

# Sharpness-Aware Minimization For Efficiently Improving Generalization

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Motivation

# Problem setting

- Notation

- Training dataset :  $S = \cup_{i=1}^n \{(x_i, y_i)\} \sim \mathcal{D}$
- Model parameter :  $w \in \mathcal{W} \subseteq \mathbb{R}^k$
- Empirical loss function :  $L_S(w) = \frac{1}{n} \sum_{i=1}^n l(w, x_i, y_i)$
- Population loss function :  $L_{\mathcal{D}}(w) = \mathbb{E}_{(x,y) \sim \mathcal{D}}[l(w, x, y)]$

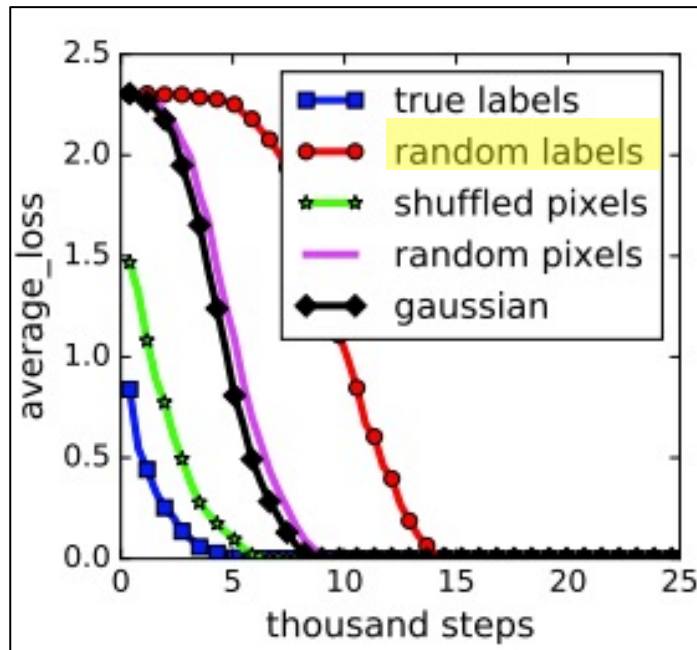
- Objective

- Select model parameter  $w$  having low population loss  $L_{\mathcal{D}}(w)$

\* Conventional approach :  $\min_w L_S(w) + \lambda \|w\|_2^2$

# Minimizing training loss is not sufficient

- Deep neural networks easily fit **random labels**
- **Explicit regularization** is not sufficient for controlling generalization error

