

APPENDIX FOR

Sharpness-Aware Minimization with Adaptive Regularization for Training Deep Neural Networks

A. Proof of Theorem 1

A significant conclusion (3) could be deduced from Hypothesis 2. If $\nabla f(\mathbf{x})$ has a Lipschitz gradient with constant $L > 0$, we have

$$\begin{aligned} f(\mathbf{x}_{k+1}) - f(\mathbf{x}_k) &\leq \langle \nabla f(\mathbf{x}_k), \mathbf{x}_{k+1} - \mathbf{x}_k \rangle + \frac{L}{2} \|\mathbf{x}_{k+1} - \mathbf{x}_k\|^2 \\ &= -\eta_k \langle \nabla f(\mathbf{x}_k), (1 - \lambda_k) \mathbf{g}(\mathbf{x}_k) + \lambda_k \mathbf{g}(\mathbf{x}_k + \boldsymbol{\epsilon}_{\mathbf{x}_k}) \rangle + \frac{L}{2} \eta_k^2 \|(1 - \lambda_k) \mathbf{g}(\mathbf{x}_k) + \lambda_k \mathbf{g}(\mathbf{x}_k + \boldsymbol{\epsilon}_{\mathbf{x}_k})\|^2 \\ &= \underbrace{-\eta_k \langle \nabla f(\mathbf{x}_k), (1 - \lambda_k) \mathbf{g}(\mathbf{x}_k) \rangle}_{:=\spadesuit} - \underbrace{\eta_k \langle \nabla f(\mathbf{x}_k), \lambda_k \mathbf{g}(\mathbf{x}_k + \boldsymbol{\epsilon}_{\mathbf{x}_k}) \rangle}_{:=\heartsuit} + \underbrace{\frac{L}{2} \eta_k^2 \|(1 - \lambda_k) \mathbf{g}(\mathbf{x}_k) + \lambda_k \mathbf{g}(\mathbf{x}_k + \boldsymbol{\epsilon}_{\mathbf{x}_k})\|^2}_{:=\clubsuit}. \end{aligned} \quad (3)$$

We calculate each of the above three parts respectively

$$\begin{aligned} \spadesuit &= -\eta_k \langle \nabla f(\mathbf{x}_k), (1 - \lambda_k) \mathbf{g}(\mathbf{x}_k) \rangle \\ &= -\eta_k (1 - \lambda_k) [\langle \nabla f(\mathbf{x}_k), \mathbf{g}(\mathbf{x}_k) - \nabla f(\mathbf{x}_k) \rangle] - \eta_k (1 - \lambda_k) \|\nabla f(\mathbf{x}_k)\|^2, \end{aligned} \quad (4)$$

$$\begin{aligned} \heartsuit &= -\eta_k \langle \nabla f(\mathbf{x}_k), \lambda_k \mathbf{g}(\mathbf{x}_k + \boldsymbol{\epsilon}_{\mathbf{x}_k}) \rangle \\ &= -\eta_k \lambda_k \langle \nabla f(\mathbf{x}_k), \mathbf{g}(\mathbf{x}_k + \boldsymbol{\epsilon}_{\mathbf{x}_k}) - \mathbf{g}(\mathbf{x}_k) \rangle - \eta_k \lambda_k \langle \nabla f(\mathbf{x}_k), \mathbf{g}(\mathbf{x}_k) - \nabla f(\mathbf{x}_k) \rangle - \eta_k \lambda_k \|\nabla f(\mathbf{x}_k)\|^2 \\ &\stackrel{(a)}{\leq} \eta_k \lambda_k L \rho \|\nabla f(\mathbf{x}_k)\| - \eta_k \lambda_k \|\nabla f(\mathbf{x}_k)\|^2 - \eta_k \lambda_k \langle \nabla f(\mathbf{x}_k), \mathbf{g}(\mathbf{x}_k) - \nabla f(\mathbf{x}_k) \rangle, \end{aligned} \quad (5)$$

$$\begin{aligned} \clubsuit &= \frac{L}{2} \eta_k^2 \|(1 - \lambda_k) \mathbf{g}(\mathbf{x}_k) + \lambda_k \mathbf{g}(\mathbf{x}_k + \boldsymbol{\epsilon}_{\mathbf{x}_k})\|^2 \\ &\stackrel{(b)}{\leq} L \eta_k^2 [(1 - \lambda_k)^2 \|\mathbf{g}(\mathbf{x}_k)\|^2 + \lambda_k^2 \|\mathbf{g}(\mathbf{x}_k + \boldsymbol{\epsilon}_{\mathbf{x}_k})\|^2], \end{aligned} \quad (6)$$

