputs f_1 otherwise such that f_1 is arbitrarily non-robust and $|\mathcal{L}(f_\epsilon^*(x), y) - \mathcal{L}(f_1(x), y)|$ is arbitrarily large (i.e., arbitrarily non-stable). This proves statement (ii). Note that while A' here suffices to prove statement (ii), we can also generate other non-stable and non-robust algorithms by noticing the essence captured in Remark 4.

We capture the essence of all the above observations in the following remark.

Remark 4. The expected risk $\mathcal{R}[f]$ and the generalization gap $\mathcal{R}[f] - \mathcal{R}_S[f]$ of a hypothesis f with a true distribution $\mathbb{P}_{(X,Y)}$ and a dataset S are completely determined by the tuple $(\mathbb{P}_{(X,Y)}, S, f)$, independently of other factors, such as a hypothesis space $\mathcal{F}$ (and hence its properties such as capacity, Rademacher complexity, pre-defined bound on norms, and flat-minima) and properties of random datasets different from the given S (e.g., stability and robustness of the learning algorithm $\mathcal{A}$). In contrast, the conventional wisdom states that these other factors are what matter. This has created the "apparent paradox" in the literature.

From these observations, we propose the following open problem:

Open Problem 2. Tightly characterize the expected risk $\mathcal{R}[f]$ or the generalization gap $\mathcal{R}[f] - \mathcal{R}_S[f]$ of a hypothesis f with a pair $(\mathbb{P}_{(X,Y)}, S)$ of a true distribution and a dataset, *producing theoretical insights,* based only on properties of the hypothesis f and the pair $(\mathbb{P}_{(X,Y)}, S)$.

Solving Open Problem 2 for deep learning implies solving Open Problem 1, but not vice versa. Open Problem 2 encapsulates the essence of Open Problem 1 and all the issues from our Theorem 1, Corollary 2 and Proposition 3.

3.1 Consistency of theory

The empirical observations in (Zhang et al., 2017) and our results above may seem to contradict the results of statistical learning theory. However, there is no contradiction, and the apparent inconsistency arises from the misunderstanding and misuse of the precise meanings of the theoretical statements.

Statistical learning theory can be considered to provide two types of statements relevant to the scope of this paper. The first type (which comes from upper bounds) is logically in the form of "p implies q," where $p :=$ "the hypothesis-space complexity is small" (or another statement about stability, robustness, or flat minima), and $q :=$ "the generalization gap is small." Notice that "p
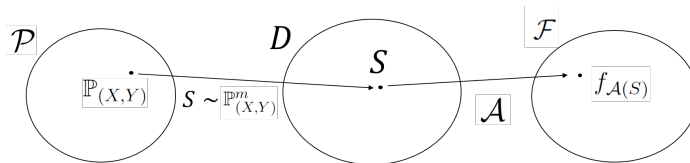
Figure 1: An illustration of differences in assumptions. Statistical learning theory analyzes the generalization behaviors of $f_{\mathcal{A}(S)}$ over randomly-drawn *unspecified* datasets $S \in D$ according to some *unspecified* distribution $\mathbb{P}_{(X,Y)} \in \mathcal{P}$. Intuitively, statistical learning theory concerns more about questions regarding a set $\mathcal{P} \times D$ because of the *unspecified* nature of $(\mathbb{P}_{(X,Y)}, S)$, whereas certain empirical studies (e.g., Zhang et al. 2017) can focus on questions regarding each *specified* point $(\mathbb{P}_{(X,Y)}, S) \in \mathcal{P} \times D$.

implies q" does not imply "q implies p." Thus, based on statements of this type, it is entirely possible that the generalization gap is small even when the hypothesis-space complexity is large or the learning mechanism is unstable, non-robust, or subject to sharp minima.

The second type (which comes from lower bounds) is logically in the following form: in a set U_{all} of all possible problem configurations, there exists a subset $U \subseteq U_{\text{all}}$ such that "q implies p" in U (with the same definitions of p and q as in the previous paragraph). For example, Mohri et al. (2012, Section 3.4) derived lower bounds on the generalization gap by showing the existence of a "bad" distribution that characterizes U. Similarly, the classical *no free lunch* theorems are the results with the existence of a worst-case distribution for each algorithm. However, if the problem instance at hand (e.g., object classification with MNIST or CIFAR-10) is not in such a U in the proofs (e.g., if the data distribution is not among the "bad" ones considered in the proofs), q does not necessarily imply p. Thus, it is still naturally possible that the generalization gap is small with large hypothesis-space complexity, instability, non-robustness, and sharp minima. Therefore, there is no contradiction or paradox.

3.2 Difference in assumptions and problem settings

Under certain assumptions, many results in statistical learning theory have been shown to be tight and insightful (e.g., Mukherjee et al. 2006; Mohri et al. 2012). Hence, the need of rethinking generalization partly comes from a difference in the assumptions and problem settings.

Figure 1 illustrates the differences in assumptions in statistical learning theory and some empirical studies. On one hand, in statistical learning theory, a distribution $\mathbb{P}_{(X,Y)}$ and a dataset S are usually unspecified except that $\mathbb{P}_{(X,Y)}$ is in some set $\mathcal{P}$ and a dataset $S \in D$ is drawn randomly according to $\mathbb{P}_{(X,Y)}$ (typically with the i.i.d. assumption). On the other hand, in most empirical studies and in our theoretical results (Theorem 1 and Proposition 3), a distribution $\mathbb{P}_{(X,Y)}$ is still unknown yet specified (e.g., via a real world process) and a dataset S is specified and usually known (e.g., CIFAR-10 or ImageNet). Intuitively, whereas statistical learning theory considers a set $\mathcal{P} \times D$ because of weak assumptions, some empirical studies can focus on a specified point $(\mathbb{P}_{(X,Y)}, S)$ in a set $\mathcal{P} \times D$ because of stronger assumptions. Therefore, by using the same terminology such as "expected risk" and "generalization" in both cases, we are susceptible to confusion and apparent contradiction.

Lower bounds, necessary conditions and tightness in statistical learning theory are typically defined via a worst-case distribution $\mathbb{P}_{(X,Y)}^{\text{worst}} \in \mathcal{P}$. For instance, classical "no free lunch" theorems and certain lower bounds on the generalization gap (e.g., Mohri et al. 2012, Section 3.4) have been

proven *for* the worst-case distribution $\mathbb{P}^{\text{worst}}_{(X,Y)} \in \mathcal{P}$. Therefore, "tight" and "necessary" typically mean "tight" and "necessary" for the set $\mathcal{P} \times D$ (e.g., through the worst or average case), but *not* for each particular point $(\mathbb{P}_{(X,Y)}, S) \in \mathcal{P} \times D$. From this viewpoint, we can understand that even if the quality of the set $\mathcal{P} \times D$ is "bad" overall, there may exist a "good" point $(\mathbb{P}_{(X,Y)}, S) \in \mathcal{P} \times D$.

Several approaches in statistical learning theory, such as the data dependent and Bayesian approaches (Herbrich and Williamson, 2002; Dziugaite and Roy, 2017), use more assumptions on the set $\mathcal{P} \times D$ to take advantage of more prior and posterior information; these have an ability to tackle Open Problem 1. However, these approaches do not apply to Open Problem 2 as they still depend on other factors than the given $(\mathbb{P}_{(X,Y)}, S, f)$. For example, data-dependent bounds with the *luckiness framework* (Shawe-Taylor et al., 1998; Herbrich and Williamson, 2002) and *empirical* Rademacher complexity (Koltchinskii and Panchenko, 2000; Bartlett et al., 2002) still depend on a concept of hypothesis spaces (or the sequence of hypothesis spaces), and the robustness approach (Xu and Mannor, 2012) depend on different datasets than a given S via the definition of robustness (i.e., in Section 2, $\zeta(S)$ is a data-dependent term, but the definition of ζ itself and Ω depend on other datasets than S).

We note that analyzing a set $\mathcal{P} \times D$ is of significant interest for its own merits and is a natural task in the field of computational complexity (e.g., categorizing a set of problem instances into subsets with or without polynomial solvability). Indeed, the situation where theory focuses more on a set and many practical studies focus on each element in the set is prevalent in computer science (see the discussion in Appendix A2 for more detail).

3.3 Practical role of generalization theory

From the discussions above, we can see that there is a *logically expected* difference between the scope in theory and the focus in practice; it is logically expected that there are problem instances where theoretical bounds are pessimistic. In order for generalization theory to have maximal impact in practice, we must be clear on a set of different roles it can play regarding practice, and then work to extend and strengthen it in each of these roles. We have identified the following practical roles for theory:

Role 1 Provide guarantees on expected risk.

Role 2 Guarantee generalization gap

    Role 2.1 to be small for a given fixed S, and/or

    Role 2.2 to approach zero with *a fixed model class* as m increases.

Role 3 Provide theoretical insights to guide the search over model classes.

4. Generalization bounds via validation

In practical deep learning, we typically adopt the training–validation paradigm, usually with a held-out validation set. We then search over hypothesis spaces by changing architectures (and other hyper-parameters) to obtain low validation error. In this view, we can conjecture the reason that deep learning can sometimes generalize well as follows: it is partially because we can obtain a good model via search using a validation dataset. Indeed, Proposition 5 states that if the validation error of a hypothesis is small, it is guaranteed to generalize well, regardless of its capacity, Rademacher

complexity, stability, robustness, and flat minima. Let $S_{m_{\text{val}}}^{(\text{val})}$ be a held-out validation dataset of size m_{val}, which is independent of the training dataset S.

