AN ADAPTIVE POLICY TO EMPLOY SHARPNESS-AWARE MINIMIZATION

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ABSTRACT

Sharpness-aware minimization (SAM), which searches for flat minima by min-max optimization, has been shown to be useful in improving model generalization. However, since each SAM update requires computing two gradients, its computational cost and training time are both doubled compared to standard empirical risk minimization (ERM). Recent state-of-the-arts reduce the fraction of SAM updates and thus accelerate SAM by switching between SAM and ERM updates randomly or periodically. In this paper, we design an adaptive policy to employ SAM based on the loss landscape geometry. Two efficient algorithms, AE-SAM and AE-LookSAM, are proposed. We theoretically show that AE-SAM has the same convergence rate as SAM. Experimental results on various datasets and architectures demonstrate the efficiency and effectiveness of the proposed method.

1 INTRODUCTION

Despite great success in many applications (He et al., 2016; Zagoruyko & Komodakis, 2016; Han et al., 2017), deep networks are often over-parameterized and capable of memorizing all training data. The training loss landscape is complex and nonconvex with many local minima of different generalization abilities. Many studies have investigated the relationship between geometry of the loss surface and generalization performance (Hochreiter & Schmidhuber, 1994; McAllester, 1999; Keskar et al., 2017; Neyshabur et al., 2017; Jiang et al., 2020), and found that flatter minima generalize better than sharper minima (Dziugaite & Roy, 2017; Petzka et al., 2021; Chaudhari et al., 2017; Keskar et al., 2017; Jiang et al., 2020).

Sharpness-aware minimization (SAM) (Foret et al., 2021) is the current state-of-the-art to seek flat minima by solving a min-max optimization problem. In the SAM algorithm, each update consists of *two* forward-backward computations: one for computing the perturbation and the other for computing the actual update direction. Since these two computations are not parallelizable, SAM doubles the computational overhead as well as the training time compared to empirical risk minimization (ERM).

Several algorithms (Du et al., 2021; Zhao et al., 2022b; Liu et al., 2022) have been proposed to improve SAM's efficiency. ESAM (Du et al., 2021) uses fewer samples to compute the gradients and updates fewer parameters, but each update still requires two gradient computations. Thus, ESAM does not alleviate the bottleneck of training speed. Instead of using the SAM update at every iteration, recent state-of-the-arts (Zhao et al., 2022b; Liu et al., 2022) proposed to use SAM randomly or periodically. Specifically, SS-SAM (Zhao et al., 2022b) selects SAM or ERM according to a Bernoulli trial, while LookSAM (Liu et al., 2022) employs SAM at every k step. Though efficiency, random or periodic policy of using SAM is suboptimal as it is not geometry-aware. Intuitively, the SAM update is more necessary for sharp regions than for flat regions.

In this paper, we propose an adaptive policy to employ SAM based on the geometry of the loss landscape. The SAM update is used when the model is in sharp regions, while the ERM update is used in flat regions for reducing the fraction of SAM updates. To measure sharpness, we use the squared stochastic gradient norm and model it as normal distribution. We estimate the distribution parameters by exponential moving average. Experimental results on standard benchmarks demonstrate the superiority of the proposed policy.

Our contributions are summarized as follows: (i) We propose an adaptive policy to employ SAM based on the loss landscape geometry. (ii) We propose an efficient algorithm, called AE-SAM, to

reduce the fraction of SAM updates. We also theoretically study its convergence rates with both batch and stochastic gradient descent. (iii) The proposed policy is general and can be combined with any SAM variant. In this paper, we integrate it with LookSAM and propose AE-LookSAM. (iv) Experimental results on various datasets and network architectures, with and without label noise, verify the superiority of AE-SAM and AE-LookSAM over existing baselines.

Notations. Vectors (e.g., $\mathbf{x}$) and matrices (e.g., $\mathbf{X}$) are denoted by lowercase and uppercase boldface letters, respectively. For a vector $\mathbf{x}$, its ℓ_2-norm is $\|\mathbf{x}\|$. $\mathcal{N}(\mu; \sigma^2)$ is the univariate normal distribution with mean μ and variance σ^2. $\mathrm{diag}(\mathbf{x})$ constructs a diagonal matrix with $\mathbf{x}$ on the diagonal.

2 Related Work

We are given a training set $\mathcal{D}$ with i.i.d. samples $\{(\mathbf{x}_i, y_i) : i = 1, \ldots, n\}$ drawn from a data distribution, Let $f(\mathbf{x}; \mathbf{w})$ be a model parameterized by $\mathbf{w}$. Its empirical risk on $\mathcal{D}$ is $\mathcal{L}(\mathcal{D}; \mathbf{w}) = \frac{1}{n}\sum_{i=1}^{n} \ell(f(\mathbf{x}_i; \mathbf{w}), y_i)$, where $\ell(\cdot, \cdot)$ is a loss (e.g., cross-entropy loss for classification). Model training aims to learn a model from the training data that generalizes well on test data.

Generalization and Flat Minima. The connection between model generalization and loss landscape geometry has been theoretically and empirically studied in (Keskar et al., 2017; Dziugaite & Roy, 2017; Jiang et al., 2020). Recently, Jiang et al. (2020) conducted large-scale experiments and found that sharpness-based measures (flatness) are related to generalization of minimizers. Although flatness can be characterized by Hessian eigenvalues (Keskar et al., 2017; Dinh et al., 2017), dealing with Hessian explicitly is computationally prohibitive. To address this issue, practical algorithms propose to seek flat minima by injecting noise in the optimizers (Zhu et al., 2019; Zhou et al., 2019; Orvieto et al., 2022; Bisla et al., 2022), introducing regularization (Chaudhari et al., 2017; Zhao et al., 2022a; Du et al., 2022), averaging model weights during training (Izmailov et al., 2018; He et al., 2019; Cha et al., 2021), or sharpness-aware minimization (SAM) (Foret et al., 2021; Kwon et al., 2021; Zhuang et al., 2021; Kim et al., 2022).

SAM. The state-of-the-art SAM (Foret et al., 2021) and its variants (Kwon et al., 2021; Zhuang et al., 2021; Kim et al., 2022) search for flat minima by solving the min-max optimization problem:

$$\min_{\mathbf{w}} \max_{\|\boldsymbol{\epsilon}\| \leq \rho} \mathcal{L}(\mathcal{D}; \mathbf{w} + \boldsymbol{\epsilon}), \tag{1}$$

where $\rho > 0$ is the radius of perturbation. The above can be rewritten as $\min_{\mathbf{w}} \mathcal{L}(\mathcal{D}; \mathbf{w}) + \mathcal{R}(\mathcal{D}; \mathbf{w})$, where $\mathcal{R}(\mathcal{D}; \mathbf{w}) \equiv \max_{\|\boldsymbol{\epsilon}\| \leq \rho} \mathcal{L}(\mathcal{D}; \mathbf{w} + \boldsymbol{\epsilon}) - \mathcal{L}(\mathcal{D}; \mathbf{w})$ is a regularizer that penalizes sharp minimizers (Foret et al., 2021). As solving the inner maximization in Eq.(1) exactly is computationally infeasible for nonconvex optimization, SAM approximately solves it by the first-order Taylor approximation and its update rule is

$$\mathbf{w}_{t+1} = \mathbf{w}_t - \eta \nabla \mathcal{L}(\mathcal{B}_t; \mathbf{w}_t + \rho_t \nabla \mathcal{L}(\mathcal{B}_t; \mathbf{w}_t)), \tag{2}$$

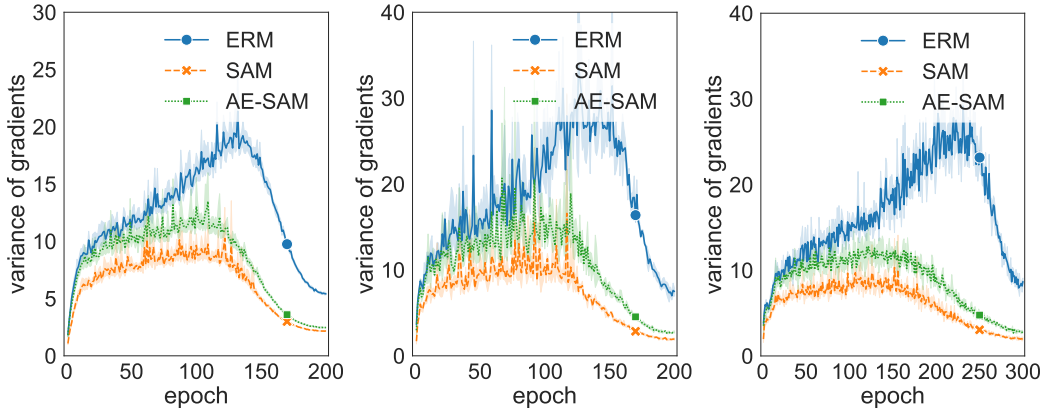
where $\mathcal{B}_t$ is a mini-batch of data, η is the step size, and $\rho_t = \frac{\rho}{\|\nabla \mathcal{L}(\mathcal{B}_t; \mathbf{w}_t)\|}$. Although SAM has shown to be effective in improving the generalization of deep networks, a major drawback is that each update in Eq.(2) requires *two* forward-backward calculations. Specifically, SAM first calculates the gradient of $\mathcal{L}(\mathcal{B}_t; \mathbf{w})$ at $\mathbf{w}_t$ to obtain the perturbation, then calculates the gradient of $\mathcal{L}(\mathcal{B}_t; \mathbf{w})$ at $\mathbf{w}_t + \rho_t \nabla \mathcal{L}(\mathcal{B}_t; \mathbf{w}_t)$ to obtain the update direction for $\mathbf{w}_t$. As a result, SAM doubles the computational overhead compared to ERM.

Efficient Variants of SAM. Several algorithms have been proposed to accelerate the SAM algorithm. ESAM (Du et al., 2021) uses fewer samples to compute the gradients and only updates part of parameters in the second step, but still requires to compute most of the gradients. Another direction is to reduce the number of SAM updates used in the training process. SS-SAM (Zhao et al., 2022b) randomly selects SAM or ERM update according to a Bernoulli trial, while LookSAM (Liu et al., 2022) employ SAM at every k iteration. Unlike the random or periodic policy of employing SAM, the proposed policy is adaptive to the loss landscape.

