EFFICIENT SHARPNESS-AWARE MINIMIZATION FOR IMPROVED TRAINING OF NEURAL NETWORKS

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ABSTRACT

Overparametrized Deep Neural Networks (DNNs) often achieve astounding performances, but may potentially result in severe generalization error. Recently, the relation between the sharpness of the loss landscape and the generalization error has been established by Foret et al. (2020), in which the Sharpness Aware Minimizer (SAM) was proposed to mitigate the degradation of the generalization. Unfortunately, SAM's computational cost is roughly double that of base optimizers, such as Stochastic Gradient Descent (SGD). This paper thus proposes *Efficient Sharpness Aware Minimizer* (ESAM), which boosts SAM's efficiency at no cost to its generalization performance. ESAM includes two novel and efficient training strategies—Stochastic Weight Perturbation and Sharpness-Sensitive Data Selection. In the former, the sharpness measure is approximated by perturbing a stochastically chosen set of weights in each iteration; in the latter, the SAM loss is optimized using only a judiciously selected subset of data that is sensitive to the sharpness. We provide theoretical explanations as to why these strategies perform well. We also show, via extensive experiments on the CIFAR and ImageNet datasets, that ESAM enhances the efficiency over SAM from requiring 100% extra computational overhead to 40% vis-à-vis base optimizers, while test accuracies are preserved or even improved.

1 INTRODUCTION

Deep learning has achieved astounding performances in many fields by relying on larger numbers of parameters and increasingly sophisticated optimization algorithms. However, DNNs with far more parameters than training samples are more prone to poor generalization. Generalization is arguably the most fundamental and yet mysterious aspect of deep learning.

Several studies have been conducted to better understand the generalization of DNNs and to train DNNs that generalize well across the natural distribution (Keskar et al., 2016; Neyshabur et al., 2017; Chaudhari et al., 2019; Zhang et al., 2019; Wu et al., 2020; Foret et al., 2020; Zhang et al., 2021). For example, Keskar et al. (2016) investigate the effect of batch size on neural networks' generalization ability. Zhang et al. (2019) propose an optimizer for training DNNs with improved generalization ability. Specifically, Hochreiter & Schmidhuber (1995), Li et al. (2017) and Dinh et al. (2017) argue that the geometry of the loss landscape affects generalization and DNNs with a flat minimum can generalize better.

The recent work by Foret et al. (2020) proposes an effective training algorithm *Sharpness Aware Minimizer (SAM)* for obtaining a flat minimum. SAM employs a base optimizer such as Stochastic Gradient Descent (Nesterov, 1983) or Adam (Kingma & Ba, 2014) to minimize both the vanilla training loss and the sharpness. The sharpness, which describes the flatness of a minimum, is characterized using eigenvalues of the Hessian matrix by Keskar et al. (2016). SAM quantifies the sharpness as the maximized change of training loss when a constraint perturbation is added to current weights. As a result, SAM leads to a flat minimum and significantly improves the generalization ability of the trained DNNs. SAM and its variants have been shown to outperform the state-of-the-art across a variety of deep learning benchmarks (Kwon et al., 2021; Chen et al., 2021; Galatolo et al., 2021; Zheng et al., 2021). Regrettably though, SAM and its variants achieve such remarkable performance at the expense of doubling the computational overhead of the given base optimizers, which minimize the training loss with a single forward and backward propagation step. SAM requires an

additional propagation step compared to the base optimizers to resolve the weight perturbation for quantifying the sharpness. The extra propagation step requires the same computational overhead as the single propagation step used by base optimizers, resulting in SAM's computational overhead being *doubled* (2×). As demonstrated in Figure 1, SAM achieves higher test accuracy (i.e., 84.46% vs. 81.89%) at the expense of sacrificing half of the training speed of the base optimizer (i.e., 276 imgs/s vs. 557 imgs/s).

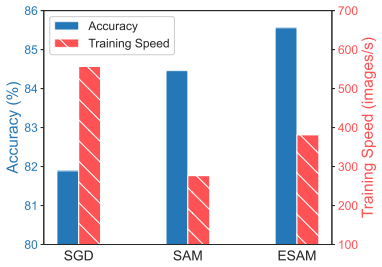

Figure 1: Training Speed vs. Accuracy of SGD, SAM and ESAM evaluated by PyramidNet on CIFAR100. ESAM improves the efficiency with better accuracy compared to SAM.

In this paper, we aim to improve the efficiency of SAM but preserve its superior performance in generalization. We propose *Efficient Sharpness Aware Minimizer (ESAM)*, which consists of two training strategies *Stochastic Weight Perturbation (SWP)* and *Sharpness-sensitive Data Selection (SDS)*, both of which reduce computational overhead and preserve the performance of SAM. On the one hand, SWP approximates the sharpness by searching weight perturbation within a stochastically chosen neighborhood of the current weights. SWP preserves the performance by ensuring that the expected weight perturbation is identical to that solved by SAM. On the other hand, SDS improves efficiency by approximately optimizing weights based on the sharpness-sensitive subsets of batches. These subsets consist of samples whose loss values increase most w.r.t. the weight perturbation and consequently can better quantify the sharpness of DNNs. As a result, the sharpness calculated over the subsets can serve as an upper bound of the SAM's sharpness, ensuring that SDS's performance is comparable to that of SAM's.

We verify the effectiveness of ESAM on the CIFAR10, CIFAR100 (Krizhevsky et al., 2009) and ImageNet (Deng et al., 2009) datasets with five different DNN architectures. The experimental results demonstrate that ESAM obtains flat minima at a cost of only 40% (vs. SAM's 100%) extra computational overhead over base optimizers. More importantly, ESAM achieves better performance in terms of the test accuracy compared to SAM. In a nutshell, our contributions are as follows:

- We propose two novel and effective training strategies *Stochastic Weight Perturbation (SWP)* and *Sharpness-sensitive Data Selection (SDS)*. Both strategies are designed to improve efficiency without sacrificing performance. The empirical results demonstrate that both of the proposed strategies can improve both the efficiency and effectiveness of SAM.
- We introduce the ESAM, which integrates SWP and SDS. ESAM improves the generalization ability of DNNs with marginally additional computational cost compared to standard training.

The rest of this paper is structured in this way. Section 2.1 introduces SAM and its computational issues. Section 2.2 and Section 2.3 discuss how the two proposed training strategies SWP and SDS are designed respectively. Section 3 verifies the effectiveness of ESAM across a variety of datasets and DNN architectures. Section 4 presents the related work and Section 5 concludes this paper.

2 Methodology

We start with recapitulating how SAM achieves a flat minimum with small sharpness, which is quantified by resolving a maximization problem. To compute the sharpness, SAM requires additional forward and backward propagation and results in the doubling of the computational overhead compared to base optimizers. Following that, we demonstrate how we derive and propose ESAM, which integrates SWP and SDS, to maximize efficiency while maintaining the performance. We introduce SWP and SDS in Sections 2.2 and 2.3 respectively. Algorithm 1 shows the overall proposed ESAM algorithm.

