EVALUATING NATURAL LANGUAGE PROCESSING MODELS WITH GENERALIZATION METRICS THAT DO NOT NEED ACCESS TO ANY TRAINING OR TESTING DATA

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Paper under double-blind review

ABSTRACT

The search for effective and robust metrics has been the focus of recent theoretical and empirical work on generalization of deep neural networks (NNs). In this paper, we discuss the performance of natural language processing (NLP) models, and we evaluate various existing and novel generalization metrics. Compared to prior studies, we (i) focus on NLP instead of computer vision (CV), (ii) focus on generalization metrics that predict test error instead of the generalization gap, (iii) focus on generalization metrics that do not need the access to data, and (iv) focus on the heavy-tail (HT) phenomenon that has received comparatively less attention in the study of deep neural networks. We extend recent HT-based work which focuses on power law (PL) distributions, and we study exponential (EXP) and exponentially truncated power law (E-TPL) fitting to the empirical spectral densities (ESDs) of weight matrices. Our empirical studies are carried on (i) hundreds of Transformers trained in different settings, in which we systematically vary the amount of data, the model size and the optimization hyperparameters, (ii) a total of 51 pretrained Transformers from eight families of Huggingface NLP models, including BERT, GPT2, ALBERT, etc., and (iii) a total of 28 existing and novel generalization metrics. From our detailed empirical analyses, we show that *shape metrics*, or the metrics obtained from fitting the shape of the ESDs, perform uniformly better at predicting generalization performance than *scale metrics* commonly studied in the literature, as measured by the *average* rank correlations with the generalization performance for all of our experiments. We also show that among the three HT distributions considered in our paper, the E-TPL fitting of ESDs performs the most robustly when the models are trained in experimental settings, while the PL fitting achieves the best performance on well-trained Huggingface models, and that both E-TPL and PL metrics (which are both shape metrics) outperform scale metrics.

1 INTRODUCTION

Recent years have seen a wide array of large-scale empirical studies on the various metrics used to quantify generalization (Dziugaite et al., 2020; Jiang et al., 2019; Martin & Mahoney, 2021a; Martin et al., 2021). On the one hand, theory-driven metrics have the potential to reveal more information than test error, bringing us one step closer to unpacking the black box of deep NNs (Frankle & Carbin, 2018; Nakkiran et al., 2019; Zhang et al., 2021). On the other hand, a wide variety of generalization metrics have been applied to predict the *quality* of pretrained models (Martin & Mahoney, 2019; Martin et al., 2021), design effective training procedures (Foret et al., 2020; Izmailov et al., 2018), improve network efficiency (Chen et al., 2020; Dong et al., 2019), quantify network robustness (Tanay & Griffin, 2016; Yang et al., 2020), improve ensemble learning techniques (Fort et al., 2019; Garipov et al., 2018), analyze and improve large-scale machine learning contests (Martin & Mahoney, 2021a), and so on.

Despite advances in the study of generalization, however, several recent papers point out the deficiencies of many of these "fantastic" generalization metrics. These include a lack of "robustness" to the changes of environmental hyperparameters (Dziugaite et al., 2020; Jiang et al., 2019) (such as data, network architecture and training schemes), or the Simpson's paradox that generalization metrics perform differently (i.e., predict opposite trends) when applied to each sub-part of a collection

of learning models or to the holistic study (Martin & Mahoney, 2021a). Another drawback is the over-reliance on experiments with CV models, which are relatively well-explored, and which are not representative of many other application areas. Despite a few counterexamples (Martin et al., 2021; Nakkiran et al., 2019; Yang et al., 2021), systematic studies of generalization in other fields, such as NLP, are largely missing.

Generalization metrics for NLP. The objective of this paper is to provide a systematic study of generalization metrics in NLP, addressing several deficiencies in prior studies (Dziugaite et al., 2020; Jiang et al., 2019; Martin et al., 2021). Compared to CV, predicting generalization in NLP has several important differences that require careful consideration. The training data from standard CV benchmarks can often be easily obtained, while NLP pretraining datasets are typically web-scale and are challenging to access. Therefore, generalization metrics that can measure the quality of learning models *without access to data* are ideal for NLP. Indeed, recent work has shown that access to training or testing data is not necessary for assessing the model quality of learning models (Martin et al., 2021), though these have yet to be evaluated at scale in the NLP domain. Furthermore, it is typically infeasible to train NLP models to interpolate the (frequently large) training set. This becomes an issue when applying most existing generalization metrics as they often estimate the *generalization gap* (i.e., the difference between training and test performance) rather than the test error itself. Metrics that focus on predicting the generalization gap include most of the well-known metrics in CV, such as those based on the PAC-Bayesian framework (McAllester, 1999; Neyshabur et al., 2018) and margins (Bartlett et al., 2017; Jiang et al., 2018; Pitas et al., 2017).

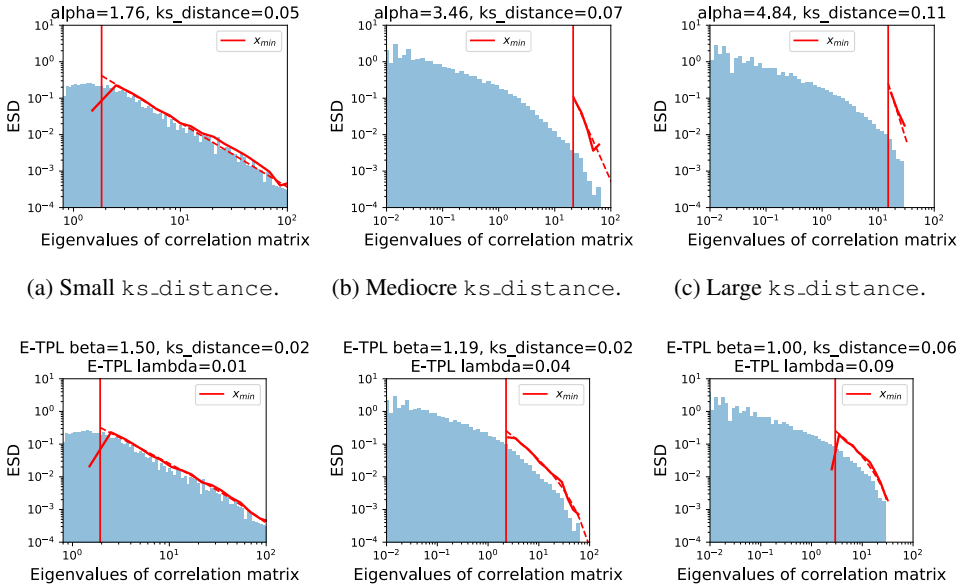
To illustrate the issue, consider the problem of model selection between two models (Jiang et al., 2020; Martin & Mahoney, 2021a). Suppose we are given two classification models. Then even if we have i) access to both models' training errors, and ii) a metric which is guaranteed to perfectly rank correlate with the generalization gap, then we still cannot determine which model as smaller test error. This is means that, if our objective is to construct a metric that correctly predicts which model has lower test error, rank correlation with the generalization gap is not sufficient. In this paper, we aim to study how generalization metrics correlate with *model quality*, for which we use test error as a close approximation. As we will demonstrate (in Figure 4), rank correlation with the generalization gap indeed does not imply rank correlation with model quality in practice, and in fact often orders models in the opposite order of their test errors. From a practical point of view, for NLP tasks, we prefer generalization metrics that can directly predict trends in test error (or similar evaluation metrics in NLP, such as the test BLEU score (Papineni et al., 2002)) rather than trends in the generalization gap.

