
Temperature Balancing, Layer-wise Weight Analysis, and Neural Network Training

Yefan Zhou^{*} ¹, Tianyu Pang^{*} ², Keqin Liu², Charles H. Martin³, Michael W. Mahoney⁴, and Yaoqing Yang¹

¹Department of Computer Science, Dartmouth College

²National Center for Applied Mathematics and Department of Mathematics, Nanjing University

³Calculation Consulting

⁴ICSI, LBNL, and Department of Statistics, University of California at Berkeley

{yefan.zhou.gr, yaoqing.yang}@dartmouth.edu

tianyupang628@gmail.com, kqliu@nju.edu.cn

charles@CalculationConsulting.com, mmahoney@stat.berkeley.edu

Abstract

Regularization in modern machine learning is crucial, and it can take various forms in algorithmic design: training set, model family, error function, regularization terms, and optimizations. In particular, the learning rate, which can be interpreted as a temperature-like parameter within the statistical mechanics of learning, plays a crucial role in neural network training. Indeed, many widely adopted training strategies basically just define the decay of the learning rate over time. This process can be interpreted as decreasing a temperature, using either a global learning rate (for the entire model) or a learning rate that varies for each parameter. This paper proposes TempBalance, a straightforward yet effective layer-wise learning rate method. TempBalance is based on Heavy-Tailed Self-Regularization (HT-SR) Theory, an approach which characterizes the implicit self-regularization of different layers in trained models. We demonstrate the efficacy of using HT-SR-motivated metrics to guide the scheduling and balancing of temperature across all network layers during model training, resulting in improved performance during testing. We implement TempBalance on CIFAR10, CIFAR100, SVHN, and TinyImageNet datasets using ResNets, VGGs and WideResNets with various depths and widths. Our results show that TempBalance significantly outperforms ordinary SGD and carefully-tuned spectral norm regularization. We also show that TempBalance outperforms a number of state-of-the-art optimizers and learning rate schedulers.

1 Introduction

Having a learning rate schedule that gradually decreases over time is crucial for the convergence and performance of state-of-the-art machine learning algorithms. Indeed, many optimization algorithms essentially boil down to designing a progression of parameter updates, as realized by different learning rate schedules [1–4]. Common schedules assign a global learning rate per epoch, where the same learning rate is used for all layers in the model. This includes the family of cyclical learning rates [3], and parameter-wise learning rate schedules like Adam [2] and its variants [5, 6]. However, such a global learning rate schedule does not take into account the structural characteristics of neural networks (NNs). At the same time, parameter-wise learning rate schedules are sometimes used, but they have long been conjectured to have worse generalization performance than carefully tuned

*First two authors contributed equally.

stochastic gradient descent (SGD) optimizers [7], and storing both first and second-order moments for each parameter can lead to substantially increased memory consumption [8]. As mentioned in [9], storing the whole Megatron-Turing NLG requires 10 terabytes of aggregate memory, and the Adam optimizer’s first and second-order moments [2] consume 40% of the memory. Nonetheless, improving parameter-wise learning rate schedules is an active field of study [4, 5, 10, 11].

A largely under-explored idea to reconcile the two extremes of setting a single global learning rate or assigning fine-grained parameter-level learning rates is to assign layer-wise learning rates. Such a learning rate assignment method does not require much storage cost, and it can assign very different training speeds to different layers. However, existing layer-wise schemes are often introduced as an additional part of hyperparameter sweeping, thus substantially increasing computational cost; and most lack a strong (or any) theoretical foundation. For instance, layer-wise learning rates can increase test accuracy in transfer learning [12] and domain adaptation [13], but these learning rates are often empirically tuned. More recently, motivated by the intuition that lower-level layers should be domain-specific and higher-level layers should be task-specific, [14] automates the search for an optimal set of learning rates. However, the authors find the nested, bi-level optimization scheme to be too computationally expensive in practice [15]. AutoLR also automatically tunes its layer-wise learning rates according to the “role” of each layer [16]. The method is validated almost entirely by empirical results, further explained by layer-wise weight variations. While the authors attempt to assign a different initial learning rate to each layer, the learning rate for each layer continues to stay largely constant throughout training. LARS [17, 18] is another method to assign layer-wise learning rate. It is based on the “trust ratio,” defined as the ratio of weight norm to gradient update norm of each layer, and it is specifically used in large batch training to avoid gradient divergence.

In this paper, we propose TempBalance, a simple yet effective layer-wise learning rate assignment (and regularization) method, grounded in Heavy-Tail Self Regularization (HT-SR) Theory [19–24]. Our approach leverages HT-SR Theory to assess the quality of each network layer. This is achieved through an analysis of the heavy-tail (HT) structure present in the Empirical Spectral Density (ESD) of NN weight matrices. Given this information, TempBalance meticulously adjusts the *temperature-like parameter* to control each layer’s quality, with the objective of ensuring consistently high quality across all layers of the network. From the *statistical physics viewpoint* on learning and optimization [24–28], a temperature-like parameter refers to some quantity related to the empirical noise/stochasticity of the learning process. This is the noise scale described by [29, 30], and it can be written as a function of learning rate, batch size, and momentum. Prior research [19, 31] has shown that temperature-like parameters significantly influence HT structure in the ESD. Our approach, TempBalance, focuses on the strategic adjustment of the learning rate as the temperature-like parameter, thereby facilitating accurate control of the quality across each network layer, as characterized by its HT ESD structure. The following paragraph will delve deeper into the importance of HT-SR, highlighting its connection to the concept of layer-wise temperature.

HT-SR Theory. HT-SR Theory [19–24] relies on the empirical fact that very well-trained models tend to exhibit strong correlations, resulting in HT structure in the ESD of each layer. To obtain this ESD, we take a NN with L layers and the corresponding weight matrices $\mathbf{W}_1, \mathbf{W}_2, \dots, \mathbf{W}_L$ with shape $n \times m$ (where $n \leq m$). For the i -th layer, we calculate the eigenvalues of its correlation matrix $\mathbf{X}_i = \mathbf{W}_i^T \mathbf{W}_i$, and then we plot the ESD for that layer. Upon training, the ESD will typically gradually change to have an HT structure [19, 22]. We can then fit a power law (PL) distribution to the HT part of the ESD, and extract its exponent as, namely, PL_Alpha. The fitted PL will have the following formula:

$$p(\lambda) \propto \lambda^{-\alpha}, \quad \lambda_{\min} < \lambda < \lambda_{\max}. \quad (1)$$

The PL_Alpha metric measures the PL exponent of the weight matrices’ ESD. Its underlying motivation stems from random matrix theory and statistical physics, as well as the empirical observation that HT ESDs are ubiquitous in well trained NN models [20, 22].

The PL_Alpha metric has been shown to predict the trends in the test accuracy of state-of-the-art models in computer vision (CV) and natural language processing (NLP), without even the need for access to training or testing data [22, 32]. According to [22], one can aggregate PL_Alpha’s for different layers either by simple averaging or weighted averaging, and each can predict test accuracy in different cases [22, 32]. Furthermore, the *layer-wise* nature of PL_Alpha makes it a fine-grained metric that can be used to assess the quality of individual layers of the network. Thus, in this paper, we extend and apply HT-SR Theory (originally designed as a predictive diagnostic for analyzing

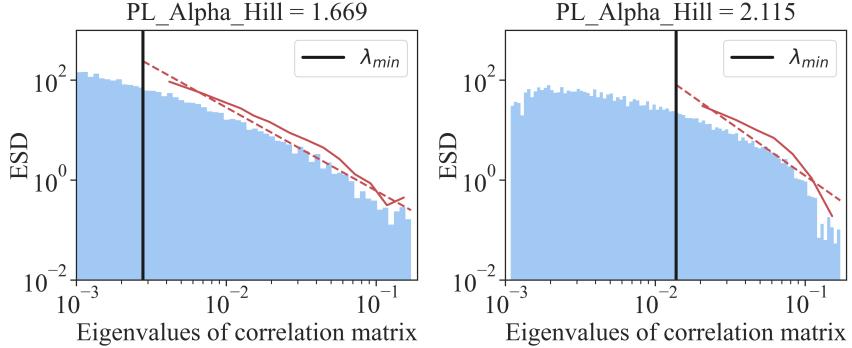


Figure 1: Examples of PL fitting. Blue histograms depict the ESDs. Vertical black lines indicate the lower threshold λ_{\min} used to truncate the full ESDs and extract the tail portion. Solid red curves represent the tail part of the ESDs truncated by λ_{\min} , while dashed red curves represent the fitted HT distributions. The left shows a more HT ESD, which requires a relatively lower learning rate. The right one shows a less HT ESD, which requires a relatively higher learning rate. Unlike prior work, we do not aim to find the “optimal” PL exponent. (Thus, we are less interested in obtaining a precise estimate than in obtaining a robust estimate.) Instead, we use the PL exponent to *rank* ESDs to find layers that need higher/lower learning rates. These two ESDs correspond to two layers of a ResNet18 model trained on TinyImageNet.

pre-trained NN models) to NN training, and we exploit the layer-wise information provided by PL_Alpha to determine the layer-wise learning rates for better test accuracy.

We note that, while it provides perhaps the most principled approach, the PL_Alpha metric is not the only way to try to measure the HT structure in NN models. Several recent papers [33–35] use different HT metrics to try to measure the spectral properties of other matrices (such as input/output covariance matrices, Fisher Information Matrices, and the Hessian). We show in Appendix A that these HT phenomena, measured in different ways on different matrices, are closely related to each other. On the other hand, this also means that (for the problems considered in this paper) the absolute numerical value of PL_Alpha is less important, as optimal PL exponents estimated by different algorithms can be different [22, 33]. What matters the most, as we show in this paper, is the layer-wise quality *ranked* by the PL exponent: layers with a smaller PL_Alpha tend to be relatively more “overtrained,” and layers with a larger PL_Alpha tend to be relatively more “undertrained.” (We emphasize that this is true for the training problem we consider in this paper—for prior HT-SR work, the actual numerical value of PL_Alpha mattered *a lot*.)

This observation leads to a simple and efficient way to *balance* layer-wise learning rates: assign a lower learning rate to more overtrained layers and a larger learning rate to more undertrained layers, using PL_Alpha (see Figure 1). In implementing this learning rate balancing approach, we use a *scale-free* method to map the PL_Alpha value of each layer to a predefined learning rate range. This range is established in relation to a *global* learning rate. Rather than depending on the absolute numerical values of PL_Alpha for each layer, this method emphasizes the importance of their relative differences and quality ranking. As a result, the learning rates assigned to individual layers remain stable and unaffected by arbitrary linear scaling of PL_Alpha estimates, whether they arise from the choice of the estimator or the presence of noisy measurements. On top of this, we can perform a grid search on the global learning rate. This is standard practice, and it is more efficient than grid-searching the layer-wise learning rates. We use this combination of assigning layer-wise learning rates using PL_Alpha and grid-searching the base global learning rate to avoid having to decide the “optimal” PL exponent, as this can be tricky due to different ways of measuring HT properties. Indeed, there are different ways to measure PL_Alpha [19], and we use the Hill estimator [36]. While not necessarily the best estimate (see [19, 22]), it shows stable performance in our experiments. We refer to our version of the PL_Alpha metric as the PL_Alpha_Hill metric, and we use it for the remainder of the paper.

Another popular way to change the ESD of weights is to constrain the spectral norm (i.e., the largest eigenvalue) using spectral norm regularization (SNR) [37, 38]. SNR provides a different form of regularization, compared to HT-SR, because it regulates the largest eigenvalue instead of the ESD slope (i.e., the PL_Alpha_Hill metric). It has been demonstrated that the spectral norm

and PL_Alpha_Hill serve distinct roles in evaluating model quality, and their combined form yields optimal predictions for test accuracy trends [19, 22, 23, 32]. To complement this, our results demonstrate that TempBalance outperforms SNR in training deep NNs in most cases. Moreover, when these two regularization methods are combined during training, they result in optimal test accuracy, thereby confirming their complementary roles. As described in [23, 32], the spectral norm and PL_Alpha_Hill measure the scale and the shape of a ESD, respectively; and regulating both the scale and shape is crucial for achieving better ESD regularization. We provide ablation studies on several layer-wise metrics for assigning layer-wise learning rates, including spectral norm, and we show that PL_Alpha_Hill performs the best among them.

Our main contributions. The following summarizes our main contributions.²

- We propose a simple yet effective layer-wise learning rate schedule, TempBalance, which is motivated by HT-SR Theory. Based on our empirical results, we obtain two main high-level insights. First, the mapping from PL_Alpha_Hill to learning rates should be scale-free, meaning that arbitrary linear scaling on the estimated PL exponent should not change the learning rate assignment. Second, searching for the minimum eigenvalue λ_{\min} , a standard practice in PL fitting [19, 39, 40], leads to unstable training. To improve stability, we instead fix λ_{\min} as the median of the ESD.
- We compare TempBalance to ordinary SGD and SNR on various training tasks. This includes (1) different network architectures, such as ResNet, VGG, WideResNet, (2) different datasets, such as CIFAR10, CIFAR100, SVHN, TinyImageNet, and (3) ablation studies, such as varying widths, depths, initial learning rates, HT-SR layer-wise metrics, and PL fitting methods. Compared to ordinary SGD, TempBalance achieves higher test accuracy by setting layer-wise learning rates. Compared to SNR, TempBalance performs better by providing a more fine-grained regularization on *shape/slope* instead of norm. We also show that combining TempBalance and SNR leads to further improved accuracy, verifying their complementary roles in informing deep learning training.
- We compare TempBalance to a range of state-of-the-art optimizers and learning rate schedulers, including SGDR [10], SGDP [41], Lookahead [42] and LARS [17, 18] on ResNet18 and ResNet34 trained on CIFAR100. We show that TempBalance achieves the highest test accuracy. We do careful hyperparameter tuning for all baselines. All results are obtained from five random seeds.
- We use ablation studies to show that PL_Alpha_Hill provides the best test accuracy among several layer-wise metrics considered by HT-SR [22, 32]. We also show that TempBalance maintains stable performance over SGD baselines when the model size changes. Furthermore, we show visualization results in Appendix B, verifying that TempBalance controls ESDs during training.

2 Related Work

Here, we give an overview of the statistical mechanics of learning and recent progress in theoretical and empirical studies on generalization metrics and their applications.

Statistical mechanics of learning and HT-SR. Our paper is motivated by statistical mechanics of learning [43–45], and especially by works that connect load-like [43, 46, 47] and temperature-like parameters [25, 48] to NNs. According to prior works in this area [24, 49], a *temperature-like parameter* represents the amount of noise/variance in an iteration of SGD, such as learning rate, weight decay parameters, and batch size. A *load-like parameter* represents the quantity and/or quality of data relative to the size of the learning model. To measure the quality of publicly-available pre-trained NNs, Martin and Mahoney [19] introduce HT-SR Theory, showing that the weight matrices of deep NNs exhibit HT ESDs, and they show that a decay coefficient of ESD, PL_Alpha, effectively gauges model quality. Subsequently, [31, 50–54] provide rigorous bounds for HT phenomenon and generalization, further adding support to HT-SR Theory. HT-SR has also been applied to predicting trends in test accuracy of large-scale NNs, in both CV and NLP [22, 23, 32], but it has yet to be systematically incorporated to novel training algorithms. Recently, more papers realize the important connections between deep NNs and statistical mechanics of learning [24]. To name a few, Yang et al. [49] use load and temperature parameters to study a wide range of loss landscapes, providing a taxonomy from the perspective of global structure of a loss landscape. On the theory side, Baity-Jesi et al. [55] investigates the glassy behavior of NNs, and Barbier et al. [56] derives the optimal generalization error of generalized linear systems. More recently, Sorscher et al. [57] studies easy versus hard samples used in training and design a “data-pruning” method; and Zhou et al. [58] establishes a

²Our code is open-sourced: <https://github.com/YefanZhou/TempBalance>.