Throughout this paper, we denote a neural network f with weight parameters θ as f_θ. The weights are contained in the vector $\theta = (\theta_1, \theta_2, \dots, \theta_N)$, where N is the number of weight units in the neural network. Given a training dataset $\mathbb{S}$ that contains samples i.i.d. drawn from a distribution $\mathcal{D}$,

Algorithm 1 Efficient SAM (ESAM)

Input: Network f_θ, $\theta = (\theta_1, \theta_2, \ldots, \theta_N)$, Training set $\mathbb{S}$, Batch size b, Learning rate $\eta > 0$, Neighborhood size $\rho > 0$, Iterations A, SWP hyperparameter β, SDS hyperparameter γ.
Output: A flat minimum solution $\hat{\theta}$.

```
for a = 1 to A do
    Sample a mini-batch B ⊂ S with size b.
    for n = 1 to N do
        if θ_n is chosen by probability β then
            ε_n ← (ρ/(1−β)) ∇_{θ_n} L_B(f_θ)                    ▷ SWP in B_1
        else
            ε_n ← 0
        ε̂ ← (ε_1, ..., ε_N)                                     ▷ Assign Weight Perturbation
        Compute ℓ(f_{θ+ε̂}, x_i, y_i) and construct B^+ with selection ratio γ (Equation 6)
        Compute gradients g = ∇_θ L_{B^+}(f_{θ+ε̂})              ▷ SDS in B_2
        Update weights θ ← θ − ηg
```

the network is trained to obtain optimal weights $\hat{\theta}$ via *empirical risk minimization* (ERM), i.e.,

$$\hat{\theta} = \arg\min_{\theta} \left\{ L_{\mathbb{S}}(f_\theta) = \frac{1}{|\mathbb{S}|} \sum_{(x_i, y_i) \in \mathbb{S}} \ell(f_\theta, x_i, y_i) \right\} \tag{1}$$

where ℓ can be an arbitrary loss function. We take ℓ to be the cross entropy loss in this paper. The *population loss* is defined as $L_{\mathcal{D}}(f_\theta) \triangleq \mathbb{E}_{(x_i, y_i) \sim \mathcal{D}}(\ell(f_\theta, x_i, y_i))$. In each training iteration, optimizers sample a mini-batch $\mathbb{B} \subset \mathbb{S}$ with size b to update parameters.

2.1 Sharpness-aware minimization and its computational drawback

To improve the generalization capability of DNNs, Foret et al. (2020) proposed the SAM training strategy for searching flat minima. SAM trains DNNs by solving the following min-max optimization problem,

$$\min_{\theta} \max_{\epsilon : \|\epsilon\|_2 \leq \rho} L_{\mathbb{S}}(f_{\theta+\epsilon}). \tag{2}$$

Given θ, the inner optimization attempts to find a weight perturbation ϵ in Euclidean ball with radius ρ that maximizes the empirical loss. The maximized loss at weights θ is the sum of the empirical loss and the sharpness, which is defined to be $R_{\mathbb{S}}(f_\theta) = \max_{\epsilon : \|\epsilon\|_2 < \rho} [L_{\mathbb{S}}(f_{\theta+\epsilon}) - L_{\mathbb{S}}(f_\theta)]$. This sharpness is quantified by the maximal change of empirical loss when a constraint perturbation ϵ is added to θ. The min-max problem encourages SAM to find flat minima.

For a certain set of weights θ, Foret et al. (2020) theoretically justifies that the population loss of DNNs can be upper-bounded by the sum of sharpness, empirical loss, and a regularization term on the norm of weights (refer to Equation 3). Thus, by minimizing the sharpness together with the empirical loss, SAM produces optimized solutions for DNNs with flat minima, and the resultant models can thus generalize better (Foret et al., 2020; Chen et al., 2021; Kwon et al., 2021).

$$L_{\mathcal{D}}(f_\theta) \leq R_{\mathbb{S}}(f_\theta) + L_{\mathbb{S}}(f_\theta) + \lambda \|\theta\|_2^2 = \max_{\epsilon : \|\epsilon\|_2 \leq \rho} L_{\mathbb{S}}(f_{\theta+\epsilon}) + \lambda \|\theta\|_2^2 \tag{3}$$

In practice, SAM first approximately solves the inner optimization by means of a single-step gradient descent method, i.e.,

$$\hat{\epsilon} = \arg\max_{\epsilon : \|\epsilon\|_2 < \rho} L_{\mathbb{S}}(f_{\theta+\epsilon}) \approx \rho \nabla_\theta L_{\mathbb{S}}(f_\theta). \tag{4}$$

The sharpness at weights θ is approximated by $R_{\mathbb{S}}(f_\theta) = L_{\mathbb{S}}(f_{\theta+\hat{\epsilon}}) - L_{\mathbb{S}}(f_\theta)$. Then, a base optimizer, such as SGD (Nesterov, 1983) or Adam (Kingma & Ba, 2014), updates the DNNs' weights to minimize $L_{\mathbb{S}}(f_{\theta+\hat{\epsilon}})$. We refer to $L_{\mathbb{S}}(f_{\theta+\hat{\epsilon}})$ as the *SAM loss*. Overall, SAM requires two forward and two backward operations to update weights once. We refer to the forward and backward propagation for approximating $\hat{\epsilon}$ as F_1 and B_1 and those for updating weights by base optimizers as F_2 and B_2

respectively. Although SAM can effectively improve the generalization of DNNs, it additionally requires one forward and one backward operation (F_1 and B_1) in each training iteration. Thus, SAM results in a *doubling* of the computational overhead compared to the use of base optimizers.

To improve the efficiency of SAM, we propose ESAM, which consists of two strategies—SWP and SDS, to accelerate the sharpness approximation phase and the weight updating phase. Specifically, on the one hand, when estimating $\hat{\epsilon}$ around weight vector θ, SWP efficiently approximates $\hat{\epsilon}$ by randomly selecting each parameter with a given probability to form a subset of weights to be perturbed. The reduction of the number of perturbed parameters results in lower computational overhead during the backward propagation. SWP rescales the resultant weight perturbation so as to assure that the expected weight perturbation equals to $\hat{\epsilon}$, and the generalization capability thus will not be significantly degraded. On the other hand, when updating weights via base optimizers, instead of computing the upper bound $L_{\mathbb{B}}(f_{\theta+\hat{\epsilon}})$ over a whole batch of samples, SDS selects a *subset* of samples, $\mathbb{B}^+$, whose loss values increase the most with respect to the perturbation $\hat{\epsilon}$. Optimizing the weights based on a fewer number of samples decreases the computational overhead (in a linear fashion). We further justify that $L_{\mathbb{B}}(f_{\theta+\hat{\epsilon}})$ can be upper bounded by $L_{\mathbb{B}^+}(f_{\theta+\hat{\epsilon}})$ and consequently the generalization capability can be preserved. In general, ESAM works much more efficiently and performs as well as SAM in terms of its generalization capability.