Naturally, we cannot expect a metric to be universally correlated with test error if evaluating the metric does not need data (otherwise, models could be trained without data). However, within certain classes of models (e.g. stages of training in one model or across pre-trained models), they may be effective at diagnosing model quality. With these objectives in mind, among the generalization metrics in the literature, we take particular interest in those derived from the heavy-tail self regularization (HT-SR) theory (Martin & Mahoney, 2019, 2021b), which (i) predicts test error directly instead of the generalization gap and (ii) does not require access to training (or testing) data.

HT-SR theory. The core principle of HT-SR theory is that HT structures arise naturally in the ESDs of the weight matrices as the result of extracting various correlations in data during optimization (Martin & Mahoney, 2019, 2021a,b; Martin et al., 2021). Its primary practical consequence is that by estimating the PL coefficient from the ESDs (requiring only weights), one can predict model quality, as smaller coefficients are reported to correspond to higher test accuracy. However, these estimators can be unstable, and so one must be careful not to rely on them alone. The quality of the PL fit itself should also point to similar conclusions (Martin & Mahoney, 2021b), which can be a sanity check.

The principles of HT-SR theory extend beyond fitting the PL coefficient, however, as ESDs can take many forms. To this end, we study three different types of distributions to fit to the ESDs of weight matrices, including power laws (PL) in Eqn. (1), exponentially truncated power laws (E-TPL) in Eqn. (2), and exponential laws (EXP) in Eqn. (3). These are all commonly considered families of distributions in classical studies of PL (Clauset et al., 2009), and it is often hard in practice to predict which family fits data the best (as we show in this paper, this is true for deep NNs especially). Figure 1 shows examples of comparing different HT fittings on the same ESD. Following Martin & Mahoney (2021a), we refer to the various metrics derived from HT-SR as *shape metrics*.

Contributions. The following summarizes our main contributions.



(a) Small `ks_distance`. (b) Mediocre `ks_distance`. (c) Large `ks_distance`.

(d) E-TPL fitting of the ESD. (e) E-TPL fitting of the ESD. (f) E-TPL fitting of the ESD.

Figure 1: Comparing PL and E-TPL fitting. **(First row).** Good, mediocre, and bad PL fittings measured by the `ks_distance`. **(Second row).** E-TPL fitting of the ESD on the same column. Blue histograms represent the ESDs. Solid vertical lines represent the lower threshold $x_{\min}$ of the PL distribution found by the fitting procedure. Solid curves represent ESDs truncated using $x_{\min}$, and dashed curves represent the fitted HT distributions.

- Deviating from prior work examining generalization metrics in CV (Dziugaite et al., 2020; Jiang et al., 2019), we provide the first systematic empirical study on various generalization metrics in NLP. Our detailed studies include:
  - 400 transformers trained with varying hyperparameters, and eight families of pretrained SOTA transformers downloaded from Huggingface (Wolf et al., 2020), including BERT (Kenton & Toutanova, 2019), GPT2 (Radford et al., 2019), ALBERT (both v1 and v2) (Lan et al., 2019), etc..
  - measuring the correlation between 28 generalization metrics and the model quality (measured by test-time performance) over three different model classes: (i) models trained with the optimal hyperparameters; (ii) a single model at different stages of training; and (iii) a model trained with different hyperparameters (similar to Jiang et al. (2019)).
- We extend prior studies on HT-SR theory and investigate alternative models to fit heavy-tail/light-tail distributions. Our results show that E-TPL fits are comparatively robust alternatives to PL fits for predicting trends in test error on suboptimally-trained models.
- Applied appropriately, we will find that shape metrics consistently perform better than scale metrics (or norm-based metrics) for predicting model quality.
- We also provide results for data-dependent metrics motivated by margins and PAC-Bayesian bounds (Dziugaite et al., 2020; Jiang et al., 2019). While these metrics perform well in predicting the generalization gap, we show that none of them satisfactorily predicts test error directly.

1.1 Preliminary of ESDs of weight matrices

Consider a NN with d layers and corresponding weight matrices $\mathbf{W}_1$, $\mathbf{W}_2$,..., $\mathbf{W}_d$. For each weight matrix $\mathbf{W}_i$ with shape $N \times M$, assume without loss of generality that $N \geq M$ (otherwise, consider $\mathbf{W}_i^\top$). We define the correlation matrix as $\mathbf{X}_i = \mathbf{W}_i^\top \mathbf{W}_i$, and denote the eigenvalues of $\mathbf{X}_i$ as $\{\lambda_j\}_{j=1}^M$, so that $\lambda_j = \sigma_j^2$, where $\{\sigma_j\}_{j=1}^M$ are the singular values of $\mathbf{W}_i$. Furthermore, we use $\lambda_{i,\max}$ to denote the maximum eigenvalue of the correlation matrix $\mathbf{X}_i$. The ESD of the weight matrix $\mathbf{W}_i$ refers to the empirical density of the eigenvalues of $\mathbf{X}_i$, typically represented through a histogram. We let $p(x)$ denote the density function to fit the ESD taking values in the interval $(x_{\min}, x_{\max})$. For

a power law, p satisfies

$$p(x) \propto x^{-\alpha}, \quad x_{\min} < x < x_{\max}. \tag{1}$$

From Martin & Mahoney (2021a), $x_{\max}$ is chosen to be the maximum eigenvalue of the correlation matrix. However, $x_{\min}$ is a variable to be optimized to improve the quality of PL fitting, and it is not equal to the minimum eigenvalue in general.