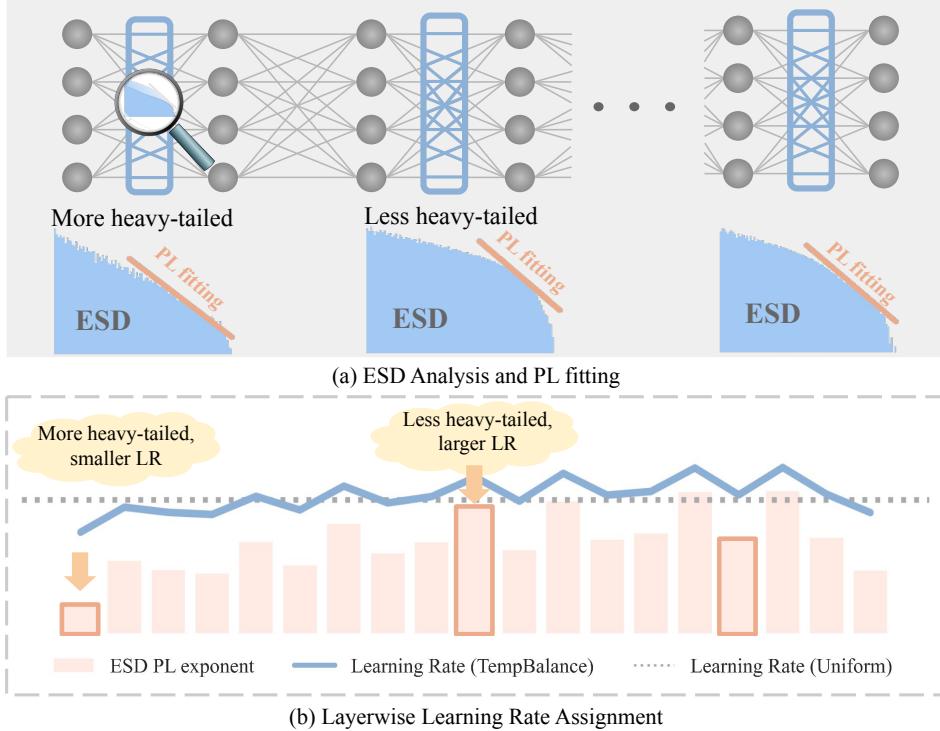


Figure 2: The pipeline diagram of TempBalance. In each epoch, TempBalance undergoes two steps: (a) Performing ESD analysis on all layers and employing PL fitting to derive the layer-wise PL_Alpha_Hill, and (b) Using the layer-wise PL_Alpha_Hill to assign learning rates to each layer using an assignment function.

“three-regime model” in network pruning, unifying multiple practical hyperparameter tuning methods in a principled way.

Generalization measures. The search for effective and robust generalization metrics (which, importantly, can be very different than model quality metrics [32]) has been the focus of several recent theoretical and empirical works [22, 32, 49, 59–61]. Several recent papers apply metric-informed training and architecture search, such as those based on the Hessian [4, 62–64], spectral norm [37, 38], stable rank [65], and the spectrum of the neural tangent kernel [66]. However, most generalization metrics, such as those based on the PAC-Bayes bounds [67–70], do not straightforwardly transfer to layer-wise quality metrics, because such generalization metrics often study the whole NN as an architecture-free function, and they lack the fine granularity to unveil the quality of each layer. Also, it has been mentioned in the literature [59] that (1) directly regularizing generalization metrics can lead to difficulty in training, (2) evaluating these regularization methods may be hard due to the existence of *implicit regularization* in SGD, and (3) these metrics, especially norm-based metrics, cannot be expected to correlate with test accuracy causally [60], making the link between these generalization metrics and practical training methods nuanced. It will be clear in the next section that we do not regularize ESD metrics directly. Instead, we change learning rates to modify ESDs.

3 The TempBalance Algorithm

In this section, we introduce our simple yet effective method TempBalance, based on the PL_Alpha_Hill metric from HT-SR Theory. For a NN, different layers tend to have different values for PL_Alpha_Hill, [19, 24]: a layer with a larger PL_Alpha_Hill indicates that layer is relatively undertrained, while a layer with a smaller PL_Alpha_Hill indicates that layer is relatively overtrained. A natural idea is to adjust the degree of learning among different layers to get a balance: for a layer whose PL_Alpha_Hill is too large, we could assign a larger learning rate to accelerate its learning, and vice versa. The intuition of our method is transferring one layer’s learning rate to another and hence, TempBalance. The pipeline is in Figure 2.

Algorithm 1: TempBalance

Input: M : Deep NN, T : Total training epoch, t : Current epoch, α_t^i : i th layer's PL_Alpha_Hill at epoch t , η_t : Baseline global learning rate at epoch t , s_1, s_2 : Minimum and maximum scaling ratio, f_t : Learning rate schedule function

- 1 Initialize model M ;
- 2 **for** $t \leftarrow 0$ to T **do**
- 3 | Compute α_t^i for all layers using the Hill estimator;
- 4 | Leverage all α_t^i and adopt f_t in (2) to assign per-layer learning rate $f_t(i)$ between $s_1\eta_t$ and $s_2\eta_t$ for the next epoch;
- 5 | Update the optimizer for the next epoch;
- 6 **end**

We provide the details of TempBalance in Algorithm 1. Based on PL_Alpha_Hill in different layers, we use the learning rate schedule function f_t to map the i -th layer to a particular learning rate $f_t(i)$ in epoch t . We adopt f_t as a linear map between the layer-wise PL_Alpha_Hill and the final layer-wise learning rate, which has the following formula:

$$f_t(i) = \eta_t \cdot \left[\frac{\alpha_t^i - \alpha_t^{\min}}{\alpha_t^{\max} - \alpha_t^{\min}} (s_2 - s_1) + s_1 \right], \quad (2)$$

where η_t means the base global learning rate in epoch t , (s_1, s_2) are the minimum and maximum learning rate scaling ratio relative to η_t , α_t^i represents the layer i 's PL_Alpha_Hill at the beginning of epoch t , and $(\alpha_t^{\min}, \alpha_t^{\max})$ denote the minimum and maximum PL_Alpha_Hill across all the layers in epoch t . Using (2), we ensure that the new learning rate $f_t(i)$ is a scaled version of the original base learning rate η_t and is always inside the interval $[s_1\eta_t, s_2\eta_t]$. Note that (s_1, s_2) serves as tunable hyperparameters in our method. We conducted ablation studies on it, which are detailed in Appendix C. The hyperparameter values used across all experiments can be found in Appendix D. Our studies reveal that the optimal results are usually achieved around (0.5, 1.5).

To fit the PL distribution $p(\lambda)$ defined in (1), we use the Hill estimator [36, 71]. (It is not the best estimator for fine-scale diagnostics based on HT-SR Theory [19, 22], but it is robust, and it suffices for our purposes.) For the i -th layer, suppose the weight matrix is \mathbf{W}_i and the correlation matrix $\mathbf{W}_i^\top \mathbf{W}_i$ has ascending eigenvalues $\{\lambda_i\}_{i=1}^n$. Then, the Hill estimator calculates PL_Alpha_Hill using the following:

$$\text{PL_Alpha_Hill} = 1 + \frac{k}{(\sum_{i=1}^k \ln \frac{\lambda_{n-i+1}}{\lambda_{n-k}})}, \quad (3)$$

where k is the adjustable parameter. We adopt $k = \frac{n}{2}$ in our experiments. Note that changing k essentially changes the lower eigenvalue threshold λ_{\min} for (truncated) PL estimation, as shown by the vertical black line in Figure 1. Choosing $k = \frac{n}{2}$ means using the largest half of the eigenvalues to estimate the slope. We empirically find that fixing k for all layers leads to more stable performance than searching k for different layers (e.g., optimizing k using the Kolmogorov–Smirnov test [40], as is needed for other applications of HT-SR Theory [19, 22]).

One advantage of mapping PL_Alpha_Hill to learning rates using (2) is that the scale of PL_Alpha_Hill is unimportant, i.e., linearly scaling PL_Alpha_Hill arbitrarily does not change the learning rate assignment because the linear scaling cancels each other in (2). This can maximally reduce the artifact of estimating the ESD PL exponent/slope due to estimation noise, which has been found to be a tricky issue in practice [19, 23].

4 Empirical results

In this section, we give full details of the experimental setup (Section 4.1) and compare our method TempBalance to a few baselines (Section 4.2), and then (Section 4.3) we perform ablation studies on varied initial learning rates, model widths, HT-SR layer-wise metrics, and PL fitting methods.

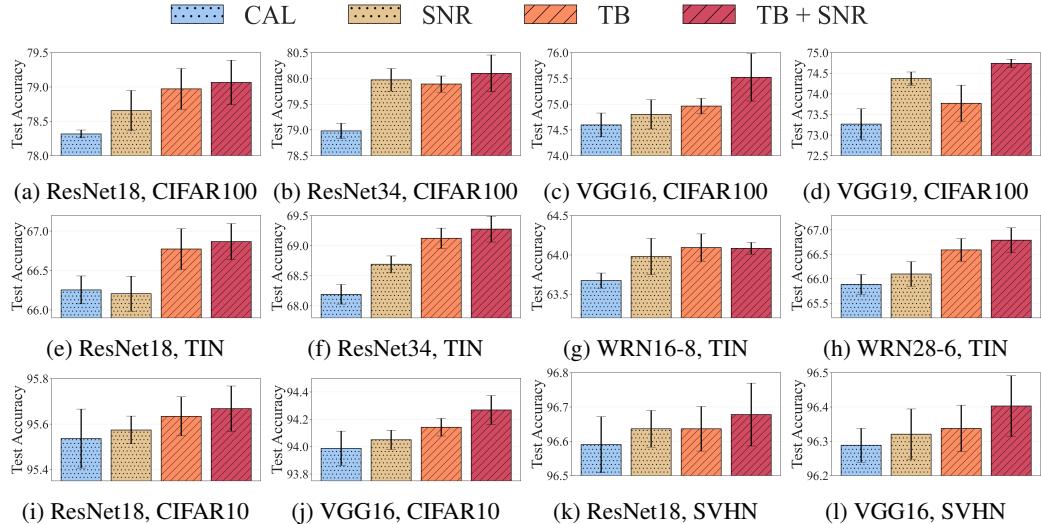


Figure 3: (Main result). Comparing our method TempBalance (TB) to CAL and SNR. Our method TempBalance outperforms CAL and SNR in almost all the settings except for VGG19 and ResNet 34 on CIFAR 100. For all experiments, combining TempBalance and SNR (TB+SNR) yields the best performance. All baselines are carefully tuned. All results are obtained by running five random seeds. See Appendix D for the details in all hyperparameters.

4.1 Experimental setup

Datasets. We consider CIFAR100, CIFAR10, SVHN and Tiny ImageNet (TIN) [72–75]. CIFAR100 consists of 50K pictures for training and 10K pictures for testing with 100 categories. CIFAR10 consists of 50K pictures for training and 10K pictures for testing with 10 categories. SVHN consists of around 73K pictures for training and around 26K pictures for testing with 10 categories. Tiny ImageNet consists of 10K pictures for training and 10K images for testing with 200 classes.

Models. We mainly consider three types of NNs: VGG, ResNet, and WideResNet (WRN) [76–78]. For each network, we consider two different size options. For VGG, we consider VGG16 and VGG19. For ResNet, we consider ResNet18 and ResNet34. For WideResNet, we consider WRN16-8 and WRN28-6. Also, for ResNet and VGG, we consider three different widths for ablation studies.

Hyperparameters. One baseline is ordinary SGD training with a cosine annealing learning rate schedule (CAL), which follows the formula: $\eta_t = \frac{\eta_0}{2} (1 + \cos(\frac{t \cdot \pi}{T}))$, where t is the current epoch, T represents the total training epochs, and η_0 is the initial learning rate. We grid search the optimal initial (base) learning rate η_0 for the CAL baseline, using the grid $\{0.05, 0.1, 0.15\}$ for ResNet and $\{0.025, 0.05, 0.1\}$ for VGG. The momentum and weight decay are 0.9 and 5×10^{-4} , respectively, which are both standard choices.

Another baseline is spectral norm regularization (SNR). Prior work [37] uses the SNR objective:

$$\min_{\Theta} \frac{1}{n} \sum_{i=1}^n l(f_{\Theta}(\mathbf{x}_i), \mathbf{y}_i) + \frac{\lambda_{sr}}{2} \sum_{l=1}^L \sigma(W_l)^2, \quad (4)$$

where λ_{sr} is the SNR coefficient, $\sigma(W_l)$ is the largest eigenvalue, i.e., spectral norm of weight matrix \mathbf{W}_l , and L is the number of layers. We use the power iteration method to calculate $\sigma(W_l)$ in our experiments. For SNR, we grid search the optimal regularization coefficient λ_{sr} , and we again adopt the CAL schedule for SNR, similar to the CAL baseline.

To make our results fully reproducible, we report in Appendix D all hyperparameters, random seeds, and all numerical values of experimental results shown in the figures.

4.2 Comparing TempBalance and multiple baseline methods.

First, we compare TempBalance to two baseline training methods. See results in Figure 3. In the figure, CAL means SGD training with a CAL learning rate schedule, and SNR means SGD trained

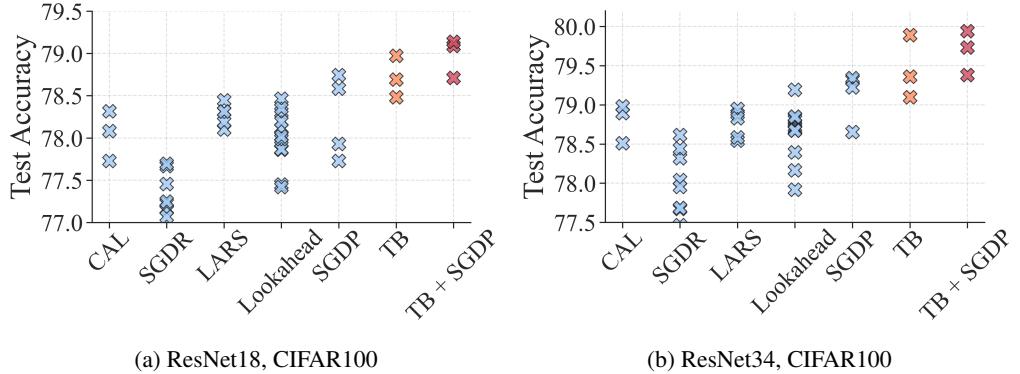


Figure 4: (More baseline optimizers). Comparing our method TempBalance (TB) to cosine annealing (CAL) baseline and other state-of-the-art optimizers and learning rate schedulers for ResNet18 and ResNet34 trained on CIFAR100. Crosses for the same method represent different hyperparameter settings. Each cross represents the mean test accuracy of five random seeds. The best performing model thus far is TB combined with SGDP.

with spectral norm regularization. TB means our method TempBalance, and TB + SNR means TempBalance combined with SNR. All error bars are obtained from five random seeds. From Figure 3, we see that TempBalance outperforms the CAL baseline in all settings. In almost all cases, it performs better than SNR baseline. When TempBalance does not outperform SNR, combining SNR with TempBalance leads to better test accuracy.

Second, we compare our method to a number of optimizers and learning rate schedulers that are not necessarily related to ESD of weights. These include SGDR [10], SGDP [41], Lookahead [42] and LARS [17, 18], and we compare these baselines with TempBalance for ResNet18 and ResNet34 trained on CIFAR100. SGDR is stochastic gradient descent with warm restarts. SGDP modifies the ordinary SGD to compensate for the effect of increasing weight norm. Lookahead [42] modifies SGD by letting each gradient update approximate the future trajectory of multiple updates. LARS assigns layer-wise learning rates based on the so-called “trust-ratio” and is the closest to our method. Results in Figure 4 show that TempBalance outperforms these baselines, and TempBalance combined with SGDP is the best-performing method. The crosses on each column represent training runs with different hyperparameters. Note that there are several other methods based on modifying the Adam optimizer [2], such as AdamW [11], AdamP [41] and LAMB [79]. However, we do not find them to provide better results than the SGD baseline with cosine annealing (CAL in Figure 4). The results are detailed in Appendix E.

4.3 Corroborating results and ablation studies.

In addition to the main results (Figures 3 and 4), we provide corroborating results and ablation studies.

Experiment one: tuning initial learning rate η_0 . We train models from scratch using TempBalance versus CAL with various initial learning rates, comparing TempBalance and the CAL baseline when both methods are allowed to search for the optimal hyperparameters. We again use ResNet18, ResNet34, VGG16 and VGG19 as our architectures and show results on CIFAR100. Results in Figure 5 show that TempBalance achieves a higher test accuracy than CAL for both ResNet and VGG.