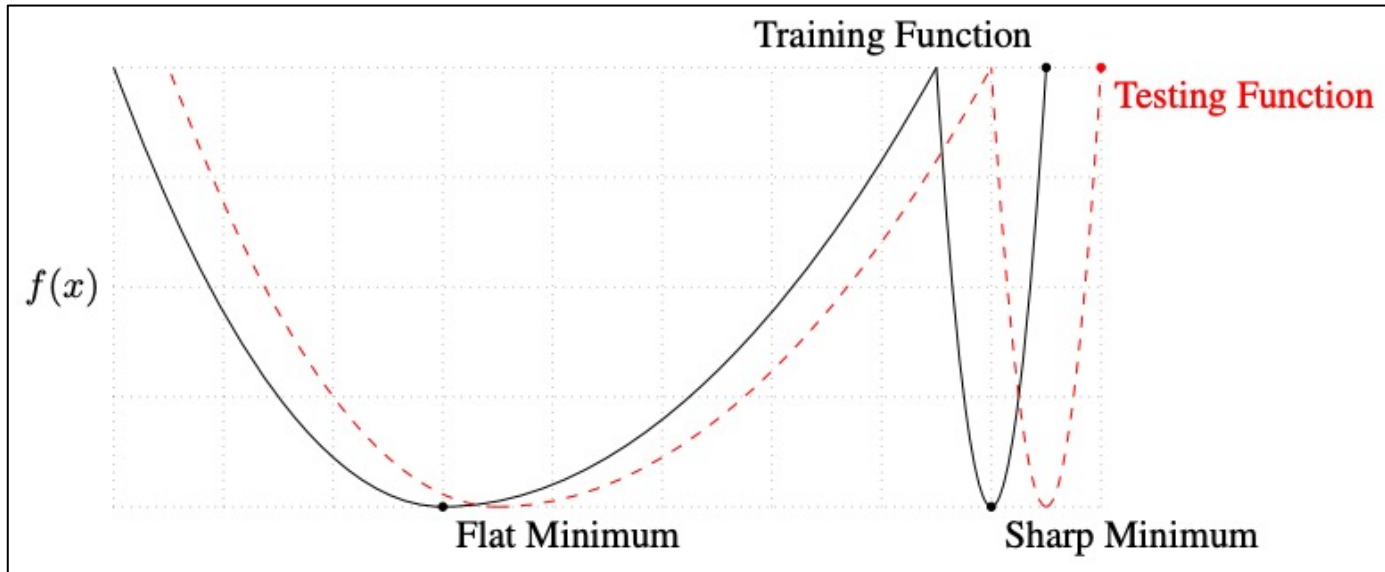


Training loss decaying with steps

data aug	dropout	weight decay	top-1 train	top-5 train	top-1 test	top-5 test
ImageNet 1000 classes with the original labels						
yes	yes	yes	92.18	99.21	77.84	93.92
yes	no	no	92.33	99.17	72.95	90.43
no	no	yes	90.60	100.0	67.18 (72.57)	86.44 (91.31)
no	no	no	99.53	100.0	59.80 (63.16)	80.38 (84.49)
Alexnet (Krizhevsky et al., 2012)			-	-	-	83.6
ImageNet 1000 classes with random labels						
no	yes	yes	91.18	97.95	0.09	0.49
no	no	yes	87.81	96.15	0.12	0.50
no	no	no	95.20	99.14	0.11	0.56

Performance on ImageNet with true labels and random labels

# Loss Landscape v.s. Generalization

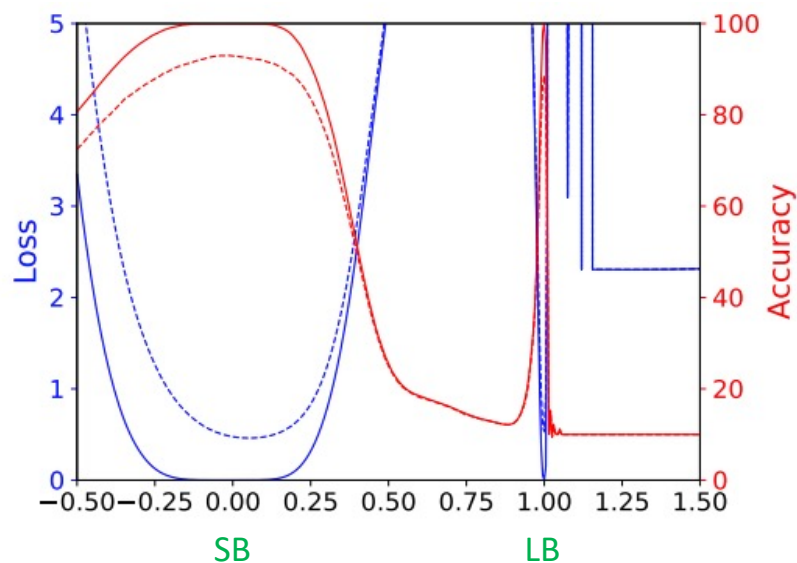


If there exists a shift from empirical loss to population loss, **flat** minimum is more robust than **sharp** minimum.

- Smoothening loss landscape : Skip connection, Batch normalization
- Escaping basins of sharp minima : Small-batch training