2.2 Stochastic Weight Perturbation

This section elaborates on the first efficiency enhancement strategy, SWP, and explains why SWP can effectively reduce computational overhead while preserving the generalization capability.

To efficiently approximate $\hat{\epsilon}(\theta, \mathbb{S})$ during the sharpness estimation phase, SWP randomly chooses a subset $\tilde{\theta} = \{\theta_{I_1}, \theta_{I_2}, \ldots\}$ from the original set of weights $\theta = (\theta_1, \ldots, \theta_N)$ to perform backpropagation B_1. Each parameter is selected to be in the subvector $\tilde{\theta}$ with some probability β, which can be tuned as a hyperparameter. SWP approximates the weight perturbation with $\rho \nabla_{\tilde{\theta}} L_{\mathbb{S}}(f_\theta)$. To be formal, we introduce a *gradient mask* $\mathbf{m} = (m_1, \ldots, m_N)$ where $m_i \overset{\text{i.i.d.}}{\sim} \text{Bern}(\beta)$ for all $i \in \{1, \ldots, N\}$. Then, we have $\rho \nabla_{\tilde{\theta}} L_{\mathbb{S}}(f_\theta) = \mathbf{m}^\top \hat{\epsilon}(\theta, \mathbb{B})$. To ensure the expected weight perturbation of SWP equals to $\hat{\epsilon}$, we scale $\rho \nabla_{\tilde{\theta}} L_{\mathbb{S}}(f_\theta)$ by a factor of $\frac{1}{1-\beta}$. Finally, SWP produces an approximate solution of the inner maximization as

$$\boldsymbol{a}(\theta, \mathbb{B}) = \frac{\mathbf{m}^\top \hat{\epsilon}(\theta, \mathbb{B})}{1 - \beta}. \tag{5}$$

Computation Ideally, SWP reduces the overall computational overhead in proportion to $1 - \beta$ in B_1. However, there exists some parameters not included in $\tilde{\theta}$ that are still required to be updated in the backpropagation step. This additional computational overhead is present due to the use of the chain rule, which calculates the entire set of gradients with respect to the parameters along a propagation path. This additional computational overhead slightly increases in deeper neural networks. Thus, the amount of reduction in the computational overhead is positively correlated to $1 - \beta$. Decreasing β can reduce the computational overhead further, but at the performance may degrade. In practice, β is tuned to maximize SWP's efficiency while maintaining a generalization performance comparable to SAM's.

Generalization We will next argue that SWP's generalization performance can be preserved when compared to SAM by showing that the expected weight perturbation $\boldsymbol{a}(\theta, \mathbb{B})$ of SWP equals to the original SAM's perturbation $\hat{\epsilon}(\theta, \mathbb{B})$ in the sense of the ℓ_2 norm and direction. We denote the expected SWP perturbation by $\bar{\boldsymbol{a}}(\theta, \mathbb{B})$, where

$$\bar{\boldsymbol{a}}(\theta, \mathbb{B})_{[i]} = \mathbb{E}[\boldsymbol{a}(\theta, \mathbb{B})_{[i]}] = \frac{1}{1-\beta} \cdot (1-\beta)\hat{\epsilon}(\theta, \mathbb{B})_{[i]} = \hat{\epsilon}(\theta, \mathbb{B})_{[i]},$$

for $i \in \{1, \ldots, N\}$. Thus, it holds that

$$\|\bar{\boldsymbol{a}}(\theta, \mathbb{B})\|_2 = \|\hat{\epsilon}(\theta, \mathbb{B})\|_2 \quad \text{and} \quad \text{CosSim}\Big(\bar{\boldsymbol{a}}(\theta, \mathbb{B}), \hat{\epsilon}(\theta, \mathbb{B})\Big) = 1,$$

showing that the expected weight perturbation of SWP is the same as that of SAM's.

2.3 Sharpness-sensitive Data Selection

In this section, we introduce the second efficiency enhancement technique, SDS, which reduces computational overhead of SAM linearly as the number of selected samples decreases. We also explain why the generalization capability of SAM is preserved by SDS.

In the sharpness estimation phase, we obtain the approximate solution $\hat{\epsilon}$ of the inner maximization. Perturbing weights along this direction significantly increases the average loss over a batch $\mathbb{B}$. To improve the efficiency but still control the upper bound $L_{\mathbb{B}}(f_{\theta+\hat{\epsilon}})$, we select a subset of samples from the whole batch. The loss values of this subset of samples increase most when the weights are perturbed by $\hat{\epsilon}$. To be specific, SDS splits the mini-batch $\mathbb{B}$ into the following two subsets

$$\begin{aligned} \mathbb{B}^{+} &:= \{(x_i, y_i) \in \mathbb{B} : \ell(f_{\theta+\hat{\epsilon}}, x_i, y_i) - \ell(f_{\theta}, x_i, y_i) > \alpha\}, \\ \mathbb{B}^{-} &:= \{(x_i, y_i) \in \mathbb{B} : \ell(f_{\theta+\hat{\epsilon}}, x_i, y_i) - \ell(f_{\theta}, x_i, y_i) < \alpha\}, \end{aligned} \tag{6}$$

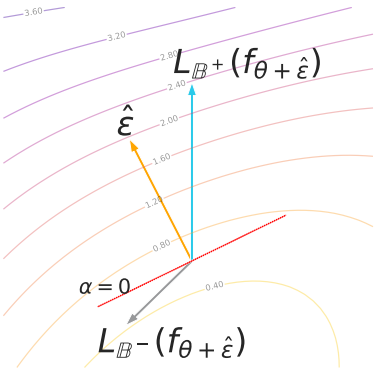

Figure 2: Illustration on the loss changes of samples in $\mathbb{B}^+$ and $\mathbb{B}^-$ along the weight perturbation $\hat{\epsilon}$. The average loss of samples in $\mathbb{B}^+$ increases the most along the perturbation $\hat{\epsilon}$.

where $\mathbb{B}^+$ is termed as the sharpness-sensitive subset and the threshold α controls the size of $\mathbb{B}^+$. We let $\gamma = |\mathbb{B}^+|/|\mathbb{B}|$ be the ratio of the number of selected samples with respect to the batch size. In practice, γ determines the exact value of α and serves as a predefined hyperparameter of SDS. As illustrated in Figure 2, when $\alpha = 0$, the gradient of the weights evaluated on $\mathbb{B}^+$ *aligns* with the direction of $\hat{\epsilon}$ and the loss values of the samples in $\mathbb{B}^+$ will increase with respect to the weight perturbation $\hat{\epsilon}$.

Computation SDS reduces the computational overhead in F_2 and B_2. The reduction is linear in $1 - \gamma$. The hyperparameter γ can be tuned to meet up distinct requirements in efficiency and performance. SDS is configured the same as SWP for maximizing efficiency with comparable performance to SAM.