3 Method

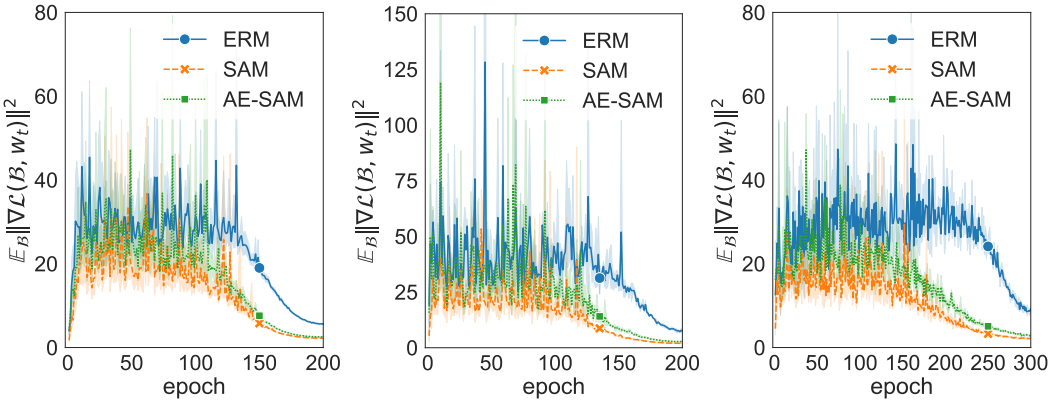
In this section, we propose an adaptive policy to employ the SAM update. The general idea is to use ERM when $\mathbf{w}_t$ is already in a flat region, and use SAM only when the loss landscape is locally sharp.

We start by introducing a sharpness measure (Section 3.1), then propose an adaptive policy based on the sharpness measure (Section 3.2). Next, we propose two algorithms (AE-SAM and AE-LookSAM) and study the convergence of AE-SAM.



(a) *ResNet-18*. (b) *WRN-28-10*. (c) *PyramidNet-110*.

Figure 1: Variance of gradients on *CIFAR-100*. Best viewed in color.



(a) *ResNet-18*. (b) *WRN-28-10*. (c) *PyramidNet-110*.

Figure 2: Squared stochastic gradient norms $\mathbb{E}_{\mathcal{B}}\|\nabla\mathcal{L}(\mathcal{B};\mathbf{w}_t)\|^2$ on *CIFAR-100*. Best viewed in color.

3.1 Sharpness Measure

Though sharpness can be characterized by the eigenvalues of Hessian (Keskar et al., 2017; Dinh et al., 2017), it is expensive to compute. A widely-used approximation is based on the gradient magnitude $\mathrm{diag}([\nabla\mathcal{L}(\mathcal{B};\mathbf{w}_t)]^2)$ (Bottou et al., 2018; Khan et al., 2018), where $[\mathbf{v}]^2$ denotes the elementwise square of $\mathbf{v}$. As $\|\nabla\mathcal{L}(\mathcal{B};\mathbf{w}_t)\|^2$ equals the trace of $\mathrm{diag}([\nabla\mathcal{L}(\mathcal{B};\mathbf{w}_t)]^2)$, it is reasonable to choose $\|\nabla\mathcal{L}(\mathcal{B};\mathbf{w}_t)\|^2$ as a sharpness measure.

$\|\nabla\mathcal{L}(\mathcal{B};\mathbf{w}_t)\|^2$ is also related to another sharpness measure, namely, the variance of gradients, which is defined as

$$\mathsf{Var}(\nabla\mathcal{L}(\mathcal{B};\mathbf{w})) \equiv \mathbb{E}_{\mathcal{B}}\|\nabla\mathcal{L}(\mathcal{B};\mathbf{w}) - \nabla\mathcal{L}(\mathcal{D};\mathbf{w})\|^2 = \mathbb{E}_{\mathcal{B}}\|\nabla\mathcal{L}(\mathcal{B};\mathbf{w})\|^2 - \|\nabla\mathcal{L}(\mathcal{D};\mathbf{w})\|^2. \quad (3)$$

With appropriate smoothness assumptions on the loss $\mathcal{L}$, both SAM and ERM can be shown theoretically to converge to critical points of $\mathcal{L}(\mathcal{D};\mathbf{w})$ (i.e., $\nabla\mathcal{L}(\mathcal{D};\mathbf{w}) = 0$) (Reddi et al., 2016; Andriushchenko & Flammarion, 2022). Thus, it follows from Eq.(3) that the squared stochastic gradient norm $\mathbb{E}_{\mathcal{B}}\|\nabla\mathcal{L}(\mathcal{B};\mathbf{w})\|^2$ indicates the variance of gradients. Jiang et al. (2020) conducted extensive experiments and empirically shows that the variance of gradients is positively correlated with the generalization gap. In other words, the smaller the $\mathsf{Var}(\nabla\mathcal{L}(\mathcal{B};\mathbf{w}))$, the better generalization is the model with parameter $\mathbf{w}$. This finding also explains why SAM generalizes better than ERM. Figure 1 shows the variance of gradients w.r.t. the number of epochs using SAM and ERM on

CIFAR-100 with various network architectures (experimental details are in Section 4.1). As can be seen, SAM always has a much smaller variance than ERM. Figure 2 shows the squared stochastic gradient norm w.r.t. the number of epochs on *CIFAR-100*. As can be seen, SAM achieves a much smaller $\mathbb{E}_{\mathcal{B}}\|\nabla\mathcal{L}(\mathcal{B};\mathbf{w}_t)\|^2$ than ERM.

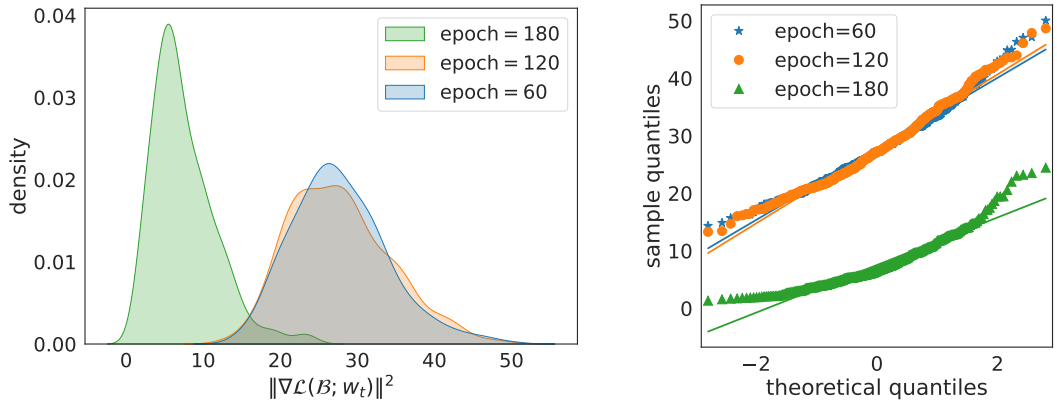
3.2 Adaptive Policy to Employ SAM

As $\mathbb{E}_{\mathcal{B}}\|\nabla\mathcal{L}(\mathcal{B};\mathbf{w}_t)\|^2$ changes over t (Figure 2), it needs to be estimated at every iteration. One can sample a large number of mini-batches and compute the mean of the corresponding stochastic gradient norms. However, this can be computationally expensive as the computational overhead is substantial. To address this problem, we model $\|\nabla\mathcal{L}(\mathcal{B};\mathbf{w}_t)\|^2$ with a distribution and estimate the distribution parameters in an online manner. Figure 3(a) shows $\|\nabla\mathcal{L}(\mathcal{B};\mathbf{w}_t)\|^2$ of 400 mini-batches at different training stages (epoch $= 60$, 120, and 180) on *CIFAR-100* using *ResNet-18*. As can be seen, the distribution follows a Bell curve. Figure 3(b) shows the corresponding quantile-quantile (Q-Q) plot, which is usually used to assess normality: the closer the curve to the line, the distribution is closer to the normal distribution. Both Figures 3(a) and 3(b) suggest that $\|\nabla\mathcal{L}(\mathcal{B};\mathbf{w}_t)\|^2$ can be modeled with a normal distribution $\mathcal{N}(\mu_t, \sigma_t^2)$. We estimate the mean and variance by an exponential moving average (EMA):

$$\mu_t = \delta\mu_{t-1} + (1-\delta)\|\nabla\mathcal{L}(\mathcal{B}_t;\mathbf{w}_t)\|^2, \tag{4}$$

$$\sigma_t^2 = \delta\sigma_{t-1}^2 + (1-\delta)(\|\nabla\mathcal{L}(\mathcal{B}_t;\mathbf{w}_t)\|^2 - \mu_t)^2, \tag{5}$$

where $\delta \in (0,1)$ controls the forgetting rate. Empirically, we use $\delta = 0.9$. Since $\nabla\mathcal{L}(\mathcal{B}_t;\mathbf{w}_t)$ is already available, EMA does not involve any additional gradient calculations (the cost for the norm operator is negligible).



(a) Distributions of stochastic gradient norms.

(b) Q-Q plots of stochastic gradient norms.

Figure 3: Stochastic gradient norms $\{\|\mathcal{L}(\mathcal{B};\mathbf{w}_t)\|^2 : \mathcal{B} \sim \mathcal{D}\}$ of *ResNet-18* on *CIFAR-100* are approximately normally distributed. Best viewed in color.

Using μ_t and σ_t^2, we employ SAM only at iterations where $\|\nabla\mathcal{L}(\mathcal{B}_t;\mathbf{w}_t)\|^2$ is relatively large. Specifically, when $\|\nabla\mathcal{L}(\mathcal{B}_t;\mathbf{w}_t)\|^2 \geq \mu_t + c_t\sigma_t$ (where c_t is a threshold), SAM is used; otherwise, ERM is used. When using the SAM update is more desirable, c_t is small (or even negative). When $c_t \to -\infty$, it reduces to SAM; when $c_t \to \infty$, it becomes ERM. Note that during the early training stage, the model is still underfitting and $\mathbf{w}_t$ is far from the region of final convergence. Thus, minimizing the empirical loss is more important than seeking a locally flat region. Andriushchenko & Flammarion (2022) also empirically observe that the SAM update is more effective in boosting performance towards the end of training. We therefore design a schedule that linearly decreases c_t from λ_2 to λ_1 (which are pre-set values): $c_t = g_{\lambda_1,\lambda_2}(t) \equiv \frac{t}{T}\lambda_1 + \left(1 - \frac{t}{T}\right)\lambda_2$, where T is the total number of iterations. The whole procedure, called Adaptive policy to Employ SAM (**AE-SAM**), is summarized in Algorithm 1.

AE-LookSAM. The proposed adaptive policy can be combined with any SAM variant. Here, we consider integrating it with LookSAM (Liu et al., 2022). When $\|\nabla\mathcal{L}(\mathcal{B}_t;\mathbf{w}_t)\|^2 \geq \mu_t + c_t\sigma_t$, SAM is used and the update direction for $\mathbf{w}_t$ is decomposed into two orthogonal directions as in LookSAM:

(i) the ERM update direction to reduce training loss, and (ii) the direction that biases the model to a flat region. When $\|\nabla\mathcal{L}(\mathcal{B}_t;\mathbf{w}_t)\|^2 < \mu_t + c_t\sigma_t$, ERM is performed and the second direction of previous SAM update is reused to compose an approximate SAM direction. The procedure, called AE-LookSAM, is also shown in Algorithm 1.

Algorithm 1 AE-SAM and AE-LookSAM.