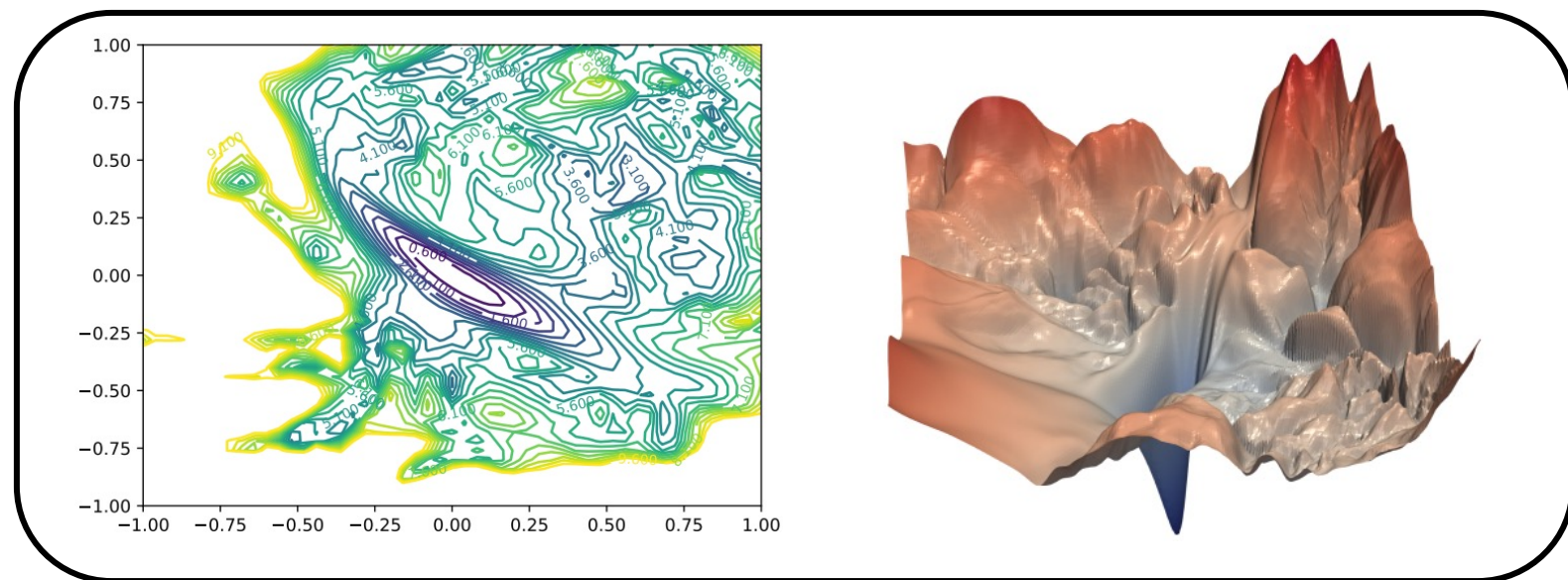
# How to analyze sharpness?

1D linear interpolation



$L(\alpha w_l^* + (1 - \alpha)w_s^*)$  with  $-1 \leq \alpha \leq 1$   
( $w_s^*$  : converged w/ Small Batch (SB) training)  
( $w_l^*$  : converged w/ Large Batch (LB) training)

2D contour plot and its 3D visualization

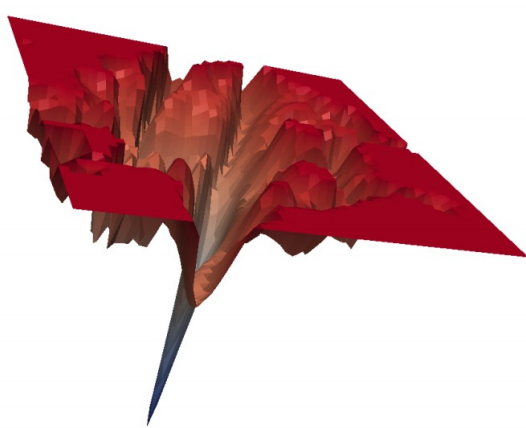


$L(w + \alpha\delta + \beta\eta)$  with  $-1 \leq \alpha, \beta \leq 1$   
( $\delta$  and  $\eta$  are random weights of the same size of  $w$ )  
(Filter-wise normalization is aware of *scale invariance* )

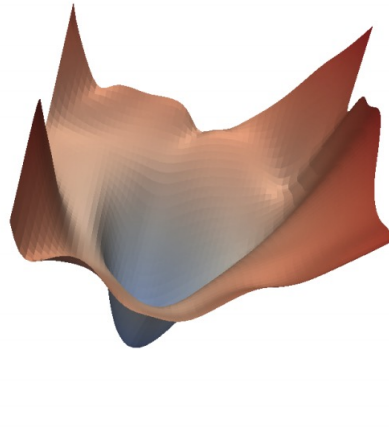
Previous studies have shown better generalization, however, yet struggle to beat a range of state-of-the-art models

# Sharpness-Aware Minimization (SAM)

- Find a wide and flat minima by simultaneously minimizing loss and **sharpness**
  - Seeks parameters that lie in **neighborhoods** having uniformly low loss
  - Conduct a rigorous empirical study across a range of widely studied computer vision tasks