Generalization For the generalization capability, we now justify that the SAM loss computing over the batch $\mathbb{B}$, $L_{\mathbb{B}}(f_{\theta+\hat{\epsilon}})$, can be approximately upper bounded by the corresponding loss evaluated only on $\mathbb{B}^+$, $L_{\mathbb{B}^+}(f_{\theta+\hat{\epsilon}})$. From Equation 3, we have

$$\begin{aligned} L_{\mathbb{B}}(f_{\theta+\hat{\epsilon}}) &= \gamma L_{\mathbb{B}^+}(f_{\theta+\hat{\epsilon}}) + (1-\gamma) L_{\mathbb{B}^-}(f_{\theta+\hat{\epsilon}}) \\ &= L_{\mathbb{B}^+}(f_{\theta+\hat{\epsilon}}) + (1-\gamma)[R_{\mathbb{B}^-}(f_\theta) - R_{\mathbb{B}^+}(f_\theta) + L_{\mathbb{B}^-}(f_\theta) - L_{\mathbb{B}^+}(f_\theta)]. \end{aligned} \tag{7}$$

On the one hand, since $R_{\mathbb{B}}(f_\theta) = \frac{1}{|\mathbb{B}|}\sum_{(x_i,y_i)\in\mathbb{B}}[\ell(f_{\theta+\hat{\epsilon}}, x_i, y_i) - \ell(f_\theta, x_i, y_i)]$ represents the average sharpness of the batch $\mathbb{B}$, by Equation 6, we have $R_{\mathbb{B}^-}(f_\theta) \leq R_{\mathbb{B}}(f_\theta) \leq R_{\mathbb{B}^+}(f_\theta)$, and

$$R_{\mathbb{B}^-}(f_\theta) - R_{\mathbb{B}^+}(f_\theta) \leq 0. \tag{8}$$

On the other hand, $\mathbb{B}^+$ and $\mathbb{B}^-$ are constructed sorting by $\ell(f_{\theta+\hat{\epsilon}}, x_i, y_i) - \ell(f_\theta, x_i, y_i)$, which is positively correlated to $l(f_\theta, x_i, y_i)$ (Li et al., 2019) (more details can be found in the Appendix A.2). Thus, we have

$$L_{\mathbb{B}^-}(f_\theta) - L_{\mathbb{B}^+}(f_\theta) \leq 0. \tag{9}$$

Therefore, by Equation 8 and Equation 9, we have

$$L_{\mathbb{B}}(f_{\theta+\hat{\epsilon}}) \leq L_{\mathbb{B}^+}(f_{\theta+\hat{\epsilon}}). \tag{10}$$

Experimental results in Figure 5 corroborate that $R_{\mathbb{B}^-}(f_\theta) - R_{\mathbb{B}^+}(f_\theta) < 0$ and $L_{\mathbb{B}^-}(f_\theta) - L_{\mathbb{B}^+}(f_\theta) < 0$. Besides, Figure 6 verifies that the selected batch $\mathbb{B}^+$ is sufficiently representative to mimic the gradients of $\mathbb{B}$ since $\mathbb{B}^+$ has a significantly higher cosine similarity with $\mathbb{B}$ compared to $\mathbb{B}^-$ in terms of the computed gradients. According to Equation 10, one can utilize $L_{\mathbb{B}^+}(f_{\theta+\hat{\epsilon}})$ as a proxy to the real objective to minimize of the overall loss $L_{\mathbb{B}}(f_{\theta+\hat{\epsilon}})$ with a smaller number of samples. As a result, SDS improves SAM's efficiency without performance degradation.

3 EXPERIMENTS

This section demonstrates the effectiveness of our proposed ESAM algorithm. We conduct experiments on several benchmark datasets: CIFAR-10 (Krizhevsky et al., 2009), CIFAR-100 (Krizhevsky et al., 2009) and ImageNet (Deng et al., 2009), using various model architectures: ResNet (He et al., 2016), Wide ResNet (Zagoruyko & Komodakis, 2016), and PyramidNet (Han et al., 2017). We demonstrate the proposed ESAM improves the efficiency of vanilla SAM by speeding up to 40.3% computational overhead with better generalization performance. We report the main results in Table 1 and Table 2. Besides, we perform an ablation study on the two proposed strategies of ESAM (i.e., SWP and SDS). The experimental results in Table 3 and Figure 3 indicate that both strategies improve SAM's efficiency and performance.

3.1 RESULTS

CIFAR10 and CIFAR100 We start from evaluating ESAM on the CIFAR-10 and CIFAR-100 image classification datasets. The evaluation is carried out on three different model architectures: ResNet-18 (He et al., 2016), WideResNet-28-10 (Zagoruyko & Komodakis, 2016) and PyramidNet-110 (Han et al., 2017). We set all the training settings, including the maximum number of training epochs, iterations per epoch, and data augmentations, the same for fair comparison among SGD, SAM and ESAM. Additionally, the other parameters of SGD, SAM and ESAM have been tuned separately for optimal test accuracies using grid search.

We train all the models with 3 different random seeds using a batch size of 128, weight decay 10^{-4} and cosine learning rate decay (Loshchilov & Hutter, 2016). The training epochs are set to be 200 for ResNet-18 (He et al., 2016), WideResNet-28-10 (Zagoruyko & Komodakis, 2016), and 300 for PyramidNet-110 (Han et al., 2017). We set $\beta = 0.6$ and $\gamma = 0.5$ for ResNet-18 and PyramidNet-110 models; and set $\beta = 0.5$ and $\gamma = 0.5$ for WideResNet-28-10. The above-mentioned β and γ are optimal for efficiency with comparable performance compared to SAM. The details of training setting are listed in Appendix A.3. We record the best test accuracies obtained by SGD, SAM and ESAM in Table 1.

The experimental results indicate that our proposed ESAM can increase the training speed by up to 40.30% in comparison with SAM. Concerning the performance, ESAM outperforms SAM in the six sets of experiments. The best efficiency of ESAM is reported in CIFAR10 trained with ResNet-18 (140.3% vs. SAM 100%). The best accuracy is reported in CIFAR100 trained with PyramidNet110 (85.56% vs. SAM 84.46%). ESAM improves efficiency and achieves better performance compared to SAM in CIFAR10/100 benchmarks.

Table 1: Classification accuracies and training speed on the CIFAR-10 and CIFAR-100 datasets. Computational overhead is quantified by #images processed per second (images/s). The numbers in parentheses $(\cdot)$ indicate the ratio of ESAM's training speed w.r.t. SAM.