2 HEAVY-TAIL SELF-REGULARIZATION THEORY

First, we provide a brief overview of the HT-SR theory, and discuss several metrics that can be derived from it. According to HT-SR theory, the ESDs of the weight matrices become more heavy-tailed during training as they become increasingly correlated. One can quantify the extent of these correlations by fitting a PL to the ESD of a weight matrix, for example, by using the open-source `WeightWatcher` tool (Martin et al., 2021). After computing the ESD of a weight matrix, we use the maximum likelihood estimate from Alstott et al. (2014) to fit the PL distribution, the specific form of which has been defined in (1). Let `PL_alpha` denote the PL coefficient averaged over layers; effectively the slope of the tail of the ESD of the pooled weights, on a log-log scale.

Correctly identifying and fitting PL distributions is well-known to be a challenge in practice. For example, a density that appears as a straight line on a log-log scale plot need not follow a power law, as there are many other distributions that could show a similar behavior, including lognormal and exponential-type distributions (Clauset et al., 2009). Nested distributions such as E-TPL, which combine the pure PL and other distributional assumptions, can often improve the quality of fitting (Alstott et al., 2014; Clauset et al., 2009). Therefore, in addition to the PL distribution defined in (1), we consider several other distribution classes from the literature.

- (`E_TPL_lambda` and `E_TPL_beta`) The ESDs are assumed to take a "nested" form.

$$p(x) \propto x^{-\beta} \exp(-\lambda x), \; x_{\min} < x < x_{\max}. \tag{2}$$

  After fitting the E-TPL, we call the exponential truncation coefficient λ the `E_TPL_lambda` metric, and we call the PL coefficient the `E_TPL_beta` metric.

- (`EXP_lambda`). The ESDs are assumed to take the following form.

$$p(x) \propto \exp(-\lambda x), \; x_{\min} < x < x_{\max}. \tag{3}$$

  After fitting the EXP, we call the exponential coefficient λ the `EXP_lambda` metric.

For more details of the various metrics considered in this paper, see Table 1. All of the metrics derived from HT-SR do not require access to data, and are relatively cheap to compute. Our primary comparisons are between shape metrics (derived from HT-SR), and scale metrics (mostly norm-based). For the precise definitions of these metrics, see Appendix A.

Issues of PL fitting. It is well-known that subtle issues can arise when fitting the ESDs (Alstott et al., 2014; Clauset et al., 2009; Martin & Mahoney, 2017, 2021a). To best mitigate these issues in PL fits, we adopt the fitting strategies used in WeightWatcher (Martin & Mahoney, 2017). For example, as in Clauset et al. (2009), it is common to choose the lower threshold $x_{\min}$ which coincides with the best quality fit under the Kolmogorov–Smirnoff statistic (referred to as `PL_ks_distance` for PL and `E_TPL_ks_distance` for E-TPL in the sequel; see Eqn. (12)). However, this method is time-consuming, especially for E-TPL as there are two parameters to fit. Instead, we adopt the *fix-finger method* (Martin & Mahoney, 2017) which selects $x_{\min}$ as the peak of the ESD when fitting E-TPLs. More than a simple speed improvement, we find this method also yields more stable results.

Comparing PL and E-TPL fitting. Referring to Figure 1, we now discuss how E-TPL could partially address these fitting issues. On the first row of Figure 1, we show three typical cases of PL fitting. In Figure 1a, the log-log scale reveals a "linear region" of the histogram, which the PL fitting correctly locates. The quality of fit, measured by the `ks_distance`, is within a typical range, as reported in Table 5 of Martin & Mahoney (2021b). In Figure 1b and Figure 1c, the ESDs do not exhibit a clear linear region on the log-log scale. Following Martin & Mahoney (2021b), it is ill-advised to consider metrics derived from a PL fit in these scenario. In practice, this typically occurs when `PL_alpha` > 4 (e.g., see Figure 1c). On the other hand, in these two cases, the corresponding E-TPL fits (shown on the second row in Figure 1) still closely match the empirical density function

Name	Eqn	Ref	Need initial weights?	Scale or shape	Need data?	Need gpu?	Predicting model quality or generalization gap?
param_norm	(4)	Jiang et al. (2019)	No	Scale	No	No	Generalization gap
fro_dist	(5)	Jiang et al. (2019)	Yes	Scale	No	No	Generalization gap
log_norm	(6)	Martin & Mahoney (2021b)	No	Scale	No	No	Generalization gap
log_spectral_norm	(7)	Martin & Mahoney (2021a)	No	Scale	No	No	Generalization gap
dist_spec_int	(8)	Jiang et al. (2019)	Yes	Scale	No	No	Generalization gap
path_norm	(9)	Neyshabur et al. (2015)	No	Scale	No	No	Generalization gap
mp_softrank	(10)	Martin & Mahoney (2021b)	No	Scale/Shape	No	No	Model quality
stable_rank	(11)	Martin & Mahoney (2021b)	No	Scale/Shape	No	No	Model quality
PL_alpha	(1)	Martin & Mahoney (2021b)	No	Shape	No	No	Model quality
E_TPL_beta	(2)	This paper WeightWatcher	No	Shape	No	No	Model quality
E_TPL_lambda	(2)	This paper WeightWatcher	No	Shape	No	No	Model quality
EXP_lambda	(3)	This paper WeightWatcher	No	Shape	No	No	Model quality
PL_ks_distance	(12)	Martin & Mahoney (2021b)	No	Shape	No	No	Model quality
E_TPL_ks_distance	(12)	This paper Martin & Mahoney (2021b)	No	Shape	No	No	Model quality
alpha_weighted	(13)	Martin & Mahoney (2021b)	No	Hybrid	No	No	Model quality
log_alpha_norm	(14)	Martin & Mahoney (2021a)	No	Hybrid	No	No	Model quality
inverse_margin	(17)	Jiang et al. (2019)	No	Scale	Yes	Maybe	Generalization gap
log_prod_of_spec_over_margin	(18)	Bartlett et al. (2017) Pitas et al. (2017)	No	Scale	Yes	Maybe	Generalization gap
log_sum_of_spec_over_margin	(19)	Bartlett et al. (2017) Pitas et al. (2017)	No	Scale	Yes	Maybe	Generalization gap
log_prod_of_fro_over_margin	(20)	Bartlett et al. (2017) Pitas et al. (2017)	No	Scale	Yes	Maybe	Generalization gap
log_sum_of_fro_over_margin	(21)	Bartlett et al. (2017) Pitas et al. (2017)	No	Scale	Yes	Maybe	Generalization gap
path_norm_over_margin	(22)	Neyshabur et al. (2015)	No	Scale	Yes	Maybe	Generalization gap
pacbayes_init	(25)	Neyshabur et al. (2017)	Yes	Scale	Yes	Yes	Generalization gap
pacbayes_orig	(26)	Neyshabur et al. (2017)	No	Scale	Yes	Yes	Generalization gap
pacbayes_flatness	(27)	Neyshabur et al. (2017)	No	Scale	Yes	Yes	Generalization gap
pacbayes_mag_init	(28)	Jiang et al. (2019)	Yes	Scale	Yes	Yes	Generalization gap
pacbayes_mag_orig	(29)	Jiang et al. (2019)	No	Scale	Yes	Yes	Generalization gap
pacbayes_mag_flatness	(30)	Jiang et al. (2019)	No	Scale	Yes	Yes	Generalization gap