Require: training set $\mathcal{D}$, stepsize η, radius ρ; λ_1 and λ_2 for $g_{\lambda_1,\lambda_2}(t)$; $\mathbf{w}_0$, $\mu_{-1}=0$, $\sigma_{-1}^2 = e^{-10}$, and α for AE-LookSAM;

for $t = 0, \ldots, T-1$ **do**
  sample a mini-batch data $\mathcal{B}_t$ from $\mathcal{D}$;
  compute $\mathbf{g} = \nabla\mathcal{L}(\mathcal{B}_t;\mathbf{w}_t)$;
  update μ_t by (4) and σ_t^2 by (5);
  compute $c_t = g_{\lambda_1,\lambda_2}(t)$;
  if $\|\nabla\mathcal{L}(\mathcal{B}_t;\mathbf{w}_t)\|^2 \geq \mu_t + c_t\sigma_t$ **then**
    $\mathbf{g}_s = \nabla\mathcal{L}(\mathcal{B}_t;\mathbf{w}_t + \rho\nabla\mathcal{L}(\mathcal{B}_t;\mathbf{w}_t))$;
    if AE-LookSAM: decompose $\mathbf{g}_s$ as $\mathbf{g}_v = \mathbf{g}_s - \frac{\mathbf{g}^\top\mathbf{g}_s}{\|\mathbf{g}\|^2}\mathbf{g}$;
  else:
    if AE-SAM: $\mathbf{g}_s = \mathbf{g}$;
    if AE-LookSAM: $\mathbf{g}_s = \mathbf{g} + \alpha\frac{\|\mathbf{g}\|}{\|\mathbf{g}_v\|}\mathbf{g}_v$;
  end if
  $\mathbf{w}_{t+1} = \mathbf{w}_t - \eta\mathbf{g}_s$;
end for
return $\mathbf{w}_T$.

3.3 Convergence Analysis

In this section, we study the convergence of the proposed AE-SAM. As AE-SAM switches between ERM and SAM, analyzing its convergence is more challenging compared with that of SAM.

The following smoothness assumption is standard in the literature on non-convex optimization (Ghadimi & Lan, 2013; Reddi et al., 2016) and SAM (Andriushchenko & Flammarion, 2022; Abbas et al., 2022; Qu et al., 2022). All proofs are in Appendix A.

Assumption 3.1 (Smoothness)**.** $\mathcal{L}(\mathcal{D};\mathbf{w})$ is β-smooth in $\mathbf{w}$, i.e., $\|\nabla\mathcal{L}(\mathcal{D};\mathbf{w}) - \nabla\mathcal{L}(\mathcal{D};\mathbf{v})\| \leq \beta\|\mathbf{w}-\mathbf{v}\|$.

The following Theorem shows that AE-SAM with full-batch gradient descent (i.e., $\mathcal{B}_t = \mathcal{D}$) reaches a critical point at an $\mathcal{O}(1/T)$ rate, which is the same as SAM (Andriushchenko & Flammarion, 2022).

Theorem 3.2. *With full-batch gradient descent, if $\rho < \frac{1}{2\beta}$ and $\eta < \frac{1}{\beta}$, AE-SAM satisfies*

$$\min_{0\leq t\leq T-1}\|\nabla\mathcal{L}(\mathcal{D};\mathbf{w}_t)\|^2 \leq \frac{2(\mathcal{L}(\mathcal{D};\mathbf{w}_0) - \mathcal{L}(\mathcal{D};\mathbf{w}_T))}{T\eta\,(1-\beta\eta)}. \tag{6}$$

Next, we study the convergence of AE-SAM with stochastic gradient descent (SGD). The following assumption on bounded variance of stochastic gradients is standard in the literature on stochastic non-convex optimization (Ghadimi & Lan, 2013; Reddi et al., 2016) and SAM with SGD (Andriushchenko & Flammarion, 2022; Abbas et al., 2022; Qu et al., 2022).

Assumption 3.3 (Bounded variance of stochastic gradients)**.** $\mathbb{E}_{(\mathbf{x}_i,y_i)\sim\mathcal{D}}\|\nabla\ell(f(\mathbf{x}_i;\mathbf{w}),y_i) - \nabla\mathcal{L}(\mathcal{D};\mathbf{w})\|^2 \leq \sigma^2$.

Theorem 3.4. *Let b be the mini-batch size. If $\eta = \frac{1}{4\beta\sqrt{T}}$ and $\rho = 1/T^{\frac{1}{4}}$, AE-SAM satisfies*

$$\min_{0\leq t\leq T-1}\mathbb{E}\|\nabla\mathcal{L}(\mathcal{D};\mathbf{w}_t)\|^2 \leq \frac{32\beta(\mathbb{E}\mathcal{L}(\mathcal{D};\mathbf{w}_0) - \mathbb{E}\mathcal{L}(\mathcal{D};\mathbf{w}_T))}{3\sqrt{T}} + \frac{4\beta\sigma^2(8+4\beta+4\beta^2)}{b\sqrt{T}}. \tag{7}$$

The $\mathcal{O}(1/\sqrt{T})$ rate is the same as SAM with SGD (Andriushchenko & Flammarion, 2022) under the same condition on ρ.

4 EXPERIMENTS

In this section, we evaluate the proposed AE-SAM and AE-LookSAM on several standard benchmarks. As the SAM update doubles the computational overhead compared to the ERM update, the training speed is mainly determined by how often the SAM update is used. Hence, we evaluate efficiency by measuring the fraction of SAM updates used:

$$\%\text{SAM} \equiv 100 \times \#\{\text{iterations using SAM}\}/T,$$

where T, the total number of iterations, is the same for all methods.

4.1 *CIFAR-10* AND *CIFAR-100*

Setup. In this section, experiments are conducted on the *CIFAR-10* and *CIFAR-100* datasets (Krizhevsky & Hinton, 2009) using three network architectures: *ResNet-18* (He et al., 2016), *WideResNet-28-10* (denoted *WRN-28-10*) (Zagoruyko & Komodakis, 2016), and *PyramidNet-110* (Han et al., 2017).

Following the setup in (Liu et al., 2022; Foret et al., 2021), we use batch size 128, initial learning rate of 0.1, cosine learning rate schedule, SGD optimizer with momentum 0.9 and weight decay 0.0001. The number of training epochs is 300 for *PyramidNet-110*, and 200 for *ResNet-18* and *WideResNet-28-10*. 10% of the training set is used as the validation set. We perform grid search on the radius ρ over $\{0.01, 0.02, 0.05, 0.1, 0.2, 0.5\}$ as in Foret et al. (2021). Similarly, α is selected by grid search over $\{0.1, 0.3, 0.6, 0.9\}$. For the c_t schedule $g_{\lambda_1,\lambda_2}(t)$, $\lambda_1 = -1$ and $\lambda_2 = 1$ for AE-SAM; $\lambda_1 = 0$ and $\lambda_2 = 2$ for AE-LookSAM.

Baselines. The proposed AE-SAM and AE-LookSAM are compared with the following baselines: (i) ERM; (ii) SAM (Foret et al., 2021); and its more efficient variants including (iii) ESAM (Du et al., 2021) which uses part of the weights to compute the perturbation and part of the samples to compute the SAM update direction. These two techniques can reduce the computational cost, but may not always accelerate SAM, particularly in parallel training (Li et al., 2020); (iv) SS-SAM (Zhao et al., 2022b), which randomly selects SAM or ERM according to a Bernoulli trial with success probability 0.5. This is the scheme with the best performance in (Zhao et al., 2022b); (v) LookSAM (Liu et al., 2022) which uses SAM at every $k = 5$ step. The experiment is repeated five times with different random seeds.

Results. Table 1 shows the testing accuracy and fraction of SAM updates (%SAM), in which methods are grouped based on %SAM. As can be seen, AE-SAM has higher accuracy than SAM while using only 20% of SAM updates. SS-SAM and AE-SAM have comparable %SAM (about 50%), and AE-SAM achieves higher accuracy than SS-SAM (which is statistically significant based on the pairwise t-test at 95% significance level). Finally, LookSAM and AE-LookSAM have comparable %SAM (about 20%), and AE-LookSAM also has higher accuracy than LookSAM. These improvements confirm the adaptive policy is better.

4.2 *ImageNet*

Setup. In this section, we perform experiments on the *ImageNet* (Russakovsky et al., 2015), which contains 1000 classes and 1.28 million images. The *ResNet-50* (He et al., 2016) is used. Following the setup in Du et al. (2021), we train the network for 90 epochs using a SGD optimizer with momentum 0.9, weight decay 0.0001, initial learning rate 0.1, cosine learning rate schedule, and batch size 512. As in (Foret et al., 2021; Du et al., 2021), $\rho = 0.05$. For the c_t schedule $g_{\lambda_1,\lambda_2}(t)$, $\lambda_1 = -1$ and $\lambda_2 = 1$ for AE-SAM; $\lambda_1 = 0$ and $\lambda_2 = 2$ for AE-LookSAM. $k = 5$ is used for LookSAM. Experiments are repeated with three different random seeds.

Results. Table 2 shows the testing accuracy and fraction of SAM updates. As can be seen, with only half of the iterations using SAM, AE-SAM achieves comparable (or even better) performance as SAM. Compared with LookSAM, AE-LookSAM has better performance (which is also statistically significant), verifying the proposed adaptive policy is more effective than LookSAM's periodic policy.

Table 1: Means and standard deviations of testing accuracy and fraction of SAM updates (%SAM) on *CIFAR-10* and *CIFAR-100*. Methods are grouped based on %SAM. The highest accuracy in each group is underlined; while the highest accuracy for each network architecture (across all groups) is in bold.

		CIFAR-10		*CIFAR-100*	
		Accuracy	%SAM	Accuracy	%SAM
ResNet-18	ERM	95.41 ±0.03	0.0 ±0.0	78.17 ±0.05	0.0 ±0.0
	SAM (Foret et al., 2021)	96.52 ±0.12	100.0 ±0.0	80.17 ±0.15	100.0 ±0.0
	ESAM (Du et al., 2021)	96.56 ±0.08	100.0 ±0.0	80.41 ±0.10	100.0 ±0.0
	SS-SAM (Zhao et al., 2022b)	96.40 ±0.16	50.0 ±0.0	80.10 ±0.16	50.0 ±0.0
	AE-SAM	**96.63** ±0.04	50.1 ±0.1	**80.48** ±0.11	49.8 ±0.0
	LookSAM (Liu et al., 2022)	96.32 ±0.12	20.0 ±0.0	79.89 ±0.29	20.0 ±0.0
	AE-LookSAM	96.56 ±0.21	20.0 ±0.1	80.29 ±0.37	20.0 ±0.0
WRN-28-10	ERM	96.34 ±0.12	0.0 ±0.0	81.56 ±0.14	0.0 ±0.0
	SAM (Foret et al., 2021)	97.27 ±0.11	100.0 ±0.0	83.42 ±0.05	100.0 ±0.0
	ESAM (Du et al., 2021)	97.29 ±0.11	100.0 ±0.0	**84.51** ±0.02	100.0 ±0.0
	SS-SAM (Zhao et al., 2022b)	97.09 ±0.11	50.0 ±0.0	82.89 ±0.02	50.0 ±0.0
	AE-SAM	**97.30** ±0.10	49.5 ±0.1	**84.51** ±0.11	49.6 ±0.0
	LookSAM (Liu et al., 2022)	97.02 ±0.12	20.0 ±0.0	83.70 ±0.12	20.0 ±0.0
	AE-LookSAM	97.15 ±0.08	20.0 ±0.0	83.92 ±0.07	20.2 ±0.0
PyramidNet-110	ERM	96.62 ±0.10	0.0 ±0.0	81.89 ±0.15	0.0 ±0.0
	SAM (Foret et al., 2021)	97.30 ±0.10	100.0 ±0.0	84.46 ±0.05	100.0 ±0.0
	ESAM (Du et al., 2021)	97.42 ±0.10	100.0 ±0.0	85.39 ±0.05	100.0 ±0.0
	SS-SAM (Zhao et al., 2022b)	97.22 ±0.10	50.0 ±0.0	84.90 ±0.05	50.0 ±0.0
	AE-SAM	**97.45** ±0.09	49.9 ±0.0	**85.58** ±0.10	49.8 ±0.1
	LookSAM (Liu et al., 2022)	97.10 ±0.11	20.0 ±0.0	84.01 ±0.06	20.0 ±0.0
	AE-LookSAM	97.22 ±0.11	20.3 ±0.0	84.80 ±0.13	20.2 ±0.1

Table 2: Means and standard deviations of testing accuracy and fraction of SAM updates (%SAM) on *ImageNet* using *ResNet-50*. Methods are grouped based on %SAM. The highest accuracy in each group is underlined; while the highest across all groups is in bold.