	CIFAR-10		**CIFAR-100**	
ResNet-18	Accuracy	images/s	Accuracy	images/s
SGD	95.41 ± 0.03	3,387	78.17 ± 0.05	3,483
SAM	96.52 ± 0.13	1,717(100.0%)	80.17 ± 0.17	1,730 (100.0%)
ESAM	**96.56** ± 0.08	2,409 (140.3%)	**80.41** ± 0.10	2,423 (140.0%)
Wide-28-10	Accuracy	images/s	Accuracy	images/s
SGD	96.34 ± 0.12	801	81.56 ± 0.13	792
SAM	97.27 ± 0.11	396 (100.0%)	83.42 ± 0.04	391 (100.0%)
ESAM	**97.29** ± 0.11	550 (138.9%)	**84.51** ± 0.01	545 (139.4%)
PyramidNet-110	Accuracy	images/s	Accuracy	images/s
SGD	96.62 ± 0.10	580	81.89 ± 0.17	555
SAM	97.30 ± 0.10	289 (100.0%)	84.46 ± 0.04	276 (100.0%)
ESAM	**97.81** ± 0.01	401 (138.7%)	**85.56** ± 0.05	381 (137.9%)

ImageNet To evaluate ESAM's effectiveness on a large-scale benchmark dataset, we conduct experiments on ImageNet Datasets.The 1000 class ImageNet dataset contains roughly 1.28 million

Table 2: Classification accuracies and training speed on the ImageNet dataset. The numbers in parentheses (·) indicate the ratio of ESAM's training speed w.r.t. SAM's. Results with * are referred to Chen et al. (2021)

	ResNet-50		**ResNet-101**	
ImageNet	Accuracy	images/s	Accuracy	images/s
SGD	76.00*	1,327	77.80*	891
SAM	76.70*	654 (100.0%)	78.60*	438 (100.0%)
ESAM	77.05	846 (129.3%)	79.09	564 (128.7%)

training images and $50,000$ validation images with 469×387 averaged resolution. The ImageNet dataset is more representative (of real-world scenarios) and persuasive (of a method's effectiveness) than CIFAR datasets. We resize the images on ImageNet to 224×224 resolution to train ResNet-50 and ResNet-110 models. We train 90 epochs and set the optimal hyperparameters for SGD, SAM and ESAM as suggested by Chen et al. (2021), and the details are listed in appendix A. We use $\beta = 0.6$ and $\gamma = 0.7$ for ResNet-50 and ResNet-101. We employ the m-sharpness strategy for both SAM and ESAM with $m = 128$, which is the same as that suggested in Zheng et al. (2021).

The experimental results are reported in Table 2. The results indicate that the performance of ESAM on large-scale datasets is consistent with the two (smaller) CIFAR datasets. ESAM outperforms SAM by 0.35% to 0.49% in accuracy and, more importantly, enjoys 28.7% faster training speed compared to SAM. As the γ we used here is larger than the one used in CIFAR datasets, the training speed of ESAM here is slightly slower than that in the CIFAR datasets.

These experiments demonstrate that ESAM outperforms SAM on a variety of benchmark datasets for widely-used DNNs' architectures in terms of training speed and classification accuracies.

3.2 Ablation and Parameter Studies

To better understand the effectiveness of SWP and SDS in improving the performance and efficiency compared to SAM, we conduct four sets of ablation studies on CIFAR-10 and CIFAR-100 datasets using ResNet-18 and WideResNet-28-10 models, respectively. We consider two variants of ESAM: (i) only with SWP, (ii) only with SDS. The rest of the experimental settings are identical to the settings described in Section 3.1. We conduct grid search over the interval $[0.3, 0.9]$ for β and the interval $[0.3, 0.9]$ for γ, with a same step size of 0.1. We report the grid search results in Figure 3. We use $\beta = 0.6$,$\gamma = 0.5$ for ResNet-18; and set $\beta = 0.5$, $\gamma = 0.5$ for WideResNet-28-10 in the four sets of ablation studies. The ablation study results are reported in Table 3.

Table 3: Ablation Study of ESAM on CIFAR-10 and CIFAR100. The numbers in brackets [·] represent the accuracy improvement in comparison to SGD. The numbers in parentheses (·) indicate the ratio of ESAM's training speed to SAM's. Green color indicates improvement compared to SAM, whereas red color suggests a degradation.

	CIFAR-10		**CIFAR-100**	
ResNet-18	Accuracy	images/s	Accuracy	images/s
SGD	95.41	3,387	78.17	3,438
SAM	96.52 [+1.11]	1,717 (100.0%)	80.17 [+2.00]	1,730 (100.0%)
+ ESAM-SWP	**96.74** [+1.33]	1,896 (110.5%)	**80.53** [+2.36]	1,887 (109.1%)
+ ESAM-SDS	96.45 [+1.04]	2,105 (122.6%)	80.38 [+2.21]	2,103 (121.5%)
ESAM	96.56 [+1.15]	**2,409** (140.3%)	80.41 [+2.24]	**2,423** (140.9%)
Wide-28-10	Accuracy	images/s	Accuracy	images/s
SGD	96.34	801	81.56	792
SAM	97.27 [+0.93]	396 (100.0%)	83.42 [+1.86]	391 (100.0%)
+ ESAM-SWP	**97.37** [+1.03]	430 (108.5%)	84.44 [+2.88]	423 (108.3%)
+ ESAM-SDS	97.24 [+0.90]	495 (124.8%)	84.46 [+2.90]	492 (125.8%)
ESAM	97.29 [+0.95]	**551** (138.9%)	**84.51** [+2.95]	**545** (139.4%)