Table 1: Overview of the generalization metrics considered. We focus on the *shape* metrics derived from the ESDs of weight matrices. See Appendix A for the details of these metrics.

(see Figure 1e and Figure 1f), and the `ks_distance` on the second row using a E-TPL fit is smaller than that for the PL fit on the first row, even when the fit on the second row clearly covers a larger part of the ESD. In these two cases, the `E_TPL_lambda` plays a similar role as the `PL_alpha` in PL fitting, and provides an effective alternative when the ESD does not exhibit a proper PL.

Between these three PL and E-TPL fittings, we would like to point out that the important thing in HT-SR is not the PL fitting *per se* but that the spectral distributions exhibit HT or other non-standard shapes; the particular forms of the distributions fit here simply constitute different ways to quantify this property in practice. These details, such as selecting the most appropriate distributional assumptions, clearly matter if we would like to engineer the tools of HT analysis to effectively measure the ground truth. However, the primary concern in predicting generalization is to measure the shape information, and the shape information is independent of the fitting procedure, although better fitting procedures may capture the shape information better.

3 Empirical Results

3.1 Experimental Setup

Dataset. We consider the WMT14 German to English (DE-EN) dataset (Bojar et al., 2014), commonly used as a benchmark for neural machine translation (Edunov et al., 2018; Ott et al., 2018; Shen et al., 2020; Vaswani et al., 2017). WMT14 consists of 4.5 million sentence pairs for training.

Hyperparameters. To capture the relationship between the generalization metrics and model quality in a number of different settings, we follow Jiang et al. (2019) and vary several hyperparameters: the number of samples (either 160K, 320K, 640K, 1.28M, 2.56M samples), the initial learning rate during training (across eight different rates), the model width (embedding dimension either 256, 384, 512, 768, or 1024), and the model depth ({4, 5, 6, 7, 8}-layer transformers). Following Jiang et al.

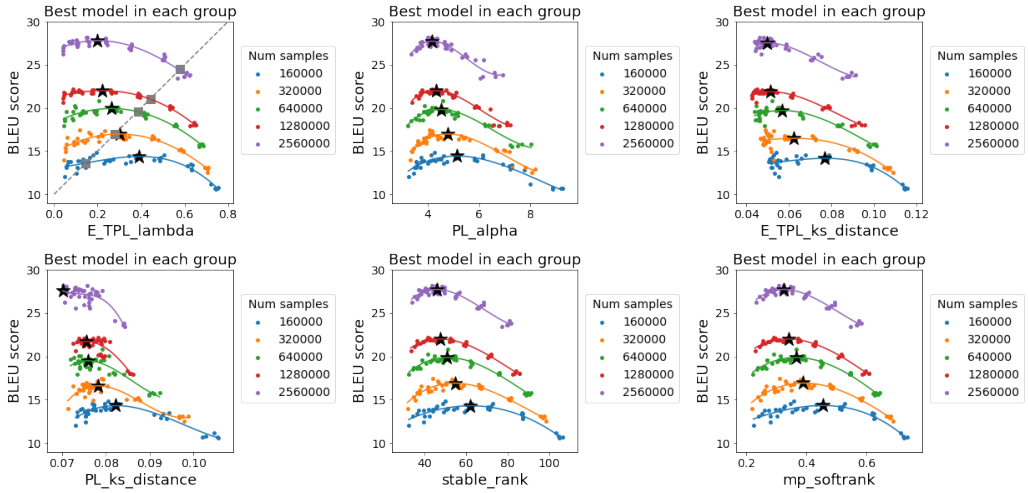


Figure 2: BLEU-score vs. six shape metrics for 200 Transformers trained on WMT14 with varying hyperparameters. HT-SR theory applies for optimally-tuned models (black stars), that is, models that have better BLEU scores exhibit heavier-tailed ESDs. For suboptimal models, the HT-SR metrics can be anti-correlated with model quality, see e.g. the grey dotted line in the first subfigure.

(2019), we construct a high-dimensional grid of different hyperparameters $\boldsymbol{\Theta} = \{(\theta_1, \ldots, \theta_K) : \theta_1 \in \boldsymbol{\Theta}_1, \ldots, \theta_K \in \boldsymbol{\Theta}_K\}$, so that we can compare models when one of the hyperparameters is varied. Two separate high-dimensional grids with dimension $K = 3$ are considered: (1) sample$\times$learning rate$\times$width; (2) sample$\times$learning rate$\times$depth. Each grid contains 5$\times$8$\times$5=200 of these training settings, and in total, there are 400 trained models. We will consider three subtasks to evaluate the considered generalization metrics.

Task one, correlation evaluated on optimally trained models. In the first task (Section 3.2.1), we study the relationship between model quality and generalization metrics on models trained with the optimal choice of hyperparameters. This task mimics the grid-search method often employed in large-scale (pre)training tasks.

Task two, correlation in time. In the second task (Section 3.2.2), we track BLEU score and generalization metrics during training, assessing time-wise correlation to model quality. This task has been considered in the literature (Bartlett et al., 2017), and from a practical point of view, capturing the time-wise dependence during training could potentially lead to better ways of early stopping or regularizing the model.

Task three, correlation when hyperparameters are varied. In the third task, we follow Jiang et al. (2019) and study the relationship between the model quality and the generalization metrics when a single hyperparameter is varied. Metrics that achieve a high (rank) correlation for all the hyperparameters are good candidates for model selection. Constrained by space, we discuss this result in details in Appendix B.