where the inequality (a) uses Lipschitz continuity $\|\mathbf{g}(\mathbf{x}_k + \boldsymbol{\epsilon}_{\mathbf{x}_k}) - \mathbf{g}(\mathbf{x}_k)\| \leq L \|\boldsymbol{\epsilon}_{\mathbf{x}_k}\|$ and the Cauchy's inequality $\langle \mathbf{x}, \mathbf{y} \rangle \leq \|\mathbf{x}\| \cdot \|\mathbf{y}\|$. The inequality (b) depends on the inequality $\|\mathbf{a} + \mathbf{b}\|^2 \leq 2\|\mathbf{a}\|^2 + 2\|\mathbf{b}\|^2$. Taking expectation on (4), (5) and (6), we can further get

$$\mathbb{E}[\spadesuit] \stackrel{(c)}{=} -\eta_k (1 - \lambda_k) \mathbb{E}[\|\nabla f(\mathbf{x}_k)\|^2], \quad (7)$$

$$\begin{aligned} \mathbb{E}[\heartsuit] &\leq \eta_k \lambda_k L \rho \mathbb{E}[\|\nabla f(\mathbf{x}_k)\|] - \eta_k \lambda_k \mathbb{E}[\|\nabla f(\mathbf{x}_k)\|^2] \\ &\stackrel{(d)}{\leq} \frac{L}{2} \rho^2 + \frac{L}{2} \eta_k^2 \lambda_k^2 [\mathbb{E}[\|\nabla f(\mathbf{x}_k)\|]^2 - \eta_k \lambda_k \mathbb{E}[\|\nabla f(\mathbf{x}_k)\|^2]] \\ &\stackrel{(e)}{\leq} \frac{L}{2} \rho^2 + \frac{L}{2} \eta_k^2 \lambda_k^2 \mathbb{E}[\|\nabla f(\mathbf{x}_k)\|^2] - \eta_k \lambda_k \mathbb{E}[\|\nabla f(\mathbf{x}_k)\|^2], \end{aligned} \quad (8)$$

$$\begin{aligned} \mathbb{E}[\clubsuit] &\leq L \eta_k^2 [(1 - \lambda_k)^2 \mathbb{E}[\|\mathbf{g}(\mathbf{x}_k)\|^2] + \lambda_k^2 \mathbb{E}[\|\mathbf{g}(\mathbf{x}_k + \boldsymbol{\epsilon}_{\mathbf{x}_k})\|^2]] \\ &\stackrel{(f)}{\leq} L \eta_k^2 [(1 - \lambda_k)^2 (\sigma^2 + \mathbb{E}[\|\nabla f(\mathbf{x}_k)\|^2]) + \lambda_k^2 (2L^2 \rho^2 + 2\sigma^2 + 2\mathbb{E}[\|\nabla f(\mathbf{x}_k)\|^2])], \end{aligned} \quad (9)$$

where the equality (c) utilizes that $\mathbf{g}(\mathbf{x}_k)$ is the unbiased estimation of $f(\mathbf{x}_k)$. The inequality (d) leverages the basic inequality $\frac{a+b}{2} \geq \sqrt{ab}$. The inequality (e) comes from the nonnegative variance property $\text{Var}(\mathbf{X}) = \mathbb{E}[\mathbf{X}^2] - [\mathbb{E}[\mathbf{X}]]^2 \geq 0$. A combination of the following results (11) and (13) leads to (f). After a simple mathematical derivation of $\|\mathbf{g}(\mathbf{x}_k)\|^2$, the following results could be derived:

$$\begin{aligned} \|\mathbf{g}(\mathbf{x}_k)\|^2 &= \|\mathbf{g}(\mathbf{x}_k) - \nabla f(\mathbf{x}_k) + \nabla f(\mathbf{x}_k)\|^2 \\ &= \|\mathbf{g}(\mathbf{x}_k) - \nabla f(\mathbf{x}_k)\|^2 + \|\nabla f(\mathbf{x}_k)\|^2 + 2\langle \mathbf{g}(\mathbf{x}_k) - \nabla f(\mathbf{x}_k), \nabla f(\mathbf{x}_k) \rangle. \end{aligned} \quad (10)$$

Taking expectation on (10), then we derive

$$\mathbb{E}[\|\mathbf{g}(\mathbf{x}_k)\|^2] \leq \sigma^2 + \mathbb{E}[\|\nabla f(\mathbf{x}_k)\|^2]. \quad (11)$$

After a plain derivation of $\|\mathbf{g}(\mathbf{x}_k + \boldsymbol{\epsilon}_{\mathbf{x}_k})\|^2$, we have

$$\begin{aligned}\|\mathbf{g}(\mathbf{x}_k + \boldsymbol{\epsilon}_{\mathbf{x}_k})\|^2 &= \|\mathbf{g}(\mathbf{x}_k + \boldsymbol{\epsilon}_{\mathbf{x}_k}) - \mathbf{g}(\mathbf{x}_k) + \mathbf{g}(\mathbf{x}_k)\|^2 \\ &\leq 2\|\mathbf{g}(\mathbf{x}_k + \boldsymbol{\epsilon}_{\mathbf{x}_k}) - \mathbf{g}(\mathbf{x}_k)\|^2 + 2\|\mathbf{g}(\mathbf{x}_k)\|^2 \\ &\leq 2L^2\rho^2 + 2\|\mathbf{g}(\mathbf{x}_k)\|^2.\end{aligned}\quad (12)$$