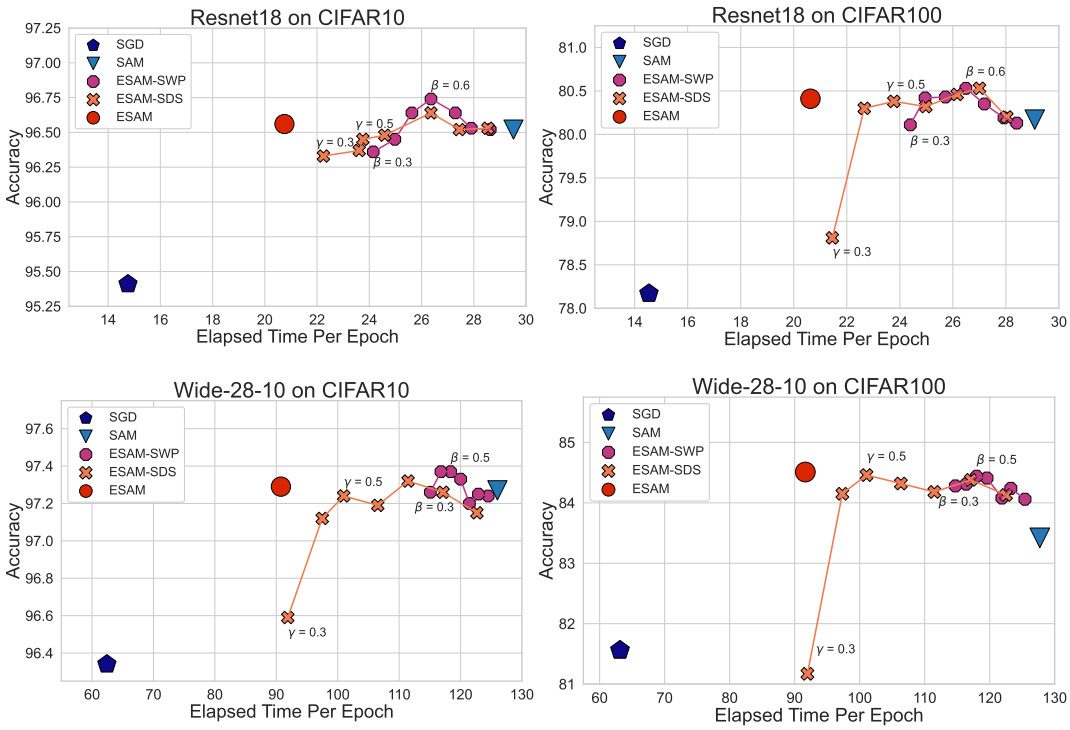

Figure 3: Parameter study of SWP and SDS. The connected dots refer to SWP and SDS with different parameters; the isolated dots refer to the final results of SGD, SAM, and ESAM.

ESAM-SWP As shwon in Table 3, SWP improves SAM's training speed by 8.3% to 10.5%, and achieves better performance at the same time. SWP can further improve the efficiency by using a smaller β. The best performance of SWP is obtained when $\beta = 0.6$ for ResNet-18 and $\beta = 0.5$ for WideResNet-28-10. The four sets of experiments indicate that β is consistent among different architectures and datasets. Therefore, we set $\beta = 0.6$ for PyramidNet in CIFAR10/100 datasets and ResNet on ImageNet datasets.

ESAM-SDS SDS also significantly improves the efficiency by 21.5% to 25.8% compared to SAM. It outperforms SAM's performance in CIFAR100 datasets, and achieves comparable performance in CIFAR10 datasets. SDS can outperform SAM in both datasets with both architectures with little degradation to the efficiency, as demonstrated in Figure 3. Across all experiments, $\gamma = 0.5$ is the smallest value that is optimal for efficiency while maintaining comparable performance to SAM.

Visualization of Loss Landscapes To visualize the sharpness of the flat minima obtained by ESAM, we plot the loss landscapes trained with SGD, SAM and ESAM on the ImageNet dataset. We display the loss landscapes in Figure 4, following the plotting algorithm in Li et al. (2017). The x- and y-axes represent two random sampled orthogonal Gaussian perturbations. We sampled 100×100 points for 10 groups random Gaussian perturbations. The displayed loss landscapes are the results we obtained by averaging over ten groups of random perturbations. It can be clearly seen that both SAM and ESAM improve the sharpness significantly in comparison to SGD.

To summarize, SWP and SDS both reduce the computational overhead and accelerate training compared to SAM. Most importantly, both these strategies achieve a comparable or better performance than SAM. In practice, by configuring the β and γ, ESAM can meet a variety of user-defined efficiency and performance requirements.

4 Related Work

The concept of regularizing sharpness for better generalization dates back to (Hochreiter & Schmidhuber, 1995). By using an MDL-based argument, which clarifies that a statistical model with fewer

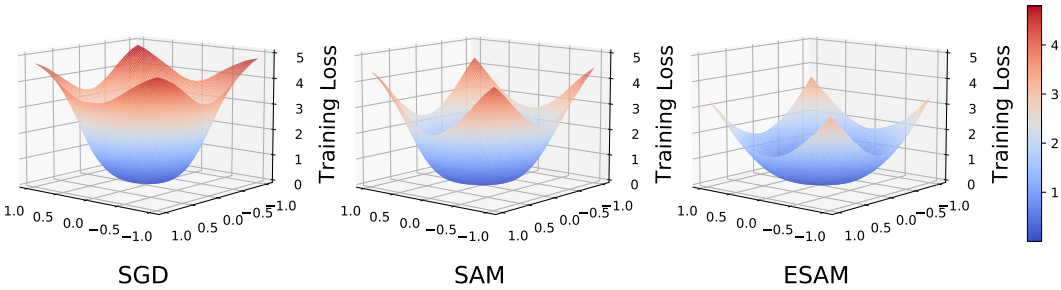

Figure 4: Cross-entropy loss landscapes of the ResNet50 model on the ImageNet dataset trained with SGD, SAM, and ESAM.

bits to describe can have better generalization ability, Hochreiter & Schmidhuber (1995) claim that a flat minimum can alleviate overfitting issues. Following that, more studies were proposed to investigate the connection between the flat minima with the generalization abilities (Keskar et al., 2016; Dinh et al., 2017; Liu et al., 2020; Li et al., 2017; Dziugaite & Roy, 2017; Jiang et al., 2019; Moosavi-Dezfooli et al., 2019). Keskar et al. (2016) starts by investigating the phenomenon that training with a larger batch size results in worse generalization ability. The authors found that the sharpness of the minimum is critical in accounting for the observed phenomenon. Keskar et al. (2016) and Dinh et al. (2017) both argue that the sharpness can be characterized using the eigenvalues of the Hessian. Although they also define specific notions and methods to quantify sharpness, they do not propose complete training strategies to find minima that are relative "flat".

SAM (Foret et al., 2020) leverages the connection between "flat" minima and the generalization error to train DNNs that generalize well across the natural distribution. Inspired by Keskar et al. (2016) and Dinh et al. (2017), SAM first proposes the quantification of the sharpness, which is achieved by solving a maximization problem. Then, SAM proposes a complete training algorithm to improve the generalization abilities of DNNs. SAM is demonstrated to achieve state-of-the-art performance in a variety of deep learning benchmarks, including image classification, natural language processing, and noisy learning (Foret et al., 2020; Chen et al., 2021; Kwon et al., 2021; Pham et al., 2021; Yuan et al., 2021; Jia et al., 2021).

A series of SAM-related works has been proposed. A work that was done contemporaneously SAM (Wu et al., 2020) also regularizes the sharpness term in adversarial training and achieves much more robust generalization performance against adversarial attacks. Many works focus on combining SAM with other training strategies or architectures (Chen et al., 2021; Wang et al., 2021; Tseng et al., 2021), or apply SAM on other tasks (Zheng et al., 2021; Damian et al., 2021; Galatolo et al., 2021). Kwon et al. (2021) improves SAM's sharpness by adaptively scaling the size of the nearby search space ρ in relation to the size of parameters. However, most of these works overlook the fact that SAM improves generalization at the expense of the doubling the computational overhead. As a result, most of the SAM-related works suffer from the same efficiency drawback as SAM. This computational cost prevents SAM from being widely used in large-scale datasets and architectures, particularly in real-world applications, which motivates us to propose ESAM to *efficiently* improve the generalization ability of DNNs.