	Accuracy	%SAM
ERM	77.11 ±0.14	0.0 ±0.0
SAM (Foret et al., 2021)	**77.47** ±0.12	100.0 ±0.0
ESAM (Du et al., 2021)	77.25 ±0.75	100.0 ±0.0
SS-SAM (Zhao et al., 2022b)	77.38 ±0.06	50.0 ±0.0
AE-SAM	77.43 ±0.06	49.4 ±0.0
LookSAM (Liu et al., 2022)	77.13 ±0.09	20.0 ±0.0
AE-LookSAM	77.29 ±0.08	20.3 ±0.0

4.3 Robustness to Label Noise

Setup. In this section, we study whether the more-efficient SAM variants will affect its robustness to training label noise. Following the setup in Foret et al. (2021), we conduct experiments on a corrupted version of *CIFAR-10*, with some of its training labels randomly flipped (while its testing set is kept clean). The *ResNet-18* and *ResNet-32* networks are used. They are trained for 200 epochs using SGD with momentum 0.9, weight decay 0.0001, batch size 128, initial learning rate 0.1, and cosine

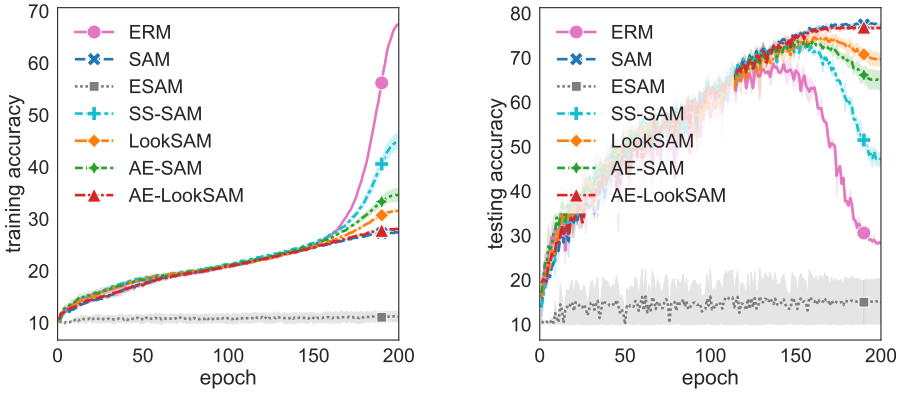
learning rate schedule. For LookSAM, the SAM update is used every $k = 2$ steps.[1] For AE-SAM and AE-LookSAM, we set $\lambda_1 = -1$ and $\lambda_2 = 1$ in their c_t schedules $g_{\lambda_1,\lambda_2}(t)$, such that their fractions of SAM updates (approximately 50%) are comparable with SS-SAM and LookSAM. Experiments are repeated with five different random seeds.

Results. Table 3 shows the testing accuracy and fraction of SAM updates[2]. As can be seen, AE-LookSAM achieves comparable performance with SAM but is faster as only half of the iterations use the SAM update. Compared with ESAM, SS-SAM and LookSAM, AE-LookSAM performs better. The improvement is particularly noticeable at the higher noise levels (e.g., 80%).

Table 3: Testing accuracy and fraction of SAM updates on *CIFAR-10* with different levels of label noise. The best accuracy is in bold and the second best is underlined.

		noise $= 20\%$		noise $= 40\%$		noise $= 60\%$		noise $= 80\%$	
		accuracy	%SAM	accuracy	%SAM	accuracy	%SAM	accuracy	%SAM
ResNet-18	ERM	87.92	0.0	70.82	0.0	49.61	0.0	28.23	0.0
	SAM (Foret et al., 2021)	**94.80**	100.0	<u>91.50</u>	100.0	**88.15**	100.0	**77.40**	100.0
	ESAM (Du et al., 2021)	94.19	100.0	91.46	100.0	81.30	100.0	15.00	100.0
	SS-SAM (Zhao et al., 2022b)	90.62	50.0	77.84	50.0	61.18	50.0	47.32	50.0
	LookSAM (Liu et al., 2022)	92.72	50.0	88.04	50.0	72.26	50.0	69.72	50.0
	AE-SAM	92.84	50.0	84.17	50.0	73.54	49.9	65.00	50.0
	AE-LookSAM	<u>94.34</u>	49.9	**91.58**	50.0	<u>87.85</u>	50.0	<u>76.90</u>	50.0
ResNet-32	ERM	87.43	0.0	70.82	0.0	46.26	0.0	29.00	0.0
	SAM (Foret et al., 2021)	**95.08**	100.0	91.01	100.0	**88.90**	100.0	**77.32**	100.0
	ESAM (Du et al., 2021)	93.42	100.0	<u>91.63</u>	100.0	82.73	100.0	10.09	100.0
	SS-SAM (Zhao et al., 2022b)	89.63	50.0	74.17	50.0	58.40	50.0	59.53	50.0
	LookSAM (Liu et al., 2022)	92.49	50.0	86.56	50.0	63.35	50.0	68.01	50.0
	AE-SAM	92.87	50.0	82.85	50.0	71.50	50.0	65.43	50.3
	AE-LookSAM	<u>94.70</u>	50.0	**91.80**	50.0	<u>88.22</u>	50.0	<u>77.03</u>	49.8

Figure 4 shows the training and testing accuracies with number of epochs at a noise level of 80% using *ResNet-18*. Results for other noise levels and *ResNet-32* are shown in Appendix B.2. As can be seen, SAM is robust to the label noise, while ERM and SS-SAM heavily suffer from overfitting. AE-SAM and LookSAM can alleviate the overfitting problem to a certain extent. AE-LookSAM, by combining the adaptive policy with LookSAM, achieves the same high level of robustness as SAM.



(a) Training accuracy. (b) Testing accuracy.

Figure 4: Accuracies with number of training epochs on *CIFAR-10* (with 80% noisy labels) using *ResNet-18*. Best viewed in color.

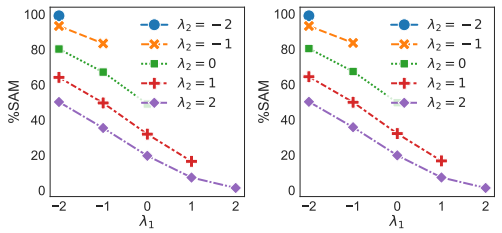
[1]The performance of LookSAM can be sensitive to the value of k. In this experiment, setting $k = 2$ leads to the best performance. Details can be found in Appendix B.2.

[2]The full table, with standard deviation on the results, is shown in Table 4 of Appendix B.2.

4.4 EFFECTS OF λ_1 AND λ_2

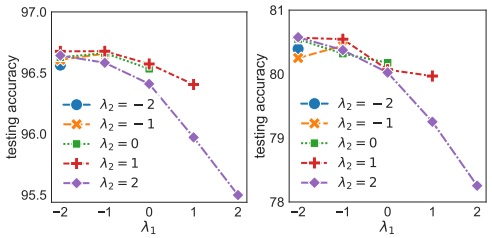
In this experiment, we study the effects of λ_1 and λ_2 on AE-SAM. A similar on AE-LookSAM is shown in Appendix B.2. We use the setup as in Section 4.1, where λ_1 and λ_2 (with $\lambda_1 \leq \lambda_2$) are chosen from $\{0, \pm 1, \pm 2\}$.

Figure 5 shows the effect on the fraction of SAM updates. For a fixed λ_2, increasing λ_1 increases the threshold c_t, and the condition $\|\nabla \mathcal{L}(\mathcal{B}_t; \mathbf{w}_t)\|^2 \geq \mu_t + c_t \sigma_t$ becomes more difficult to satisfy. Thus, as can be seen, the fraction of SAM updates is reduced. The same applies when λ_2 increases. Figure 6 shows the effect on the testing accuracy. For $\lambda_2 \in \{0, 1, 2\}$ (particularly, $\lambda_2 = 2$), increasing λ_1 leads to a reduction in testing accuracy as SAM updates are fewer. For $\lambda_2 \in \{-2, -1\}$, their accuracies are similar as the SAM update is used frequently (%SAM $\geq 80\%$ as shown in Figure 5).



(a) *CIFAR-10*. (b) *CIFAR-100*.

Figure 5: Effects of λ_1 and λ_2 on fraction of SAM updates using *ResNet-18*.

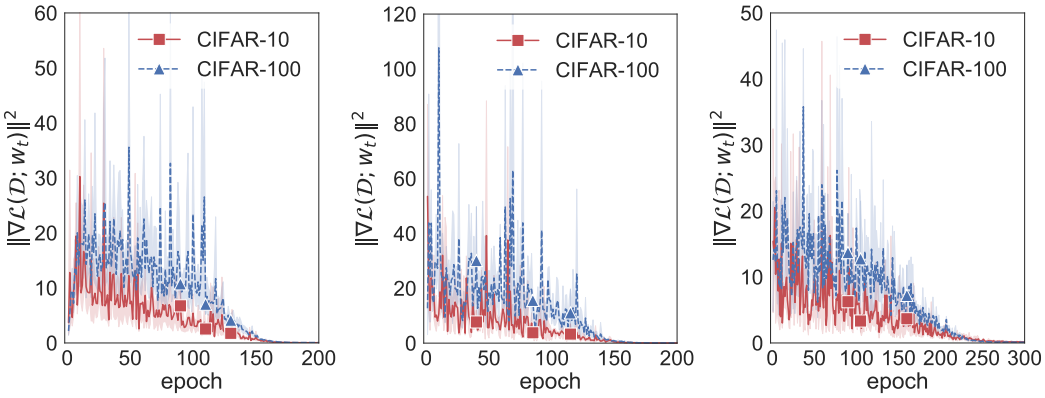


(a) *CIFAR-10*. (b) *CIFAR-100*.