Proposition 5. (generalization guarantee via validation error) *Assume that $S_{m_{\text{val}}}^{(\text{val})}$ is generated by i.i.d. draws according to a true distribution $\mathbb{P}_{(X,Y)}$. Let $\kappa_{f,i} = \mathcal{R}[f] - \mathcal{L}(f(x_i), y_i)$ for $(x_i, y_i) \in S_{m_{\text{val}}}^{(\text{val})}$. Suppose that $\mathbb{E}[\kappa_{f,i}^2] \leq \gamma^2$ and $|\kappa_{f,i}| \leq C$ almost surely, for all $(f, i) \in \mathcal{F}_{\text{val}} \times \{1, \ldots, m_{\text{val}}\}$. Then, for any $\delta > 0$, with probability at least $1 - \delta$, the following holds for all $f \in \mathcal{F}_{\text{val}}$:*

$$\mathcal{R}[f] \leq \mathcal{R}_{S_{m_{\text{val}}}^{(\text{val})}}[f] + \frac{2C \ln(\frac{|\mathcal{F}_{\text{val}}|}{\delta})}{3m_{\text{val}}} + \sqrt{\frac{2\gamma^2 \ln(\frac{|\mathcal{F}_{\text{val}}|}{\delta})}{m_{\text{val}}}}.$$

Here, $\mathcal{F}_{\text{val}}$ is defined as a set of models f that is independent of a held-out validation dataset $S_{m_{\text{val}}}^{(\text{val})}$, but can depend on the training dataset S. For example, $\mathcal{F}_{\text{val}}$ can contain a set of models f such that each element f is a result at the end of each epoch during training with at least 99.5% *training* accuracy. In this example, $|\mathcal{F}_{\text{val}}|$ is at most (the number of epochs) × (the cardinality of the set of possible hyper-parameter settings), and is likely much smaller than that because of the 99.5% training accuracy criteria and the fact that a space of many hyper-parameters is narrowed down by using the training dataset as well as other datasets from different tasks. If a hyper-parameter search depends on the validation dataset, $\mathcal{F}_{\text{val}}$ must be the possible space of the search instead of the space actually visited by the search. We can also use a sequence $\{\mathcal{F}_{\text{val}}^{(j)}\}_j$ (see Appendix A).

The bound in Proposition 5 is non-vacuous and tight enough to be practically meaningful. For example, consider a classification task with 0–1 loss. Set $m_{\text{val}} = 10,000$ (e.g., MNIST and CIFAR-10) and $\delta = 0.1$. Then, even in the worst case with $C = 1$ and $\gamma^2 = 1$ and even with $|\mathcal{F}_{\text{val}}| = 1,000,000,000$, we have with probability at least 0.9 that $\mathcal{R}[f] \leq \mathcal{R}_{S_{m_{\text{val}}}^{(\text{val})}}[f] + 6.94\%$ for all $f \in \mathcal{F}_{\text{val}}$. In a non-worst-case scenario, for example, with $C = 1$ and $\gamma^2 = (0.05)^2$, we can replace 6.94% by 0.49%. With a larger validation set (e.g., ImageNet) and/or more optimistic C and γ^2, we can obtain much better bounds.

Although Proposition 5 poses the concern of increasing the generalization bound when using a single validation dataset with too large $|\mathcal{F}_{\text{val}}|$, the rate of increase is only $\ln |\mathcal{F}_{\text{val}}|$ and $\sqrt{\ln |\mathcal{F}_{\text{val}}|}$. We can also avoid dependence on the cardinality of $\mathcal{F}_{\text{val}}$ using Remark 6.

Remark 6. Assume that $S_{m_{\text{val}}}^{(\text{val})}$ is generated by i.i.d. draws according to $\mathbb{P}_{(X,Y)}$. Let $\mathcal{L}_{\mathcal{F}_{\text{val}}} = \{g : f \in \mathcal{F}_{\text{val}}, g(x, y) := \mathcal{L}(f(x), y)\}$. By applying (Mohri et al., 2012, Theorem 3.1) to $\mathcal{L}_{\mathcal{F}_{\text{val}}}$, if the codomain of $\mathcal{L}$ is in $[0, 1]$, with probability at least $1 - \delta$, for all $f \in \mathcal{F}_{\text{val}}$, $\mathcal{R}[f] \leq \mathcal{R}_{S_{m_{\text{val}}}^{(\text{val})}}[f] + 2\mathfrak{R}_m(\mathcal{L}_{\mathcal{F}_{\text{val}}}) + \sqrt{(\ln 1/\delta)/m_{\text{val}}}$.

Unlike the standard use of Rademacher complexity with a training dataset, the set $\mathcal{F}_{\text{val}}$ cannot depend on the validation set $S_{m_{\text{val}}}$, but can depend on the training dataset S in any manner, and hence $\mathcal{F}_{\text{val}}$ differs significantly from the typical hypothesis space defined by the parameterization of models. We can thus end up with a very different effective capacity and hypothesis complexity (as selected by model search using the validation set) depending on whether the training data are random or have interesting structure which the neural network can capture.

5. Direct analyses of neural networks

Unlike the previous section, this section analyzes the generalization gap with a training dataset S. In Section 3, we extended Open Problem 1 to Open Problem 2, and identified the different assumptions

in theoretical and empirical studies. Accordingly, this section aims to address these problems to some extent, both in the case of particular specified datasets and the case of random unspecified datasets. To achieve this goal, this section presents a *direct analysis* of neural networks, rather than deriving results about neural networks from more generic theories based on capacity, Rademacher complexity, stability, or robustness.

Sections 5.2 and 5.3 deals with the squared loss, while Section 5.4 considers 0-1 loss with multi-labels.

5.1 Model description via deep paths

We consider general neural networks of any depth that have the structure of a directed acyclic graph (DAG) with ReLU nonlinearity and/or max pooling. This includes any structure of a feedforward network with convolutional and/or fully connected layers, potentially with skip connections. For pedagogical purposes, we first discuss our model description for layered networks without skip connections, and then describe it for DAGs.

Layered nets without skip connections Let $z^{[l]}(x, w) \in \mathbb{R}^{n_l}$ be the pre-activation vector of the l-th hidden layer, where n_l is the width of the l-th hidden layer, and w represents the trainable parameters. Let $L - 1$ be the number of hidden layers. For layered networks without skip connections, the pre-activation (or pre-nonlinearity) vector of the l-th layer can be written as

$$z^{[l]}(x, w) = W^{[l]} \sigma^{(l-1)} \left(z^{[l-1]}(x, w) \right),$$

with a boundary definition $\sigma^{(0)} \left(z^{[0]}(x, w) \right) \equiv x$, where $\sigma^{(l-1)}$ represents nonlinearity via ReLU and/or max pooling at the $(l - 1)$-th hidden layer, and $W^{[l]} \in \mathbb{R}^{n_l \times n_{l-1}}$ is a matrix of weight parameters connecting the $(l - 1)$-th layer to the l-th layer. Here, $W^{[l]}$ can have *any* structure (e.g., shared and sparse weights to represent a convolutional layer). Let $\dot{\sigma}^{[l]}(x, w)$ be a vector with each element being 0 or 1 such that $\sigma^{[l]} \left(z^{[l]}(x, w) \right) = \dot{\sigma}^{[l]}(x, w) \circ z^{[l]}(x, w)$, which is an element-wise product of the vectors $\dot{\sigma}^{[l]}(x, w)$ and $z^{[l]}(x, w)$. Then, we can write the pre-activation of the k-th output unit at the last layer $l = L$ as

$$z_k^{[L]}(x, w) = \sum_{j_{L-1}=1}^{n_{L-1}} W_{k j_{L-1}}^{[L]} \dot{\sigma}_{j_{L-1}}^{(L-1)}(x, w) z_{j_{L-1}}^{[L-1]}(x, w).$$

By expanding $z^{[l]}(x, w)$ repeatedly and exchanging the sum and product via the distributive law of multiplication,

$$z_k^{[L]}(x, w) = \sum_{j_{L-1}=1}^{n_{L-1}} \sum_{j_{L-2}=1}^{n_{L-2}} \cdots \sum_{j_0=1}^{n_0} \overline{W}_{k j_{L-1} j_{L-2} \dots j_0} \dot{\sigma}_{j_{L-1} j_{L-2} \dots j_1}(x, w) x_{j_0},$$

where $\overline{W}_{k j_{L-1} j_{L-2} \dots j_0} = W_{k j_{L-1}}^{[L]} \prod_{l=1}^{L-1} W_{j_l j_{l-1}}^{[l]}$ and $\dot{\sigma}_{j_{L-1} j_{L-2} \dots j_1}(x, w) = \prod_{l=1}^{L-1} \dot{\sigma}_{j_l}^{[l]}(x, w)$. By merging the indices $j_0, \dots, j_{L-1}$ into j with some bijection between $\{1, \dots, n_0\} \times \cdots \times \{1, \dots, n_{L-1}\} \ni (j_0, \dots, j_{L-1})$ and $\{1, \dots, n_0 n_1 \cdots n_{L-1}\} \ni j$,

$$z_k^{[L]}(x, w) = \sum_j \bar{w}_{k,j} \bar{\sigma}_j(x, w) \bar{x}_j,$$

where $\bar{w}_{k,j}, \bar{\sigma}_j(x,w)$ and $\bar{x}_j$ represent $\overline{W}_{k j_{L-1} j_{L-2} \ldots j_0}, \dot{\sigma}_{j_{L-1} j_{L-2} \ldots j_1}(x,w)$ and x_{j_0} respectively with the change of indices (i.e., $\sigma_j(x,w)$ and $\bar{x}_j$ respectively contain the n_0 numbers and $n_1 \cdots n_{L-1}$ numbers of the same copy of each $\dot{\sigma}_{j_{L-1} j_{L-2} \ldots j_1}(x,w)$ and x_{j_0}). Note that $\sum_j$ represents summation over all the paths from the input x to the k-th output unit.