5 Conclusion

In this paper, we propose the *Efficient Sharpness Aware Minimizer* (ESAM) to enhance the efficiency of vanilla SAM. The proposed ESAM integrates two novel training strategies, namely, SWP and SDS, both of which are derived based on theoretical underpinnings and are evaluated over a variety of datasets and DNN architectures. Both SAM and ESAM are two-step training strategies consisting of sharpness estimation and weight updating. In each step, gradient back-propagation is performed to compute the weight perturbation or updating. In future research, we will explore how to combine the two steps into one by utilizing the information of gradients in previous iterations so that the computational overhead of ESAM can be reduced to the same as base optimizers.

Reproducibility Statement To ensure the reproducibility of our proposed ESAM formulation and algorithm, we will submit our source codes implemented in the PyTorch framework (Paszke et al., 2017) together with the supplementary material. The source codes contains the ESAM training algorithm codes, documents on how to apply ESAM, and examples of the application of ESAM on the CIFAR benchmark datasets. We will also release our ESAM codes that embedded into TIMM (Wightman, 2019) framework to the public.

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A APPENDIX

A.1 THE ALGORITHM OF SAM

The algorithm of SAM is demonstrated in Algorithm 2.

Algorithm 2 SGD vs. SAM

Input: Network f_θ, $\theta = (\theta_1, \theta_1, \ldots, \theta_N)$, Training set $\mathbb{S}$, Batch size b, Learning rate η, Neighborhood size ρ, Iterations A.
Output: A minimum solution $\tilde{\theta}$.

for $a = 1$ to A **do**
  Sample $\mathbb{B}$ with size b that $\mathbb{B} \subset \mathbb{S}$,
  if SGD **then**
    $\hat{\epsilon} \leftarrow 0$ ▷ No addtional computational overhead for $\hat{\epsilon}$
  else if SAM **then**
    $\hat{\epsilon} \leftarrow \nabla_\theta L_{\mathbb{B}}(f_\theta)$ ▷ additional F_1 and B_1 to compute $\hat{\epsilon}$
  Compute $g = \nabla_\theta L_{\mathbb{B}}(f_{\theta+\hat{\epsilon}})$ ▷ F_2 and B_2
  update the weights $\theta \leftarrow \theta - \eta g$

A.2 OPTIMIZING OVER SUBSET $\mathbb{B}^+$ IS REPRESENTATIVE

The sharpness-sensitive subset $\mathbb{B}^+$ are constructed sorting by $\ell(f_{\theta+\hat{\epsilon}}, x_i, y_i) - \ell(f_\theta, x_i, y_i)$, which is positively correlated to $l(f_\theta, x_i, y_i)$. By the first-order Taylor series approximation,

$$\ell(f_{\theta+\hat{\epsilon}}, x_i, y_i) - \ell(f_\theta, x_i, y_i) = \hat{\epsilon} \cdot \nabla_\theta \ell(f_\theta, x_i, y_i) + o(\|\hat{\epsilon}\|)$$

By Equation 4, $\hat{\epsilon}$ is the aggregated gradients of each instance in the complete dataset $\mathbb{B}$, i.e.,

$$\hat{\epsilon} = \underset{\epsilon:\|\epsilon\|_2<\rho}{\arg\max}\, L_{\mathbb{S}}(f_{\theta+\epsilon}) \approx \rho \nabla_\theta L_{\mathbb{S}}(f_\theta) = \sum_{i=1}^{|\mathbb{B}|} \nabla_\theta \ell(f_\theta, x_i, y_i)$$

which indicates that $\ell(f_{\theta+\hat{\epsilon}}, x_i, y_i) - \ell(f_\theta, x_i, y_i)$ is positively correlated to the gradient $\nabla_\theta \ell(f_\theta, x_i, y_i)$. Li et al. (2019) claims that the hard examples in deep learning (the training samples with high training loss) produce gradients with larger magnitudes. Therefore, $\ell(f_{\theta+\hat{\epsilon}}, x_i, y_i) - \ell(f_\theta, x_i, y_i)$ is positively correlated to $l(f_\theta, x_i, y_i)$. We also demonstrate the correlation empirically.

We conduct experiments to verify Equation 9 and Equation 10. We plot four losses in Figure 5, $L_{\mathbb{B}^+}(f_\theta)$, $L_{\mathbb{B}^-}(f_\theta)$, $L_{\mathbb{B}^+}(f_{\theta+\hat{\epsilon}})$, and $L_{\mathbb{B}^-}(f_{\theta+\hat{\epsilon}})$. The experimental results verify that Equation 9 and Equation 10 hold for every training epoch.

Moreover, we conduct experiments to demonstrate the optimizing over the subset $\mathbb{B}^+$ is representative enough to substitute for $\mathbb{B}$. We compare the updating gradients computed over $\mathbb{B}^+$ and $\mathbb{B}^-$ to those computed over $\mathbb{B}$ by calculating the cosine similarity, i.e.

$$\text{CosSim}(\nabla_\theta L_{\mathbb{B}^+}(f_{\theta+\hat{\epsilon}}), \nabla_\theta L_{\mathbb{B}}(f_{\theta+\hat{\epsilon}}))$$

$$\text{CosSim}(\nabla_\theta L_{\mathbb{B}^-}(f_{\theta+\hat{\epsilon}}), \nabla_\theta L_{\mathbb{B}}(f_{\theta+\hat{\epsilon}}))$$

The above gradients are computed by the SAM loss. We also compare the gradients computed by the vanilla empirical loss,

$$\text{CosSim}(\nabla_\theta L_{\mathbb{B}^+}(f_\theta), \nabla_\theta L_{\mathbb{B}}(f_\theta))$$

$$\text{CosSim}(\nabla_\theta L_{\mathbb{B}^-}(f_\theta), \nabla_\theta L_{\mathbb{B}}(f_\theta))$$

In Figure 6, we plot the cosine similarities in each training epoch with ResNet-18, Wide-28-10 on CIFAR10. It can be clearly seen that $\mathbb{B}^+$ has higher cosine similarities with $\mathbb{B}$ than $\mathbb{B}^-$ in terms of the computed gradients.

