Using noise resilience for ranking generalization of deep neural networks

Depen Morwani  
Department of Computer Science  
Indian Institute of Technology Madras  
Chennai, 600036  
cs19s002@smail.iitm.ac.in

Rahul Vashisht  
Department of Computer Science  
Indian Institute of Technology Madras  
Chennai, 600036  
cs18d006@smail.iitm.ac.in

Harish G. Ramaswamy  
Department of Computer Science  
Indian Institute of Technology Madras  
Chennai, 600036  
hariguru@cse.iitm.ac.in

Abstract

Recent papers have shown that sufficiently overparameterized neural networks can perfectly fit even random labels. Thus, it is crucial to understand the underlying reason behind the generalization performance of a network on real-world data. In this work, we propose several measures to predict the generalization error of a network given the training data and its parameters. Using one of these measures, based on noise resilience of the network, we secured 5th position in the predicting generalization in deep learning (PGDL) competition at NeurIPS 2020.

1 Introduction

Deep learning models have achieved tremendous success in a wide variety of tasks related to computer vision (CV) and natural language processing (NLP). However, we still do not have a clear understanding regarding the generalization behavior of these models. Generalization is defined as the ability of classifiers to perform well on unseen data. It is desirable for real-world deployment of deep models in real-world applications such as healthcare. Recently, Goodfellow et al. [2015] showed that neural networks can misclassify an example even with perturbations imperceptible to human eye, and Zhang et al. [2017] demonstrated that sufficiently overparameterized neural networks can even fit random labels. Both of these observations question the ability of a neural network to generalize well. Moreover, in both the cases, cross entropy loss on the training dataset remained small, indicating that it cannot be a predictor of generalization. Thus it is crucial to understand the reason behind generalization of neural networks.

A lot of generalization bounds have been proposed for deep networks based on margin and weight norms [Bartlett et al., 2017; Konstantinos et al., 2017]. In a recent work, Jiang et al. [2020] studied the capability of these bounds to predict the generalization gap of a network. In this work, we propose a few other measures based on noise stability and hidden layer margins of the network.

2 Notation

A neural network is represented as a function $f$ that is given by $f(x) = W_l(\sigma(W_{l-1}...(W_1x + b_1) + b_2)...)) + b_l$, where $l$ represents the number of layers in the network, $x \in \mathbb{R}^d$ represents

Preprint. Under review.
the input to the network, \( \sigma \) represents the non-linearity in the network operating element-wise and \( W_j \in \mathbb{R}^{h_j \times h_{j-1}}, b_j \in \mathbb{R}^{h_j} \) represent the weights and biases of the network with \( h_j \) representing the width of the \( j^{th} \) hidden layer. This representation suffices for a convolutional network as well, because convolution operation can be replaced by a sparse weight matrix. The pre-activations and activations at the \( j^{th} \) layer are represented by \( z_j(x) \) and \( a_j(x) \) respectively. Using this notation, the neural network can be defined as

\[
\begin{align*}
a_0(x) &= x \\
z_j(x) &= W_j a_{j-1}(x) + b_j \\
a_j(x) &= \sigma(z_j(x))
\end{align*}
\]

\( \|W\|_2 \) and \( \|W\|_F \) represent the spectral and frobenius norm respectively, of a matrix \( W \). The training dataset is represented by \( D = \{ (x_i, y_i) \}_{i=1}^n \), where \( n \) represents the number of points in the training dataset. Let the set of all classes in the dataset be denoted by \( \mathcal{Y} \). \( \mathcal{N}(\mu, \Sigma) \) represents the normal distribution with mean \( \mu \) and covariance \( \Sigma \). \( \mathbb{E}(X) \) represents the expectation of a random variable \( X \).

### 3 Methodology

The measures used can be broadly divided into three different categories: Noise-based, Margin-based and Norm-based. In this section, we will provide the description of these methods and their results in the PGDL competition will be discussed in the following section.