Training and model setup. For the details of the training settings, see Appendix C.

3.2 Evaluating the metrics on Transformers trained in different settings

In this subsection, we study 28 generalization metrics (with details provided in Table 1), and examine their correlations with BLEU score (Papineni et al., 2002): the most commonly used metric to evaluate machine translation. We also consider correlation between these metrics and the generalization gap, defined as the BLEU score for training data subtracted by the BLEU score for test data.

3.2.1 Task one: Evaluating correlations on optimally trained models only

Here, we group models using the number of training samples, and select the best model from each group when the model depth and the learning rate are varied. In Figure 2, each curve represents a group of models trained with a certain number of training samples. The black star on each curve

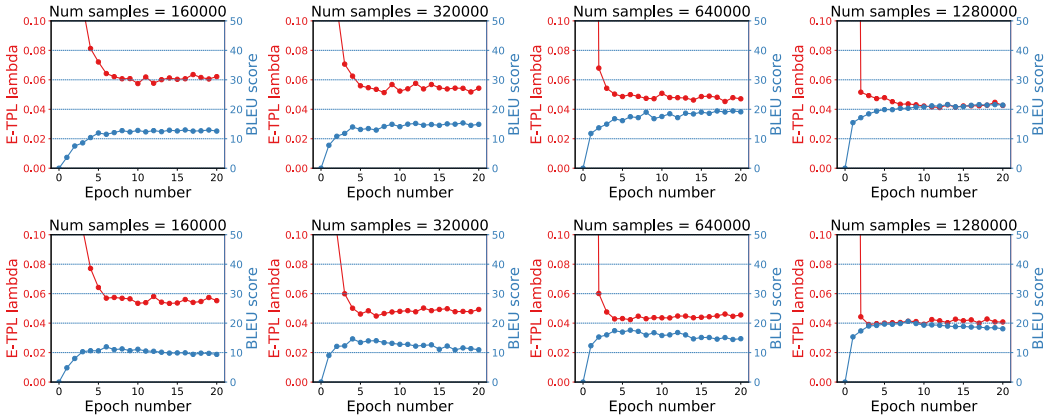
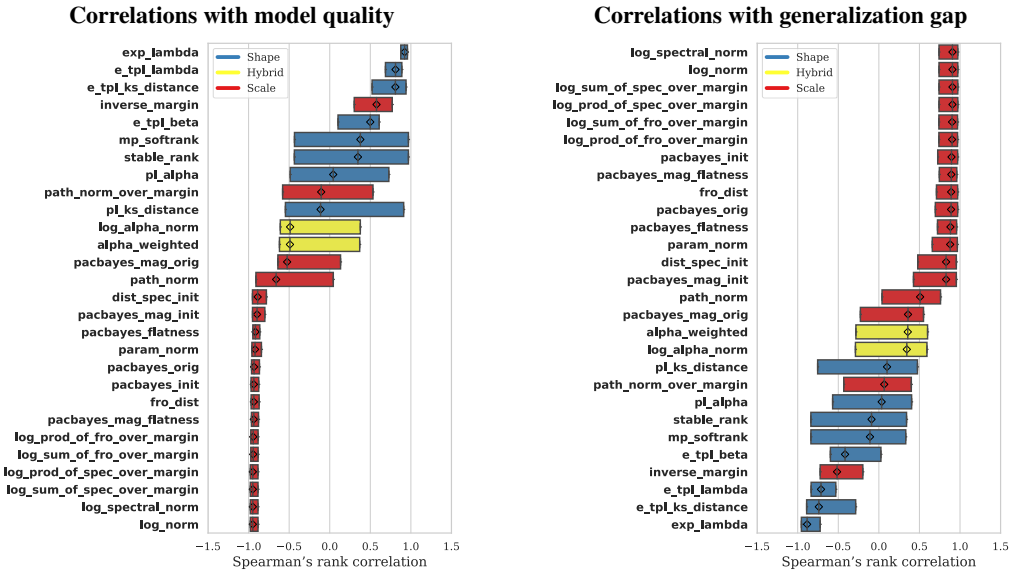


Figure 3: E_TPL_lambda closely tracks the BLEU score, i.e., BLEU score increases when the E_TPL_lambda drops. Results are shown for Transformers trained on WMT14 with different number of samples. **(First row).** Training with dropout 0.1. **(Second row).** Training without dropout.

represents the model trained with the optimal choice of hyperparameters (learning rate and depth in our setting), obtained by searching for the optimum on a third-order polynomial fit of each curve. From Figure 2, we see that the shape metrics always correctly predict the model quality, i.e., the BLEU scores should be higher when the metric values are smaller.

3.2.2 Task two: Time-wise correlations and rank correlation Results



(a) **Correlations with model quality.** Spearman's rank correlation between various generalization metrics and BLEU.

(b) **Correlations with generalization gap.** Spearman's rank correlation between various generalization metrics and the generalization gap.

Figure 4: Comparing multiple generalization metrics for predicting BLEU score (on the left) or the generalization gap (on the right). Lines on each box delineate the 25/50/75 percentiles of the rank correlations in 400 different settings (including different amount of data, different network depths, different network widths, and different initial learning rates).

In this subsection, we study time-wise correlation between our chosen metrics and the BLEU scores.

E_TPL_lambda tracks the BLEU score. As a warm-up, we consider the E_TPL_lambda metric defined in (2) to track the BLEU score (recalling that E_TPL_lambda assumes the ESDs follow

E-TPLs). We use training with and without dropout to study the effect of training schemes, and consider different quantities of data to test robustness in the dataset. In Figure 3, the first row considers models trained with dropout, while the second row considers models trained without dropout. The multiple columns track `E_TPL_lambda` and the BLEU score throughout training for different amounts of data. We can see that `E_TPL_lambda` not only successfully tracks BLEU scores but also differentiates underfitting (first row, with dropout) from overfitting (second row, without dropout) in this experiment.

Shape metrics predict model quality, while scale metrics predict the generalization gap. Now we consider the rank correlations between our chosen metrics and the test BLEU score. The rank correlations are evaluated across training, i.e., for each of the 400 settings of the hyperparameters, we calculate the Spearman's rank correlation between BLEU scores and the values of each generalization metric over all epochs. The summarized results are presented in Figure 4a. A positive Spearman's rank correlation (with BLEU) suggests that the generalization metric is useful in tracking BLEU during training. A negative Spearman's rank correlation, on the other hand, implies that the metric often gives the incorrect prediction. In Figure 4a, we use the average rank correlations for all settings to study the effectiveness of each metric, and present 25% quantile rank correlations to indicate robustness across runs.