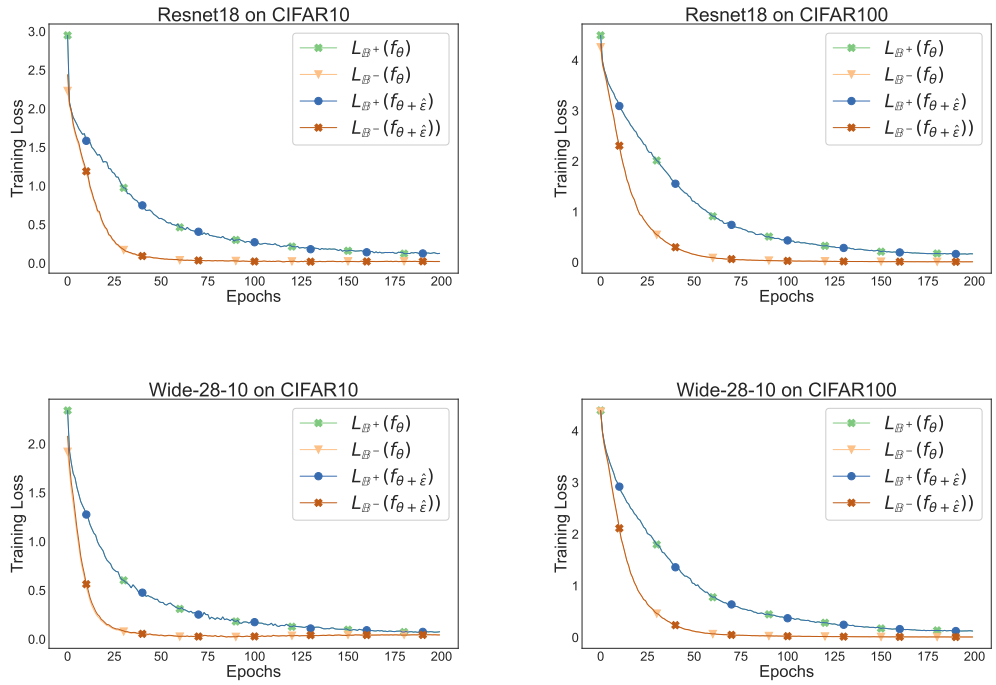

Figure 5: The SAM loss and the empirical loss calculated over the selected subsets $\mathbb{B}^+$, $\mathbb{B}^-$, changes w.r.t the epochs, with ResNet-18, Wide-28-10 on CIFAR10 and CIFAR100. The subset $\mathbb{B}^+$ selected by SDS has much higher SAM loss and empirical loss than $\mathbb{B}^-$ among all the four groups of experiments.

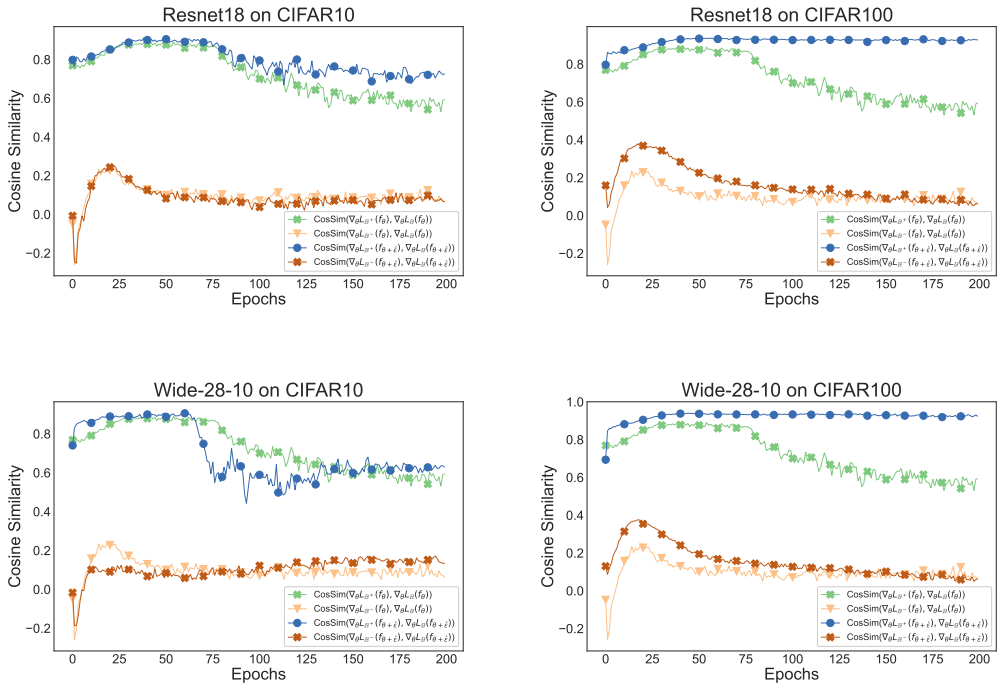

Figure 6: The cosine similarity between the gradients calculated on subsets $\mathbb{B}^+$, $\mathbb{B}^-$ with $\mathbb{B}$, evaluated with ResNet-18, Wide-28-10 on CIFAR10 and CIFAR100. The subset $\mathbb{B}^+$ selected by SDS has much higher cosine similarity with $\mathbb{B}$ in terms of calculated gradients than $\mathbb{B}^-$ among all the four groups of experiments.

A.3 TRAINING DETAILS

We tune the training parameters of SGD, SAM, and ESAM, by using grid searches. The learning rate is chosen from the set $\{0.01, 0.05, 0.1, 0.2\}$, the weight decay from the set $\{5 \times 10^{-4}, 1 \times 10^{-3}\}$, and the batch size from the set $\{64, 128, 256\}$. This is done to attain the best accuracies. The exact training hyperparameters are reported in Table 4. On the ImageNet datasets, limited by the computing resource, we follow and slightly modify the optimal hyperparameters as suggested by Chen et al. (2021) for SGD, SAM and ESAM. The exact training hyperparameters are reported in Table 5.

Table 4: Hyperparameters for training from scratch on CIFAR10 and CIFAR100

	CIFAR-10			**CIFAR-100**		
ResNet-18	SGD	SAM	ESAM	SGD	SAM	ESAM
Epoch		200			200	
Batch size		128			128	
Data augmentation		Basic			Basic	
Peak learning rate		0.05			0.05	
Learning rate decay		Cosine			Cosine	
Weight decay	5×10^{-4}	1×10^{-3}	1×10^{-3}	5×10^{-4}	1×10^{-3}	1×10^{-3}
ρ	-	0.05	0.05	-	0.05	0.05
Wide-28-10	SGD	SAM	ESAM	SGD	SAM	ESAM
Epoch		200			200	
Batch size		256			256	
Data augmentation		Basic			Basic	
Peak learning rate		0.05			0.05	
Learning rate decay		Cosine			Cosine	
Weight decay	5×10^{-4}	1×10^{-3}	1×10^{-3}	5×10^{-4}	1×10^{-3}	1×10^{-3}
ρ	-	0.1	0.1	-	0.1	0.1
PyramidNet-110	SGD	SAM	ESAM	SGD	SAM	ESAM
Epoch		300			300	
Batch size		256			256	
Data augmentation		Basic			Basic	
Peak learning rate		0.1			0.1	
Learning rate decay		Cosine			Cosine	
Weight decay		5×10^{-4}			5×10^{-4}	
ρ	-	0.2	0.2	-	0.2	0.2

Table 5: Hyperparameters for training from scratch on ImageNet

	ResNet-50			**ResNet-110**		
ImageNet	SGD	SAM	ESAM	SGD	SAM	ESAM
Epoch		90			90	
Batch size		512			512	
Data augmentation		Inception-style			Inception-style	
Peak learning rate		0.2			0.2	
Learning rate decay		Cosine			Cosine	
Weight decay		1×10^{-4}			1×10^{-4}	
ρ	-	0.05	0.05	-	0.05	0.05
Input resolution		224×224			224×224	