DAGs Remember that every DAG has at least one topological ordering, which can be used to to create a layered structure with possible skip connections (e.g., see Healy and Nikolov 2001; Neyshabur et al. 2015b). In other words, we consider DAGs such that the pre-activation vector of the l-th layer can be written as

$$z^{[l]}(x,w) = \sum_{l'=0}^{l-1} W^{(l,l')} \sigma^{[l']}\left(z^{[l']}(x,w)\right)$$

with a boundary definition $\sigma^{(0)}\left(z^{[0]}(x,w)\right) \equiv x$, where $W^{(l,l')} \in \mathbb{R}^{n_l \times n_{l'}}$ is a matrix of weight parameters connecting the l'-th layer to the l-th layer. Again, $W^{(l,l')}$ can have *any* structure. Thus, in the same way as with layered networks without skip connections, for all $k \in \{1, \ldots, d_y\}$,

$$z_k^{[L]}(x,w) = \sum_j \bar{w}_{k,j} \bar{\sigma}_j(x,w) \bar{x}_j,$$

where $\sum_j$ represents the summation over all paths from the input x to the k-th output unit; i.e., $\bar{w}_{k,j} \bar{\sigma}_j(x,w) \bar{x}_j$ is the contribution from the j-th path to the k-th output unit. Each of $\bar{w}_{k,j}, \bar{\sigma}_j(x,w)$ and $\bar{x}_j$ is defined in the same manner as in the case of layered networks without skip connections. In other words, the j-th path weight $\bar{w}_{k,j}$ is the product of the weight parameters in the j-th path, and $\bar{\sigma}_j(x,w)$ is the product of the 0-1 activations in the j-th path, corresponding to ReLU nonlinearity and max pooling; $\bar{\sigma}_j(x,w) = 1$ if all units in the j-th path are active, and $\bar{\sigma}_j(x,w) = 0$ otherwise. Also, $\bar{x}_j$ is the input used in the j-th path. Therefore, for DAGs, including layered networks without skip connections,

$$z_k^{[L]}(x,w) = [\bar{x} \circ \bar{\sigma}(x,w)]^\top \bar{w}_k, \tag{1}$$

where $[\bar{x} \circ \bar{\sigma}(x,w)]_j = \bar{x}_j \bar{\sigma}_j(x,w)$ and $(\bar{w}_k)_j = \bar{w}_{k,j}$ are the vectors of the size of the number of the paths.

5.2 Theoretical insights via tight theory for every pair $(\mathbb{P}, S)$

Theorem 7 solves Open Problem 2 (and hence Open Problem 1) for neural networks with squared loss by stating that the generalization gap of a w with respect to a problem $(\mathbb{P}_{(X,Y)}, S)$ is tightly analyzable with theoretical insights, based only on the quality of the w and the pair $(\mathbb{P}_{(X,Y)}, S)$. We do *not* assume that S is generated randomly based on some relationship with $\mathbb{P}_{(X,Y)}$; the theorem holds for any dataset, regardless of how it was generated. Let w^S and $\bar{w}_k^S$ be the parameter vectors w and $\bar{w}_k$ learned with a dataset S. Let $\mathcal{R}[w^S]$ and $\mathcal{R}_S[w^S]$ be the expect risk and empirical risk of the model with the learned parameter w^S. Let $z_i = [\bar{x}_i \circ \bar{\sigma}(x_i, w^S)]$. Let $G = \mathbb{E}_{x,y \sim \mathbb{P}_{(X,Y)}}[zz^\top] - \frac{1}{m} \sum_{i=1}^m z_i z_i^\top$ and $v = \frac{1}{m} \sum_{i=1}^m y_{ik} z_i - \mathbb{E}_{x,y \sim \mathbb{P}_{(X,Y)}}[y_k z]$. Given a matrix M, let $\lambda_{\max}(M)$ be the largest eigenvalue of M.

Theorem 7. *Let $\{\lambda_j\}_j$ and $\{u_j\}_j$ be a set of eigenvalues and a corresponding orthonormal set of eigenvectors of G. Let $\theta_{\bar{w}_k,j}^{(1)}$ be the angle between u_j and $\bar{w}_k$. Let $\theta_{\bar{w}_k}^{(2)}$ be the angle between v and*

$\bar{w}_k$. *Then (deterministically),*

$$\mathcal{R}[w^S] - \mathcal{R}_S[w^S] - c_y = \sum_{k=1}^{d_y} \left(2\|v\|_2 \|\bar{w}_k^s\|_2 \cos\theta_{\bar{w}_k^s}^{(2)} + \|\bar{w}_k^s\|_2^2 \sum_j \lambda_j \cos^2\theta_{\bar{w}_k^s,j}^{(1)} \right)$$

$$\leq \sum_{k=1}^{d_y} \left(2\|v\|_2 \|\bar{w}_k^s\|_2 + \lambda_{\max}(G)\|\bar{w}_k^s\|_2^2 \right),$$

where $c_y = \mathbb{E}_y[\|y\|_2^2] - \frac{1}{m}\sum_{i=1}^{m}\|y_i\|_2^2$.

Proof idea. From Equation (1) with squared loss, we can decompose the generalization gap into three terms:

$$\mathcal{R}[w^S] - \mathcal{R}_S[w^S] = \sum_{k=1}^{d_y} \left[(\bar{w}_k^s)^\top \left(\mathbb{E}[zz^\top] - \frac{1}{m}\sum_{i=1}^{m} z_i z_i^\top \right) \bar{w}_k^s \right] \tag{2}$$

$$+ 2\sum_{k=1}^{d_y} \left[\left(\frac{1}{m}\sum_{i=1}^{m} y_{ik} z_i^\top - \mathbb{E}[y_k z^\top] \right) \bar{w}_k^s \right]$$

$$+ \mathbb{E}[y^\top y] - \frac{1}{m}\sum_{i=1}^{m} y_i^\top y_i.$$

By manipulating each term, we obtain the desired statement. See Appendix C3 for a complete proof.
$\square$

In Theorem 7, there is no concept of a hypothesis space. Instead, it indicates that if the norm of the weights $\|\bar{w}_k^s\|_2$ at the end of learning process with the actual given S is small, then the generalization gap is small, even if the norm $\|\bar{w}_k^s\|_2$ is unboundedly large at anytime with any dataset other than S.

Importantly, in Theorem 7, there are two other significant factors in addition to the norm of the weights $\|\bar{w}_k^s\|_2$. First, the eigenvalues of G and v measure the concentration of the given dataset S with respect to the (unknown) $\mathbb{P}_{(X,Y)}$ in the space of the learned representation $z_i = [\bar{x}_i \circ \bar{\sigma}(x_i, w^S)]$. Here, we can see the benefit of deep learning from the viewpoint of "deep-path" feature learning: even if a given S is not concentrated in the original space, optimizing w can result in concentrating it in the space of z. Similarly, c_y measures the concentration of $\|y\|_2^2$, but c_y is independent of w and unchanged after a pair $(\mathbb{P}_{(X,Y)}, S)$ is given. Second, the $\cos\theta$ terms measure the similarity between $\bar{w}_k^s$ and these concentration terms. Because the norm of the weights $\|\bar{w}_k^s\|_2$ is multiplied by those other factors, the generalization gap can remain small, even if $\|\bar{w}_k^s\|_2$ is large, as long as some of those other factors are small.

Based on a generic bound-based theory, Neyshabur et al. (2015a,b) proposed to control the norm of the *path* weights $\|\bar{w}_k\|_2$, which is consistent with our direct bound-less result (and which is as computationally tractable as a standard forward-backward pass[1]). Unlike the previous results, we do *not* require a pre-defined bound on $\|\bar{w}_k\|_2$ over different datasets, but depend only on its final

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1. From the derivation of Equation (1), one can compute $\|\bar{w}_k^s\|_2^2$ with a single forward pass using element-wise squared weights, an identity input, and no nonlinearity. One can also follow the previous paper (Neyshabur et al., 2015a) for its computation.
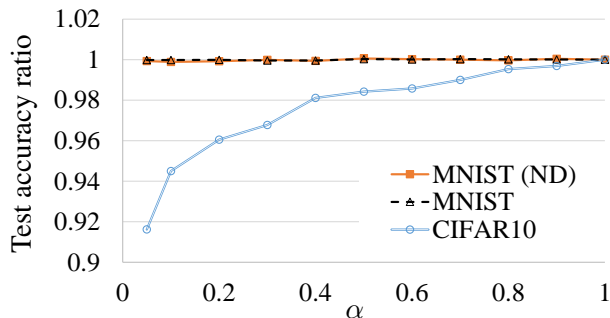
Figure 2: Test accuracy ratio (Two-phase/Base). Notice that the y-axis starts with high initial accuracy, even with a very small dataset size αm for learning w_σ.

value with each S as desired, in addition to more tight insights (besides the norm) via equality as discussed above. In addition to the pre-defined norm bound, these previous results have an explicit exponential dependence on the depth of the network, which does not appear in our Theorem 4. Similarly, some previous results specific to layered networks without skip connections (Sun et al., 2016; Xie et al., 2015) contain the 2^{L-1} factor *and* a bound on the product of the norm of weight matrices, $\prod_{l=1}^{L} \|W^{(l)}\|$, instead of $\sum_k \|\bar{w}_k^s\|_2$. Here, $\sum_k \|\bar{w}_k\|_2^2 \leq \prod_{l=1}^{L} \|W^{(l)}\|_F^2$ because the latter contains all of the same terms as the former as well as additional non-negative additive terms after expanding the sums in the definition of the norms.