Figure 6: Effects of λ_1 and λ_2 on testing accuracy using *ResNet-18*.

4.5 CONVERGENCE

In this experiment, we validate whether $\mathbf{w}_t$'s, where t is the number of epochs, obtained from AE-SAM can reach critical points of $\mathcal{L}(\mathcal{D}; \mathbf{w})$, as suggested in Theorem 3.4. From the experimental results in Section 4.1, Figure 7 shows $\|\nabla \mathcal{L}(\mathcal{D}; \mathbf{w}_t)\|^2$ w.r.t. t. As can be seen, in all settings, $\|\nabla \mathcal{L}(\mathcal{D}; \mathbf{w}_t)\|^2$ converges to 0. Figure 8 in Appendix B.1 also verifies the convergence of AE-SAM's training loss on *CIFAR-10* and *CIFAR-100*.



(a) *ResNet-18*. (b) *WRN-28-10*. (c) *PyramidNet-110*.

Figure 7: Squared gradient norms of AE-SAM with number of epochs. Best viewed in color.

5 CONCLUSION

In this paper, we proposed an adaptive policy to employ SAM based on the loss landscape geometry. Using the policy, we proposed an efficient AE-SAM algorithm to reduce the fraction of SAM updates during training. We theoretically and empirically analyzed the convergence of AE-SAM. Experimental results on a number of datasets and network architectures verify the advantage of the proposed policy. Moreover, the adaptive policy is general and can be combined with SAM variant, as demonstrated by the success of AE-LookSAM.

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A PROOFS

Let $\mathbb{I}_A(x)$ be an indicator function, i.e., $\mathbb{I}_A(x) = 1$ if $x \in A$ otherwise 0.

Lemma A.1 (Lemma 7 in Andriushchenko & Flammarion (2022))**.** *Let $\mathcal{L}(\mathcal{D}; \mathbf{w})$ be a β-smooth function. For any $\rho > 0$, we have*

$$\nabla\mathcal{L}(\mathcal{D}; \mathbf{w})^\top \nabla\mathcal{L}(\mathcal{D}; \mathbf{w} + \rho\nabla\mathcal{L}(\mathcal{D}; \mathbf{w})) \geq (1 - \rho\beta)\|\nabla\mathcal{L}(\mathcal{D}; \mathbf{w})\|^2. \tag{8}$$

A.1 PROOF OF THEOREM 3.2

Theorem 3.2. *Under Assumption 3.1, with full-batch gradient descent, if $\rho < \frac{1}{2\beta}$ and $\eta < \frac{1}{\beta}$, AE-SAM satisfies*

$$\min_{0\leq t\leq T-1} \|\nabla\mathcal{L}(\mathcal{D}; \mathbf{w}_t)\|^2 \leq \frac{2(\mathcal{L}(\mathcal{D}; \mathbf{w}_0) - \mathcal{L}(\mathcal{D}; \mathbf{w}_T))}{T\eta\,(1 - \beta\eta)}. \tag{9}$$

Proof. Let $\xi_t \equiv \mathbb{I}_{\{\mathbf{w}:\|\nabla\mathcal{L}(\mathcal{D};\mathbf{w})\|\geq\mu_t+c_t\sigma_t\}}(\mathbf{w}_t)$ be a variable indicates whether the SAM update or the ERM update is used at step t: $\xi_t = 1$ if SAM otherwise $\xi_t = 0$. Let $\mathbf{g}_t \equiv \nabla\mathcal{L}(\mathcal{D}; \mathbf{w}_t)$ and $\mathbf{h}_t \equiv \nabla\mathcal{L}(\mathcal{D}; \mathbf{w}_t + \rho\nabla\mathcal{L}(\mathcal{D}; \mathbf{w}_t))$ be the update direction of ERM and SAM, respectively. By Taylor expansion and $\mathcal{L}(\mathcal{D}; \mathbf{w})$ is β-smooth, we have

$$\begin{aligned}
&\mathcal{L}(\mathcal{D}; \mathbf{w}_{t+1}) \\
&\leq \mathcal{L}(\mathcal{D}; \mathbf{w}_t) + \mathbf{g}_t^\top(\mathbf{w}_{t+1} - \mathbf{w}_t) + \frac{\beta}{2}\|\mathbf{w}_{t+1} - \mathbf{w}_t\|^2 \\
&\leq \mathcal{L}(\mathcal{D}; \mathbf{w}_t) - \eta\mathbf{g}_t^\top\left((1 - \xi_t)\mathbf{g}_t + \xi_t\mathbf{h}_t\right) + \frac{\beta\eta^2}{2}\|(1 - \xi_t)\mathbf{g}_t + \xi_t\mathbf{h}_t\|^2 \\
&= \mathcal{L}(\mathcal{D}; \mathbf{w}_t) - \eta(1-\xi_t)\|\mathbf{g}_t\|^2 - \eta\xi_t\mathbf{g}_t^\top\mathbf{h}_t + \frac{\beta\eta^2}{2}\left((1-\xi_t)\|\mathbf{g}_t\|^2 + \xi_t\|\mathbf{h}_t\|^2 + \underbrace{2\xi_t(1-\xi_t)\mathbf{g}_t^\top\mathbf{h}_t}_{=0}\right) && (10) \\
&= \mathcal{L}(\mathcal{D}; \mathbf{w}_t) - \eta\left(1 - \xi_t - \frac{\beta\eta(1 - \xi_t)}{2}\right)\|\mathbf{g}_t\|^2 + \frac{\beta\eta^2\xi_t}{2}\|\mathbf{h}_t\|^2 - \eta\xi_t\mathbf{g}_t^\top\mathbf{h}_t, && (11)
\end{aligned}$$

where we have used $\xi_t(1 - \xi_t) = 0$ as $\xi_t \in \{0, 1\}$, $\xi_t^2 = \xi_t$, and $(1 - \xi_t)^2 = 1 - \xi_t$ to obtain Eq.(10).

As $\|\mathbf{h}_t\|^2 = \|\mathbf{h}_t - \mathbf{g}_t\|^2 - \|\mathbf{g}_t\|^2 + 2\mathbf{g}_t^\top \mathbf{h}_t$, it follows from Eq. (11) that

$$
\begin{aligned}
&\mathcal{L}(\mathcal{D}; \mathbf{w}_{t+1}) \\
=&\mathcal{L}(\mathcal{D}; \mathbf{w}_t) - \eta\left(1 - \xi_t - \frac{\beta\eta(1-\xi_t)}{2}\right)\|\mathbf{g}_t\|^2 + \frac{\beta\eta^2\xi_t}{2}\left(\|\mathbf{h}_t - \mathbf{g}_t\|^2 - \|\mathbf{g}_t\|^2 + 2\mathbf{g}_t^\top \mathbf{h}_t\right) - \eta\xi_t \mathbf{g}_t^\top \mathbf{h}_t \\
\leq&\mathcal{L}(\mathcal{D}; \mathbf{w}_t) - \eta\left(1 - \xi_t - \frac{\beta\eta(1-\xi_t)}{2} + \frac{\beta\eta\xi_t}{2}\right)\|\mathbf{g}_t\|^2 + \frac{\beta\eta^2\xi_t}{2}\|\mathbf{h}_t - \mathbf{g}_t\|^2 - \eta(1-\beta\eta)\xi_t \mathbf{g}_t^\top \mathbf{h}_t \\
\leq&\mathcal{L}(\mathcal{D}; \mathbf{w}_t) - \eta\left(1 - \xi_t - \frac{\beta\eta(1-\xi_t)}{2} + \frac{\beta\eta\xi_t}{2}\right)\|\mathbf{g}_t\|^2 + \frac{\beta^3\eta^2\rho^2\xi_t}{2}\|\mathbf{g}_t\|^2 - \eta(1-\beta\eta)\xi_t \mathbf{g}_t^\top \mathbf{h}_t \quad (12) \\
=&\mathcal{L}(\mathcal{D}; \mathbf{w}_t) - \eta\left(1 - \xi_t - \frac{\beta\eta(1-\xi_t)}{2} + \frac{\beta\eta\xi_t}{2} + \frac{\beta^3\eta\rho^2\xi_t}{2} + (1-\beta\eta)(1-\beta\rho)\xi_t\right)\|\mathbf{g}_t\|^2 \quad (13) \\
=&\mathcal{L}(\mathcal{D}; \mathbf{w}_t) - \eta\left(1 - \frac{\beta\eta(1-\xi_t)}{2} + \frac{\beta\eta\xi_t}{2} + \frac{\beta^3\eta\xi_t\rho^2}{2} - \beta\eta\xi_t - \beta\rho\xi_t + \beta^2\eta\rho\xi_t\right)\|\mathbf{g}_t\|^2 \\
\leq&\mathcal{L}(\mathcal{D}; \mathbf{w}_t) - \eta\left(1 - \frac{\beta\eta}{2} - \beta\rho\xi_t\right)\|\mathbf{g}_t\|^2, \quad (14)
\end{aligned}
$$

where we have used $\|\mathbf{h}_t - \mathbf{g}_t\|^2 = \|\nabla\mathcal{L}(\mathcal{D}; \mathbf{w}_t + \rho\nabla\mathcal{L}(\mathcal{D}; \mathbf{w}_t)) - \nabla\mathcal{L}(\mathcal{D}; \mathbf{w}_t)\|^2 \leq \beta^2\rho^2\|\nabla\mathcal{L}(\mathcal{D}; \mathbf{w}_t)\|^2 = \beta^2\rho^2\|\mathbf{g}_t\|^2$ to obtain (12), and Lemma A.1 to obtain (13).