Experiment two: varying channel width. We view the fraction of model width in Experiment one as “100%,” and we experiment with models with varied widths in [50%, 100%, 150%]. We again used ResNet18, ResNet34, VGG16 and VGG19, and trained on CIFAR100, and we grid search for the optimal learning rate for each width to get the best accuracy. Results in Figure 6 show we find that TempBalance outperforms the baseline for all widths.

Experiment three: varying HT-SR metric. We use different HT-SR metrics to assign layer-wise learning rates. That is, we replace the layer-wise PL_Alpha_Hill in (2) with other HT-SR metrics including SpectralNorm and AlphaWeighted [22]. Results in Figure 7 show that PL_Alpha_Hill achieves the optimal test accuracy.

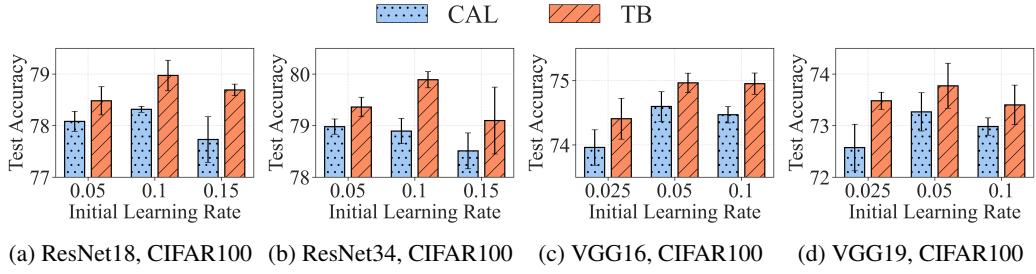


Figure 5: (Tuning initial learning rate). Comparing the test accuracy of TempBalance (red) and CAL baseline (blue) for varying initial learning rate. Our method TempBalance outperforms CAL for both ResNet and VGG trained on CIFAR100. All results are obtained by running five random seeds.

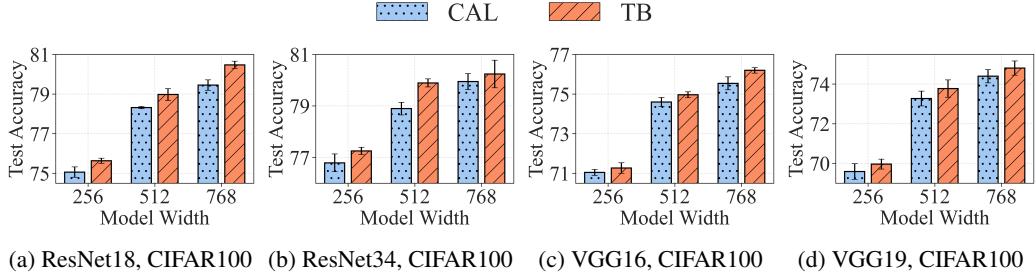


Figure 6: (Different widths). Comparing TempBalance and the CAL baseline for different network widths. Our method TempBalance consistently outperforms the CAL baseline across various network widths for both ResNet and VGG trained on CIFAR100. All results are obtained by running five random seeds.

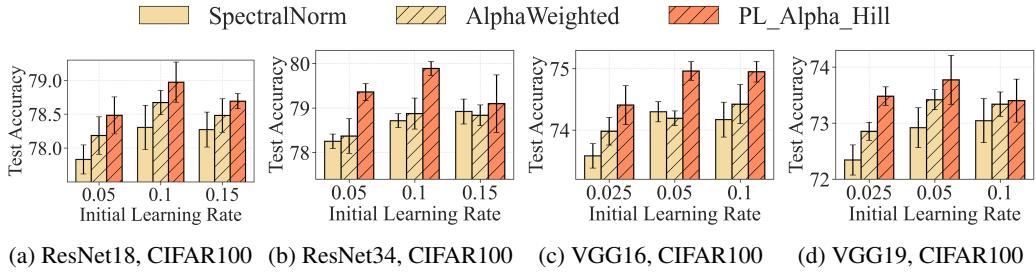


Figure 7: (Different HT-SR metrics). Comparing PL_Alpha_Hill with multiple HT-SR metrics. PL_Alpha_Hill achieves the best test accuracy among these metrics. All results are obtained by running five random seeds.

Experiment four: varying PL fitting methods. The HT-SR metric PL_Alpha_Hill is derived through PL fitting, which is influenced by the choice of hyperparameter λ_{\min} . More specifically, this involves determining the adjustable parameter k as per Equation 3. Past research has employed various methods to select λ_{\min} based on the task, such as performance prediction. For instance, Martin et al. [22], Clauset et al. [39] choose λ_{\min} that aligns with the best fit according to the Kolmogorov-Smirnov statistic [40], a method termed Goodness-of-fit. Meanwhile, Yang et al. [32] adopted the Fix-finger approach, which identifies λ_{\min} at the peak of the ESD. In our study, we designate λ_{\min} as the median of all eigenvalues present in the ESD for TempBalance. As depicted in Figure 8, our fitting method, termed Median, not only ensures optimal test accuracy but also notably decreases computation time. This shows that this PL fitting method is suited for the design of learning rate schedulers that demand low computation overhead.

Empirical analysis results. We conduct an empirical analysis of TempBalance to discuss why it provides improvement. Our first analysis involves visualization to demonstrate how TempBalance

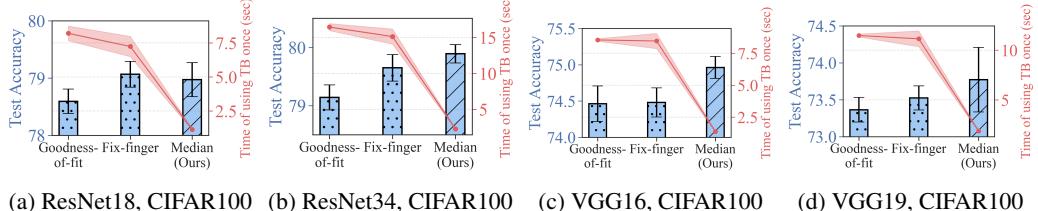


Figure 8: (Varying PL fitting method to determine the λ_{\min}). Results of using different PL fitting methods. The blue bar plot and the left y -axis label denote the test accuracy (higher the better), and the red line plots and the right y -axis label denote the time in seconds of using TempBalance once (lower the better). Our design (Median) used in the proposed method achieves higher test accuracy and takes lower computation times compared to Goodness-of-fit and Fix-finger. The test accuracy is averaged over five random seeds and computation time is averaged over ten times.

effectively regularizes ESDs by scheduling the learning rate (see Appendix B). The second analysis strengthens the connections between TempBalance and HT structure, illustrating that the observed improvements are not due to indirectly addressing other training issues, such as gradient excursions [80] (see Appendix F).

Corroborating results on other tasks. We extend our evaluation of TempBalance to two additional tasks: object detection and language modeling, the details of which can be found in Appendix G. Across these tasks, TempBalance consistently outperforms the baseline CAL in terms of generalization.

5 Conclusion

Our extensive empirical evaluations demonstrate that TempBalance offers a straightforward yet effective layer-wise learning rate schedule. Our approach for balancing layer-wise temperature confirms the following: (i) HT-SR-motivated metric PL_Alpha_Hill helps layers achieve temperature balance during training, exhibits strong correlations with model quality, and yields improved performance during testing; (ii) temperature balancing is a novel and essential aspect of NN training, and HT-SR Theory provides a strong theoretical support for balancing temperatures; and (iii) layer-wise learning rate schedules are cheap and effective to apply, and it is useful to study these layer-wise learning rate schedules further. Our method provides insights into the study of layer-wise tuning approaches and load-temperature balancing in deep NN training, as it serves both as a layer-wise learning rate schedule and an effective regularization technique based on HT-SR Theory.

Future directions, limitations, and societal impacts. Our paper leaves many future directions to explore, of which we mention just a few.

- Can HT-SR metrics be extended to parameter-wise learning rate schedules, global learning rate schedules, or other hyperparameters? It would be of interest to observe how HT-SR can assist in acquiring a comprehensive set of hyperparameter tuning tools.
- Is it possible to accelerate the computation of ESDs and PL_Alpha_Hill to achieve a more adaptive learning rate scheduler? Currently, we calculate layer-wise PL_Alpha_Hill once per epoch, resulting in a minimal increase in computational cost. Consider the example of training ResNet18 for 200 epochs on CIFAR100. Calculating layer-wise PL_Alpha_Hill takes 1.14 seconds for each epoch, leading to 3.8 minutes in total. Training CIFAR100 on 1 Quadro RTX 6000 takes 59 minutes, and thus using TB increases 6% of training time. However, if we can significantly decrease the expense of computing ESDs, it might enable an optimizer that adjusts the learning rate every few gradient updates. A study on computation overhead is detailed in Appendix H.

Our research centers around developing a generic algorithm for optimizing NNs. Although TempBalance could be applied to learning models with adverse applications, we do not see any immediate negative societal impacts stemming from the algorithm itself. Indeed, we see a lot of societal value in using a practical, predictive, and quantitative theory, such as HT-SR Theory, as opposed to developing a method that relies on a theory that provides vacuous upper bounds and then relies on extremely expensive hyperparameter tuning to obtain good results.

Acknowledgements. WeightWatcher is a publicly available tool distributed under Apache License 2.0 with a copyright held by Calculation Consulting. Our conclusions do not necessarily reflect the position or the policy of our sponsors, and no official endorsement should be inferred.

References

- [1] John Duchi, Elad Hazan, and Yoram Singer. Adaptive subgradient methods for online learning and stochastic optimization. *Journal of Machine Learning Research*, 12(61):2121–2159, 2011.
- [2] Diederik P Kingma and Jimmy Ba. Adam: A method for stochastic optimization. In *International Conference on Learning Representations*, 2014.
- [3] Leslie N Smith. Cyclical learning rates for training neural networks. In *2017 IEEE Winter Conference on Applications of Computer Vision*, pages 464–472, 2017.
- [4] Zhewei Yao, Amir Gholami, Sheng Shen, Mustafa Mustafa, Kurt Keutzer, and Michael Mahoney. Adahessian: An adaptive second order optimizer for machine learning. In *Proceedings of the AAAI Conference on Artificial Intelligence*, 2021.
- [5] Juntang Zhuang, Tommy Tang, Yifan Ding, Sekhar C Tatikonda, Nicha Dvornek, Xenophon Papademetris, and James Duncan. Adabelief optimizer: Adapting stepsizes by the belief in observed gradients. *Advances in Neural Information Processing Systems*, 2020.
- [6] Liyuan Liu, Haoming Jiang, Pengcheng He, Weizhu Chen, Xiaodong Liu, Jianfeng Gao, and Jiawei Han. On the variance of the adaptive learning rate and beyond. In *International Conference on Learning Representations*, 2020.
- [7] Ashia C Wilson, Rebecca Roelofs, Mitchell Stern, Nati Srebro, and Benjamin Recht. The marginal value of adaptive gradient methods in machine learning. In *Advances in Neural Information Processing Systems*, 2017.
- [8] Bharat Singh, Soham De, Yangmuzi Zhang, Thomas Goldstein, and Gavin Taylor. Layer-specific adaptive learning rates for deep networks. In *IEEE 14th International Conference on Machine Learning and Applications*, 2015.
- [9] Shaden Smith, Mostofa Patwary, Brandon Norick, Patrick LeGresley, Samyam Rajbhandari, Jared Casper, Zhun Liu, Shrimai Prabhumoye, George Zerveas, Vijay Korthikanti, Elton Zhang, Rewon Child, Reza Yazdani Aminabadi, Julie Bernauer, Xia Song, Mohammad Shoeybi, Yuxiong He, Michael Houston, Saurabh Tiwary, and Bryan Catanzaro. Using deepspeed and megatron to train megatron-turing nlg 530b, a large-scale generative language model. *arXiv preprint arXiv:2201.11990*, 2022.
- [10] Ilya Loshchilov and Frank Hutter. Sgdr: Stochastic gradient descent with warm restarts. In *International Conference on Learning Representations*, 2017.
- [11] Ilya Loshchilov and Frank Hutter. Decoupled weight decay regularization. In *International Conference on Learning Representations*, 2019.
- [12] Jeremy Howard and Sebastian Ruder. Universal language model fine-tuning for text classification. In *Proceedings of the 56th Annual Meeting of the Association for Computational Linguistics*.
- [13] Mingsheng Long, Yue Cao, Jianmin Wang, and Michael Jordan. Learning transferable features with deep adaptation networks. In *International Conference on Machine Learning*, 2015.
- [14] Yixiong Chen, Jingxian Li, Hua Jiang, Li Liu, and Chris Ding. Metalr: Layer-wise learning rate based on meta-learning for adaptively fine-tuning medical pre-trained models. In *Medical Image Computing and Computer Assisted Intervention*, 2023.
- [15] Luca Franceschi, Paolo Frasconi, Saverio Salzo, Riccardo Grazzi, and Massimiliano Pontil. Bilevel programming for hyperparameter optimization and meta-learning. In *International Conference on Machine Learning*, 2018.

- [16] Youngmin Ro and Jin Young Choi. Autolr: Layer-wise pruning and auto-tuning of learning rates in fine-tuning of deep networks. In *Proceedings of the AAAI Conference on Artificial Intelligence*, 2021.
- [17] Yang You, Igor Gitman, and Boris Ginsburg. Scaling SGD batch size to 32k for ImageNet training. *arXiv preprint arXiv:1708.03888*, 6(12):6, 2017.
- [18] Yang You, Zhao Zhang, Cho-Jui Hsieh, James Demmel, and Kurt Keutzer. Imagenet training in minutes. In *Proceedings of the 47th International Conference on Parallel Processing*, 2018.
- [19] 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, 2021.
- [20] Charles H Martin and Michael W Mahoney. Traditional and heavy tailed self regularization in neural network models. In *International Conference on Machine Learning*, 2019.
- [21] Charles H Martin and Michael W Mahoney. Heavy-tailed universality predicts trends in test accuracies for very large pre-trained deep neural networks. In *SIAM International Conference on Data Mining*, 2020.
- [22] 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.
- [23] 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, 2021.
- [24] 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.
- [25] Hyunjune Sebastian Seung, Haim Sompolinsky, and Naftali Tishby. Statistical mechanics of learning from examples. *Physical Review A*, 45(8):6056–6091, 1992.
- [26] Timothy L. H. Watkin, Albrecht Rau, and Michael Biehl. The statistical mechanics of learning a rule. *Rev. Mod. Phys.*, 65:499–556, Apr 1993.
- [27] David Haussler, H. Sebastian Seung, Michael Kearns, and Naftali Tishby. Rigorous learning curve bounds from statistical mechanics. In *Proceedings of the Seventh Annual Conference on Computational Learning Theory*, page 76–87, 1994.
- [28] Andreas Engel and Christian Van den Broeck. *Statistical mechanics of learning*. Cambridge University Press, 2001.
- [29] Samuel L Smith and Quoc V Le. A bayesian perspective on generalization and stochastic gradient descent. In *International Conference on Learning Representations*, 2018.
- [30] Samuel L. Smith, Pieter-Jan Kindermans, and Quoc V. Le. Don’t decay the learning rate, increase the batch size. In *International Conference on Learning Representations*, 2018.
- [31] Mert Gurbuzbalaban, Umut Simsekli, and Lingjiong Zhu. The heavy-tail phenomenon in sgd. In *International Conference on Machine Learning*, 2021.
- [32] Yaoqing Yang, Ryan Theisen, Liam Hodgkinson, Joseph E Gonzalez, Kannan Ramchandran, Charles H Martin, and Michael W Mahoney. Test accuracy vs. generalization gap: Model selection in nlp without accessing training or testing data. In *Proceedings of the 29th ACM SIGKDD Conference on Knowledge Discovery and Data Mining*, pages 3011–3021, 2023.
- [33] Kumar K Agrawal, Arnab Kumar Mondal, Arna Ghosh, and Blake Richards. $\$\\alpha\$$ -req : Assessing representation quality in self-supervised learning by measuring eigenspectrum decay. In *Advances in Neural Information Processing Systems*, 2022.