Therefore, unlike previous bounds, Theorem 7 generates these new theoretical insights based on *the tight equality* (in the first line of the equation in Theorem 7). Notice that without manipulating the generalization gap, we can always obtain equality. However, the question answered here is whether or not we can obtain competitive theoretical insights (the path norm bound) via equality instead of inequality. From a practical view point, if the obtained insights are the same (e.g., regularize the norm), then equality-based theory has the obvious advantage of being more precise.

5.3 Probabilistic bound over random datasets

While the previous subsection tightly analyzed each given point $(\mathbb{P}_{(X,Y)}, S)$, this subsection considers the set $\mathcal{P} \times D \ni (\mathbb{P}_{(X,Y)}, S)$, where D is the set of possible datasets S endowed with an i.i.d. product measure $\mathbb{P}_{(X,Y)}^m$ where $\mathbb{P}_{(X,Y)} \in \mathcal{P}$ (see Section 3.2).

In Equation (2), the generalization gap is decomposed into three terms, each of which contains the difference between a sum of *dependent* random variables and its expectation. The dependence comes from the fact that $z_i = [\bar{x}_i \circ \bar{\sigma}(x_i, w^S)]$ are dependent over the sample index i, because of the dependence of w^S on the entire dataset S. We then observe the following: in $z_k^{[L]}(x, w) = [\bar{x} \circ \bar{\sigma}(x, w)]^\top \bar{w}$, the derivative of $z = [\bar{x} \circ \bar{\sigma}(x, w)]$ with respect to w is zero everywhere (except for the measure zero set, where the derivative does not exist). Therefore, each step of the (stochastic) gradient decent greedily chooses the best direction in terms of $\bar{w}$ (with the current $z = [\bar{x} \circ \bar{\sigma}(x, w)]$), but not in terms of w in $z = [\bar{x} \circ \bar{\sigma}(x, w)]$ (see Appendix A3 for more detail). This observation leads to a conjecture that the dependence of $z_i = [\bar{x}_i \circ \bar{\sigma}(x_i, w^S)]$ via the training process with the whole dataset S is not entirely "bad" in terms of the concentration of the sum of the terms with z_i.

5.3.1 EMPIRICAL OBSERVATIONS

As a first step to investigate the dependence of z_i, we evaluated the following novel *two-phase* training procedure that explicitly breaks the dependence of z_i over the sample index i. We first train a network in a standard way, but only using a *partial* training dataset $S_{\alpha m} = \{(x_1, y_1), \ldots, (x_{\alpha m}, y_{\alpha m})\}$ of size αm, where $\alpha \in (0, 1)$ (standard phase). We then assign the value of $w^{S_{\alpha m}}$ to a new placeholder $w_\sigma := w^{S_{\alpha m}}$ and freeze w_σ, meaning that as w changes, w_σ does not change. At this point, we have that $z_k^{[L]}(x, w^{S_{\alpha m}}) = [\bar{x} \circ \bar{\sigma}(x, w_\sigma)]^\top \bar{w}_k^{S_{\alpha m}}$. We then keep training only the $\bar{w}_k^{S_{\alpha m}}$ part with the entire training dataset of size m (freeze phase), yielding the final model via this two-phase training procedure as

$$\tilde{z}_k^{[L]}(x, w^S) = [\bar{x} \circ \bar{\sigma}(x, w_\sigma)]^\top \bar{w}_k^S. \tag{3}$$

Note that the vectors $w_\sigma = w^{S_{\alpha m}}$ and $\bar{w}_k^S$ contain the untied parameters in $\tilde{z}_k^{[L]}(x, w^S)$. See Appendix A4 for a simple implementation of this two-phase training procedure that requires at most (approximately) twice as much computational cost as the normal training procedure.

We implemented the two-phase training procedure with the MNIST and CIFAR-10 datasets. The test accuracies of the standard training procedure (base case) were 99.47% for MNIST (ND), 99.72% for MNIST, and 92.89% for CIFAR-10. MNIST (ND) indicates MNIST with no data augmentation. The experimental details are in Appendix B.

Our source code is available at: http://lis.csail.mit.edu/code/gdl.html

Figure 2 presents the test accuracy ratios for varying α: the test accuracy of the two-phase training procedure divided by the test accuracy of the standard training procedure. The plot in Figure 2 begins with $\alpha = 0.05$, for which $\alpha m = 3000$ in MNIST and $\alpha m = 2500$ in CIFAR-10. Somewhat surprisingly, using a much smaller dataset for learning w_σ still resulted in competitive performance. A dataset from which we could more easily obtain a better generalization (i.e., MNIST) allowed us to use smaller αm to achieve competitive performance, which is consistent with our discussion above.

5.3.2 THEORETICAL RESULTS

We now prove a probabilistic bound for the hypotheses resulting from the two-phase training algorithm. Let $\tilde{z}_i = [\bar{x}_i \circ \bar{\sigma}(x_i, w_\sigma)]$ where $w_\sigma := w^{S_{\alpha m}}$, as defined in the two-phase training procedure above. Our two-phase training procedure forces $\tilde{z}_{\alpha m+1}, \ldots, \tilde{z}_m$ *over samples* to be independent random variables (each $\tilde{z}_i$ is dependent *over coordinates*, which is taken care of in our proof), while maintaining the competitive practical performance of the output model $\tilde{z}_k^{[L]}(\cdot, w^S)$. As a result, we obtain the following bound on the generalization gap for the practical deep models $\tilde{z}_k^{[L]}(\cdot, w^S)$. Let $m_\sigma = (1 - \alpha)m$. Given a matrix M, let $\|M\|_2$ be the spectral norm of M.

Assumption 1. *Let $G^{(i)} = \mathbb{E}_x[\tilde{z}\tilde{z}^\top] - \tilde{z}_i\tilde{z}_i^\top$, $V_{kk'}^{(i)} = y_{ik}\tilde{z}_{i,k'} - \mathbb{E}_{x,y}[y_k\tilde{z}_{k'}]$, and $c_y^{(i)} = \mathbb{E}_y[\|y\|_2^2] - \|y_i\|_2^2$. Assume that for all $i \in \{\alpha m + 1, \ldots, m\}$,*

- $C_{zz} \geq \lambda_{\max}(G^{(i)})$ *and* $\gamma_{zz}^2 \geq \|\mathbb{E}_x[(G^{(i)})^2]\|_2$

- $C_{yz} \geq \max_{k,k'} |V_{kk'}^{(i)}|$ *and* $\gamma_{yz}^2 \geq \max_{k,k'} \mathbb{E}_x[(V_{kk'}^{(i)})^2])$

- $C_y \geq |c_y^{(i)}|$ *and* $\gamma_y^2 \geq \mathbb{E}_x[(c_y^{(i)})^2]$.

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Theorem 8. *Suppose that Assumption 1 holds. Assume that $S \setminus S_{\alpha m}$ is generated by i.i.d. draws according to true distribution $\mathbb{P}_{(X,Y)}$. Assume that $S \setminus S_{\alpha m}$ is independent of $S_{\alpha m}$. Let $f_{\mathcal{A}(S)}$ be the model learned by the two-phase training procedure with S. Then, for each $w_\sigma := w^{S_{\alpha m}}$, for any $\delta > 0$, with probability at least $1 - \delta$,*

$$\mathcal{R}[f_{\mathcal{A}(S)}] - \mathcal{R}_{S \setminus S_{\alpha m}}[f_{\mathcal{A}(S)}] \le \beta_1 \sum_{k=1}^{d_y} \left\| \bar{w}_k^S \right\|_1 + 2\beta_2 \sum_{k=1}^{d_y} \left\| \bar{w}_k^S \right\|_2^2 + \beta_3,$$

where $\beta_1 = \frac{2C_{zz}}{3m_\sigma} \ln \frac{3d_z}{\delta} + \sqrt{\frac{2\gamma_{zz}^2}{m_\sigma} \ln \frac{3d_z}{\delta}}$, $\beta_2 = \frac{2C_{yz}}{3m_\sigma} \ln \frac{6d_y d_z}{\delta} + \sqrt{\frac{\gamma_{yz}^2}{m_\sigma} \ln \frac{6d_y d_z}{\delta}}$, and $\beta_2 = \frac{2C_y}{3m_\sigma} \ln \frac{3}{\delta} + \sqrt{\frac{2\gamma_y^2}{m_\sigma} \ln \frac{3}{\delta}}$.

Our proof does *not* require independence over the coordinates of $\tilde{z}_i$ and the entries of the random matrices $\tilde{z}_i \tilde{z}_i^\top$ (see the proof of Theorem 8).

The bound in Theorem 8 is data-dependent because the norms of the weights $\bar{w}_k^S$ depend on each particular S. Similarly to Theorem 7, the bound in Theorem 8 does not contain a pre-determined bound on the norms of weights and can be independent of the concept of hypothesis space, as desired; i.e., Assumption 1 can be also satisfied without referencing a hypothesis space of w, because $\tilde{z} = [\bar{x}_i \circ \bar{\sigma}(x_i, w_\sigma)]$ with $\bar{\sigma}_j(x_i, w_\sigma) \in \{0, 1\}$. However, unlike Theorem 7, Theorem 8 *implicitly* contains the properties of datasets different from a given S, via the pre-defined bounds in Assumption 1. This is expected since Theorem 8 makes claims about the set of random datasets S instead of each instantiated S. Therefore, while Theorem 8 presents a strongly-data-dependent bound (over random datasets), Theorem 7 is tighter for each given S; indeed, the main equality of Theorem 7 is as tight as possible.