Summing over t from $t = 0$ to $T - 1$ on both sides of Eq.(14) and rearranging, we have

$$
\sum_{t=0}^{T-1} \eta\left(1 - \frac{\beta\eta}{2} - \beta\rho\xi_t\right)\|\mathbf{g}_t\|^2 \leq \mathcal{L}(\mathcal{D}; \mathbf{w}_0) - \mathcal{L}(\mathcal{D}; \mathbf{w}_T). \quad (15)
$$

As $\rho < \frac{1}{2\beta}$ and $\eta < \frac{1}{\beta}$, it follows that $1 - \frac{\beta\eta}{2} - \beta\rho\xi_t > 0$ for all t. Thus, Eq. (15) implies

$$
\begin{aligned}
\min_{0\leq t\leq T-1}\|\mathbf{g}_t\|^2 \leq \frac{\mathcal{L}(\mathbf{w}_0) - \mathcal{L}(\mathcal{D}; \mathbf{w}_T)}{\sum_{t=0}^{T-1}\eta\left(1 - \frac{\beta\eta}{2} - \xi_t\beta\rho\right)} &= \frac{\mathcal{L}(\mathcal{D}; \mathbf{w}_0) - \mathcal{L}(\mathcal{D}; \mathbf{w}_T)}{T\eta\left(1 - \frac{\beta\eta}{2} - \beta\rho\zeta\right)} \\
&\leq \frac{2(\mathcal{L}(\mathcal{D}; \mathbf{w}_0) - \mathcal{L}(\mathcal{D}; \mathbf{w}_T))}{T\eta\,(1-\beta\eta)},
\end{aligned} \quad (16)
$$

where $\zeta = \frac{1}{T}\sum_{t=0}^{T-1}\xi_t = \frac{1}{T}\sum_{t=0}^{T-1}\mathbb{I}_{\{\mathbf{w}:\|\nabla\mathcal{L}(\mathcal{D};\mathbf{w})\|\geq\mu_t + c_t\sigma_t\}}(\mathbf{w}_t) \in [0, 1]$ and we conclude that AE-SAM reaches critical points at an $\mathcal{O}\left(\frac{1}{T}\right)$ rate. □

A.2 Proof of Theorem 3.4

Theorem 3.4. *Under Assumptions 3.1 and 3.3, let b be the mini-batch size. If $\eta = \frac{1}{4\beta\sqrt{T}}$ and $\rho = 1/T^{\frac{1}{4}}$, AE-SAM satisfies*

$$
\min_{0\leq t\leq T-1}\mathbb{E}\|\nabla\mathcal{L}(\mathcal{D}; \mathbf{w}_t)\|^2 \leq \frac{32\beta(\mathbb{E}\mathcal{L}(\mathcal{D}; \mathbf{w}_0) - \mathbb{E}\mathcal{L}(\mathcal{D}; \mathbf{w}_T))}{3\sqrt{T}} + \frac{4\beta\sigma^2(8 + 4\beta + 4\beta^2)}{b\sqrt{T}}. \quad (17)
$$

Lemma A.2 ((Andriushchenko & Flammarion, 2022))**.** *Under Assumptions 3.1 and 3.3 for all t and $\rho > 0$, we have*

$$
\mathbb{E}\nabla\mathcal{L}(\mathcal{B}_t; \mathbf{w} + \rho\nabla\mathcal{L}(\mathcal{B}_t; \mathbf{w}))^\top\nabla\mathcal{L}(\mathcal{D}; \mathbf{w}) \geq \left(\frac{1}{2} - \rho\beta\right)\|\nabla\mathcal{L}(\mathcal{D}; \mathbf{w})\|^2 - \frac{\beta^2\rho^2\sigma^2}{2b}. \quad (18)
$$

Proof. Let $\mathbf{g}_t \equiv \frac{1}{b}\sum_{(\mathbf{x}_i, y_i)\in\mathcal{B}_t}\nabla\ell(f(\mathbf{x}_i; \mathbf{w}_t), y_i)$, $\mathbf{h}_t \equiv \frac{1}{b}\sum_{(\mathbf{x}_i, y_i)\in\mathcal{B}_t}\nabla\ell(f(\mathbf{x}_i; \mathbf{w}_t + \rho\mathbf{g}_t), y_i)$, and $\hat{\mathbf{g}}_t \equiv \nabla\mathcal{L}(\mathcal{D}; \mathbf{w}_t)$. Let $\xi_t \equiv \mathbb{I}_{\{\mathbf{w}:\|\nabla\mathcal{L}(\mathcal{D};\mathbf{w})\|\geq\mu_t + c_t\sigma_t\}}(\mathbf{w}_t)$ as above.

By Taylor expansion and $\mathcal{L}(\mathcal{D};\mathbf{w})$ is β-smooth, we have

$$\begin{aligned}
&\mathcal{L}(\mathcal{D};\mathbf{w}_{t+1})\\
\leq&\mathcal{L}(\mathcal{D};\mathbf{w}_t)+\hat{\mathbf{g}}_t^\top(\mathbf{w}_{t+1}-\mathbf{w}_t)+\frac{\beta}{2}\|\mathbf{w}_{t+1}-\mathbf{w}_t\|^2\\
\leq&\mathcal{L}(\mathcal{D};\mathbf{w}_t)-\eta\hat{\mathbf{g}}_t^\top\left((1-\xi_t)\mathbf{g}_t+\xi_t\mathbf{h}_t\right)+\frac{\beta\eta^2}{2}\|(1-\xi_t)\mathbf{g}_t+\xi_t\mathbf{h}_t\|^2\\
=&\mathcal{L}(\mathcal{D};\mathbf{w}_t)-\eta(1-\xi_t)\hat{\mathbf{g}}_t^\top\mathbf{g}_t-\eta\xi_t\hat{\mathbf{g}}_t^\top\mathbf{h}_t+\frac{\beta\eta^2}{2}\left((1-\xi_t)\|\mathbf{g}_t\|^2+\xi_t\|\mathbf{h}_t\|^2+\underbrace{2\xi_t(1-\xi_t)\mathbf{g}_t^\top\mathbf{h}_t}_{=0}\right) \quad (19)\\
=&\mathcal{L}(\mathcal{D};\mathbf{w}_t)-\eta(1-\xi_t)\hat{\mathbf{g}}_t^\top\mathbf{g}_t-\eta\xi_t\hat{\mathbf{g}}_t^\top\mathbf{h}_t+\frac{\beta\eta^2}{2}\left((1-\xi_t)\|\mathbf{g}_t\|^2+\xi_t\|\mathbf{h}_t\|^2\right), \quad (20)
\end{aligned}$$

where we have used $\xi_t(1-\xi_t)=0$ as $\xi_t\in\{0,1\}$, $\xi_t^2=\xi_t$, and $(1-\xi_t)^2=1-\xi_t$ to obtain Eq.(19). Taking expectation w.r.t. $\mathbf{w}_t$ on both sides of (20), we have

$$\mathbb{E}\mathcal{L}(\mathcal{D};\mathbf{w}_{t+1})\leq\mathbb{E}\mathcal{L}(\mathcal{D};\mathbf{w}_t)-\eta(1-\xi_t)\mathbb{E}\|\hat{\mathbf{g}}_t\|^2-\eta\xi_t\mathbb{E}\hat{\mathbf{g}}_t^\top\mathbf{h}_t+\frac{\beta\eta^2(1-\xi_t)}{2}\mathbb{E}\|\mathbf{g}_t\|^2+\frac{\beta\eta^2\xi_t}{2}\mathbb{E}\|\mathbf{h}_t\|^2. \quad (21)$$

Claim 1: $\mathbb{E}\|\mathbf{g}_t\|^2=\mathbb{E}\|\mathbf{g}_t-\hat{\mathbf{g}}_t\|^2+\mathbb{E}\|\hat{\mathbf{g}}_t\|^2=\frac{\sigma^2}{b}+\mathbb{E}\|\hat{\mathbf{g}}_t\|^2$, which follows from Assumption 3.3.

Claim 2: $\mathbb{E}\|\mathbf{h}_t\|^2\leq 2(1+\rho^2\beta^2)\frac{\sigma^2}{b}-(1-2\rho^2\beta^2)\mathbb{E}\|\hat{\mathbf{g}}_t\|^2+2\mathbb{E}\hat{\mathbf{g}}_t^\top\mathbf{h}_t$, which is derived as follows:

$$\begin{aligned}
\mathbb{E}\|\mathbf{h}_t\|^2&=\mathbb{E}\|\mathbf{h}_t-\hat{\mathbf{g}}_t\|^2-\mathbb{E}\|\hat{\mathbf{g}}_t\|^2+2\mathbb{E}\hat{\mathbf{g}}_t^\top\mathbf{h}_t\\
&=2\mathbb{E}\|\mathbf{h}_t-\mathbf{g}_t\|^2+2\mathbb{E}\|\mathbf{g}_t-\hat{\mathbf{g}}_t\|^2-\mathbb{E}\|\hat{\mathbf{g}}_t\|^2+2\mathbb{E}\hat{\mathbf{g}}_t^\top\mathbf{h}_t\\
&\leq 2\rho^2\beta^2\mathbb{E}\|\mathbf{g}_t\|^2+\frac{2\sigma^2}{b}-\mathbb{E}\|\hat{\mathbf{g}}_t\|^2+2\mathbb{E}\hat{\mathbf{g}}_t^\top\mathbf{h}_t \quad (22)\\
&\leq 2\rho^2\beta^2\left(\frac{\sigma^2}{b}+\mathbb{E}\|\hat{\mathbf{g}}_t\|^2\right)+\frac{2\sigma^2}{b}-\mathbb{E}\|\hat{\mathbf{g}}_t\|^2+2\mathbb{E}\hat{\mathbf{g}}_t^\top\mathbf{h}_t \quad (23)\\
&=2(1+\rho^2\beta^2)\frac{\sigma^2}{b}-(1-2\rho^2\beta^2)\mathbb{E}\|\hat{\mathbf{g}}_t\|^2+2\mathbb{E}\hat{\mathbf{g}}_t^\top\mathbf{h}_t, \quad (24)
\end{aligned}$$

where Eq.(22) follows from $\|\mathbf{h}_t-\mathbf{g}_t\|\leq\rho\beta\|\mathbf{g}_t\|$ and Assumption 3.3, Eq.(23) follows from the above Claim 1.

Substituting Claims 1 and 2 into (21), we obtain

$$\begin{aligned}
&\mathbb{E}\mathcal{L}(\mathcal{D};\mathbf{w}_{t+1})\\
&\leq\mathbb{E}\mathcal{L}(\mathcal{D};\mathbf{w}_t)-\eta\left(1-\xi_t\right)\mathbb{E}\|\hat{\mathbf{g}}_t\|^2-\eta\xi_t\mathbb{E}\hat{\mathbf{g}}_t^\top\mathbf{h}_t+\frac{\beta\eta^2(1-\xi_t)}{2}\left(\frac{\sigma^2}{b}+\mathbb{E}\|\hat{\mathbf{g}}_t\|^2\right)\\
&\quad+\frac{\beta\eta^2\xi_t}{2}\left(2(1+\rho^2\beta^2)\frac{\sigma^2}{b}-(1-2\rho^2\beta^2)\mathbb{E}\|\hat{\mathbf{g}}_t\|^2+2\mathbb{E}\hat{\mathbf{g}}_t^\top\mathbf{h}_t\right) \quad (25)\\
&=\mathbb{E}\mathcal{L}(\mathcal{D};\mathbf{w}_t)-\eta\left(1-\xi_t-\frac{\beta\eta(1-\xi_t)}{2}+\frac{\beta\eta\xi_t(1-2\rho^2\beta^2)}{2}\right)\mathbb{E}\|\hat{\mathbf{g}}_t\|^2-\eta\xi_t\left(1-\eta\beta\right)\mathbb{E}\hat{\mathbf{g}}_t^\top\mathbf{h}_t\\
&\quad+\left(\frac{\beta\eta^2(1-\xi_t)}{2}+\beta\eta^2\xi_t(1+\rho^2\beta^2)\right)\frac{\sigma^2}{b}\\
&\leq\mathbb{E}\mathcal{L}(\mathcal{D};\mathbf{w}_t)-\eta\left(1-\xi_t-\frac{\beta\eta(1-\xi_t)}{2}+\frac{\beta\eta\xi_t(1-2\rho^2\beta^2)}{2}+\xi_t\left(1-\eta\beta\right)\left(\frac{1}{2}-\rho\beta\right)\right)\mathbb{E}\|\hat{\mathbf{g}}_t\|^2\\
&\quad+\left(\frac{\beta\eta^2(1-\xi_t)}{2}+\beta\eta^2\xi_t(1+\rho^2\beta^2)+\eta\xi_t\left(1-\eta\beta\right)\frac{\beta^2\rho^2}{2}\right)\frac{\sigma^2}{b} \quad (26)\\
&\leq\mathbb{E}\mathcal{L}(\mathcal{D};\mathbf{w}_t)-\eta\left(1-(1+\beta\eta-2\rho\beta)\frac{\xi_t}{2}-\frac{\beta\eta}{2}\right)\mathbb{E}\|\hat{\mathbf{g}}_t\|^2\\
&\quad+\left(\eta+\xi_t(\eta+2\eta\rho^2\beta^2+\beta\rho^2-\eta\beta^2\rho^2)\right)\frac{\eta\beta\sigma^2}{2b}, \quad (27)
\end{aligned}$$

where Eq.(25) follows from Claims 1 and 2, Eq.(26) follows from Lemma A.2 and $1-\eta\beta>0$. As $\eta<\frac{1}{2\beta}$, we have $1+\beta\eta-2\rho\beta\leq 3/2$ and $\beta\eta<1/2$, thus, $1-(1+\beta\eta-2\rho\beta)\frac{\xi_t}{2}-\frac{\beta\eta}{2}>0$.