Taking expectation on (12) gives us

$$\mathbb{E}[\|\mathbf{g}(\mathbf{x}_k + \boldsymbol{\epsilon}_{\mathbf{x}_k})\|^2] \leq 2L^2\rho^2 + 2\mathbb{E}[\|\mathbf{g}(\mathbf{x}_k)\|^2]. \quad (13)$$

Taking expectation on (3) combining (7), (8), (9), (11) and (13), we can get

$$\begin{aligned}\mathbb{E}[f(\mathbf{x}_{k+1}) - f(\mathbf{x}_k)] &\leq \mathbb{E}[\spadesuit] + \mathbb{E}[\heartsuit] + \mathbb{E}[\clubsuit] \\ &\leq -\eta_k(1 - \lambda_k)\mathbb{E}[\|\nabla f(\mathbf{x}_k)\|^2] + \frac{L}{2}\rho^2 + \frac{L}{2}\eta_k^2\lambda_k^2\mathbb{E}[\|\nabla f(\mathbf{x}_k)\|^2] - \eta_k\lambda_k\mathbb{E}[\|\nabla f(\mathbf{x}_k)\|^2] \\ &\quad + L\eta_k^2\left[(1 - \lambda_k)^2(\sigma^2 + \mathbb{E}[\|\nabla f(\mathbf{x}_k)\|^2]) + \lambda_k^2(2L^2\rho^2 + 2\sigma^2 + 2\mathbb{E}[\|\nabla f(\mathbf{x}_k)\|^2])\right].\end{aligned}\quad (14)$$

Rearranging these terms and dividing the constant η_k on both sides of (14) yields

$$\begin{aligned}\underbrace{\left[1 - \frac{5}{2}L\eta_k\lambda_k^2 - L\eta_k(1 - \lambda_k)^2\right]}_{:=M_k}\mathbb{E}[\|\nabla f(\mathbf{x}_k)\|^2] &\leq 2L\eta_k\lambda_k^2\sigma^2 + \frac{L\rho^2}{2\eta_k} + L\eta_k(1 - \lambda_k)^2\sigma^2 \\ &\quad + 2L^3\eta_k\lambda_k^2\rho^2 + \frac{\mathbb{E}[f(\mathbf{x}_k) - f(\mathbf{x}_{k+1})]}{\eta_k}.\end{aligned}$$

It holds that $\lambda_k \in (0, 1)$ according to the update rule in Algorithm 1. Thus we have $1 - \frac{5}{2}L\eta_k \leq M_k = 1 - \frac{5}{2}L\eta_k\lambda_k^2 - L\eta_k(1 - \lambda_k)^2 \leq 1 - \frac{5}{7}L\eta_k$, $M_k \geq \nu = 1 - \frac{5L\eta_0}{2\sqrt{K}}$ with $\eta_k = \frac{\eta_0}{\sqrt{K}}$ and $\rho = \frac{\rho_0}{\sqrt{K}}$. Consequently, we further get

$$\begin{aligned}\mathbb{E}[\|\nabla f(\mathbf{x}_k)\|^2] &\leq \frac{1}{\nu}\left[2L\eta_k\sigma^2 + \frac{L\rho^2}{2\eta_k} + L\eta_k\sigma^2 + 2L^3\eta_k\rho^2 + \frac{\mathbb{E}[f(\mathbf{x}_k) - f(\mathbf{x}_{k+1})]}{\eta_k}\right] \\ &= \frac{1}{\nu}\left[\frac{2L\eta_0\sigma^2}{\sqrt{K}} + \frac{L\rho_0^2}{2\eta_0\sqrt{K}} + \frac{L\eta_0\sigma^2}{\sqrt{K}} + \frac{2L^3\eta_0\rho_0^2}{K^{\frac{3}{2}}} + \frac{\mathbb{E}[f(\mathbf{x}_k) - f(\mathbf{x}_{k+1})]}{\eta_0}\sqrt{K}\right].\end{aligned}\quad (15)$$