#### 3.1 Noise-based measures

The noise stability of the \( j^{th} \) layer with respect to \((j-1)^{th}\) layer is measured by adding Gaussian noise to the activations of \((j-1)^{th}\) layer and quantifying its propagation to the pre-activations of the \( j^{th} \) layer. Precisely, let \( Y \sim \mathcal{N}(0, I) \), where \( Y \in \mathbb{R}^{h_{j-1}} \). Then, define

\[
\begin{align*}
a_{j-1}'(x) &= a_{j-1}(x) + \sqrt{\frac{\nu}{d_{j-1}}} \|a_{j-1}(x)\| Y \\
z_j'(x) &= W_j a_{j-1}'(x) + b_j
\end{align*}
\]

where \( \nu \) controls the standard deviation of the Gaussian noise and the other factors ensure that \( \mathbb{E}(\|\mathbf{a}_{j-1}'(\mathbf{x})\|^2) = (1 + \nu)\mathbb{E}(\|\mathbf{a}_{j-1}(\mathbf{x})\|^2) \), thus making the noise proportional to the scale of the inputs. In this case, noise stability \( (\beta_j(x)) \) of layer \( j \) with respect to layer \( j-1 \) is defined as

\[
\beta_j(x) = \frac{1}{\nu} \frac{\|z_j'(x) - z_j(x)\|^2}{\|z_j(x)\|^2}
\]

Two measures defined using \( \beta_j(x) \) are given below

\[
\text{mean-noise-stability} = \frac{1}{n \times l} \sum_{i=1}^n \sum_{j=1}^l \beta_j(x_i)
\]

\[
\text{geometric-mean-noise-stability} = \frac{1}{n \times l} \sum_{i=1}^n \sum_{j=1}^l \log(\beta_j(x_i))
\]

Two other measures can be defined similarly (mean-noise-stability-output and geometric-mean-noise-stability-output), using the noise stability of the output with respect to the input. Variations of this measure have been used in recent papers [Arora et al., 2018, Nagarajan and Kolter, 2019] for establishing data-dependent generalization bounds.

---

1 Code available: https://github.com/VASHISHT-RAHUL/Generalization_performance_of_neural_networks
3.2 Margin-based measures

Multiple generalization bounds based on the output-layer margin have been established for deep networks [Jiang* et al., 2020]. However, margin can be defined at intermediate layers as well [Elsayed et al., 2018]. Moreover, a linear parametric model with these margins as inputs has been shown to predict the generalization gap reasonably well, given a constant depth [Jiang et al., 2019]. However, with varying depth, determining the inputs for the parametric model is tricky and moreover, we explicitly wanted to avoid parametric models and focus on theoretically grounded measures.

3.2.1 Input-layer margin (γ_{inp})

It is defined as the minimum perturbation that needs to be added to an input \( x \) so that the perturbed input is misclassified by the network [Elsayed et al., 2018]. It was approximated using the first-order Taylor expansion of the network around the input.

3.2.2 All-layer-margin (γ_{all})

Consider a neural network represented as a composition of \( l \) functions denoted by \( f_1, \ldots, f_l \). Let \( \delta_1, \ldots, \delta_l \) represent the perturbations applied at each layer. Then the perturbed network output (\( F(x, \delta) \)) is given by

\[
g_1(x, \delta) = f(x) + \delta_1 \|x\|_2 \\
g_j(x, \delta) = f_j(g_{j-1}(x, \delta)) + \delta_j \|g_{j-1}(x, \delta)\|_2 \\
F(x, \delta) = g_l(x, \delta)
\]

Then, all-layer-margin [Wei and Ma, 2020] is defined as

\[
\gamma_{all}(x, y) = \min_{\delta_1, \ldots, \delta_l} \sqrt{\sum_{j=1}^{l} \|\delta_j\|^2} \\
\text{subject to } \text{arg max}_{y' \in \mathcal{Y}} F(x, \delta)_{y'} = y
\]

It was approximated by performing gradient ascent on the loss function with respect to the parameters \( \delta_1, \ldots, \delta_l \).