Summing over t on both sides of Eq.(27) and rearranging, we obtain

$$\begin{aligned}
\min_{0\leq t\leq T-1}\mathbb{E}\|\hat{\mathbf{g}}_t\|^2 &\leq \frac{\mathbb{E}\mathcal{L}(\mathcal{D};\mathbf{w}_0)-\mathbb{E}\mathcal{L}(\mathcal{D};\mathbf{w}_T)}{\eta\sum_{t=0}^{T-1}\left(1-(1+\beta\eta-2\rho\beta)\frac{\xi_t}{2}-\frac{\beta\eta}{2}\right)} \\
&\quad+\frac{\sum_{t=0}^{T-1}\left(\eta+\xi_t(\eta+\eta\rho^2\beta^2+\beta\rho^2)\right)}{\sum_{t=0}^{T-1}\left(1-(1+\beta\eta-2\rho\beta)\frac{\xi_t}{2}-\frac{\beta\eta}{2}\right)}\frac{\beta\sigma^2}{2b} \\
&=\frac{\mathbb{E}\mathcal{L}(\mathcal{D};\mathbf{w}_0)-\mathbb{E}\mathcal{L}(\mathcal{D};\mathbf{w}_T)}{T\eta(1-\frac{\gamma\zeta}{2}-\frac{\beta\eta}{2})}+\frac{T(\eta+\eta\kappa\zeta+\beta\rho^2\zeta)\beta\sigma^2}{2bT(1-\frac{\gamma\zeta}{2}-\frac{\beta\eta}{2})} \qquad (28)\\
&=\frac{\mathbb{E}\mathcal{L}(\mathcal{D};\mathbf{w}_0)-\mathbb{E}\mathcal{L}(\mathcal{D};\mathbf{w}_T)}{T\eta(1-\frac{\gamma\zeta}{2}-\frac{\beta\eta}{2})}+\frac{(1+\kappa\zeta+\beta\zeta)\beta\sigma^2}{b\sqrt{T}(2-\gamma\zeta-\beta\eta)} \qquad (29)\\
&\leq\frac{2(\mathbb{E}\mathcal{L}(\mathcal{D};\mathbf{w}_0)-\mathbb{E}\mathcal{L}(\mathcal{D};\mathbf{w}_T))}{T\eta(1-\beta\eta)}+\frac{(2+\beta+\beta^2)\beta\sigma^2}{b\sqrt{T}(\frac{1}{2}-\beta\eta)}, \qquad (30)
\end{aligned}$$

where $\gamma=1+\beta\eta-2\rho\beta\leq 3/2$, $\kappa=1+\rho^2\beta^2$, $\rho^2=1/\sqrt{T}$, and $\zeta=\frac{1}{T}\sum_{t=0}^{T-1}\xi_t=\frac{1}{T}\sum_{t=0}^{T-1}\mathbb{I}_{\{\mathbf{w}:\|\nabla\mathcal{L}(\mathcal{B}_t;\mathbf{w})\|\geq\mu_t+c_t\sigma_t\}}(\mathbf{w}_t)\in[0,1]$.

As $\frac{1}{2}-\beta\eta\geq\frac{1}{2}-\frac{1}{4}=\frac{1}{4}$ and $\eta(1-\beta\eta)=\frac{1}{4\beta\sqrt{T}}(1-\frac{\beta}{4\beta\sqrt{T}})\geq\frac{3}{16\beta\sqrt{T}}$, the upper bound in Eq.(30) can be simplified as

$$\min_{0\leq t\leq T-1}\mathbb{E}\|\hat{\mathbf{g}}_t\|^2\leq\frac{32\beta(\mathbb{E}\mathcal{L}(\mathcal{D};\mathbf{w}_0)-\mathbb{E}\mathcal{L}(\mathcal{D};\mathbf{w}_T))}{3\sqrt{T}}+\frac{4\beta\sigma^2(8+4\beta+4\beta^2)}{b\sqrt{T}}, \qquad (31)$$

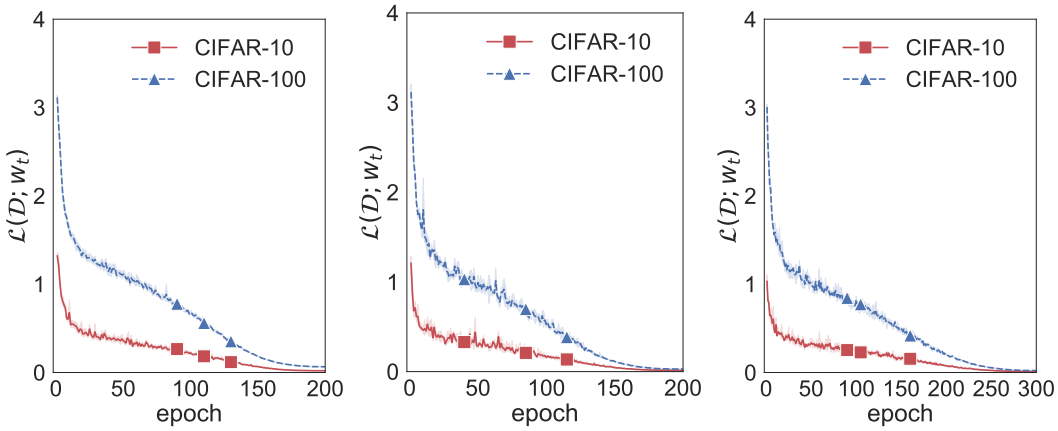
and we finish the proof.

□

B Additional Experiments

B.1 Additional Experimental Results on *CIFAR-10* and *CIFAR-100*

Figure 8 shows the convergence of AE-SAM's training loss on *CIFAR-10* and *CIFAR-100* datasets. As can be seen, AE-SAM achieves convergence in various network architectures.



(a) *ResNet-18*. (b) *WRN-28-10*. (c) *PyramidNet-110*.

Figure 8: Training loss of AE-SAM with number of epochs on *CIFAR-10* and *CIFAR-100*. Best viewed in color.

B.2 ADDITIONAL EXPERIMENTAL RESULTS ON *CIFAR-10* WITH LABEL NOISE

Table 4 reports the testing accuracy and fraction of SAM updates on *CIFAR-10* with label noise.

Table 4: Testing accuracy and fraction of SAM updates on *CIFAR-10* with different levels of label noise. The best accuracy is in bold and the second best is underlined.

		noise = 20%		noise = 40%		noise = 60%		noise = 80%	
		Accuracy	%SAM	Accuracy	%SAM	Accuracy	%SAM	Accuracy	%SAM
ResNet-18	ERM	87.92 ±0.02	0.0 ±0.0	70.82 ±0.33	0.0 ±0.0	49.61 ±0.39	0.0 ±0.0	28.23 ±0.40	0.0 ±0.0
	SAM (Foret et al., 2021)	**94.80** ±0.05	100.0 ±0.0	<u>91.50</u> ±0.22	100.0 ±0.0	**88.15** ±0.23	100.0 ±0.0	**77.40** ±0.21	100.0 ±0.0
	ESAM (Du et al., 2021)	94.19 ±0.10	100.0 ±0.0	91.46 ±0.49	100.0 ±0.0	81.29 ±0.69	100.0 ±0.0	15.00 ±4.89	100.0 ±0.0
	SS-SAM (Zhao et al., 2022b)	90.62 ±0.37	50.0 ±0.0	77.84 ±0.56	50.0 ±0.0	61.18 ±0.87	50.0 ±0.0	47.32 ±1.50	50.0 ±0.0
	AE-SAM	92.84 ±0.25	50.0 ±0.1	84.17 ±0.53	50.0 ±0.0	73.54 ±0.50	49.9 ±0.0	65.00 ±2.25	50.0 ±0.0
	LookSAM (Liu et al., 2022)	92.72 ±0.18	50.0 ±0.0	88.04 ±0.40	50.0 ±0.0	72.26 ±1.75	50.0 ±0.0	69.72 ±1.52	50.0 ±0.0
	AE-LookSAM	<u>94.34</u> ±0.29	49.9 ±0.0	**91.58** ±0.54	50.0 ±0.0	<u>87.85</u> ±0.23	50.0 ±0.0	<u>76.90</u> ±0.32	50.0 ±0.0
ResNet-32	ERM	87.43 ±0.0	0.0 ±0.00	70.82 ±0.98	0.0 ±0.0	46.26 ±0.18	0.0 ±0.0	29.00 ±1.79	0.0 ±0.0
	SAM (Foret et al., 2021)	**95.08** ±0.23	100.0 ±0.0	91.01 ±0.41	100.0 ±0.0	**88.90** ±0.39	100.0 ±0.0	**77.32** ±0.12	100.0 ±0.0
	ESAM (Du et al., 2021)	93.42 ±0.50	100.0 ±0.0	<u>91.63</u> ±0.29	100.0 ±0.0	82.73 ±1.21	100.0 ±0.0	10.09 ±0.10	100.0 ±0.0
	SS-SAM (Zhao et al., 2022b)	89.63 ±0.26	50.0 ±0.0	74.17 ±0.47	50.0 ±0.0	58.40 ±2.95	50.0 ±0.0	59.53 ±1.63	50.0 ±0.0
	AE-SAM	92.87 ±0.17	50.0 ±0.0	82.85 ±2.16	50.0 ±0.0	71.50 ±0.74	50.0 ±0.0	65.43 ±3.19	50.3 ±0.0
	LookSAM (Liu et al., 2022)	92.49 ±0.05	50.0 ±0.0	86.56 ±0.92	50.0 ±0.0	63.35 ±0.48	50.0 ±0.0	68.01 ±5.37	50.0 ±0.0
	AE-LookSAM	<u>94.70</u> ±0.10	50.0 ±0.0	**91.80** ±0.87	50.0 ±0.0	<u>88.22</u> ±0.27	50.0 ±0.0	<u>77.03</u> ±0.16	49.8 ±0.1

Effects of k on LookSAM. We conduct an additional experiment on *CIFAR-10* with label noise to show that the performance of LookSAM is sensitive to the choice of k. Table 5 reports the testing accuracy and fraction of SAM updates using LookSAM with different $k \in \{2, 3, 4, 5\}$ for *ResNet-18*. As can be seen, $k = 2$ yields better performance than $k = 3, 4$, or 5, particularly in the higher noisy levels (e.g., 80%).