Summing (15) from $k = 0$ to $K - 1$, we have

$$\begin{aligned}\frac{1}{K}\sum_{k=0}^{K-1}\mathbb{E}[\|\nabla f(\mathbf{x}_k)\|^2] &\leq \frac{1}{\nu}\left[\frac{2L\eta_0\sigma^2}{\sqrt{K}} + \frac{L\rho_0^2}{2\eta_0\sqrt{K}} + \frac{L\eta_0\sigma^2}{\sqrt{K}} + \frac{2L^3\eta_0\rho_0^2}{K^{\frac{3}{2}}} + \frac{\mathbb{E}[f(\mathbf{x}_0) - f(\mathbf{x}_K)]}{\eta_0\sqrt{K}}\right] \\ &\leq \frac{1}{\nu}\left[\frac{f(\mathbf{x}_0) - f_{\inf}}{\eta_0\sqrt{K}} + \frac{L\rho_0^2}{2\eta_0\sqrt{K}} + \frac{3L\eta_0\sigma^2}{\sqrt{K}} + \frac{2L^3\eta_0\rho_0^2}{K^{\frac{3}{2}}}\right].\end{aligned}\quad (16)$$

As to $\frac{1}{K}\sum_{k=0}^{K-1}\mathbb{E}[\|\nabla f(\mathbf{x}_k + \boldsymbol{\epsilon}_{\mathbf{x}_k})\|^2]$, which could be derived by leveraging on (16). After an ordinary derivation of $\|\nabla f(\mathbf{x}_k + \boldsymbol{\epsilon}_{\mathbf{x}_k})\|^2$, we are then led to

$$\begin{aligned}\|\nabla f(\mathbf{x}_k + \boldsymbol{\epsilon}_{\mathbf{x}_k})\|^2 &= \|\nabla f(\mathbf{x}_k + \boldsymbol{\epsilon}_{\mathbf{x}_k}) - \nabla f(\mathbf{x}_k) + \nabla f(\mathbf{x}_k)\|^2 \\ &\leq 2\|\nabla f(\mathbf{x}_k + \boldsymbol{\epsilon}_{\mathbf{x}_k}) - \nabla f(\mathbf{x}_k)\|^2 + 2\|\nabla f(\mathbf{x}_k)\|^2 \\ &\leq 2L^2\rho^2 + 2\|\nabla f(\mathbf{x}_k)\|^2.\end{aligned}\quad (17)$$

Utilizing (17), we have

$$\begin{aligned}\frac{1}{K}\sum_{k=0}^{K-1}\mathbb{E}[\|\nabla f(\mathbf{x}_k + \boldsymbol{\epsilon}_{\mathbf{x}_k})\|^2] &\leq 2L^2\rho^2 + \frac{2}{K}\sum_{k=0}^{K-1}\mathbb{E}[\|\nabla f(\mathbf{x}_k)\|^2] \\ &\leq \frac{2}{\nu}\left[\frac{f(\mathbf{x}_0) - f_{\inf}}{\eta_0\sqrt{K}} + \frac{L\rho_0^2}{2\eta_0\sqrt{K}} + \frac{3L\eta_0\sigma^2}{\sqrt{K}} + \frac{2L^3\eta_0\rho_0^2}{K^{\frac{3}{2}}}\right] + \frac{2L^2\rho_0^2}{K}.\end{aligned}\quad (18)$$

TABLE III
HYPERPARAMETERS SETTING USED TO PRODUCE THE RESULTS OF CIFAR10/CIFAR100

Dataset	Model	Optimizer	Lr	ρ	θ	γ	χ
CIFAR10	ResNet-34	SAMAR	0.3	0.10	-	1.550	1.100
		SGD	0.3	-	-	-	-
		SAM	0.3	0.10	-	-	-
		VaSSO	0.3	0.10	0.9	-	-
	Wide-Resnet-34-10	SAMAR	0.1	0.10	-	1.400	1.050
		SGD	0.1	-	-	-	-
		SAM	0.1	0.10	-	-	-
		VaSSO	0.1	0.10	0.9	-	-
CIFAR100	ResNet-34	SAMAR	0.3	0.10	-	1.400	1.075
		SGD	0.3	-	-	-	-
		SAM	0.3	0.10	-	-	-
		VaSSO	0.3	0.10	0.9	-	-
	Wide-Resnet-34-10	SAMAR	0.3	0.15	-	1.500	1.000
		SGD	0.3	-	-	-	-
		SAM	0.3	0.15	-	-	-
		VaSSO	0.3	0.15	0.9	-	-

B. Hyperparameters for experiments

The hyperparameters throughout the experiment are noteworthy. Since every model is only trained for 100 epochs, we set a slightly larger initial learning rate to ensure that all models converge after training 100 epochs. Referring to the hyperparameters in the relevant literature [5, 6, 11–13, 16], and combining them with the changes in experimental results we observed while finetuning the hyperparameters, the hyperparameters in experiments are shown in Table III. Following [12], VaSSO adopts $\theta = 0.9$. To reduce the effort of finetuning the hyperparameters, we take $\lambda_0 = 1$, $\delta = 0.01$ for SAMAR, and weight decay is 0.0005 in all experiments.