- [34] Josue Nassar, Piotr Sokol, SueYeon Chung, Kenneth D Harris, and Il Memming Park. On 1/n neural representation and robustness. In *Advances in Neural Information Processing Systems*, 2020.
- [35] Zeke Xie, Qian-Yuan Tang, Yunfeng Cai, Mingming Sun, and Ping Li. On the power-law hessian spectrums in deep learning. *arXiv preprint arXiv:2201.13011*, 2022.
- [36] Bruce M Hill. A simple general approach to inference about the tail of a distribution. *The Annals of Statistics*, pages 1163–1174, 1975.
- [37] Yuichi Yoshida and Takeru Miyato. Spectral norm regularization for improving the generalizability of deep learning. *arXiv preprint arXiv:1705.10941*, 2017.
- [38] Takeru Miyato, Toshiki Kataoka, Masanori Koyama, and Yuichi Yoshida. Spectral normalization for generative adversarial networks. In *International Conference on Learning Representations*, 2018.
- [39] Aaron Clauset, Cosma Rohilla Shalizi, and Mark EJ Newman. Power-law distributions in empirical data. *SIAM review*, 51(4):661–703, 2009.
- [40] Jeff Alstott, Ed Bullmore, and Dietmar Plenz. Powerlaw: a python package for analysis of heavy-tailed distributions. *PloS one*, 9(1):e85777, 2014.
- [41] Byeongho Heo, Sanghyuk Chun, Seong Joon Oh, Dongyo Han, Sangdoo Yun, Gyuwan Kim, Youngjung Uh, and Jung-Woo Ha. Adamp: Slowing down the slowdown for momentum optimizers on scale-invariant weights. In *International Conference on Learning Representations*, 2021.
- [42] Michael Zhang, James Lucas, Jimmy Ba, and Geoffrey E Hinton. Lookahead optimizer: k steps forward, 1 step back. In *Advances in Neural Information Processing Systems*, 2019.
- [43] John J Hopfield. Neural networks and physical systems with emergent collective computational abilities. *Proceedings of the National Academy of Sciences*, 1982.
- [44] Haim Sompolinsky. Statistical mechanics of neural networks. *Physics Today*, 41(21):70–80, 1988.
- [45] LM Rasdi Rere, Mohamad Ivan Fanany, and Aniati Murni Arymurthy. Simulated annealing algorithm for deep learning. *Procedia Computer Science*, 72:137–144, 2015.
- [46] Adriano Barra and Francesco Guerra. About the ergodic regime in the analogical hopfield neural networks: moments of the partition function. *Journal of Mathematical Physics*, 49(12):125217, 2008.
- [47] Adriano Barra, Alberto Bernacchia, Enrica Santucci, and Pierluigi Contucci. On the equivalence of hopfield networks and boltzmann machines. *Neural Networks*, 34:1–9, 2012.
- [48] Stephen G. Brush. History of the lenz-ising model. *Reviews of Modern Physics*, 39:883–893, 1967.
- [49] 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 *Advances in Neural Information Processing Systems*, 2021.
- [50] Umut Simsekli, Levent Sagun, and Mert Gurbuzbalaban. A tail-index analysis of stochastic gradient noise in deep neural networks. In *International Conference on Machine Learning*, pages 5827–5837, 2019.
- [51] Umut Simsekli, Ozan Sener, George Deligiannidis, and Murat A Erdogdu. Hausdorff dimension, heavy tails, and generalization in neural networks. *Advances in Neural Information Processing Systems*, 33:5138–5151, 2020.
- [52] Liam Hodgkinson and Michael W Mahoney. Multiplicative noise and heavy tails in stochastic optimization. In *International Conference on Machine Learning*, pages 4262–4274, 2021.

- [53] Liam Hodgkinson, Umut Simsekli, Rajiv Khanna, and Michael Mahoney. Generalization bounds using lower tail exponents in stochastic optimizers. In *International Conference on Machine Learning*, pages 8774–8795, 2022.
- [54] Anant Raj, Lingjiong Zhu, Mert Gurbuzbalaban, and Umut Simsekli. Algorithmic stability of heavy-tailed sgd with general loss functions. In *International Conference on Machine Learning*, pages 28578–28597, 2023.
- [55] Marco Baity-Jesi, Levent Sagun, Mario Geiger, Stefano Spigler, Gérard Ben Arous, Chiara Cammarota, Yann LeCun, Matthieu Wyart, and Giulio Biroli. Comparing dynamics: Deep neural networks versus glassy systems. In *International Conference on Machine Learning*, pages 314–323, 2018.
- [56] Jean Barbier, Florent Krzakala, Nicolas Macris, Léo Miolane, and Lenka Zdeborová. Optimal errors and phase transitions in high-dimensional generalized linear models. *Proceedings of the National Academy of Sciences*, 116(12):5451–5460, 2019.
- [57] Ben Sorscher, Robert Geirhos, Shashank Shekhar, Surya Ganguli, and Ari Morcos. Beyond neural scaling laws: beating power law scaling via data pruning. In *Advances in Neural Information Processing Systems*, 2022.
- [58] Yefan Zhou, Yaoqing Yang, Arin Chang, and Mahoney W Michael. A three-regime model of network pruning. In *International Conference on Machine Learning*, 2023.
- [59] 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.
- [60] 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. In *Advances in Neural Information Processing Systems*, 2020.
- [61] Peter Bartlett, Dylan Foster, and Matus Telgarsky. Spectrally-normalized margin bounds for neural networks. In *Advances in Neural Information Processing Systems*, 2017.
- [62] Huanrui Yang, Xiaoxuan Yang, Neil Zhenqiang Gong, and Yiran Chen. Hero: Hessian-enhanced robust optimization for unifying and improving generalization and quantization performance. In *Proceedings of the 59th ACM/IEEE Design Automation Conference*, 2022.
- [63] 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*, 2019.
- [64] Sheng Shen, Zhen Dong, Jiayu Ye, Linjian Ma, Zhewei Yao, Amir Gholami, Michael W Mahoney, and Kurt Keutzer. Q-BERT: Hessian based ultra low precision quantization of bert. In *AAAI Conference on Artificial Intelligence*, 2020.
- [65] Amartya Sanyal, Philip H. Torr, and Puneet K. Dokania. Stable rank normalization for improved generalization in neural networks and gans. In *International Conference on Learning Representations*, 2020.
- [66] 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*, 2021.
- [67] David A McAllester. Some pac-bayesian theorems. In *Proceedings of the Eleventh Annual Conference on Computational Learning Theory*, 1998.
- [68] John Langford and John Shawe-Taylor. Pac-bayes & margins. In *Advances in Neural Information Processing Systems*, 2002.
- [69] Gintare Karolina Dziugaite and Daniel M Roy. Computing nonvacuous generalization bounds for deep (stochastic) neural networks with many more parameters than training data. In *Annual Conference on Uncertainty in Artificial Intelligence*, 2017.

- [70] 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.
- [71] Xuanzhe Xiao, Zeng Li, Chuanlong Xie, and Fengwei Zhou. Heavy-tailed regularization of weight matrices in deep neural networks. *arXiv preprint arXiv:2304.02911*, 2023.
- [72] Alex Krizhevsky, Vinod Nair, and Geoffrey Hinton. Cifar-10 and cifar-100 datasets. 2009.
- [73] Pierre Sermanet, Koray Kavukcuoglu, and Yann LeCun. Traffic signs and pedestrians vision with multi-scale convolutional networks. In *Snowbird Machine Learning Workshop*, 2011.
- [74] Jia Deng, Wei Dong, Richard Socher, Li-Jia Li, Kai Li, and Li Fei-Fei. Imagenet: A large-scale hierarchical image database. In *IEEE Conference on Computer Vision and Pattern Recognition*, 2009.
- [75] Ya Le and Xuan Yang. Tiny imagenet visual recognition challenge. *CS 231N*, 7(7):3, 2015.
- [76] Karen Simonyan and Andrew Zisserman. Very deep convolutional networks for large-scale image recognition. *arXiv preprint arXiv:1409.1556*, 2014.
- [77] Kaiming He, Xiangyu Zhang, Shaoqing Ren, and Jian Sun. Deep residual learning for image recognition. In *IEEE Conference on Computer Vision and Pattern Recognition*, 2016.
- [78] Sergey Zagoruyko and Nikos Komodakis. Wide residual networks. In *Proceedings of the British Machine Vision Conference*, 2016.
- [79] Yang You, Jing Li, Sashank Reddi, Jonathan Hseu, Sanjiv Kumar, Srinadh Bhojanapalli, Xiaodan Song, James Demmel, Kurt Keutzer, and Cho-Jui Hsieh. Large batch optimization for deep learning: Training bert in 76 minutes. In *International Conference on Learning Representations*, 2020.
- [80] Razvan Pascanu, Tomas Mikolov, and Yoshua Bengio. On the difficulty of training recurrent neural networks. In *International Conference on Machine Learning*, pages 1310–1318, 2013.
- [81] Ryo Karakida, Shotaro Akaho, and Shun-ichi Amari. Pathological spectra of the fisher information metric and its variants in deep neural networks. *Neural Computation*, 33:2274–2307, 2019.
- [82] Ryo Karakida, Shotaro Akaho, and Shun-ichi Amari. Universal statistics of fisher information in deep neural networks: Mean field approach. In *the 22nd International Conference on Artificial Intelligence and Statistics*, 2019.
- [83] Ka-Veng Yuen. *Bayesian methods for structural dynamics and civil engineering*. John Wiley & Sons, 2010.
- [84] Yudi Pawitan. *In all likelihood: statistical modelling and inference using likelihood*. Oxford University Press, 2001.
- [85] Bohang Zhang, Du Jiang, Di He, and Liwei Wang. Rethinking lipschitz neural networks and certified robustness: A boolean function perspective. In *Advances in Neural Information Processing Systems*, 2022.
- [86] Li Deng. The mnist database of handwritten digit images for machine learning research. *IEEE Signal Processing Magazine*, 29(6):141–142, 2012.
- [87] Zhewei Yao, Amir Gholami, Kurt Keutzer, and Michael W Mahoney. PyHessian: Neural networks through the lens of the hessian. In *IEEE International Conference on Big Data*, pages 581–590, 2020.
- [88] Arthur Jacot, Franck Gabriel, and Clément Hongler. Neural tangent kernel: Convergence and generalization in neural networks. In *Advances in Neural Information Processing Systems*, 2018.

- [89] Lingyu Gu, Yongqi Du, Yuan Zhang, Di Xie, Shiliang Pu, Robert Qiu, and Zhenyu Liao. "lossless" compression of deep neural networks: A high-dimensional neural tangent kernel approach. In *Advances in Neural Information Processing Systems*, 2022.
- [90] Zeke Xie, Qian-Yuan Tang, Zheng He, Mingming Sun, and Ping Li. Rethinking the structure of stochastic gradients: Empirical and statistical evidence. *arXiv preprint arXiv:2212.02083*, 2022.
- [91] Aitor Lewkowycz, Yasaman Bahri, Ethan Dyer, Jascha Sohl-Dickstein, and Guy Gur-Ari. The large learning rate phase of deep learning: the catapult mechanism. *arXiv preprint arXiv:2003.02218*, 2020.
- [92] Ethan Dyer and Guy Gur-Ari. Asymptotics of wide networks from feynman diagrams. In *International Conference on Learning Representations*, 2020.
- [93] Peter L Bartlett, Philip M Long, Gábor Lugosi, and Alexander Tsigler. Benign overfitting in linear regression. In *Proceedings of the National Academy of Sciences*, 2020.
- [94] Romain Couillet and Zhenyu Liao. *Random Matrix Methods for Machine Learning*. Cambridge University Press, 2022.
- [95] Mark Everingham, Luc Van Gool, Christopher KI Williams, John Winn, and Andrew Zisserman. The pascal visual object classes (voc) challenge. *International Journal of Computer Vision*, 88: 303–338, 2010.
- [96] Joseph Redmon, Santosh Divvala, Ross Girshick, and Ali Farhadi. You only look once: Unified, real-time object detection. In *Proceedings of the IEEE Conference on Computer Vision and Pattern Recognition*, pages 779–788, 2016.
- [97] Tsung-Yi Lin, Michael Maire, Serge Belongie, James Hays, Pietro Perona, Deva Ramanan, Piotr Dollár, and C Lawrence Zitnick. Microsoft coco: Common objects in context. In *Computer Vision–ECCV 2014: 13th European Conference, Zurich, Switzerland, September 6–12, 2014, Proceedings, Part V 13*, pages 740–755, 2014.
- [98] Mitchell P. Marcus, Beatrice Santorini, and Mary Ann Marcinkiewicz. Building a large annotated corpus of English: The Penn Treebank. *Computational Linguistics*, 19(2):313–330, 1993.
- [99] Xindian Ma, Peng Zhang, Shuai Zhang, Nan Duan, Yuexian Hou, Ming Zhou, and Dawei Song. A tensorized transformer for language modeling. *Advances in neural information processing systems*, 32, 2019.

Appendix

A Heavy-tail phenomena in different DNN matrices are closely related

Recently, several papers have separately studied HT structures in different types of matrices, including the Hessian, the Fisher Information Matrix (FIM), and input/output covariance matrices [35, 81, 82]. The results confirm that when NNs are well-trained, various matrices have HT properties. Among these works, there are two major ways to characterize the HT spectrum, namely the HT-shaped ESDs (such as PL_Alpha_Hill), or HT-shaped decaying eigenvalues [33–35]. Our paper mainly uses the first way of characterizing the HT structure. On the other hand, the second way is to sort eigenvalues from largest to smallest and study the PL phenomena between the ordered eigenvalues and their index. Our experiments show fruitful connections between the PL phenomena manifested in different DNN matrices; if one matrix shows a PL spectrum, the other matrices often show something similar [35]. Thus, it is meaningful to ask why and how the PL phenomena in different prior works correlate.

This section first establishes the connections between input/output covariance matrices, the FIM and the Hessian in subsection A.1. We find that if one of these matrices shows the PL phenomenon, the other two matrices have a high chance to exhibit a similar PL phenomenon. Then, in subsection A.2, we derive the connection between our metric PL_Alpha_Hill and the PL exponent on decaying eigenvalues, showing a simple reciprocal relationship between these two.

A.1 Connections between different matrices

Consider a NN $f_\theta : \mathbb{R}^d \rightarrow \mathbb{R}^C$, where $\theta \in \mathbb{R}^P$ is the vectorized weights, d is the input dimension, and C is the output dimension. When the NN is used for a classifying task, C is also the number of classes. We denote the input data as $\{(x_i, y_i)\}_{i=1}^n$, where $x_i \in \mathbb{R}^d$, and the number of samples is n . We denote the loss function as $L(\theta) = \frac{1}{n} \sum_{i=1}^n l(y_i, f_\theta(x_i))$.

Covariance matrices. We denote the output covariance matrix as $\mathbb{E}[f_\theta(x)f_\theta^\top(x)]$, where the expectation is taken over the input distribution. We tend to consider the following empirical covariance matrix:

$$C(\theta) := \frac{1}{n} \sum_{i=1}^n f_\theta(x_i) f_\theta^\top(x_i) \in \mathbb{R}^{C \times C}. \quad (5)$$

Fisher Information Matrices. We denote the (output) FIM as

$$\mathbb{E}[\nabla_\theta f_\theta(x) \nabla_\theta f_\theta(x)^\top] = \sum_{k=1}^C \mathbb{E}[\nabla_\theta f_\theta^{(k)}(x) \nabla_\theta f_\theta^{(k)}(x)^\top], \quad (6)$$

where $f_\theta^{(k)}(x)$ is the k -th entry of the vector function $f(x)$. We also consider the empirical version of the FIM:

$$F(\theta) := \sum_{k=1}^C \frac{1}{n} \sum_{i=1}^n \nabla_\theta f_\theta^{(k)}(x_i) \nabla_\theta f_\theta^{(k)}(x_i)^\top \in \mathbb{R}^{P \times P}. \quad (7)$$

Note that (7) can be equally written as

$$F(\theta) := \frac{1}{n} \nabla_\theta \tilde{f}_\theta(x) \nabla_\theta \tilde{f}_\theta(x)^\top, \quad (8)$$

where $\nabla_\theta \tilde{f}_\theta(x)$ has the following form:

$$\begin{bmatrix} \frac{\partial f_\theta^{(1)}(x_1)}{\partial \theta_1} \dots \frac{\partial f_\theta^{(1)}(x_n)}{\partial \theta_1} & \dots & \frac{\partial f_\theta^{(C)}(x_1)}{\partial \theta_1} \dots \frac{\partial f_\theta^{(C)}(x_n)}{\partial \theta_1} \\ \vdots & \ddots & \vdots \\ \frac{\partial f_\theta^{(1)}(x_1)}{\partial \theta_P} \dots \frac{\partial f_\theta^{(1)}(x_n)}{\partial \theta_P} & \dots & \frac{\partial f_\theta^{(C)}(x_1)}{\partial \theta_P} \dots \frac{\partial f_\theta^{(C)}(x_n)}{\partial \theta_P} \end{bmatrix} \in \mathbb{R}^{P \times Cn}.$$

Hessian Matrices. We denote the Hessian as $\mathbb{E} \left[\frac{\partial^2 l(y, f_\theta(x))}{\partial \theta^2} \right]$, and we tend to consider the empirical Hessian Matrices:

$$H(\theta) := \frac{\partial^2 L(\theta)}{\partial \theta^2} \in R^{P \times P}, \quad (9)$$

where $L(\theta)$ is the empirical loss function $L(\theta) = \frac{1}{n} \sum_{i=1}^n l(y_i, f_\theta(x_i))$.