Theorems 7 and 8 provide generalization bounds for practical deep learning models that do not necessarily have explicit dependence on the number of weights, or exponential dependence on depth or effective input dimensionality. Although the size of the vector $\bar{w}_k^S$ can be exponentially large in the depth of the network, the norms of the vector need not be. Because $\tilde{z}_k^{[L]}(x, w^S) = \|\bar{x} \circ \bar{\sigma}(x, w_\sigma)\|_2 \|\bar{w}_k^S\|_2 \cos\theta$, we have that $\|\bar{w}_k^S\|_2 = z_k^{[L]}(x, w)/(\|\bar{x} \circ \bar{\sigma}(x, w_\sigma)\|_2 \cos\theta)$ (unless the denominator is zero), where θ is the angle between $\bar{x} \circ \bar{\sigma}(x, w_\sigma)$ and $\bar{w}_k^S$. Additionally, as discussed in Section 5.2, $\sum_k \|\bar{w}_k\|_2^2 \le \prod_{l=1}^{L} \|W^{(l)}\|_F^2$.

5.4 Probabilistic bound for 0-1 loss with multi-labels

For the 0–1 loss with multi-labels, the two-phase training procedure in Section 5.3 yields the generalization bound in Theorem 9. Similarly to the bounds in Theorems 7 and 8, the generalization bound in Theorem 9 does not necessarily have dependence on the number of weights, and exponential dependence on depth and effective input dimensionality.

Theorem 9. *Assume that $S \setminus S_{\alpha m}$ is generated by i.i.d. draws according to true distribution $\mathbb{P}_{(X,Y)}$. Assume that $S \setminus S_{\alpha m}$ is independent of $S_{\alpha m}$. Fix $\rho > 0$ and w_σ. Let $\mathcal{F}$ be the set of the models with the two-phase training procedure. Suppose that $\mathbb{E}_x[\|\bar{x} \circ \bar{\sigma}(x, w_\sigma)\|_2^2] \le C_\sigma^2$ and $\max_k \|\bar{w}_k\|_2 \le C_w$ for all $f \in \mathcal{F}$. Then, for any $\delta > 0$, with probability at least $1 - \delta$, the following holds for all $f \in \mathcal{F}$:*

$$\mathcal{R}[f] \le \mathcal{R}_{S \setminus S_{\alpha m}}^{(\rho)}[f] + \frac{2d_y^2(1-\alpha)^{-1/2} C_\sigma C_w}{\rho \sqrt{m_\sigma}} + \sqrt{\frac{\ln \frac{1}{\delta}}{2m_\sigma}}.$$

Here, the empirical margin loss $\mathcal{R}_S^{(\rho)}[f]$ is defined as $\mathcal{R}_S^{(\rho)}[f] = \frac{1}{m}\sum_{i=1}^m \mathcal{L}_{\text{margin},\rho}(f(x_i), y_i)$, where $\mathcal{L}_{\text{margin},\rho}$ is defined as follows:

$$\mathcal{L}_{\text{margin},\rho}(f(x), y) = \mathcal{L}^{(2)}_{\text{margin},\rho}(\mathcal{L}^{(1)}_{\text{margin},\rho}(f(x), y))$$

where

$$\mathcal{L}^{(1)}_{\text{margin},\rho}(f(x), y) = z_y^{[L]}(x) - \max_{y \neq y'} z_{y'}^{[L]}(x) \in \mathbb{R},$$

and

$$\mathcal{L}^{(2)}_{\text{margin},\rho}(t) = \begin{cases} 0 & \text{if } \rho \leq t \\ 1 - t/\rho & \text{if } 0 \leq t \leq \rho \\ 1 & \text{if } t \leq 0. \end{cases}$$

6. Discussions and open problems

It is very difficult to make a detailed characterization of how well a specific hypotheses generated by a certain learning algorithm will generalize, in the absence of detailed information about the given problem instance. Traditional learning theory addresses this very difficult question and has developed bounds that are as tight as possible given the generic information available. In this paper, we have worked toward drawing stronger conclusions by developing theoretical analyses tailored for the situations with more detailed information, including actual neural network structures, and actual performance on a validation set.

Optimization and generalization in deep learning are closely related via the following observation: if we make optimization easier by changing model architectures, generalization performance can be degraded, and vice versa. Hence, non-pessimistic generalization theory discussed in this paper might allow more architectural choices and assumptions in optimization theory.

Define the partial order of problem instances $(\mathbb{P}, S, f)$ as

$$(\mathbb{P}, S, f) \leq (\mathbb{P}', S', f') \quad \Leftrightarrow \quad \mathcal{R}_{\mathbb{P}}[f] - \mathcal{R}_S[f] \leq \mathcal{R}_{\mathbb{P}'}[f'] - \mathcal{R}_{S'}[f']$$

where $\mathcal{R}_{\mathbb{P}}[f]$ is the expected risk with probability measure $\mathbb{P}$. Then, any theoretical insights without the partial order preservation can be misleading as it can change the ranking of the preference of $(\mathbb{P}, S, f)$. For example, theoretically motivated algorithms can degrade actual performances when compared with heuristics, if the theory does not preserve the partial order of $(\mathbb{P}, S, f)$. This observation suggests the following open problem.

Open Problem 3. Tightly characterize the expected risk $\mathcal{R}[f]$ or the generalization gap $\mathcal{R}[f] - \mathcal{R}_S[f]$ of a hypothesis f with a pair $(\mathbb{P}, S)$, producing theoretical insights while partially yet provably preserving the partial order of $(\mathbb{P}, S, f)$.

Theorem 7 partially addresses Open Problem 3 by preserving the exact ordering via equality without bounds. However, it would be beneficial to consider a weaker notion of order preservation to gain analyzability with more useful insights as stated in Open Problem 3.

Our discussion with Proposition 5 and Remark 6 suggests another open problem: analyzing the role and influence of *human intelligence* on generalization. For example, human intelligence seems to be able to often find good architectures (and other hyper-parameters) that get low validation errors (without non-exponentially large $|\mathcal{F}_{\text{val}}|$ in Proposition 5, or a low complexity of $\mathcal{L}_{\mathcal{F}_{\text{val}}}$ in Remark

6). A close look at the deep learning literature seems to suggest that this question is fundamentally related to the process of science and engineering, because many successful architectures have been designed based on the physical properties and engineering priors of the problems at hand (e.g., hierarchical nature, convolution, architecture for motion such as that by Finn et al. 2016, memory networks, and so on). While this is a hard question, understanding it would be beneficial to further automate the role of human intelligence towards the goal of artificial intelligence.

Acknowledgements

A. Appendix: Additional discussions

Theorem 7 address Open Problem 2 with the limited applicability to certain neural networks with squared loss. In contrast, a parallel study (Kawaguchi and Bengio, 2018) presents a novel generic learning theory to address Open Problem 2 for general cases in machine learning. It would be beneficial to explore both a generic analysis (Kawaguchi and Bengio, 2018) and a concrete analysis in deep learning to get theoretical insights that are tailored for each particular case.

In previous bounds with a hypothesis space $\mathcal{F}$, if we try different hypothesis spaces $\mathcal{F}$ depending on S, the basic proof breaks down. An easy recovery at the cost of an extra quantity in a bound is to take a union bound over all possible $\mathcal{F}_j$ for $j = 1, 2, \ldots$, where we pre-decide $\{\mathcal{F}_j\}_j$ without dependence on S (because simply considering the "largest" $\mathcal{F} \supseteq \mathcal{F}_j$ can result in a very loose bound for each $\mathcal{F}_j$). Similarly, if we need to try many $w_\sigma := w^{S_{\alpha m}}$ depending on the whole S in Theorem 8, we can take a union bound over $w_\sigma^{(j)}$ for $j = 1, 2, \ldots$, where we pre-determine $\{w_\sigma^{(j)}\}_j$ without dependence on $S \setminus S_{\alpha m}$ but with dependence on $S_{\alpha m}$. We can do the same with Proposition 5 and Remark 6 to use many $\mathcal{F}_{\text{val}}$ depending on the validation dataset $S_{m_{\text{val}}}^{(\text{val})}$ with a predefined sequence.

A1 Simple regularization algorithm

In general, theoretical bounds from statistical learning theory can be too loose to be directly used in practice. In addition, many theoretical results in statistical learning theory end up suggesting to simply regularize some notion of smoothness of a hypothesis class. Indeed, by upper bounding a distance between two functions (e.g., a hypothesis and the ground truth function corresponding to expected true labels), one can immediately see *without statistical learning theory* that regularizing some notion of smoothness of the hypothesis class helps guarantees on generalization. Then, by the Occam's razor argument, one might prefer a simpler (yet still rigor) theory and a corresponding simpler algorithm.

Accordingly, this subsection examines another simple regularization algorithm that directly regularize smoothness of the learned hypothesis. In this subsection, we focus on multi-class classification problems with d_y classes, such as object classification with images. Accordingly, we analyze the

Table 1: Test error (%)

Method	MNIST	CIFAR-10
Baseline	0.26	3.52
DARC1	0.20	3.43

Table 2: Test error ratio (DARC1/Base)

	MNIST (ND)		MNIST		CIFAR-10	
	mean	stdv	mean	stdv	mean	stdv
Ratio	0.89	0.61	0.95	0.67	0.97	0.79

expected risk with 0–1 loss as $\mathcal{R}[f] = \mathbb{E}_x[\mathbb{1}\{f(x) = y(x)\}]$, where $f(x) = \text{argmax}_{k \in \{1,...,d_y\}}($ $z_k^{[L]}(x))$ is the model prediction, and $y(x) \in \{1, \ldots, d_y\}$ is the true label of x.