3.2.3 Margin-jacobian

This measure was defined by combining the output-layer margin (\( \gamma_{out} \)) with the Jacobian of the output with respect to the intermediate layers.

\[
\text{margin-jacobian} = \left( \frac{1}{\gamma_{out}^2} \right)^{\frac{1}{4}} + \sum_{i=1}^{n} \sum_{j=1}^{l} \| \frac{\partial f(x_i)}{\partial a_j} \|_F \\
\frac{1}{nl^2 \gamma_{out}}
\]

The first term normalizes the margin by the depth and was inspired from one of the bounds in [Jiang* et al., 2020]. \( \sum_{i=1}^{n} \sum_{j=1}^{l} \frac{\| \frac{\partial f(x_i)}{\partial a_j} \|_F}{nl^2 \gamma_{out}} \) represents the average Jacobian norm, that is further normalized by depth and margin. We found that the sum of these terms works better empirically than the individual terms.

3.3 Norm-based Measures

Multiple bounds based on spectral and frobenius norms have been proposed recently for feed-forward as well as convolutional networks [Bartlett et al., 2017, Konstantinos et al., 2017]. The capability of these bounds to predict the generalization gap has also been explored in [Jiang* et al., 2020]. We provide an efficient way of evaluating the spectral norm of weight matrices in case of convolutional networks.

Converting the weight matrix of a convolution operator to the sparse weight matrix of a linear operator is time-consuming task. Instead, for calculating the spectral norm, or any eigenvalues of the convolution operator, we used the Power Method, that works for any linear operator, whether or not
it is defined explicitly by a weight matrix (for more details, refer to the code). This trick allowed us to evaluate these bounds for deep networks within the time limit of the competition.

Based on this faster method of evaluation, the one metric based on spectral norm that we tried was

$$\text{fast-log-spec} = (1 - \frac{1}{7}) \sum_{i=1}^{l} \log(\|W_i\|_2^2) - \log(\gamma_{out}^2)$$

This is based on the generalization bound for convolutional networks from Konstantinos et al. [2017].

4 Results in PGDL

The PGDL competition had three different kind of datasets - public, development and private. Public dataset had two different tasks - Task 1 and Task 2, and was completely accessible to the competitors, i.e, we could access the final test error of the networks as well as the final scores on these tasks. Development dataset had two different tasks - Task 4 and Task 5, and was partially accessible, i.e, we could just access the final scores on these tasks. Private dataset had 4 tasks - Task 6, Task 7, Task 8 and Task 9, and was significantly more complex as compared to public and development datasets. Participants were allowed limited submissions on this dataset and the final score was only revealed after the competition ended.

Each task consisted of a dataset and a set of neural networks with varying hyperparameters such as depth, dropout etc., that were trained to almost 100% accuracy on the training dataset. The aim was to come up with a measure that can predict the test error of the network, given the training data and its parameters. The evaluation metric used was the mutual information between the predicted measure and the generalization error, conditioned on the hyperparameters. More details regarding the competition can be found on the PGDL website.

The results for development and public dataset for all the measures (except for one that we did not try on the development dataset) are given in Table 1. As limited submissions were allowed on private dataset, results for a few of these measures on the private dataset are shown in Table 2 (for exact hyperparameter settings, refer to the code).

As can be clearly seen, geometric-mean-noise-stability clearly beats the other measures on the private dataset. However, its performance on a particular task - Private Task 8 is poor. Similarly, on development and public datasets, it doesn’t perform as well as other measures. This clearly indicates a non-uniformity in the measure that is predictive of generalization on a particular task.

5 Conclusion

Although noise resilience based measure beats other measures on the private dataset, the same does not hold for public and development datasets. This clearly indicates a non-uniformity in the measure required to predict generalization for a given task, that can be explored further, if the data of these tasks is made available to the competitors.
### Table 2: Results on private dataset

| Method                          | Private Task 6 | Private Task 7 | Private Task 8 | Private Task 9 |
|---------------------------------|----------------|----------------|----------------|----------------|
| geometric-mean-noise-stability  | 6.51           | 7.76           | 8.02           | 9.58           |
| mean-noise-stability-output     | 2.10           | 0.07           | 0.80           | 5.77           |
| input-layer-margin              | 1.34           | 1.18           | 2.74           | 0.62           |
| all-layer-margin                | 2.50           | 3.15           | 2.21           | 0.63           |
| margin-jacobian                 | 4.01           | 8.50           | 2.02           | 2.67           |