In Figure 4a, we find shape metrics, such as `EXP_lambda`, `E_TPL_lambda`, `E_TPL_ks_distance`, and `E_TPL_beta`, exhibit some of the highest rank correlations with BLEU score. The `EXP_lambda` metric, which assumes a EXP distribution on the ESDs, achieves the highest median rank correlation, while the `E_TPL_lambda` metric, which assumes a E-TPL distribution on the ESDs, achieves the second highest. We discuss the `inverse_margin` metric in Appendix D.

In Figure 4b, we plot the rank correlations to the generalization gap across our chosen metrics. While it is encouraging that most existing generalization metrics yield correct predictions, as previously discussed, correct predictions of the generalization gap do not imply accurate predictions on the best-performing models here.

Rank-correlation results when varying a hyperparameter. We also assess whether the generalization metrics can predict trends in BLEU score when a single hyperparameter is changed (Jiang et al., 2019). Our findings are shown in Appendix B. Again, shape metrics have better rank correlations with model quality, while scale metrics are better correlated with the generalization gap.

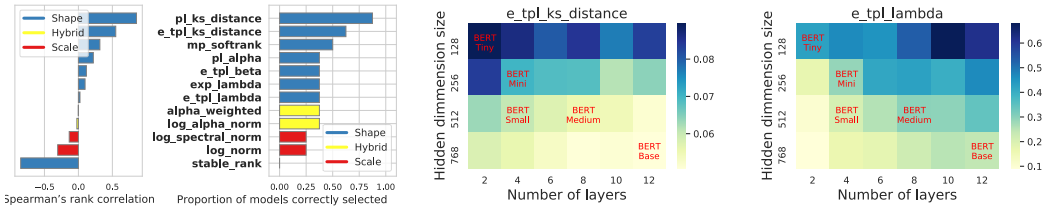
3.3 Evaluating the generalization metrics using Huggingface Transformers

Finally, we evaluate the data-free generalization metrics on pretrained Transformers. Eight series of models downloaded from Huggingface (Wolf et al., 2020) are considered—see Table 2 for details. We also include 24 BERT models from the "Smaller BERT" series (Turc et al., 2019) produced from a "pretrained distillation" pipeline that combines masked language modeling pretraining (Kenton & Toutanova, 2019) and knowledge distillation from a single BERT teacher model. In total, there are 51 pretrained Transformers.

Model series	Models
BERT (Kenton & Toutanova, 2019)	BERT-Tiny, BERT-Mini, BERT-Small, BERT-Medium, BERT-Base, BERT-Large
Smaller BERT (Turc et al., 2019)	24 smaller BERT models (English only, uncased, trained with WordPiece masking)
GPT2 (Radford et al., 2019)	GPT2, GPT2-medium, GPT2-large, GPT2-xl
ALBERTv1 (Lan et al., 2019)	ALBERT-base-v1, ALBERT-large-v1, ALBERT-xlarge-v1, ALBERT-xxlarge-v1
ALBERTv2 (Lan et al., 2019)	ALBERT-base-v2, ALBERT-large-v2, ALBERT-xlarge-v2, ALBERT-xxlarge-v2
T5 (Raffel et al., 2020)	T5-small, T5-base, T5-large
DialoGPT (Zhang et al., 2020)	DialoGPT-small, DialoGPT-medium, DialoGPT-large
FlauBERT (Le et al., 2020)	FlauBERT_small_cased, FlauBERT_base_cased, FlauBERT_large_cased
Funnel Transformer (Dai et al., 2020)	FunnelModel-small, FunnelModel-medium, FunnelModel-intermediate FunnelModel-large, FunnelModel-xlarge

Table 2: Pretrained Transformers considered in this paper.

We report rank-correlations averaged over these 8 model series in Figure 5a (left subplot), i.e., larger/deeper models should have smaller generalization metric values. Again, we find that the shape metrics outperform scale metrics (except for `stable_rank`, which is strongly influenced by the size of the weight matrix). The hybrid models achieve performance in-between the shape and scale metrics. In Figure 5a (right subplot), we compare different metrics in their ability to select the best



(a) Model selection on Huggingface Transformers. Metrics on the left and right are aligned.

(b) `E_TPL_ks_distance` evaluated on BERT models of different size.

(c) `E_TPL_lambda` evaluated on BERT models of different size.

Figure 5: Generalization metrics evaluated on pretrained Transformers. (a) Model selection results on eight Huggingface Transformer model series: BERT, GPT2, ALBERTv1, ALBERTv2, T5, DialoGPT, FlauBERT, Funnel Transformer. Left shows the rank correlation averaged over different Transformers. Right shows the proportion of the best Transformers correctly selected using different metrics. Shape metrics outperform scale metric only except `stable_rank` which is strongly influenced by the matrix size. (b and c) Evaluating two metrics on the "Smaller BERT" series. While `E_TPL_ks_distance` predicts the correct trends, `E_TPL_lambda` shows the reversed trends with depth.

model. That is, we report for each metric the proportion that the best model is selected from one model series when this metric is used as the model selection criterion. Note that the rankings of metrics on the two subplots in Figure 5a are the same.

From Figure 5a, we can see that, while the shape metrics perform better than scale metrics, none show a particularly strong rank correlation. To understand this, we examine the "Smaller BERT" series (Turc et al., 2019), which contains a more fine-grained structure of different model sizes. Specifically, these models are arranged in a 4-by-6 grid, where 6 represents {2,4,6,8,10,12} transformer layers and 4 means different hidden embedding sizes {128,256,512,768}. From Figure 5b, we see that the `E_TPL_ks_distance` correctly predicts the trend that wider and deeper models perform better. On the other hand, from Figure 5c, `E_TPL_lambda` correctly predicts that wider models are better, but incorrectly predicts that shallower models are better (another form of Simpson's paradox (Martin & Mahoney, 2021a)).

Another curious observation from Figure 5a is that, for the pretrained transformers, PL metrics, such as `PL_alpha` and `PL_ks_distance`, outperform E-TPL metrics, such as `E_TPL_lambda`, `E_TPL_beta` and `E_TPL_ks_distance`. This phenomenon may seem surprising as one may expect E-TPL fits to be more flexible than PL fits. These pretrained models are likely trained with much larger datasets and over many more epochs than the models we have otherwise considered. Here, PLs appear to provide a more natural fit.