This subsection proposes the following family of simple regularization algorithms: given any architecture and method, add a new regularization term for each mini-batch as

$$\text{loss} = \text{original loss} + \frac{\lambda}{\bar{m}} \left| \max_k \sum_{i=1}^{\bar{m}} \xi_i z_k^{[L]}(x_i) \right|,$$

where x_i is drawn from some distribution approximating the true distribution of x, $\xi_1, \ldots, \xi_{\bar{m}}$ are independently and uniformly drawn from $\{-1, 1\}$, $\bar{m}$ is a mini-batch size and λ is a hyper-parameter. Importantly, the approximation of the true distribution of x is only used for regularization purposes and hence needs not be precisely accurate (as long as it plays its role for regularization). For example, it can be approximated by populations generated by a generative neural network and/or an extra data augmentation process. For simplicity, we call this family of methods as Directly Approximately Regularizing Complexity (DARC).

In this paper, we evaluated only a very simple version of the proposed family of methods as a first step. That is, our experiments employed the following simple and easy-to-implement method, called DARC1:

$$\text{loss} = \text{original loss} + \frac{\lambda}{\bar{m}} \left(\max_k \sum_{i=1}^{\bar{m}} |z_k^{[L]}(x_i)| \right), \tag{A.1}$$

where x_i is the i-th sample in the training mini-batch. The additional computational cost and programming effort due to this new regularization is almost negligible because $z_k^{[L]}(x_i)$ is already used in computing the original loss. This simplest version was derived by approximating the true distribution of x with the empirical distribution of the training data.

We evaluated the proposed method (DARC1) by simply adding the new regularization term in equation (A.1) to existing standard codes for MNIST and CIFAR-10. A standard variant of LeNet (LeCun et al., 1998) and ResNeXt-29(16×64d) (Xie et al., 2016) are used for MNIST and CIFAR-10, and compared with the addition of the studied regularizer. For all the experiments, we fixed $(\lambda/\bar{m}) = 0.001$ with $\bar{m} = 64$. We used a single model without ensemble methods. The experimental details are in Appendix B. The source code is available at: http://lis.csail.mit.edu/code/gdl.html

Table 3: Values of $\frac{1}{m}\left(\max_k \sum_{i=1}^{m} |z_k^{[L]}(x_i)|\right)$

Method	MNIST (ND)		MNIST		CIFAR-10	
	mean	stdv	mean	stdv	mean	stdv
Base	17.2	2.40	8.85	0.60	12.2	0.32
DARC1	1.30	0.07	1.35	0.02	0.96	0.01

Table 1 shows the error rates comparable with previous results. To the best of our knowledge, the previous state-of-the-art classification error is 0.23% for MNIST with a single model (Sato et al., 2015) (and 0.21% with an ensemble by Wan et al. 2013). To further investigate the improvement, we ran 10 random trials with computationally less expensive settings, to gather mean and standard deviation (stdv). For MNIST, we used fewer epochs with the same model. For CIFAR-10, we used a smaller model class (pre-activation ResNet with only 18 layers). Table 2 summarizes the improvement ratio: the new model's error divided by the base model's error. We observed the improvements for all cases. The test errors (standard deviations) of the base models were 0.53 (0.029) for MNIST (ND), 0.28 (0.024) for MNIST, and 7.11 (0.17) for CIFAR-10 (all in %).

Table 3 summarizes the values of the regularization term $\frac{1}{m}(\max_k \sum_{i=1}^{m} |z_k^{[L]}(x_i)|)$ for each obtained model. The models learned with the proposed method were significantly different from the base models in terms of this value. Interestingly, a comparison of the base cases for MNIST (ND) and MNIST shows that data augmentation by itself *implicitly* regularized what we explicitly regularized in the proposed method.

A2 Relationship to other fields

The situation where theoretical studies focus on a set of problems and practical applications care about each element in the set is prevalent in machine learning and computer science literature, not limited to the field of learning theory. For example, for each practical problem instance $q \in Q$, the size of the set Q that had been analyzed in theory for optimal exploration in Markov decision processes (MDPs) were demonstrated to be frequently too pessimistic, and a methodology to partially mitigate the issue was proposed (Kawaguchi, 2016b). Bayesian optimization would suffer from a pessimistic set Q regarding each problem instance $q \in Q$, the issue of which was partially mitigated (Kawaguchi et al., 2015).

Moreover, characterizing a set of problems Q only via a worst-case instance $q' \in Q$ (i.e., worst-case analysis) is known to have several issues in theoretical computer science, and so-called *beyond worst-case analysis* (e.g., smoothed analysis) is an active area of research to mitigate the issues.

A3 SGD chooses direction in terms of $\bar{w}$

Recall that

$$z_k^{[L]}(x, w) = z^\top \bar{w} = [\bar{x} \circ \bar{\sigma}(x, w)]^\top \bar{w}.$$

Note that $\sigma(x, w)$ is 0 or 1 for max-pooling and/or ReLU nonlinearity. Thus, the derivative of $z = [\bar{x} \circ \bar{\sigma}(x, w)]$ with respect to w is zero everywhere (except at the measure zero set where the derivative does not exists). Thus, by the chain rule (and power rule), the gradient of the loss with

respect to w only contain the contribution from the derivative of $z_k^{[L]}$ with respect to $\bar{w}$, but not with respect to w in z.

A4 Simple implementation of two-phase training procedure

Directly implementing Equation (3) requires the summation over all paths, which can be computationally expensive. To avoid it, we implemented it by creating two deep neural networks, one of which defines $\bar{w}$ paths hierarchically, and another of which defines w_σ paths hierarchically, resulting in the computational cost at most (approximately) twice as much as the original cost of training standard deep learning models. We tied w_σ and $\bar{w}$ in the two networks during standard phase, and untied them during freeze phase.

Our source code is available at: http://lis.csail.mit.edu/code/gdl.html

The computation of the standard network without skip connection can be re-written as:

$$z^{[l]}(x, w) = \sigma^{[l]}(W^{[l]} z^{[l-1]}(x, w))$$
$$= \dot{\sigma}^{[l]}(W^{[l]} z^{[l-1]}(x, w)) \circ W^{[l]} z^{[l-1]}(x, w)$$
$$= \dot{\sigma}^{[l]}(W_\sigma^{[l]} z_\sigma^{[l-1]}(x, w)) \circ W^{[l]} z^{[l-1]}(x, w)$$

where $W_\sigma^{[l]} := W^{[l]}$, $z_\sigma^{[l-1]} := \sigma(W_\sigma^{[l]} z_\sigma^{[l-1]}(x, w))$ and $\dot{\sigma}_j^{[l]}(W^{[l]} z^{[l-1]}(x, w)) = 1$ if the j-th unit at the l-th layer is active, $\dot{\sigma}_j^{[l]}(W^{[l]} z^{[l-1]}(x, w)) = 0$ otherwise. Note that because $W_\sigma^{[l]} = W^{[l]}$, we have that $z_\sigma^{[l-1]} = z^{[l]}$ in standard phase and standard models.

In the two-phase training procedure, we created two networks for $W_\sigma^{[l]} z_\sigma^{[l-1]}(x, w)$ and $W^{[l]} z^{[l-1]}(x, w)$ separately. We then set $W_\sigma^{[l]} = W^{[l]}$ during standard phase, and frozen $W_\sigma^{[l]}$ and only trained $W^{[l]}$ during freeze phase. By following the same derivation of Equation (1), we can see that this defines the desired computation without explicitly computing the summation over all paths. By the same token, this applies to DAGs.

B. Appendix: Experimental details

For MNIST:

We used the following fixed architecture:

  (i) Convolutional layer with 32 filters with filter size of 5 by 5, followed by max pooling of size of 2 by 2 and ReLU.

 (ii) Convolution layer with 32 filters with filter size of 5 by 5, followed by max pooling of size of 2 by 2 and ReLU.

(iii) Fully connected layer with output 1024 units, followed by ReLU and Dropout with its probability being 0.5.

 (iv) Fully connected layer with output 10 units.

Layer 4 outputs $z^{[L]}$ in our notation. For training purpose, we use softmax of $z^{[L]}$. Also, $f(x) = \operatorname{argmax}(z^{[L]}(x))$ is the label prediction.

We fixed learning rate to be 0.01, momentum coefficient to be 0.5, and optimization algorithm to be (standard) stochastic gradient decent (SGD). We fixed data augmentation process as: random crop with size 24, random rotation up to ± 15 degree, and scaling of 15%. We used 3000 epochs for Table 1, and 1000 epochs for Tables 2 and 3.

For CIFAR-10:

For data augmentation, we used random horizontal flip with probability 0.5 and random crop of size 32 with padding of size 4.

For Table 1, we used ResNeXt-29(16×64d) (Xie et al., 2016). We set initial learning rate to be 0.05 and decreased to 0.005 at 150 epochs, and to 0.0005 at 250 epochs. We fixed momentum coefficient to be 0.9, weight decay coefficient to be 5×10^{-4}, and optimization algorithm to be stochastic gradient decent (SGD) with Nesterov momentum. We stopped training at 300 epochs.

For Tables 2 and 3, we used pre-activation ResNet with only 18 layers (pre-activation ResNet-18) (He et al., 2016). We fixed learning rate to be 0.001 and momentum coefficient to be 0.9, and optimization algorithm to be (standard) stochastic gradient decent (SGD). We used 1000 epochs.

C. Appendix: Proofs

We use the following lemma in the proof of Theorem 7.