Hessian and FIM are equivalent under certain conditions. FIM can be defined in alternative ways different from (6). For instance, from classic statistical knowledge, we have the standard FIM (sFIM) in the following form:

$$sFIM := \mathbb{E}[\nabla_\theta \log P(y|x; \theta) \nabla_\theta \log P(y|x; \theta)^T], \quad (10)$$

where $P(y|x; \theta)$ represents the likelihood. After simple derivations, one can show that sFIM also has the following form [83, 84]:

$$sFIM = -\mathbb{E} \left[\frac{\partial^2 \log P(y|x; \theta)}{\partial \theta^2} \right]. \quad (11)$$

Therefore, when the loss function is defined as the negative log-likelihood, the sFIM in (11) is equivalent to Hessian defined in (9).

Why is the FIM defined in (6) equivalent to (10). Back to deep learning, the FIM is often defined as (6). It is thus meaningful to derive the equivalence between these two forms. Suppose $P(y|x; \theta)$ here means the conditional probability distribution of output y given input data x . If $P(y|x; \theta)$ is assumed to take the following form:

$$P(y|x; \theta) = \frac{1}{\sqrt{2\pi}} \exp \left(-\frac{1}{2} \|y - f_\theta(x)\|^2 \right), \quad (12)$$

then the MSE estimator $\min_\theta \frac{1}{2} \|y - f_\theta(x)\|^2$ is equivalent to the maximum likelihood estimation of $P(y|x; \theta)$. Then, plugging (12) into (10), we have:

$$sFIM_{mse} = \mathbb{E}[\|y - f_\theta(x)\|^2 \nabla_\theta f_\theta(x) \nabla_\theta f_\theta(x)^T]. \quad (13)$$

We now expand $sFIM_{mse}$ by the definition of expectation, and we have the following [81]:

$$sFIM_{mse} = \int_{\mathbb{R}} \int_{\mathbb{R}} \|y - f_\theta(x)\|^2 \nabla_\theta f_\theta(x) \nabla_\theta f_\theta(x)^T p(x, y; \theta) dy dx \quad (14)$$

$$= \int_{\mathbb{R}} \int_{\mathbb{R}} \|y - f_\theta(x)\|^2 \nabla_\theta f_\theta(x) \nabla_\theta f_\theta(x)^T P(y|x; \theta) q(x) dy dx \quad (15)$$

$$= \int_{\mathbb{R}} \left[\int_{\mathbb{R}} \frac{1}{\sqrt{2\pi}} \|y - f_\theta(x)\|^2 \exp \left(-\frac{1}{2} \|y - f_\theta(x)\|^2 \right) dy \right] \nabla_\theta f_\theta(x) \nabla_\theta f_\theta(x)^T q(x) dx \quad (16)$$

$$= \int_{\mathbb{R}} \nabla_\theta f_\theta(x) \nabla_\theta f_\theta(x)^T q(x) dx \quad (17)$$

$$= \mathbb{E}[\nabla_\theta f_\theta(x) \nabla_\theta f_\theta(x)^T], \quad (18)$$

where (14) follows from the definition of expectation, $q(x)$ is input distribution, and (17) holds because the integral of y in the brackets [] equals 1 due to the property of Gamma function $\Gamma(\cdot)$.

Therefore, from (18), we find that $sFIM_{mse}$ is just equal to FIM, defined in (6). Also, plugging (12) into $\mathbb{E} \left[\frac{\partial^2 \log P(y|x; \theta)}{\partial \theta^2} \right]$ and taking the loss function $L(\theta)$ as the mean-square loss, we will again find that $\mathbb{E} \left[\frac{\partial^2 \log P(y|x; \theta)}{\partial \theta^2} \right]$ is equal to $H(\theta)$. Therefore, jointly considering (11), we can see that FIM is equal to the Hessian $H(\theta)$.

PL in the covariance matrix and PL in Hessian are tightly correlated. Next, we consider the relationship between the covariance matrix and the Hessian. Suppose the NN function f_θ is a Lipschitz function [85]. Then, it can be seen that the covariance matrix (5) may be controlled and estimated by FIM defined in (6), which is equivalent to being controlled by Hessian.

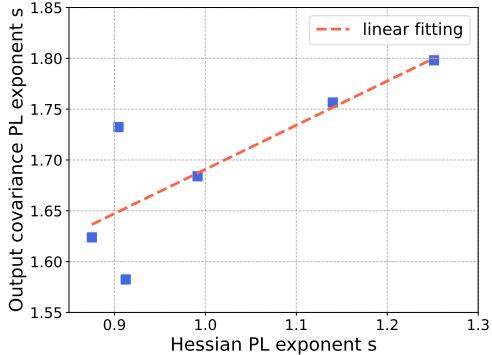


Figure 9: We train a MLP for 50 epochs and fit PL exponent s for both the output covariance and the Hessian. For models trained with epochs $\{1, 10, 20, 30, 40, 50\}$, we see their PL exponents s show a strong correlation.

Although deriving an exact equivalent between these two can be hard, we numerically show that the PL in one matrix informs the PL in the other. To visualize their relationship in the presence of PL, we train a simple MLP on MNIST [86] with one hidden layer and 2000 neurons for 50 epochs. We leverage the spectral regularization from Nassar et al. [34] to make the output covariance matrix exhibit a PL spectrum. Meanwhile, we calculate the top eigenvalues of the covariance and the Hessian [87], fit the PL exponent s for each matrix, and compare the PL exponents against each other. More specifically, we take trained NNs from epochs $\{1, 10, 20, 30, 40, 50\}$ and plot the Hessian PL exponent s versus the output covariance PL exponent s . From the results shown in Figure 9, we can see that their PL exponent s shows a strong correlation, which supports our claim that the PL phenomena in one matrix can inform the other.

Connections to the NTK matrix. Interestingly, if we ignore the constant in (8) and switch the two matrices multiplied together, we obtain $\nabla_\theta \tilde{f}_\theta(x)^T \nabla_\theta \tilde{f}_\theta(x)$. This matrix is equal to Neural Tangent Kernel(NTK) [88], which is a kernel used to approximate the deep NN when NN’s width is infinite. We thus conjecture that NTK should show PL when the NN is well trained [89]. Indeed, Karakida et al. [81] and Karakida et al. [82] study the eigenvalues of NTK, showing a PL trend. Some other work on stochastic gradient [90] claim that the so-called “stochastic gradient matrix” (which is similar to the NTK matrix) shows a PL spectrum as well, which matches our expectations. Also, Lewkowycz et al. [91], Dyer and Gur-Ari [92] show that the eigenvalues of NTK are similar to those in the Hessian, which again meets our expectation because the Hessian tends to be PL when NNs are well-trained [35].

In summary, this section investigates different “important matrices” and shows that they are tightly correlated to each other in terms of the PL trends: if one matrix shows a PL spectrum, there is a high chance that the other ones show something similar.

A.2 Connections between PL in ESD and PL in decaying eigenvalues

Next, we derive the connection between our PL_Alpha_Hill metric and the exponent of PL distribution on decaying eigenvalues. Take the covariance matrix (5) as an instance. According to Nassar et al. [34], the HT phenomenon in the output covariance matrix is similar to the layer-wise covariance matrices. Thus, without the loss of generality, we can consider the case when there is only one layer in the NN. We assume the weight matrix L is in $\mathbf{R}^{N \times Q}$. According to prior works, when L is well-trained, the ESD follows a PL distribution:

$$p(\lambda) = \frac{1}{H} \lambda^{-\alpha}, \quad \lambda_{\min} < \lambda < \lambda_{\max}. \quad (19)$$

Here, H is a normalizing constant, and α is the PL exponent.

Another way to characterize the PL phenomenon is to consider eigenvalues directly following a PL series. For example, Xie et al. [35] show that the decaying eigenvalues follows the following PL

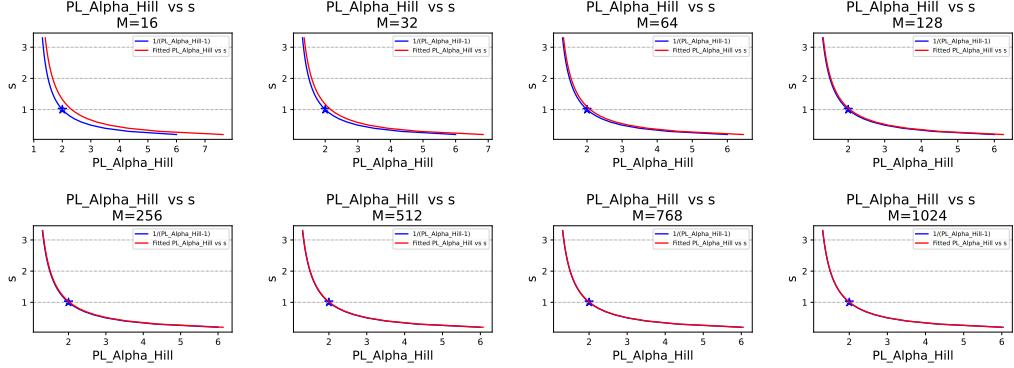


Figure 10: We show the connection between $\text{PL}_{\text{Alpha}}_{\text{Hill}}$ and the PL exponent of the decaying eigenvalues (denoted as s) satisfy $s = \frac{1}{\text{PL}_{\text{Alpha}}_{\text{Hill}} - 1}$. Results are shown for different matrix size Q . In particular, we see that $\text{PL}_{\text{Alpha}}_{\text{Hill}} = 2$ [19] is equivalent to $s = 1$ [33] in the linear case.

series:

$$\lambda_k = \lambda_1 k^{-s}, k = 1, 2, \dots, Q, \quad (20)$$

where λ_1 is the same as λ_{\max} used in the main paper.

Now, we will analytically and empirically show that these two ways of characterizing PL are strongly related. Furthermore, the two PL coefficients satisfy $s = \frac{1}{\alpha - 1}$.

An analytical way to show that $s = \frac{1}{\alpha - 1}$. The derivation is actually quite simple. Consider the case that $\lambda_k = \lambda_1 k^{-s}$ (i.e., (20) holds), and suppose Λ is a random variable distributed according to the empirical distribution from these eigenvalues $\lambda_k = \lambda_1 k^{-s}$. Now, from (20), we can see that the distribution function takes the following form:

$$\mathbb{P}(\Lambda > \lambda_1 k^{-s}) = \frac{k}{Q}. \quad (21)$$

By changing variables $\lambda_1 k^{-s} = \lambda$, we get the cumulative distribution function of Λ :

$$\mathbb{P}(\Lambda > \lambda) \sim \lambda^{-\frac{1}{s}}. \quad (22)$$

After that, we take the derivative with respect to λ , and we get the ESD:

$$p(\lambda) \sim \lambda^{-(\frac{1}{s} + 1)}. \quad (23)$$

In other words, we have $\lambda^{-(\frac{1}{s} + 1)} = \lambda^{-\alpha}$, which means $s = \frac{1}{\alpha - 1}$.

An empirical way to show that $s = \frac{1}{\alpha - 1}$. We consider matrices of size $Q \times Q$, where we choose Q in $\{16, 32, 64, 128, 256, 512, 768, 1024\}$, and we assign the parameters such that the decaying eigenvalues obey the formula $\lambda_1 k^{-s}$, for s in $\{0.2, 0.3, 0.4, \dots, 3.2\}$. Then, we fit the ESD and get our estimate $\text{PL}_{\text{Alpha}}_{\text{Hill}}$. We plot the relationship between $\text{PL}_{\text{Alpha}}_{\text{Hill}}$ and s in Figure 10. From Figure 10, we find that the connection between $\text{PL}_{\text{Alpha}}_{\text{Hill}}$ and s shows a good fit with the formula $s = \frac{1}{\alpha - 1}$. With increasing matrix size Q , the fitting becomes increasingly accurate.

When $s = \frac{1}{\alpha - 1}$, $s = 1$ corresponds to $\alpha = 2$. Some prior works Nassar et al. [34], Xie et al. [35], Bartlett et al. [93] measure the HT phenomena from the perspective of decaying eigenvalues with PL exponent s , and they show either theoretically or empirically that $s = 1$ is the *optimal* exponent. Now that we have $s = \frac{1}{\alpha - 1}$ in the linear case, and from the theory of NTK[88], the infinite wide NN is approximated as a linear model, we tend to believe that $\alpha = 2$ satisfies a similar property. Indeed, one of the main contributions of Martin and Mahoney [19] is to establish different HT families of ESDs, and $\alpha = 2$ is believed to be the boundary between ‘‘moderately HT’’ and ‘‘very HT,’’ corresponding to the best models. Martin and Mahoney [19] further argue that the optimal exponent for PL_{Alpha} is in the range $[2, 4]$. Combining the perspective from Nassar et al. [34], Xie et al. [35], Bartlett et al. [93] and those from Martin and Mahoney [19], it is reasonable to believe that the optimal exponent for PL_{Alpha} is around 2. When PL_{Alpha} is much higher or lower than 2,

the NN probably has some issue in training. Although we argued in the main paper that the absolute numerical value of PL_Alpha is unimportant in implementing our TempBalance algorithm, it is, however, helpful to have an “optimal” PL_Alpha value to test if our algorithm actually works in controlling the ESDs. We will show visualization results in Appendix B that TempBalance leads to a better distribution of our estimated PL_Alpha_Hill.

In summary, this section explores two distinct methods for determining PL fit. We demonstrate that, although these two methods yield numerically distinct PL exponents, they essentially capture the same underlying phenomenon. Moreover, it is noteworthy that the “optimal” values of the PL exponents reported in various papers are consistent with one another [19, 34, 35, 93].

B Visualization results: how does TempBalance control ESDs

We demonstrate that the proposed method, TempBalance, effectively controls the shape of ESDs, resulting in a more favorable distribution of PL_Alpha_Hill among the layers of NNs compared to the baseline method CAL. This observation elucidates the superior performance of TempBalance over CAL in our main experiment, as presented in Section 4.2.

We evaluate the models reported in the main paper. For each individual NN, we compute and aggregate PL_Alpha_Hill values across all layers, excluding the first and last layers that have an extremely small number of eigenvalues and thus cause inaccurate PL_Alpha_Hill estimation. We aggregate the PL_Alpha_Hill values from five models trained using different random seeds for each method. Figure 11 shows the distribution of PL_Alpha_Hill of TempBalance and the baseline CAL. Comparing TempBalance with CAL, we see that TempBalance consistently yields a more concentrated distribution. Furthermore, TempBalance causes the median and mean of the distribution to approach 2 (shown in each subplot respectively as the middle vertical line and the red star). The value 2 represents the theoretically optimal PL_Alpha_Hill value, as we have justified in Appendix A.

Next, in Figure 12, we group the models into different subgroups based on their architectures and/or datasets, aggregating the PL_Alpha_Hill values and comparing the distributions of the two methods TempBalance and CAL. Once again, we observe that TempBalance results in a more concentrated distribution, with a larger number of samples (layers) having PL_Alpha_Hill values closer to 2.

We provide visualization to demonstrate how the learning rates are distributed over layers during the training. In Figure 13, we report the learning rate and PL_Alpha_Hill every epoch throughout the 200-epoch training duration. The key observation includes the following.