4 Conclusion

After conducting large-scale empirical studies on a variety of metrics, we find that shape metrics derived from HT-SR theory are more effective for model selection without access to training or testing data. Poor correlations between existing generalization metrics and test-time performance have been reported in prior work (Dziugaite et al., 2020; Jiang et al., 2019; Nagarajan & Kolter, 2019). Rather than providing a "lump sum" to rank existing and novel generalization metrics (Figure 4), we evaluated these metrics in several ways: quantifying correlations only on optimally-trained models (Figure 2); examining the time-wise correlation during training (Figure 3); differentiating between the correlation with test accuracy versus generalization gap (Figure 4); evaluating these metrics on pretrained Transformer models where we do not have any control over the training process (Figure 5); and thoroughly investigating the rich correlational structures when different hyperparameters are varied (Figures 6 to 11 in the appendix). By thorough empirical investigations, we show that shape metrics perform consistently better than scale metrics in model selection—they correlate primarily with test accuracy instead of generalization gap, and display better correlations with models' test performance. These metrics provide value to practitioners, allowing one to assess pretrained NLP models without training or testing data, even when their corresponding training loss is not small. We expect these studies to be relevant and useful for improving existing generalization metrics in NLP moving forward.

REFERENCES

Jeff Alstott, Ed Bullmore, and Dietmar Plenz. Powerlaw: a python package for analysis of heavy-tailed distributions. *PloS one*, 9(1):e85777, 2014.

Peter Bartlett, Dylan Foster, and Matus Telgarsky. Spectrally-normalized margin bounds for neural networks. *Advances in Neural Information Processing Systems*, 30:6241–6250, 2017.

Paul T Boggs and Janet E Rogers. Orthogonal distance regression. *Contemporary Mathematics*, 112: 183–194, 1990.

Ondřej Bojar, Christian Buck, Christian Federmann, Barry Haddow, Philipp Koehn, Johannes Leveling, Christof Monz, Pavel Pecina, Matt Post, Herve Saint-Amand, et al. Findings of the 2014 workshop on statistical machine translation. In *Proceedings of the ninth workshop on statistical machine translation*, pp. 12–58, 2014.

Wuyang Chen, Xinyu Gong, and Zhangyang Wang. Neural architecture search on imagenet in four gpu hours: A theoretically inspired perspective. In *International Conference on Learning Representations*, 2020.

Aaron Clauset, Cosma Rohilla Shalizi, and Mark EJ Newman. Power-law distributions in empirical data. *SIAM review*, 51(4):661–703, 2009.

Zihang Dai, Guokun Lai, Yiming Yang, and Quoc Le. Funnel-transformer: Filtering out sequential redundancy for efficient language processing. *Advances in neural information processing systems*, 33:4271–4282, 2020.

Zhen Dong, Zhewei Yao, Amir Gholami, Michael W Mahoney, and Kurt Keutzer. HAWQ: Hessian aware quantization of neural networks with mixed-precision. In *IEEE/CVF International Conference on Computer Vision*, pp. 293–302, 2019.

Gintare Karolina Dziugaite, Alexandre Drouin, Brady Neal, Nitarshan Rajkumar, Ethan Caballero, Linbo Wang, Ioannis Mitliagkas, and Daniel M Roy. In search of robust measures of generalization. *Advances in Neural Information Processing Systems*, 33, 2020.

Sergey Edunov, Myle Ott, Michael Auli, and David Grangier. Understanding back-translation at scale. In *Proceedings of the 2018 Conference on Empirical Methods in Natural Language Processing*, pp. 489–500, 2018.

Gamaleldin Elsayed, Dilip Krishnan, Hossein Mobahi, Kevin Regan, and Samy Bengio. Large margin deep networks for classification. *Advances in Neural Information Processing Systems*, 31:842–852, 2018.

Pierre Foret, Ariel Kleiner, Hossein Mobahi, and Behnam Neyshabur. Sharpness-aware minimization for efficiently improving generalization. In *International Conference on Learning Representations*, 2020.

Stanislav Fort, Huiyi Hu, and Balaji Lakshminarayanan. Deep ensembles: A loss landscape perspective. Technical Report Preprint: arXiv:1912.02757, 2019.

Jonathan Frankle and Michael Carbin. The lottery ticket hypothesis: Finding sparse, trainable neural networks. In *International Conference on Learning Representations*, 2018.

Timur Garipov, Pavel Izmailov, Dmitrii Podoprikhin, Dmitry Vetrov, and Andrew Gordon Wilson. Loss surfaces, mode connectivity, and fast ensembling of dnns. In *Conference on Neural Information Processing Systems*, pp. 8803–8812, 2018.

P Izmailov, AG Wilson, D Podoprikhin, D Vetrov, and T Garipov. Averaging weights leads to wider optima and better generalization. In *Conference on Uncertainty in Artificial Intelligence*, pp. 876–885, 2018.

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*, 2018.

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*, 2019.

Yiding Jiang, Pierre Foret, Scott Yak, Daniel M Roy, Hossein Mobahi, Gintare Karolina Dziugaite, Samy Bengio, Suriya Gunasekar, Isabelle Guyon, and Behnam Neyshabur. Neurips 2020 competition: Predicting generalization in deep learning. *arXiv preprint arXiv:2012.07976*, 2020.

Jacob Devlin Ming-Wei Chang Kenton and Lee Kristina Toutanova. BERT: Pre-training of deep bidirectional transformers for language understanding. In *Proceedings of the Annual Conference of the North American Chapter of the Association for Computational Linguistics: Human Language Technologies*, pp. 4171–4186, 2019.

Zhenzhong Lan, Mingda Chen, Sebastian Goodman, Kevin Gimpel, Piyush Sharma, and Radu Soricut. ALBERT: A lite BERT for self-supervised learning of language representations. In *International Conference on Learning Representations*, 2019.

Hang Le, Loïc Vial, Jibril Frej, Vincent Segonne, Maximin Coavoux, Benjamin Lecouteux, Alexandre Allauzen, Benoit Crabbé, Laurent Besacier, and Didier Schwab. FlauBERT: Unsupervised language model pre-training for French. In *Proceedings of the 12th Language Resources and Evaluation Conference*, pp. 2479–2490, 2020.

Liyuan Liu, Xiaodong Liu, Jianfeng Gao, Weizhu Chen, and Jiawei Han. Understanding the difficulty of training transformers. *arXiv preprint arXiv:2004.08249*, 2020.