Lemma 10. (Matrix Bernstein inequality: corollary to theorem 1.4 in Tropp 2012) *Consider a finite sequence $\{M_i\}$ of independent, random, self-adjoint matrices with dimension d. Assume that each random matrix satisfies that $\mathbb{E}[M_i] = 0$ and $\lambda_{\max}(M_i) \leq R$ almost surely. Let $\gamma^2 = \|\sum_i \mathbb{E}[M_i^2]\|_2$. Then, for any $\delta > 0$, with probability at least $1 - \delta$,*

$$\lambda_{\max}\left(\sum_i M_i\right) \leq \frac{2R}{3}\ln\frac{d}{\delta} + \sqrt{2\gamma^2 \ln\frac{d}{\delta}}.$$

Proof. Theorem 1.4 by Tropp (2012) states that for all $t \geq 0$,

$$\mathbb{P}\left[\lambda_{\max}\left(\sum_i M_i\right) \geq t\right] \leq d \cdot \exp\left(\frac{-t^2/2}{\gamma^2 + Rt/3}\right).$$

Setting $\delta = d\exp\left(-\frac{t^2/2}{\gamma^2 + Rt/3}\right)$ implies

$$-t^2 + \frac{2}{3}R(\ln d/\delta)t + 2\gamma^2 \ln d/\delta = 0.$$

Solving for t with the quadratic formula and bounding the solution with the subadditivity of square root on non-negative terms (i.e., $\sqrt{a + b} \leq \sqrt{a} + \sqrt{b}$ for all $a, b \geq 0$),

$$t \leq \frac{2}{3}R(\ln d/\delta) + 2\gamma^2 \ln d/\delta.$$

$\square$

C1 Proof of Theorem 1

Proof. For any matrix M, let $\mathrm{Col}(M)$ and $\mathrm{Null}(M)$ be the column space and null space of M. Since $\mathrm{rank}(\Phi) \geq m$ and $\Phi \in \mathbb{R}^{m \times n}$, the set of its columns span $\mathbb{R}^m$, which proves statement (i). Let $w^* = w_1^* + w_2^*$ where $\mathrm{Col}(w_1^*) \subseteq \mathrm{Col}(M^T)$ and $\mathrm{Col}(w_2^*) \subseteq \mathrm{Null}(M)$. For statement (ii), set the parameter as $w := w_1^* + \epsilon C_1 + \alpha C_2$ where $\mathrm{Col}(C_1) \subseteq \mathrm{Col}(M^T)$, $\mathrm{Col}(C_2) \subseteq \mathrm{Null}(M)$, $\alpha \geq 0$ and $C_2 = \frac{1}{\alpha} w_2^* + \bar{C}_2$. Since $\mathrm{rank}(M) < n$, $\mathrm{Null}(M) \neq \{0\}$ and there exist non-zero $\bar{C}_2$. Then,

$$\hat{Y}(w) = Y + \epsilon \Phi C_1,$$

and

$$\hat{Y}_{\text{test}}(w) = Y_{\text{test}} + \epsilon \Phi_{\text{test}} C_1.$$

By setting $A = \Phi C_1$ and $B = \Phi_{\text{test}} C_1$ with a proper normalization of C_1 yields (a) and (b) in statement (ii) (note that C_1 has an arbitrary freedom in the bound on its scale because its only condition is $\mathrm{Col}(C_1) \subseteq \mathrm{Col}(M^T)$). At the same time with the same parameter, since $\mathrm{Col}(w_1^* + \epsilon C_1) \perp \mathrm{Col}(C_2)$,

$$\|w\|_F^2 = \|w_1^* + \epsilon C_1\|_F^2 + \alpha^2 \|C_2\|_F^2,$$

and

$$\|w - w^*\|_F^2 = \|\epsilon C_1\|_F^2 + \alpha^2 \|\bar{C}_2\|_F^2,$$

which grows unboundedly as $\alpha \to \infty$ without changing A and B, proving (c) in statement (ii). $\qquad\square$

C2 Proof of Corollary 2

Proof. It follows the fact that the proof in Theorem 1 uses the assumption of $n > m$ and $\mathrm{rank}(\Phi) \geq m$ only for statement (i). $\qquad\square$

C3 Proof of Theorem 7

Proof. From Equation (1), the squared loss of deep models for each point (x, y) can be rewritten as

$$\sum_{k=1}^{d_y} (z^\top \bar{w}_k - y_k)^2 = \sum_{k=1}^{d_y} \bar{w}_k^\top (zz^\top) \bar{w}_k - 2 y_k z^\top \bar{w}_k + y_k^2.$$

Thus, from Equation (1) with the squared loss, we can decompose the generalization gap into three terms as

$$\begin{aligned}
\mathcal{R}[w^S] - \mathcal{R}_S[w^S] = {} & \sum_{k=1}^{d_y} \left[(\bar{w}_k^S)^\top \left(\mathbb{E}[zz^\top] - \frac{1}{m} \sum_{i=1}^{m} z_i z_i^\top \right) \bar{w}_k^S \right] \\
& + 2 \sum_{k=1}^{d_y} \left[\left(\frac{1}{m} \sum_{i=1}^{m} y_{ik} z_i^\top - \mathbb{E}[y_k z^\top] \right) \bar{w}_k^S \right] \\
& + \mathbb{E}[y^\top y] - \frac{1}{m} \sum_{i=1}^{m} y_i^\top y_i.
\end{aligned}$$

As G is a real symmetric matrix, we denote an eigendecomposition of G as $G = U\Lambda U^\top$ where the diagonal matrix Λ contains eigenvalues as $\Lambda_{jj} = \lambda_j$ with the corresponding orthogonal eigenvector matrix U; u_j is the j-th column of U. Then,

$$(\bar{w}_k^s)^\top G \bar{w}_k^s = \sum_j \lambda_j (u_j^\top \bar{w}_k^s)^2 = \|\bar{w}_k^s\|_2^2 \sum_j \lambda_j \cos^2 \theta_{\bar{w}_k^s, j}^{(1)},$$

and

$$\sum_j \lambda_j (u_j^\top \bar{w}_k^s)^2 \leq \lambda_{\max}(G)\|U^\top \bar{w}_k^s\|_2^2 = \lambda_{\max}(G)\|\bar{w}_k^s\|_2^2.$$

Also,

$$v^\top \bar{w}_k^s = \|v\|_2 \|\bar{w}_k^s\|_2 \cos \theta_{\bar{w}_k^s}^{(2)} \leq \|v\|_2 \|\bar{w}_k^s\|_2.$$

By using these,

$$\mathcal{R}[w^s] - \mathcal{R}_S[w^s] - c_y$$
$$= \sum_{k=1}^{d_y} \left(2\|v\|_2 \|\bar{w}_k^s\|_2 \cos \theta_{\bar{w}_k^s}^{(2)} + \|\bar{w}_k^s\|_2^2 \sum_j \lambda_j \cos^2 \theta_{\bar{w}_k^s, j}^{(1)} \right)$$
$$\leq \sum_{k=1}^{d_y} \left(2\|v\|_2 \|\bar{w}_k^s\|_2 + \lambda_{\max}(G)\|\bar{w}_k^s\|_2^2 \right).$$

$\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad$ $\square$

C4 Proof of Theorem 8

Proof. We do *not* require the independence over the coordinates of $\tilde{z}_i$ and the entries of random matrices $\tilde{z}_i \tilde{z}_i^\top$ because of the definition of independence required for matrix Bernstein inequality (for $\frac{1}{m_\sigma} \sum_{i=1}^{m_\sigma} \tilde{z}_i \tilde{z}_i^\top$) (e.g., see section 2.2.3 of Tropp et al. 2015) and because of a union bound over coordinates (for $\frac{1}{m_\sigma} \sum_{i=1}^{m_\sigma} y_{ik} \tilde{z}_i$). We use the fact that $\tilde{z}_{\alpha m+1}, \ldots, \tilde{z}_m$ are independent random variables *over the sample index (although dependent over the coordinates)*, because a $w_\sigma := w^{S_{\alpha m}}$ is fixed and independent from $x_{\alpha m+1}, \ldots, x_m$.

From Equation (2), with the definition of induced matrix norm and the Cauchy-Schwarz inequality,

$$\mathcal{R}[f_{\mathcal{A}(S)}] - \mathcal{R}_{S \setminus S_{\alpha m}}[f_{\mathcal{A}(S)}] \qquad\qquad\qquad\qquad\qquad\qquad\text{(C.1)}$$
$$\leq \sum_{k=1}^{d_y} \|\bar{w}_k^S\|_2^2 \lambda_{\max} \left(\mathbb{E}[\tilde{z}\tilde{z}^\top] - \frac{1}{m_\sigma} \sum_{i=\alpha m+1}^m \tilde{z}_i \tilde{z}_i^\top \right)$$
$$+ 2 \sum_{k=1}^{d_y} \|\bar{w}_k^S\|_1 \left\| \frac{1}{m_\sigma} \sum_{i=\alpha m+1}^m y_{ik} \tilde{z}_i - \mathbb{E}[y_k \tilde{z}] \right\|_\infty$$
$$+ \mathbb{E}[y^\top y] - \frac{1}{m_\sigma} \sum_{i=\alpha m+1}^m y_i^\top y_i.$$

In the below, we bound each term of the right-hand side of the above with concentration inequalities.

<u>For the first term:</u> Matrix Bernstein inequality (Lemma 10) states that for any $\delta > 0$, with probability at least $1 - \delta/3$,

$$\lambda_{\max}\left(\mathbb{E}[\tilde{z}\tilde{z}^\top] - \frac{1}{m_\sigma}\sum_{i=\alpha m+1}^{m} \tilde{z}_i\tilde{z}_i^\top\right) \le \frac{2C_{zz}}{3m_\sigma}\ln\frac{3d_z}{\delta} + \sqrt{\frac{2\gamma_{zz}^2}{m_\sigma}\ln\frac{3d_z}{\delta}}.$$

Here, Matrix Bernstein inequality was applied as follows. Let $M_i = (\frac{1}{m_\sigma}G^{(i)})$. Then, $\sum_{i=\alpha m+1}^{m} M_i = \mathbb{E}[\tilde{z}\tilde{z}^\top] - \frac{1}{m_\sigma}\sum_{i=\alpha m+1}^{m} \tilde{z}_i\tilde{z}_i^\top$. We have that $\mathbb{E}[M_i] = 0$ for all i. Also, $\lambda_{\max}(M_i) \le \frac{1}{m_\sigma}C_{zz}$ and $\|\sum_i \mathbb{E}[M_i^2]\|_2 \le \frac{1}{m_\sigma}\gamma_{zz}^2$.