1. **How does the learning rate vary across layers?** We observed a correlation between the layer-wise learning rate and the layer-wise PL_Alpha_Hill distribution: layers with larger PL_Alpha_Hill are allocated larger learning rates, whereas those with smaller PL_Alpha_Hill receive smaller learning rates.
2. **How does the layer-wise learning rate evolve during training?** The variations in layer-wise learning rates closely reflect shifts in the layer-wise PL_Alpha_Hill distribution. Initially, the PL_Alpha_Hill distributes uniformly across layers but eventually converge to a layer-wise pattern where earlier layers have smaller PL_Alpha_Hill and later layers have larger ones.

We present visualizations of how PL_Alpha_Hill and learning rate evolve through training. In Figure 14, we show PL_Alpha_Hill and learning rate of two layers within the same ResNet18 during the training process. The two layers are layer1.0.conv2 (index=1) and layer4.0.conv2 (index=15). From Figure 14b and 14d, we can see that with the baseline CAL scheduler (blue curves), the earlier layer (index=1) achieves a smaller PL_Alpha_Hill value compared to the larger PL_Alpha_Hill value of the later layer (index=15). In contrast, TempBalance (orange curves) narrows this gap, indicating our approach balances the undertraining/overtraining levels (as signified by PL_Alpha_Hill) of different layers. This balancing effect is further corroborated by Figures 11 and 12, where our method consistently refines the layer-wise PL_Alpha_Hill distribution. Regarding the learning rate plots in Figure 14a and 14c, TempBalance allocates a lower learning rate for earlier layers and a higher one for later layers than the baseline does. This leads to a more balanced PL_Alpha_Hill distribution between layers as mentioned above. Additionally, we noted

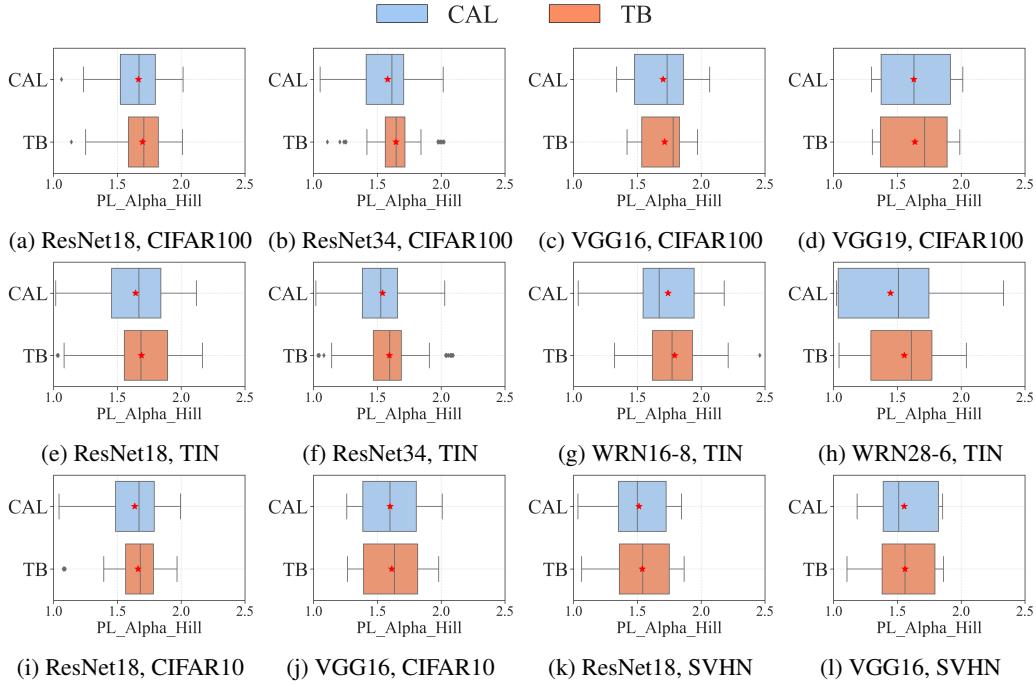


Figure 11: Comparing the distribution of PL_Alpha_Hill of NNs trained by our method TempBalance (TB) and CAL. The mean of each distribution is indicated by a red star marker. Each distribution aggregates the PL_Alpha_Hill values from models trained using five different random seeds. Across all experiments, our method TempBalance consistently yields a more concentrated distribution, resulting in the mean and median approaching the theoretically optimal PL_Alpha_Hill value of 2, as supported in Appendix A.

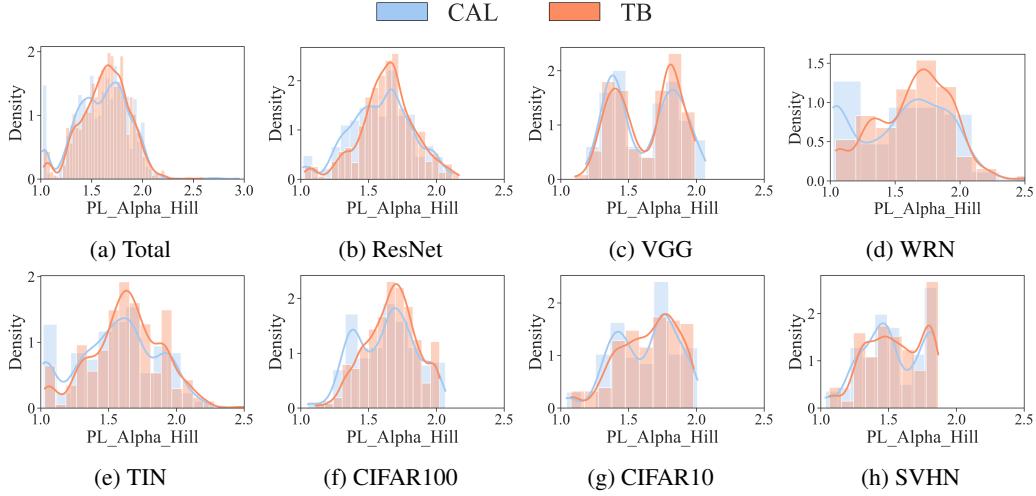


Figure 12: Comparing our method TempBalance (TB) to CAL in terms of the distribution of PL_Alpha_Hill of aggregating NNs into different architectures and datasets. Each distribution aggregates the PL_Alpha_Hill of models trained with five random seeds. Across all subgroups, our method TempBalance consistently exhibits a more concentrated distribution, accompanied by a higher number of layers approaching a PL_Alpha_Hill value close to 2. This value of 2 corresponds to the theoretically optimal PL_Alpha_Hill value, as justified in Appendix A.

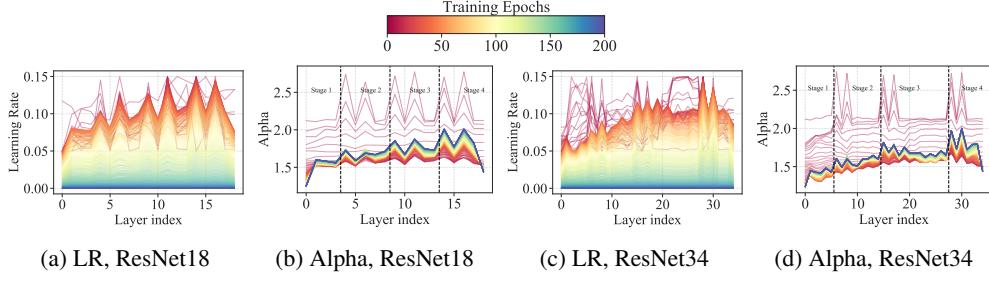


Figure 13: **(Visualization of layer-wise learning rate (LR) and PL_Alpha_Hill (Alpha) over training).** (a-b) The layer-wise LR and PL_Alpha_Hill of ResNet18 over training. (c-d) The layer-wise LR and PL_Alpha_Hill of ResNet34 over training.

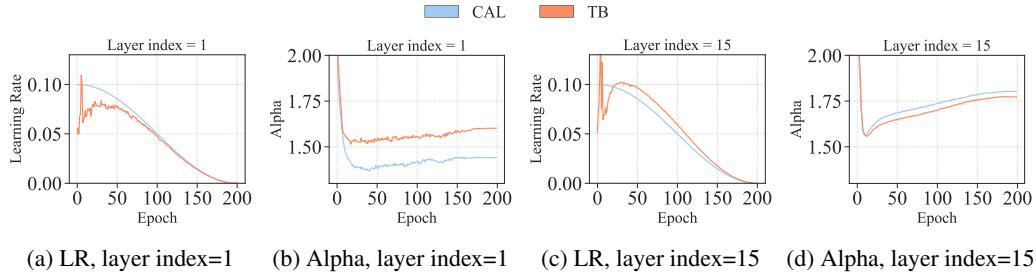


Figure 14: **(Visualization of learning rate (LR) and PL_Alpha_Hill (Alpha) of two layers during training)** (a-b) LR and PL_Alpha_Hill of one layer with index = 1 in ResNet18. (c-d) LR and PL_Alpha_Hill of one layer with index = 15 in ResNet18. The ResNet18 is trained on CIFAR100.

instability in the learning rate curves during early training phases, while smoother transitions emerge in later phases.

C Ablation studies

We provide additional ablation studies on the choices of learning rate assignment function, assignment hyperparameters.

Varying LR assignment function. For TempBalance, we selected the linear interpolation (Equation 2) for learning rate assignment function f_t , based on its superior performance in our ablation study.

We evaluated three alternative learning rate assignment functions: Square root (Sqrt), Log2, and Step:

- Sqrt : $f_t(i) = \eta_t \frac{\sqrt{\alpha_t^i}}{\frac{1}{L} \sum_{j=1}^L \sqrt{\alpha_t^j}}$,
- Log2: $f_t(i) = \eta_t \frac{\log(\alpha_t^i)}{\frac{1}{L} \sum_{j=1}^L \log(\alpha_t^j)}$,
- Step: For layer i with k -th minimum PL_Alpha_Hill among all the layers,

$$f_t(i) = \eta_t(s_1 + (k-1) \frac{s_2 - s_1}{L-1})$$

Here, η_t denotes the base global learning rate at epoch t , (s_1, s_2) represents the minimum and maximum learning rate scaling ratios relative to η_t , α_t^i is the PL_Alpha_Hill estimate of the layer i at epoch t , and L is the total number of model layers. All these notations are consistently used in the main paper.

As depicted in Figure 15, TempBalance (TB), with the current assignment function, surpasses the other designs when tested on VGG and ResNet architectures on CIFAR100. All hyperparameters are consistent with the main paper. Each experiment was conducted with five random seeds.

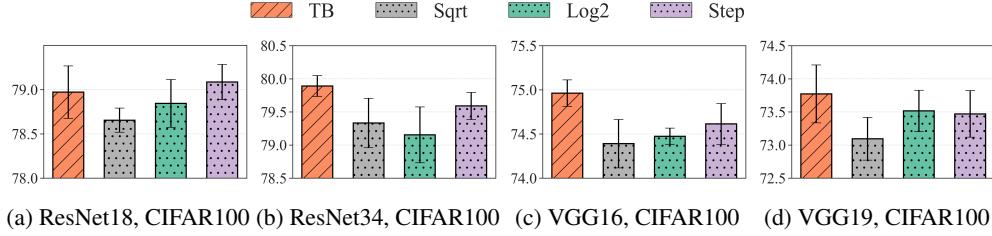


Figure 15: (**Different designs for learning rate assignment function.**) Results of using different learning rate assignment functions on different architectures and CIFAR-100. Our design in the main paper TempBalance (TB) outperforms others. Reporting mean/std over five random seeds.

Varying LR assignment function hyperparameters. We provide additional results of a hyperparameter study on (s_1, s_2) , in which we consider five different settings for (s_1, s_2) : $[(0.5, 1.5), (0.6, 1.4), (0.7, 1.3), (0.8, 1.2), (0.9, 1.1)]$. We run tasks on CIFAR100 with four VGG and ResNet architectures, each with five random seeds. Our results in Figure 16 show that a larger learning rate scaling range $(0.5, 1.5)$ performs best. This hyperparameter setting is the default setting used in our paper. All hyperparameters are consistent with those described in the main paper.

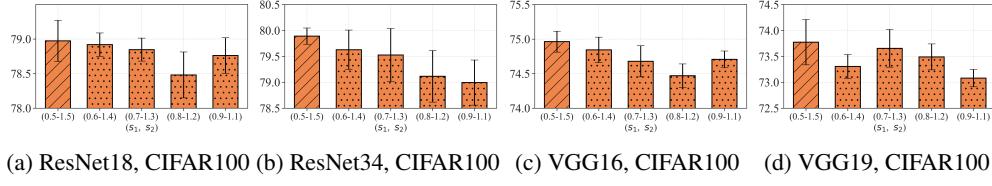


Figure 16: (**Hyperparameter study on (s_1, s_2) .**) Search for hyperparameters (s_1, s_2) with different architectures on CIFAR100. The current hyperparameter choice $(0.5, 1.5)$ used in the paper performs best among all the cases. Reporting mean/std over five random seeds.

D Hyperparameter settings for reproducing our results

We report all hyperparameters, random seeds and all numerical values of experimental results shown in the main paper (in Section 4).

First, we report the common hyperparameters shared by all the experiments: the default optimizer is SGD, trained with batch size 128, number of training epochs 200, weight decay 5e-4, and momentum 0.9. The default HT-SR metric used in TempBalance is PL_Alpha_Hill. For each experimental setting, we use five random seeds, which are always 43, 37, 13, 51, 71, and we report the mean and standard deviation of the test accuracy across these seeds.

First, Table 1 reports the details of experiments shown in Figure 3. We carefully tune the initial learning rate η_0 and λ_{sr} for the two baseline methods CAL and SNR. Then, Table 2 reports the detailed hyperparameter settings of the experiments shown in Figure 4. We again carefully tune the hyperparameters of various baseline optimizers and schedulers, as specified in their papers. Finally, Table 3, Table 4, Table 5 and Table 6 respectively report the details of the experiments shown in Figure 5, Figure 6, Figure 7 and Figure 8.

Table 1: Parameter settings of the experiment reported in Section 4.2 Figure 3. The hyperparameter in bold is the best hyperparameter selection reported in the main paper. The five random seeds for each setting are $\{43, 37, 13, 51, 71\}$, and the means and standard deviations of the test accuracy among the five seeds are reported.