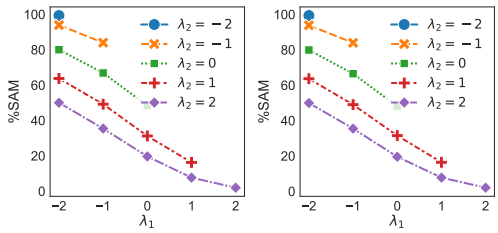
Table 5: Effects of k in LookSAM on *CIFAR-10* with different levels of label noise using *ResNet-18*.

	noise = 20%		noise = 40%		noise = 60%		noise = 80%	
	accuracy	%SAM	accuracy	%SAM	accuracy	%SAM	accuracy	%SAM
LookSAM ($k = 5$)	88.57	20.0	73.90	20.0	56.80	20.0	51.82	20.0
LookSAM ($k = 4$)	89.00	25.0	74.12	25.0	58.17	25.0	52.28	25.0
LookSAM ($k = 3$)	89.07	33.3	75.38	33.3	63.79	33.3	53.87	33.3
LookSAM ($k = 2$)	**92.72**	50.0	**88.04**	50.0	**72.26**	50.0	**69.72**	50.0

Effects of λ_1 and λ_2 on AE-LookSAM. We study the effects of λ_1 and λ_2 on AE-LookSAM. We conduct an experiment on *CIFAR-10* with label noise (80% noisy level), where AE-LookSAM achieves comparable performance.

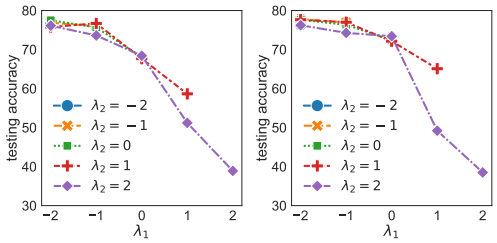
Figure 9 shows the effects of λ_1 and λ_2 on fraction of SAM updates. As can be seen, again, for a fixed λ_2, increasing λ_1 always reduces the fraction of SAM updates.

Figure 10 shows the effects of λ_1 and λ_2 on testing accuracy of AE-SAM. We can see that for a fixed $\lambda_2 \in \{0, 1, 2\}$ (particularly $\lambda_2 = 2$), increasing λ_1 always leads a reduction in testing accuracy.



(a) *ResNet-18*. (b) *ResNet-32*.

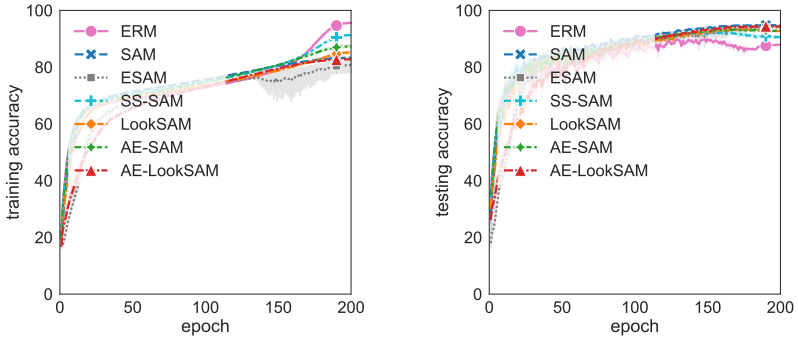
Figure 9: Effects of λ_1 and λ_2 on fraction of SAM updates on *CIFAR-10* with label noise (noisy level of 80%).



(a) *ResNet-18*. (b) *ResNet-32*.

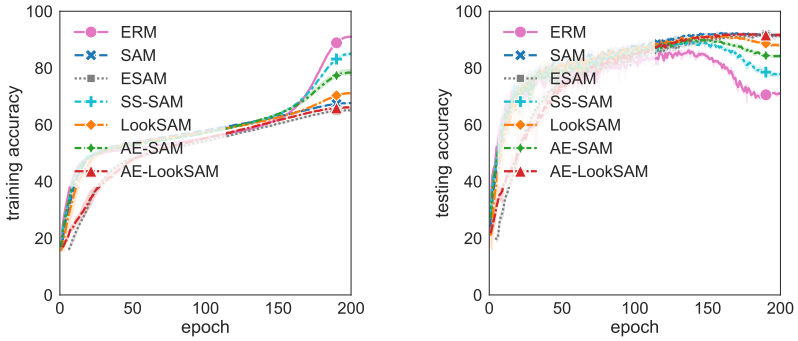
Figure 10: Effects of λ_1 and λ_2 on testing accuracy on *CIFAR-10* with label noise (noisy level of 80%).

Curves of training and testing accuracy. For *ResNet-18*, Figures 11, 12, and 13 show the curves of accuracies at noise levels of 20%, 40%, and 60%, respectively; For *ResNet-32*, Figures 14, 15, , 16, and 17 show the curves of accuracies at noise levels of 20%, 40%, 60%, and 80%, respectively. As can be seen, in all settings, AE-LookSAM is robust to labels noise like SAM.



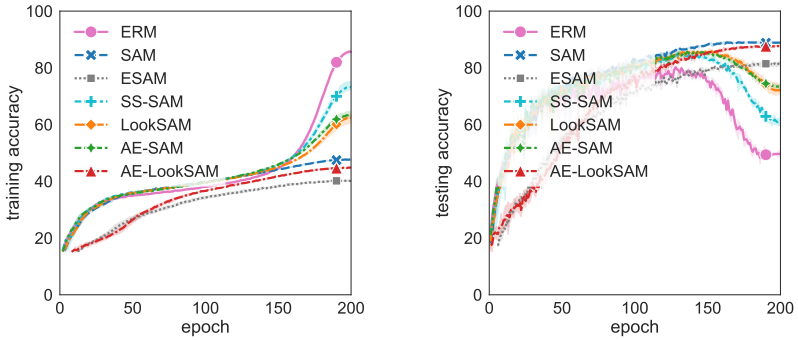
(a) Training. (b) Testing.

Figure 11: Accuracies with number of epochs on CIFAR-10 with 20% noisy level using *ResNet-18*.



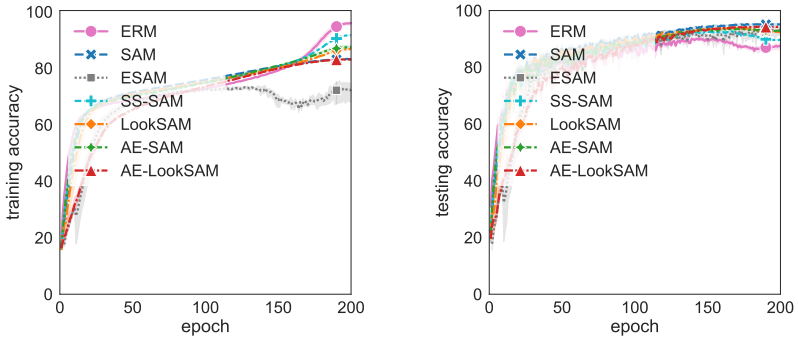
(a) Training. (b) Testing.

Figure 12: Accuracies with number of epochs on CIFAR-10 with 40% noisy level using *ResNet-18*.



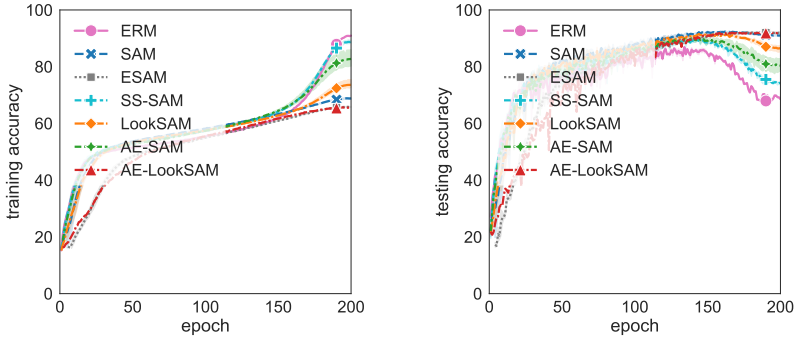
(a) Training. (b) Testing.

Figure 13: Accuracies with number of epochs on CIFAR-10 with 60% noisy level using *ResNet-18*.



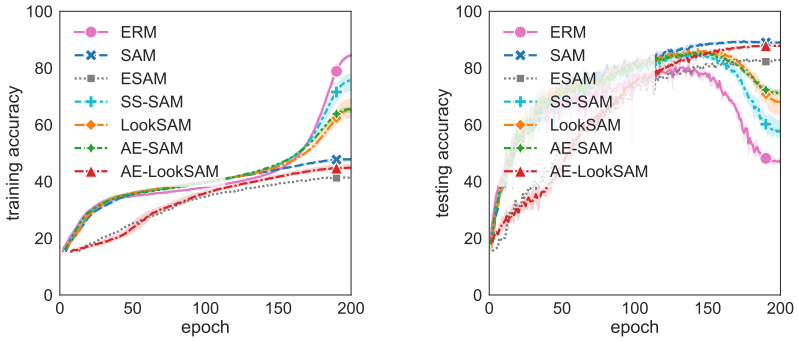
(a) Training. (b) Testing.

Figure 14: Accuracies with number of epochs on CIFAR-10 with 20% noisy level using *ResNet-32*.



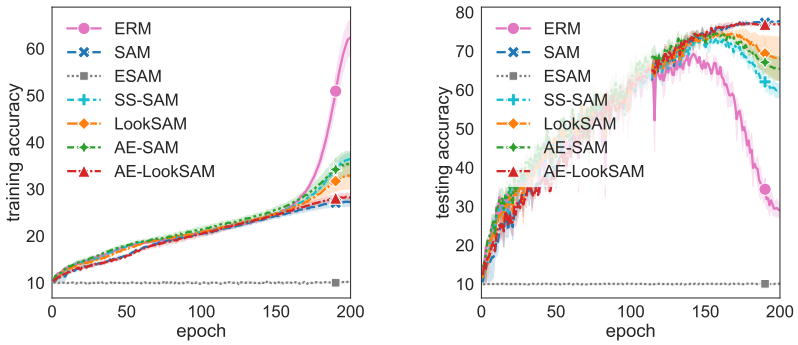
(a) Training. (b) Testing.

Figure 15: Accuracies with number of epochs on CIFAR-10 with 40% noisy level using *ResNet-32*.



(a) Training. (b) Testing.

Figure 16: Accuracies with number of epochs on CIFAR-10 with 60% noisy level using *ResNet-32*.



(a) Training. (b) Testing.

Figure 17: Accuracies with number of epochs on CIFAR-10 with 80% noisy level using *ResNet-32*.