<u>For the second term:</u> We apply Bernstein inequality to each $(k, k') \in \{1, \ldots, d_y\} \times \{1, \ldots, d_z\}$ and take union bound over $d_y d_z$ events, obtaining that for any $\delta > 0$, with probability at least $1 - \delta/3$, for all $k \in \{1, 2, \ldots, d_y\}$,

$$\left\|\frac{1}{m_\sigma}\sum_{i=\alpha m+1}^{m} y_{ik}\tilde{z}_i - \mathbb{E}[y_k\tilde{z}]\right\|_\infty \le \frac{2C_{yz}}{3m_\sigma}\ln\frac{6d_y d_z}{\delta} + \sqrt{\frac{\gamma_{yz}^2}{m_\sigma}\ln\frac{6d_y d_z}{\delta}}$$

<u>For the third term:</u> From Bernstein inequality, with probability at least $1 - \delta/3$,

$$\mathbb{E}[y^\top y] - \frac{1}{m_\sigma}\sum_{i=\alpha m+1}^{m} y_i^\top y_i \le \frac{2C_y}{3m}\ln\frac{3}{\delta} + \sqrt{\frac{2\gamma_y^2}{m}\ln\frac{3}{\delta}}.$$

<u>Putting together:</u> Putting together, for a fixed (or frozen) w_σ, with probability at least $1 - \delta$ (probability over $S \setminus S_{\alpha m} = \{(x_{\alpha m+1}, y_{\alpha m+1}), \ldots, (x_m, y_m)\}$), we have that

$$\lambda_{\max}\left(\mathbb{E}[\tilde{z}\tilde{z}^\top] - \frac{1}{m_\sigma}\sum_{i=\alpha m+1}^{m} \tilde{z}_i\tilde{z}_i^\top\right) \le \beta_1$$

, $\left\|\frac{1}{m_\sigma}\sum_{i=\alpha m+1}^{m} y_{ik}\tilde{z}_i - \mathbb{E}[y_k\tilde{z}]\right\|_\infty \le \beta_2$ (for all k), and

$$\mathbb{E}[y^\top y] - \frac{1}{m_\sigma}\sum_{i=\alpha m+1}^{m} y_i^\top y_i \le \beta_3.$$

Since Equation (C.1) always hold deterministically (with or without such a dataset), the desired statement of this theorem follows. $\qquad\square$

C5 Proof of Theorem 9

Proof. Define S_{m_σ} as

$$S_{m_\sigma} = S \setminus S_{\alpha m} = \{(x_{\alpha m+1}, y_{\alpha m+1}), \ldots, (x_m, y_m)\}.$$

Recall the following fact: using the result by Koltchinskii and Panchenko (2002), we have that for any $\delta > 0$, with probability at least $1 - \delta$, the following holds for all $f \in \mathcal{F}$:

$$\mathcal{R}[f] \le \mathcal{R}_{S_{m_\sigma}, \rho}[f] + \frac{2d_y^2}{\rho m_\sigma}\mathfrak{R}'_{m_\sigma}(\mathcal{F}) + \sqrt{\frac{\ln\frac{1}{\delta}}{2m_\sigma}},$$

where $\mathfrak{R}'_{m_\sigma}(\mathcal{F})$ is Rademacher complexity defined as

$$\mathfrak{R}'_{m_\sigma}(\mathcal{F}) = \mathbb{E}_{S_{m_\sigma},\xi}\left[\sup_{k,w}\sum_{i=1}^{m_\sigma}\xi_i z_k^{[L]}(x_i,w)\right].$$

Here, ξ_i is the Rademacher variable, and the supremum is taken over all $k \in \{1,\ldots,d_y\}$ and all w allowed in $\mathcal{F}$. Then, for our parameterized hypothesis spaces with any frozen w_σ,

$$\begin{aligned}
\mathfrak{R}'_{m_\sigma}(\mathcal{F}) &= \mathbb{E}_{S_{m_\sigma},\xi}\left[\sup_{k,\bar{w}_k}\sum_{i=1}^{m_\sigma}\xi_i[\bar{x}_i \circ \bar{\sigma}(x_i,w_\sigma)]^\top \bar{w}_k\right]\\
&\le \mathbb{E}_{S_{m_\sigma},\xi}\left[\sup_{k,\bar{w}_k}\left\|\sum_{i=1}^{m_\sigma}\xi_i[\bar{x}_i \circ \bar{\sigma}(x_i,w_\sigma)]\right\|_2 \|\bar{w}_k\|_2\right]\\
&\le C_w \mathbb{E}_{S_{m_\sigma},\xi}\left[\left\|\sum_{i=1}^{m_\sigma}\xi_i[\bar{x}_i \circ \bar{\sigma}(x_i,w_\sigma)]\right\|_2\right].
\end{aligned}$$

Because square root is concave in its domain, by using Jensen's inequality and linearity of expectation,

$$\begin{aligned}
&\mathbb{E}_{S_{m_\sigma},\xi}\left[\left\|\sum_{i=1}^{m_\sigma}\xi_i[\bar{x}_i \circ \bar{\sigma}(x_i,w_\sigma)]\right\|_2\right]\\
&\le \left(\mathbb{E}_{S_{m_\sigma}}\sum_{i=1}^{m_\sigma}\sum_{j=1}^{m_\sigma}\mathbb{E}_\xi[\xi_i\xi_j][\bar{x}_i \circ \bar{\sigma}(x_i,w_\sigma)]^\top[\bar{x}_j \circ \bar{\sigma}(x_j,w_\sigma)]\right)^{1/2}\\
&= \left(\sum_{i=1}^{m_\sigma}\mathbb{E}_{S_{m_\sigma}}\left[\|[\bar{x}_i \circ \bar{\sigma}(x_i,w_\sigma)]\|_2^2\right]\right)^{1/2}\\
&\le C_\sigma\sqrt{m_\sigma}.
\end{aligned}$$

Putting together, we have that $\mathfrak{R}'_m(\mathcal{F}) \le C_\sigma C_w \sqrt{m_\sigma}$. $\qquad\square$

C6 Proof of Proposition 5

Proof. Consider a single fixed $f \in \mathcal{F}_{\text{val}}$. Since $\mathcal{F}_{\text{val}}$ is independent from the validation dataset, $\kappa_{f,1},\ldots,\kappa_{f,m_{\text{val}}}$ are independent zero-mean random variables, given a fixed $f \in \mathcal{F}_{\text{val}}$. Thus, we can apply Bernstein inequality, yielding

$$\mathbb{P}\left(\frac{1}{m_{\text{val}}}\sum_{i=1}^{m_{\text{val}}}\kappa_{f,i} > \epsilon\right) \le \exp\left(-\frac{\epsilon^2 m_{\text{val}}/2}{\gamma^2 + \epsilon C/3}\right).$$

By taking union bound over all elements in $\mathcal{F}_{\text{val}}$,

$$\mathbb{P}\left(\cup_{f\in\mathcal{F}_{\text{val}}}\left\{\frac{1}{m_{\text{val}}}\sum_{i=1}^{m_{\text{val}}}\kappa_{f,i} > \epsilon\right\}\right) \le |\mathcal{F}_{\text{val}}|\exp\left(-\frac{\epsilon^2 m_{\text{val}}/2}{\gamma^2 + \epsilon C/3}\right).$$

By setting $\delta = |\mathcal{F}_{\text{val}}| \exp\left(-\frac{\epsilon^2 m_{\text{val}}/2}{\gamma^2 + \epsilon C/3}\right)$ and solving for ϵ (via quadratic formula),

$$\epsilon = \frac{2C \ln(\frac{|\mathcal{F}_{\text{val}}|}{\delta})}{6m_{\text{val}}} \pm \frac{1}{2}\sqrt{\left(\frac{2C \ln(\frac{|\mathcal{F}_{\text{val}}|}{\delta})}{3m_{\text{val}}}\right)^2 + \frac{8\gamma^2 \ln(\frac{|\mathcal{F}_{\text{val}}|}{\delta})}{m_{\text{val}}}}.$$

By noticing that the solution of ϵ with the minus sign results in $\epsilon < 0$, which is invalid for Bernstein inequality, we obtain the valid solution with the plus sign. Then, we have

$$\epsilon \leq \frac{2C \ln(\frac{|\mathcal{F}_{\text{val}}|}{\delta})}{3m_{\text{val}}} + \sqrt{\frac{2\gamma^2 \ln(\frac{|\mathcal{F}_{\text{val}}|}{\delta})}{m_{\text{val}}}},$$

where we used that $\sqrt{a+b} \leq \sqrt{a} + \sqrt{b}$. By tanking the negation of the statement, we obtain that for any $\delta > 0$, with probability at least $1 - \delta$, for all $f \in \mathcal{F}_{\text{val}}$,

$$\frac{1}{m_{\text{val}}}\sum_{i=1}^{m_{\text{val}}} \kappa_{f,i} \leq \frac{2C \ln(\frac{|\mathcal{F}_{\text{val}}|}{\delta})}{3m_{\text{val}}} + \sqrt{\frac{2\gamma^2 \ln(\frac{|\mathcal{F}_{\text{val}}|}{\delta})}{m}},$$

where $\frac{1}{m_{\text{val}}}\sum_{i=1}^{m_{\text{val}}} \kappa_{f,i} = \mathcal{R}[f] - \mathcal{R}_{S_{m_{\text{val}}}^{(\text{val})}}[f]$. $\qquad\square$

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