Index	Dataset	Model	Method	Initial learning rate η_0	λ_{sr}	Test Acc (best hyperparam.)	scaling ratio (s_1, s_2)
0	CIFAR100	ResNet18	CAL	0.05, 0.1 , 0.15	-	78.31 \pm 0.05	-
1		ResNet18	SNR	0.1	0.001, 0.005, 0.01 , 0.015	78.65 \pm 0.29	-
2		ResNet18	TB	0.1	-	78.97 \pm 0.29	(0.5, 1.5)
3		ResNet18	TB + SNR	0.1	0.001	79.06 \pm 0.32	(0.6, 1.4)
4		ResNet34	CAL	0.05 , 0.1, 0.15	-	78.98 \pm 0.14	-
5		ResNet34	SNR	0.1	0.001, 0.005, 0.01, 0.015	79.97 \pm 0.21	-
6		ResNet34	TB	0.1	-	79.89 \pm 0.15	(0.5, 1.5)
7		ResNet34	TB + SNR	0.1	0.005	80.09 \pm 0.35	(0.6, 1.4)
8		VGG16	CAL	0.025, 0.05 , 0.1	-	74.59 \pm 0.23	-
9		VGG16	SNR	0.05	0.001, 0.005 , 0.01, 0.015	74.80 \pm 0.28	-
10		VGG16	TB	0.05	-	74.96 \pm 0.15	(0.5, 1.5)
11		VGG16	TB + SNR	0.05	0.005	75.52 \pm 0.46	(0.6, 1.4)
12		VGG19	CAL	0.025, 0.05 , 0.1	-	73.26 \pm 0.37	-
13		VGG19	SNR	0.05	0.001, 0.005, 0.01 , 0.015	74.37 \pm 0.16	-
14		VGG19	TB	0.05	-	73.77 \pm 0.43	(0.5, 1.5)
15		VGG19	TB + SNR	0.05	0.01	74.74 \pm 0.10	(0.5, 1.5)
16	TinyImageNet	ResNet18	CAL	0.05, 0.1 , 0.15	-	66.25 \pm 0.17	-
17		ResNet18	SNR	0.1	0.001, 0.005, 0.01 , 0.015	66.20 \pm 0.22	-
18		ResNet18	TB	0.1	-	66.77 \pm 0.25	(0.6, 1.4)
19		ResNet18	TB + SNR	0.1	0.001	66.86 \pm 0.22	(0.6, 1.4)
20		ResNet34	CAL	0.05, 0.1 , 0.15	-	68.19 \pm 0.16	-
21		ResNet34	SNR	0.1	0.001, 0.005, 0.01 , 0.015	68.69 \pm 0.13	-
22		ResNet34	TB	0.1	-	69.12 \pm 0.16	(0.6, 1.4)
23		ResNet34	TB + SNR	0.1	0.001	69.27 \pm 0.21	(0.6, 1.4)
24		WRN16-8	CAL	0.05, 0.1 , 0.15	-	63.67 \pm 0.09	-
25		WRN16-8	SNR	0.1	0.00005, 0.0001 , 0.001	63.98 \pm 0.23	-
26		WRN16-8	TB	0.1	-	64.09 \pm 0.17	(0.6, 1.4)
27		WRN16-8	TB + SNR	0.1	0.0001	64.08 \pm 0.07	(0.6, 1.4)
28		WRN28-6	CAL	0.05 , 0.1, 0.15	-	65.88 \pm 0.20	-
29		WRN28-6	SNR	0.1	0.00005, 0.0001 , 0.001	66.09 \pm 0.25	-
30		WRN28-6	TB	0.1	-	66.58 \pm 0.23	(0.6, 1.4)
31		WRN28-6	TB + SNR	0.1	0.0001	66.79 \pm 0.25	(0.6, 1.4)
32	CIFAR10	ResNet18	CAL	0.05, 0.1 , 0.15	-	95.53 \pm 0.12	-
33		ResNet18	SNR	0.1	0.001 , 0.005, 0.01, 0.015	95.57 \pm 0.06	-
34		ResNet18	TB	0.1	-	95.63 \pm 0.08	(0.5, 1.5)
35		ResNet18	TB + SNR	0.1	0.001	95.66 \pm 0.09	(0.6, 1.4)
36		VGG16	CAL	0.025, 0.05, 0.1	-	93.98 \pm 0.12	-
37		VGG16	SNR	0.05	0.001, 0.005 , 0.01, 0.015	94.04 \pm 0.07	-
38		VGG16	TB	0.05	-	94.14 \pm 0.06	(0.5, 1.5)
39		VGG16	TB + SNR	0.05	0.005	94.26 \pm 0.10	(0.6, 1.4)
40		ResNet18	CAL	0.05, 0.1 , 0.15	-	96.59 \pm 0.08	-
41		ResNet18	SNR	0.1	0.001, 0.005 , 0.015, 0.01	96.65 \pm 0.12	-
42		ResNet18	TB	0.1	-	96.63 \pm 0.06	(0.5, 1.5)
43		ResNet18	TB + SNR	0.1	0.01	96.67 \pm 0.09	(0.6, 1.4)
44	SVHN	VGG16	CAL	0.025, 0.05 , 0.1	-	96.28 \pm 0.04	-
45		VGG16	SNR	0.05	0.001, 0.005, 0.015 , 0.01	96.32 \pm 0.07	-
46		VGG16	TB	0.05	-	96.33 \pm 0.06	(0.5, 1.5)
47		VGG16	TB + SNR	0.05	0.005	96.40 \pm 0.08	(0.6, 1.4)

Table 2: Parameter settings of the experiment reported in Section 4.2 Figure 4. The hyperparameter in bold is the best hyperparameter selection reported in the main paper. The five random seeds for each setting are $\{43, 37, 13, 51, 71\}$, and the means and standard deviations of the test accuracy among the five seeds are reported.

Index	Dataset	Model	Method	Initial learning rate η_0	SGDR (T_0, T_{mut})	Lookahead k	Lookahead α	Test Acc (best hyperparams.)	scaling ratio (s_1, s_2)
0	CIFAR100	ResNet18	CAL	0.05, 0.1 , 0.15	-	-	-	78.31 \pm 0.05	-
1		ResNet18	SGDR	0.05, 0.1 , 0.15	(100,1), (10, 2), (1, 2)	-	-	77.69 \pm 0.20	-
2		ResNet18	LARS	26, 28 , 30, 32, 34	-	-	-	78.44 \pm 0.12	-
3		ResNet18	Lookahead	0.05, 0.1 , 0.15	-	10 , 5	0.8 , 0.5	78.46 \pm 0.18	-
4		ResNet18	SGDP	0.01, 0.05, 0.1 , 0.15, 0.2	-	-	-	78.74 \pm 0.11	-
5		ResNet18	TB	0.05, 0.1 , 0.15	-	-	-	78.97 \pm 0.29	(0.5, 1.5)
6		ResNet18	TB + SGDP	0.05, 0.1 , 0.15	-	-	-	79.13 \pm 0.15	(0.5, 1.5)
7		ResNet34	CAL	0.05 , 0.1, 0.15	-	-	-	78.98 \pm 0.14	-
8		ResNet34	SGDR	0.05, 0.1, 0.15	(100,1), (10, 2), (1, 2)	-	-	78.61 \pm 0.20	-
9		ResNet34	LARS	26, 28, 30, 32 , 34	-	-	-	78.94 \pm 0.19	-
10		ResNet34	Lookahead	0.05, 0.1, 0.15	-	10 , 5	0.8 , 0.5	79.19 \pm 0.12	-
11		ResNet34	SGDP	0.01, 0.05, 0.1 , 0.15, 0.2	-	-	-	79.34 \pm 0.21	-
12		ResNet34	TB	0.05, 0.1 , 0.15	-	-	-	79.89 \pm 0.15	(0.5, 1.5)
13		ResNet34	TB + SGDP	0.05, 0.1 , 0.15	-	-	-	79.94 \pm 0.30	(0.5, 1.5)

Table 3: Parameter settings of the experiment reported in Section 4.3 Figure 5. The five random seeds for each setting are $\{43, 37, 13, 51, 71\}$, and the means and standard deviations of the test accuracy among the five seeds are reported.

Index	Dataset	Model	Method	Initial learning rate η_0		Test Acc	scaling ratio (s_1, s_2)
				0.05, 0.1, 0.15	78.08 \pm 0.19, 78.31 \pm 0.05, 77.72 \pm 0.44		
0	CIFAR100	ResNet18	CAL	0.05, 0.1, 0.15	78.48 \pm 0.27, 78.97 \pm 0.29, 78.69 \pm 0.11	-	(0.5, 1.5)
1		ResNet18	TB	0.05, 0.1, 0.15	78.98 \pm 0.14, 78.89 \pm 0.24, 78.51 \pm 0.34	-	(0.5, 1.5)
2		ResNet34	CAL	0.05, 0.1, 0.15	79.36 \pm 0.18, 79.89 \pm 0.15, 79.09 \pm 0.64	(0.5, 1.5)	-
3		ResNet34	TB	0.025, 0.05, 0.1	73.96 \pm 0.27, 74.59 \pm 0.23, 74.46 \pm 0.12	-	(0.5, 1.5)
4		VGG16	CAL	0.025, 0.05, 0.1	74.40 \pm 0.31, 74.96 \pm 0.15, 74.94 \pm 0.16	(0.5, 1.5)	-
5		VGG16	TB	0.025, 0.05, 0.1	72.57 \pm 0.45, 73.26 \pm 0.37, 72.98 \pm 0.16	-	(0.5, 1.5)
6		VGG19	CAL	0.025, 0.05, 0.1	73.47 \pm 0.16, 73.77 \pm 0.43, 73.40 \pm 0.38	-	(0.5, 1.5)
7		VGG19	TB	0.025, 0.05, 0.1	73.47 \pm 0.16, 73.77 \pm 0.43, 73.40 \pm 0.38	-	(0.5, 1.5)

Table 4: Parameter settings of the experiment reported in Section 4.3 Figure 6. The five random seeds for each setting are $\{43, 37, 13, 51, 71\}$, and the means and standard deviations of the test accuracy among the five seeds are reported.

Index	Dataset	Model	Method	Initial learning rate η_0		Width	Test Acc	scaling ratio (s_1, s_2)
				0.1	256, 512, 768			
0	CIFAR100	ResNet18	CAL	0.1	75.05 \pm 0.26, 78.31 \pm 0.05, 79.44 \pm 0.26	-	-	(0.5, 1.5)
1		ResNet18	TB	0.1	75.63 \pm 0.12, 78.97 \pm 0.29, 80.47 \pm 0.18	-	-	(0.5, 1.5)
2		ResNet34	CAL	0.1	76.79 \pm 0.34, 78.89 \pm 0.24, 79.94 \pm 0.31	-	-	(0.5, 1.5)
3		ResNet34	TB	0.1	77.25 \pm 0.14, 79.89 \pm 0.15, 80.23 \pm 0.53	-	-	(0.5, 1.5)
4		VGG16	CAL	0.05	71.04 \pm 0.14, 74.59 \pm 0.23, 75.53 \pm 0.32	-	-	(0.5, 1.5)
5		VGG16	TB	0.05	71.26 \pm 0.26, 74.96 \pm 0.15, 76.19 \pm 0.14	-	-	(0.5, 1.5)
6		VGG19	CAL	0.05	69.58 \pm 0.39, 73.26 \pm 0.37, 74.39 \pm 0.33	-	-	(0.5, 1.5)
7		VGG19	TB	0.05	69.96 \pm 0.25, 73.77 \pm 0.43, 74.80 \pm 0.35	-	-	(0.5, 1.5)

Table 5: Parameter settings of the experiment reported in Section 4.3 Figure 7. The five random seeds for each setting are $\{43, 37, 13, 51, 71\}$, and the means and standard deviations of the test accuracy among the five seeds are reported.

Index	Dataset	Model	Method	HT-SR Metric	Initial learning rate η_0		Test Acc	scaling ratio (s_1, s_2)
					0.05, 0.1, 0.15	77.83 \pm 0.21, 78.30 \pm 0.32, 78.27 \pm 0.25		
0	CIFAR100	ResNet18	TB	SpectralNorm	0.05, 0.1, 0.15	78.18 \pm 0.27, 78.67 \pm 0.17, 78.48 \pm 0.24	-	(0.5, 1.5)
1		ResNet18	TB	AlphaWeighted	0.05, 0.1, 0.15	78.48 \pm 0.27, 78.97 \pm 0.29, 78.69 \pm 0.11	-	(0.5, 1.5)
2		ResNet18	TB	PL_Alpha_Hill	0.05, 0.1, 0.15	78.25 \pm 0.16, 78.71 \pm 0.15, 78.92 \pm 0.28	-	(0.5, 1.5)
3		ResNet34	TB	SpectralNorm	0.05, 0.1, 0.15	78.36 \pm 0.39, 78.87 \pm 0.34, 78.83 \pm 0.23	-	(0.5, 1.5)
3		ResNet34	TB	AlphaWeighted	0.05, 0.1, 0.15	79.36 \pm 0.18, 79.89 \pm 0.15, 79.09 \pm 0.64	-	(0.5, 1.5)
3		ResNet34	TB	PL_Alpha_Hill	0.05, 0.1, 0.15	73.58 \pm 0.19, 74.29 \pm 0.16, 74.17 \pm 0.28	-	(0.5, 1.5)
4		VGG16	TB	SpectralNorm	0.025, 0.05, 0.1	73.97 \pm 0.22, 74.19 \pm 0.11, 74.42 \pm 0.31	-	(0.5, 1.5)
5		VGG16	TB	AlphaWeighted	0.025, 0.05, 0.1	74.40 \pm 0.31, 74.96 \pm 0.15, 74.94 \pm 0.16	-	(0.5, 1.5)
5		VGG16	TB	PL_Alpha_Hill	0.025, 0.05, 0.1	72.34 \pm 0.26, 72.91 \pm 0.35, 73.04 \pm 0.39	-	(0.5, 1.5)
6		VGG19	TB	SpectralNorm	0.025, 0.05, 0.1	72.85 \pm 0.16, 73.41 \pm 0.17, 73.33 \pm 0.21	-	(0.5, 1.5)
7		VGG19	TB	AlphaWeighted	0.025, 0.05, 0.1	73.47 \pm 0.16, 73.77 \pm 0.43, 73.40 \pm 0.38	-	(0.5, 1.5)

Table 6: Parameter settings of the experiment reported in Section 4.3 Figure 8. The five random seeds for each setting are $\{43, 37, 13, 51, 71\}$, and the means and standard deviations of the test accuracy among the five seeds, the means and standard deviations of the computation time of using TB among the 10 times are reported.

Index	Dataset	Model	Method	PL fitting method	Initial learning rate η_0		Test Acc	Computation Time (sec)	scaling ratio (s_1, s_2)
					0.1	78.59 \pm 0.21			
0	CIFAR100	ResNet18	TB	Goodness-of-fit	0.1	79.06 \pm 0.22	8.20 \pm 0.53	8.20 \pm 0.53	(0.5, 1.5)
1		ResNet18	TB	Fix-finger	0.1	79.97 \pm 0.22	7.24 \pm 0.74	7.24 \pm 0.74	(0.5, 1.5)
1		ResNet18	TB	Median	0.1	78.97 \pm 0.29	1.14 \pm 0.04	1.14 \pm 0.04	(0.5, 1.5)
2		ResNet34	TB	Goodness-of-fit	0.1	79.13 \pm 0.21	16.45 \pm 0.48	16.45 \pm 0.48	(0.5, 1.5)
3		ResNet34	TB	Fix-finger	0.1	79.64 \pm 0.22	15.13 \pm 1.05	15.13 \pm 1.05	(0.5, 1.5)
3		ResNet34	TB	Median	0.1	79.89 \pm 0.15	2.27 \pm 0.06	2.27 \pm 0.06	(0.5, 1.5)
4		VGG16	TB	Goodness-of-fit	0.05	74.46 \pm 0.24	8.54 \pm 0.10	8.54 \pm 0.10	(0.5, 1.5)
5		VGG16	TB	Fix-finger	0.05	74.48 \pm 0.20	8.45 \pm 0.59	8.45 \pm 0.59	(0.5, 1.5)
5		VGG16	TB	Median	0.05	74.96 \pm 0.15	1.37 \pm 0.05	1.37 \pm 0.05	(0.5, 1.5)
6		VGG19	TB	Goodness-of-fit	0.05	73.36 \pm 0.16	11.48 \pm 0.15	11.48 \pm 0.15	(0.5, 1.5)
7		VGG19	TB	Fix-finger	0.05	73.52 \pm 0.16	11.15 \pm 0.79	11.15 \pm 0.79	(0.5, 1.5)
7		VGG19	TB	Median	0.05	73.77 \pm 0.43	1.85 \pm 0.05	1.85 \pm 0.05	(0.5, 1.5)

E Comparison with more baselines

In Figure 17, we provide additional results by comparing TempBalance with LAMB and Adam. We found that our method outperforms both baseline methods. Furthermore, we also found that the Adam-based methods do not provide better results than the SGD baseline with cosine annealing (CAL) in our experiment setting, which was mentioned in Section 4.2. For Adam, we searched the initial learning rate over $\{0.00005, 0.0001, 0.001, 0.01, 0.1\}$, and we used $\epsilon = 10^{-8}$. For LAMB, we searched the initial learning rate over $\{0.005, 0.01, 0.02\}$, and we used $\epsilon = 10^{-6}$. Both methods used weight decay 5.0×10^{-4} , $\beta_1 = 0.9$, $\beta_2 = 0.999$, learning rate decay with cosine annealing. Each experiment was conducted with five random seeds.

We also discuss the difference between TempBalance and these two types of learning rate scheduling.

- **Compared to layer-wise learning rate scheduling (e.g., LARS):** TempBalance uses a more precise model quality metric, PL_Alpha_Hill from HT-SR Theory, to enhance the performance of deep models during training. This “shape-based” metric estimates the shape of the eigenspectrum of weight matrices. In contrast, LARS uses a “norm-based” metric, such as the layer-wise gradient norm. A recent study in HT-SR [22] has shown that the shape-based metrics surpasses norm-based ones in assessing model quality and performance. Figure 3 confirms that our method outperforms the layer-wise scheduler LARS in test accuracy.
- **Compared to parameter-wise learning rate scheduling (e.g., Adam):** Similarly, our method employs the “shape-based” metric PL_Alpha_Hill to improve the generalization, an approach not incorporated in traditional parameter-wise methods.