Charles H Martin and Michael W Mahoney. Rethinking generalization requires revisiting old ideas: statistical mechanics approaches and complex learning behavior. Technical Report Preprint: arXiv:1710.09553, 2017.

Charles H Martin and Michael W Mahoney. Traditional and heavy tailed self regularization in neural network models. In *International Conference on Machine Learning*, pp. 4284–4293, 2019.

Charles H Martin and Michael W Mahoney. Post-mortem on a deep learning contest: a Simpson's paradox and the complementary roles of scale metrics versus shape metrics. Technical Report Preprint: arXiv:2106.00734, 2021a.

Charles H Martin and Michael W Mahoney. Implicit self-regularization in deep neural networks: Evidence from random matrix theory and implications for learning. *Journal of Machine Learning Research*, 22(165):1–73, 2021b.

Charles H Martin, Tongsu Serena Peng, and Michael W Mahoney. Predicting trends in the quality of state-of-the-art neural networks without access to training or testing data. *Nature Communications*, 12(1):1–13, 2021.

David A McAllester. PAC-Bayesian model averaging. In *Annual Conference on Computational Learning Theory*, pp. 164–170, 1999.

Vaishnavh Nagarajan and J Zico Kolter. Uniform convergence may be unable to explain generalization in deep learning. *Advances in Neural Information Processing Systems*, 32, 2019.

Preetum Nakkiran, Gal Kaplun, Yamini Bansal, Tristan Yang, Boaz Barak, and Ilya Sutskever. Deep double descent: Where bigger models and more data hurt. In *International Conference on Learning Representations*, 2019.

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

Behnam Neyshabur, Srinadh Bhojanapalli, David Mcallester, and Nati Srebro. Exploring generalization in deep learning. *Advances in Neural Information Processing Systems*, 30:5947–5956, 2017.

Behnam Neyshabur, Srinadh Bhojanapalli, and Nathan Srebro. A PAC-Bayesian approach to spectrally-normalized margin bounds for neural networks. In *International Conference on Learning Representations*, 2018.

Myle Ott, Sergey Edunov, David Grangier, and Michael Auli. Scaling neural machine translation. In *Proceedings of the Third Conference on Machine Translation: Research Papers*, pp. 1–9, 2018.

Kishore Papineni, Salim Roukos, Todd Ward, and Wei-Jing Zhu. BLEU: a method for automatic evaluation of machine translation. In *Proceedings of the 40th annual meeting of the Association for Computational Linguistics*, pp. 311–318, 2002.

Konstantinos Pitas, Mike Davies, and Pierre Vandergheynst. Pac-bayesian margin bounds for convolutional neural networks. Technical Report Preprint: arXiv:1801.00171, 2017.

Alec Radford, Jeffrey Wu, Rewon Child, David Luan, Dario Amodei, Ilya Sutskever, et al. Language models are unsupervised multitask learners. *OpenAI blog*, 1(8):9, 2019.

Colin Raffel, Noam Shazeer, Adam Roberts, Katherine Lee, Sharan Narang, Michael Matena, Yanqi Zhou, Wei Li, Peter J Liu, et al. Exploring the limits of transfer learning with a unified text-to-text transformer. *Journal of Machine Learning Research*, 21(140):1–67, 2020.

Dinghan Shen, Mingzhi Zheng, Yelong Shen, Yanru Qu, and Weizhu Chen. A simple but tough-to-beat data augmentation approach for natural language understanding and generation. Technical Report Preprint: arXiv:2009.13818, 2020.

Thomas Tanay and Lewis Griffin. A boundary tilting persepective on the phenomenon of adversarial examples. Technical Report Preprint: arXiv:1608.07690, 2016.

Iulia Turc, Ming-Wei Chang, Kenton Lee, and Kristina Toutanova. Well-read students learn better: On the importance of pre-training compact models. Technical Report Preprint: arXiv:1908.08962, 2019.

Ashish Vaswani, Noam Shazeer, Niki Parmar, Jakob Uszkoreit, Llion Jones, Aidan N Gomez, Łukasz Kaiser, and Illia Polosukhin. Attention is all you need. In *Advances in neural information processing systems*, pp. 5998–6008, 2017.

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*, 2019.

Thomas Wolf, Lysandre Debut, Victor Sanh, Julien Chaumond, Clement Delangue, Anthony Moi, Pierric Cistac, Tim Rault, Rémi Louf, Morgan Funtowicz, Joe Davison, Sam Shleifer, Patrick von Platen, Clara Ma, Yacine Jernite, Julien Plu, Canwen Xu, Teven Le Scao, Sylvain Gugger, Mariama Drame, Quentin Lhoest, and Alexander M. Rush. Transformers: State-of-the-art natural language processing. In *Proceedings of the 2020 Conference on Empirical Methods in Natural Language Processing: System Demonstrations*, pp. 38–45. Association for Computational Linguistics, October 2020.

Ruibin Xiong, Yunchang Yang, Di He, Kai Zheng, Shuxin Zheng, Chen Xing, Huishuai Zhang, Yanyan Lan, Liwei Wang, and Tieyan Liu. On layer normalization in the transformer architecture. In *International Conference on Machine Learning*, pp. 10524–10533. PMLR, 2020.

Yaoqing Yang, Rajiv Khanna, Yaodong Yu, Amir Gholami, Kurt Keutzer, Joseph E Gonzalez, Kannan Ramchandran, and Michael W Mahoney. Boundary thickness and robustness in learning models. *Advances in Neural Information Processing Systems*, 33, 2020.

Yaoqing Yang, Liam Hodgkinson, Ryan Theisen, Joe Zou, Joseph E Gonzalez, Kannan Ramchandran, and Michael W Mahoney. Taxonomizing local versus global structure in neural network loss landscapes. In *Thirty-Fifth Conference on Neural Information Processing Systems*, 2021.

Chiyuan Zhang, Samy Bengio, Moritz Hardt, Benjamin Recht, and Oriol Vinyals. Understanding deep learning (still) requires rethinking generalization. *Communications of the ACM*, 64(3):107–115, 2021.

Yizhe Zhang, Siqi Sun, Michel Galley, Yen-Chun Chen, Chris Brockett, Xiang Gao, Jianfeng Gao, Jingjing Liu, and William B Dolan. DIALOGPT: Large-scale generative pre-training for conversational response generation. In *Proceedings of the 58th Annual Meeting of the Association for Computational Linguistics: System Demonstrations*, pp. 270–278, 2020.