## References

Ian Goodfellow, Jonathon Shlens, and Christian Szegedy. Explaining and harnessing adversarial examples. In *International Conference on Learning Representations*, 2015. URL [http://arxiv.org/abs/1412.6572](http://arxiv.org/abs/1412.6572)

Chiyuan Zhang, Samy Bengio, Moritz Hardt, Benjamin Recht, and Oriol Vinyals. Understanding deep learning requires rethinking generalization. In *5th International Conference on Learning Representations, ICLR 2017, Toulon, France, April 24-26, 2017, Conference Track Proceedings*. OpenReview.net, 2017. URL [https://openreview.net/forum?id=Sy8gdB9xx](https://openreview.net/forum?id=Sy8gdB9xx)

Peter L. Bartlett, Dylan J Foster, and Matus J Telgarsky. Spectrally-normalized margin bounds for neural networks. In I. Guyon, U. V. Luxburg, S. Bengio, H. Wallach, R. Fergus, S. Vishwanathan, and R. Garnett, editors, *Advances in Neural Information Processing Systems*, volume 30, pages 6240–6249. Curran Associates, Inc., 2017. URL [https://proceedings.neurips.cc/paper/2017/file/b22b257ad0519d4500539da3c0bcf4dd-Paper.pdf](https://proceedings.neurips.cc/paper/2017/file/b22b257ad0519d4500539da3c0bcf4dd-Paper.pdf)

Pitas Konstantinos, Mike Davies, and Pierre Vandergheynst. Pac-bayesian margin bounds for convolutional neural networks - technical report. 12 2017.

Yiding Jiang*, Behnam Neyshabur*, Hossein Mobahi, Dilip Krishnan, and Samy Bengio. Fantastic generalization measures and where to find them. In *International Conference on Learning Representations*, 2020. URL [https://openreview.net/forum?id=SJgIPJBFvH](https://openreview.net/forum?id=SJgIPJBFvH)

Sanjeev Arora, Rong Ge, Behnam Neyshabur, and Yi Zhang. Stronger generalization bounds for deep nets via a compression approach. In Jennifer Dy and Andreas Krause, editors, *Proceedings of the 35th International Conference on Machine Learning*, volume 80 of *Proceedings of Machine Learning Research*, pages 254–263, Stockholmsmässan, Stockholm Sweden, 10–15 Jul 2018. PMLR. URL [http://proceedings.mlr.press/v80/arora18b.html](http://proceedings.mlr.press/v80/arora18b.html)

Vaishnavh Nagarajan and Zico Kolter. Deterministic PAC-bayesian generalization bounds for deep networks via generalizing noise-resilience. In *International Conference on Learning Representations*, 2019. URL [https://openreview.net/forum?id=Hygn2o0qKX](https://openreview.net/forum?id=Hygn2o0qKX)

Gamaleldin Elsayed, Dilip Krishnan, Hossein Mobahi, Kevin Regan, and Samy Bengio. Large margin deep networks for classification. In S. Bengio, H. Wallach, H. Larochelle, K. Grauman, N. Cesa-Bianchi, and R. Garnett, editors, *Advances in Neural Information Processing Systems*, volume 31, pages 842–852. Curran Associates, Inc., 2018. URL [https://proceedings.neurips.cc/paper/2018/file/42998cf32d552343bc8e460416382dca-Paper.pdf](https://proceedings.neurips.cc/paper/2018/file/42998cf32d552343bc8e460416382dca-Paper.pdf)

Yiding Jiang, Dilip Krishnan, Hossein Mobahi, and Samy Bengio. Predicting the generalization gap in deep networks with margin distributions. In *International Conference on Learning Representations*, 2019. URL [https://openreview.net/forum?id=HJ1QfnCqkX](https://openreview.net/forum?id=HJ1QfnCqkX)

Colin Wei and Tengyu Ma. Improved sample complexities for deep neural networks and robust classification via an all-layer margin. In *International Conference on Learning Representations*, 2020. URL [https://openreview.net/forum?id=HJe_yR4Fw](https://openreview.net/forum?id=HJe_yR4Fw)