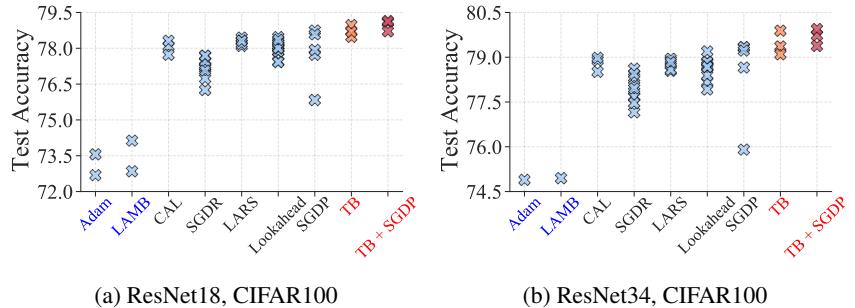


Figure 17: **(Comparison with additional baselines).** Comparing our method, TempBalance (TB), with other baselines such as parameter-wise learning rate schedulers Adam and LAMB, using ResNet18/34 trained on CIFAR100. Each cross represents the mean test accuracy of five random seeds.

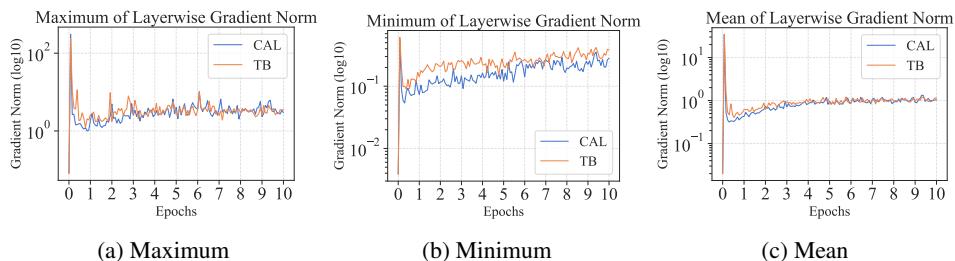


Figure 18: **(Layerwise gradient norm during training).** From left to right: maximum, minimum, and mean of the layerwise gradient norm at every 30 iterations for the first 10 epochs. ResNet18 on CIFAR-100.

F Does addressing other training issues lead to TempBalance’s improvement?

We discuss whether the improvement from the proposed method, TempBalance, is due to indirectly addressing another fundamental training issue that could distort the ESD, specifically the gradient

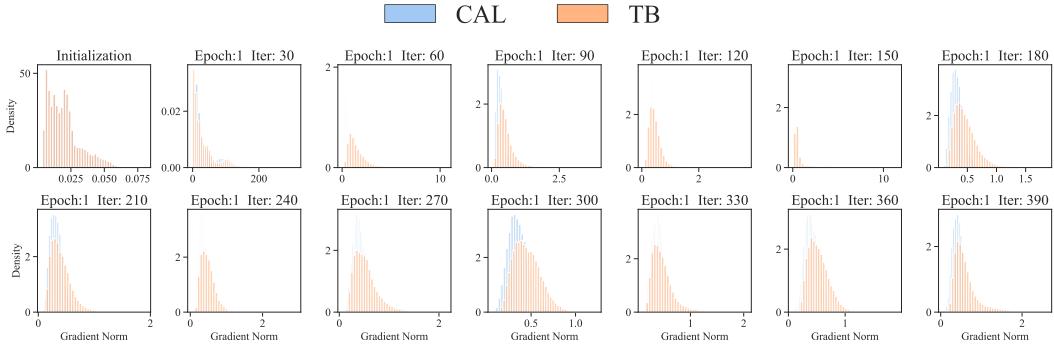


Figure 19: **(Histogram of gradient norm distribution during first epoch).** ResNet18 on CIFAR-100.

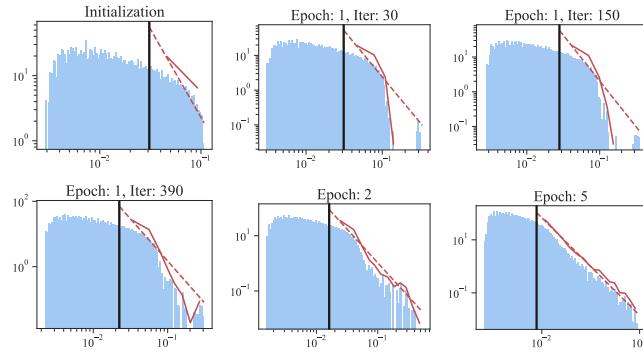


Figure 20: **(Impact of large rank-1 updates on ESD).** Large rank-1 updates result in the spikes of ESD, observed exclusively during the first epoch. From the second epoch onward, the ESD exhibits a heavy-tailed distribution. ResNet18 on CIFAR-100.

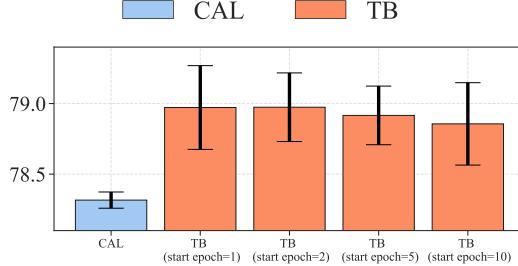


Figure 21: **(Varying the starting epoch of applying TempBalance (TB)).** Postponing the usage of TempBalance to Epochs 2, 5, and 10 doesn't affect the performance of TempBalance (originally starting from Epoch 1).

magnitude excursions [80] (explosion/vanishing). This discussion further strengthens the connection between our method and the HT structure, as discussed in the Sections 1, A, and B.

We first summarize the questions and the corresponding primary findings, with subsequent detailing of our experiment and supporting results.

- **Does gradient excursion exist?** We discovered that gradient explosion does exist, but it is confined to the first epoch out of a total of 200 training epochs, leading us to believe it does not significantly impact the test accuracy. We observed no gradient vanishing.
- **Does the observed gradient explosion impact the estimation of PL_Alpha_Hill?** We discovered that the large rank-1 updates resulting from the gradient explosion do indeed

affect the ESD as well as the PL_Alpha_Hill estimation. However, this effect is again restricted to the first epoch.

- **Does TempBalance boil down to addressing gradient explosion?** We found that postponing the use of TempBalance until the epoch when neither the gradient explosion nor the PL_Alpha_Hill estimation is affected does not compromise the test accuracy.

To support the above answers, we conducted three experiments. We discuss the setup of these experiments first and then analyze the results.

- (Figures 18, 19) We aim to detect gradient excursion by tracking the gradient norm across layers during training. We examine the model every 30 iterations over the first 10 epochs, calculating the L_2 norm of each gradient update across layers using the training batches of size 128. This produces an empirical gradient norm distribution with a total sample size of update numbers \times layer numbers. Figure 18 presents the maximum/minimum/mean of the distribution, while Figure 19 visualizes these distributions for several iterations of Epoch 1.
- (Figure 20) We aim to assess the impact of gradient explosion on PL_Alpha_Hill estimation by monitoring the ESD. Figure 20 examines the change of the ESD of a single weight matrix over several iterations, tracked in the experiment depicted in Figures 18 and 19.
- (Figure 21) We aim to see if TempBalance enhances generalization by implicitly addressing gradient explosion. Since the gradient explosion and its effect on PL_Alpha_Hill estimation only transpire in the first epoch, we postpone the starting epoch of TempBalance to Epochs 2, 5, and 10 and see if it affects the test accuracy.

Our answers to the above questions are supported by the results obtained from the three experiments:

- **First question (Figure 18 and 19):** We observed that the notable exploding gradients only occur in the initial 200 iterations of the first epoch. In Figure 18, we pinpoint a singular peak of maximum gradient norm within the first epoch. This aligns with the abnormal distribution with a large gradient norm in the subfigure of Figure 19 titled “Epoch 1, iteration 30.”
- **Second question (Figure 20):** Note that large rank-one updates have been studied in random matrix theory, which manifests as a “bulk+spike” pattern. This has been analyzed in, e.g., Theorem 2.13 of [94]. Figure 20 shows this “bulk+spike” pattern, but only in the first epoch. The ESD exhibits a heavy-tail distribution in subsequent epochs, suggesting the influence of rank-one updates is limited.
- **Third question (Figure 21):** Delaying the application of TempBalance until after the first epoch does not adversely affect the test accuracy. Figure 21 illustrates that applying TempBalance from Epochs 2, 5, and 10 results in test performance comparable to when TempBalance is applied from Epoch 1. Since the gradient explosion only occurs in the first epoch and its effect on PL_Alpha_Hill estimation diminishes after this, the effectiveness of TempBalance does not rely on addressing gradient explosion or biased PL_Alpha_Hill estimation from large rank-one updates.
- **Third question:** We compare TempBalance with the baseline method LARS, which uses gradient norms to determine layer-wise learning rates in combating gradient vanishing/explosion issues. As illustrated in Figure 4, TempBalance outperforms LARS in terms of generalization performance.

G Corroborating results on other tasks

We provide corroborating results of applying TempBalance to two different tasks: object detection (OD) and language modeling (LM). In both tasks, TempBalance consistently improves generalization, outperforming the baseline scheduler cosine annealing (CAL) when both are combined with Adam/AdamW optimizers.

For OD, we studied the PASCAL VOC2007 [95] dataset with YOLO series [96] pre-trained model. We compared TempBalance with the baseline scheduler CAL with both applied to Adam/AdamW optimizer. For both scheduler methods, we trained for 200 epochs with batch size 64, and we set the same hyperparameter for the optimizers: $\beta_1 = 0.9$, $\beta_2 = 0.999$, $\epsilon = 10^{-8}$, weight decay = 5.0×10^{-4} . We searched the initial learning rate for all methods among $\{7.5 \times 10^{-6}, 1 \times 10^{-5}, 2.5 \times 10^{-5}\}$. For metrics we use the COCO [97] version mean Average Precision (mAP, higher is better), which is calculated for 10 IOUs varying in a range of 0.5 to 0.95 with steps of 0.05. We

report the mean of mAP over five random seeds on the test set. We set the scaling factors (s_1, s_2) of TempBalance to be $(0.6, 1.4)$.

Here are the experimental settings for LM. We studied the Penn Treebank (PTB) dataset [98] using a three-layer “tensorized transformer core-1” [99]. We compared TempBalance with the baseline scheduler CAL with both applied to Adam optimizer. For both scheduler methods, we trained the models for 40K iterations with a batch size of 120, and a dropout rate of 0.3. We searched the initial learning rate for baseline methods among $\{1.25 \times 10^{-4}, 2.5 \times 10^{-4}, 5 \times 10^{-4}, 1 \times 10^{-3}, 1.25 \times 10^{-3}, 2.5 \times 10^{-3}, 5 \times 10^{-3}\}$ for baseline CAL. The hyperparameters for Adam are $\beta_1 = 0.9, \beta_2 = 0.999, \epsilon = 10^{-8}$. The mean of perplexity (PPL, lower is better) across five random seeds on the test set is reported. We observed improved performance of TempBalance in this task when extending our hyperparameter search to include the scaling factors $(s_1, s_2) \in \{(0.5, 1.5), (1.0, 2.0)\}$, the power-law fitting hyperparameter λ_{\min} index $k \in \{\frac{n}{2}, \frac{n}{1.25}\}$, and the TempBalance update interval over $\{10, 25, 50\}$ iterations.

Table 7: (a) Object Detection (OD): mean Average Precision (mAP) on PASCAL VOC 2007 using model Yolov8n. (b) Language Modeling (LM): test perplexity (PPL) on Penn TreeBank (PTB) using the tensorized transformer. TempBalance (TB) consistently outperforms the CAL in different tasks.

CAL + Adam	TB + Adam	CAL + AdamW	TB + AdamW	CAL + Adam	TB + Adam
59.59	60.03 (+0.44)	59.68	59.96 (+0.28)	49.94	47.30 (-2.64)

(a) OD, VOC2007, mAP (\uparrow)

(b) LM, PTB, PPL (\downarrow)

We present additional results in Figure 22, showing the application of our method TempBalance to ResNet 101 on CIFAR-100, and we compare it with the baseline (CAL). We searched the initial learning rate among $\{0.05, 0.1, 0.15\}$ for both the baseline and our method. The results report the mean and standard deviation across five seeds. We found that TempBalance offers improvements for the larger ResNet101 model comparable to those observed for ResNet18/34, demonstrating its potential for larger models.

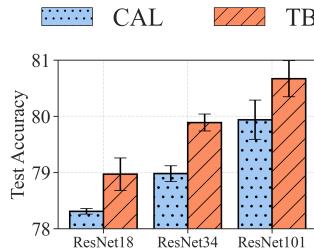


Figure 22: **(Applying the TempBalance (TB) to different sizes of ResNets).** TempBalance consistently outperforms the baseline CAL method in the larger model ResNet101. The dataset is CIFAR100. Reporting mean/std over five random seeds.

H Analysis of computation overhead

We conducted a study on the computational overhead of TempBalance, demonstrating that our method is both applicable and scalable for large models. To do so, we conducted a scaling experiment to demonstrate that the computational cost remains low for different sizes of models. We recorded the duration of a single training epoch and the time taken to apply our method once. From this, we calculated the percentage increase in time when using TempBalance once per epoch, using this as an indicator of computational overhead. The experiment setup is based on ResNet-series on CIFAR100. We studied models of depth in $\{18, 34, 50, 101\}$ and ResNet18 models of width in $\{512, 768, 1024, 2048\}$. We report the mean and the standard deviation of the results over 10 runs. The test platform was one Quadro RTX 6000 GPU with Intel Xeon Gold 6248 CPU. The results are presented in Figure 23. Our findings reveal that the computational overhead remains low (less than 9%) even when applied to exceptionally wide or deep models (ResNet18 with width 2048 or ResNet101). The

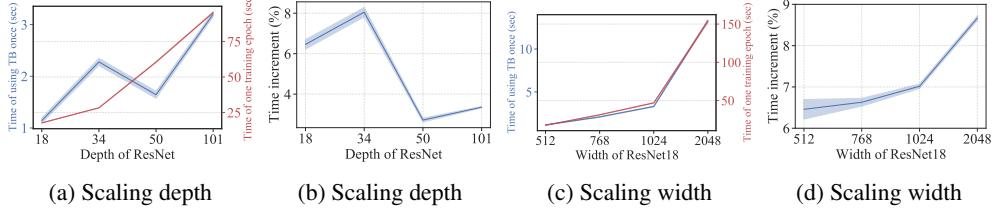


Figure 23: **(Computation overhead of TempBalance (TB) in scaling the model depth/width).** (a)(c) Time duration (second) of one training epoch (blue) and using TempBalance once (red). (b)(d) Time increment of using TempBalance once per epoch. The dataset is CIFAR100, reporting mean/std over 10 epochs. The computational overhead of using TempBalance remains low (less than 9%) even when applied to exceptionally wide or deep models.

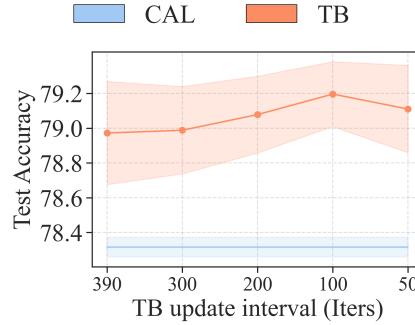


Figure 24: **(Varying the TempBalance (TB) update interval).** Reducing the update interval from 390 iters (used in the paper) brings mild improvement in test accuracy. Both use ResNet18 on CIFAR100. Reporting mean/std over five random seeds.

computation overhead is not large because: 1) we select the efficient PL fitting method to obtain PL_Alpha_Hill, which is demonstrated in Figure 8; and 2) the most computation-intensive part of our method is SVD decomposition, which we have optimized using GPU implementation and batch processing.

We conducted an experiment on reducing the update interval of the learning rate schedule to see if it affects the test accuracy of TempBalance. Figure 24 shows the experiments conducted with ResNet18 on CIFAR-100. We reduce the update interval from 390 iterations used in our paper (equivalent to one epoch) to 300, 200, 100, and 50. We observed that there indeed exists a trade-off between the computation time and test accuracy, but reducing the update interval only brings mild improvement.