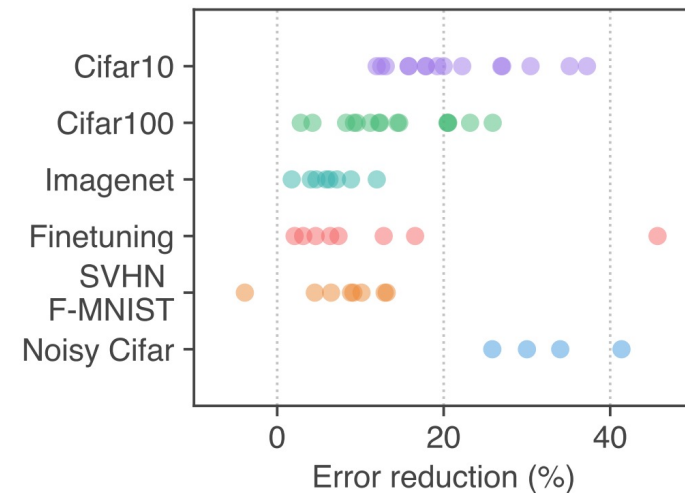


(a) Without SAM



(b) With SAM

3D visualization of the loss landscape  
around the converged solutions



Error rate reduction by switching to SAM  
(dataset / model / augmentation)



Preliminary

# PAC versus PAC-bayes

- PAC (Probably Approximately Correct)

With probability greater than  $1 - \delta$ ,

$$L_{\mathcal{D}}(w) \leq L_S(w) + \sqrt{\frac{1}{2n} \left( \ln |\mathcal{H}| + \ln \left( \frac{2}{\delta} \right) \right)}$$

- PAC-bayes

With probability greater than  $1 - \delta$ ,

$$\mathbb{E}_{w \sim Q}[L_{\mathcal{D}}(w)] \leq \mathbb{E}_{w \sim Q}[L_S(w)] + \sqrt{\frac{1}{2(n-1)} \left( KL(Q|P) + \ln \left( \frac{n}{\delta} \right) \right)}$$

# Component-wise level bound

$$[\mathbb{E}_{w \sim Q} L_{\mathcal{D}}(w)] \leq \mathbb{E}_{w \sim Q} [L_S(w)] + \sqrt{\frac{1}{2(n-1)} \left( KL(Q|P) + \ln\left(\frac{n}{\delta_j}\right) \right)}$$



Let  $P = \mathcal{N}\left(0, c \exp\left(\frac{1-j}{k}\right) I\right)$  for  $j \in \mathbb{N}$  and  $Q = \mathcal{N}(w, \sigma^2 I)$

- $KL(Q|P) \leq \frac{1}{2} \left[ 1 + k \log\left(1 + \frac{\|w\|_2^2}{k\sigma^2}\right) \right]$

- $\ln\left(\frac{n}{\delta_j}\right) \leq \log\left(\frac{n}{\delta}\right) + 2 \log(6n + 3k)$



Please refer to Appendix in paper

$$\mathbb{E}_{\epsilon \sim \mathcal{N}(0, \sigma^2 I)} [L_{\mathcal{D}}(w + \epsilon)] \leq \mathbb{E}_{\epsilon \sim \mathcal{N}(0, \sigma^2 I)} [L_S(w + \epsilon)] + \sqrt{\frac{1}{2(n-1)} \left( \frac{1}{2} \left[ 1 + k \log\left(1 + \frac{\|w\|_2^2}{k\sigma^2}\right) \right] + \log\left(\frac{n}{\delta}\right) + 2 \log(6n + 3k) \right)}$$

# How can we constrain the neighborhood?

- Directly constraining  $\epsilon$  is not intuitive due to high-dimensional nature
- Rather propose to use norm

If  $\epsilon \sim \mathcal{N}(0, \sigma^2 I)$ , then  $\|\epsilon\|_2^2 \sim \chi^2(k\sigma^2)$

$$\Pr(\|\epsilon\|_2^2 - k\sigma^2 \geq 2\sigma^2\sqrt{kt} + 2t\sigma^2) \leq \exp(-t)$$

With probability greater than  $1 - 1/\sqrt{n}$ ,

$$\begin{aligned} \|\epsilon\|_2^2 &\leq k\sigma^2 + 2\sigma^2\sqrt{kt} + 2t\sigma^2 = k\sigma^2(1 + 2\sqrt{t/k} + 2t/k) \\ &= k\sigma^2 \left( 1 + 2\sqrt{\ln \sqrt{n} / k} + 2 \ln \sqrt{n} / k \right) (:= \rho^2) \end{aligned}$$

# PAC-bayes Generalization Bound for SAM

$$\mathbb{E}_{\epsilon \sim \mathcal{N}(0, \sigma^2 I)}[L_{\mathcal{D}}(w + \epsilon)]$$

$$\leq \mathbb{E}_{\epsilon \sim \mathcal{N}(0, \sigma^2 I)}[L_S(w + \epsilon)] + \sqrt{\frac{1}{2(n-1)} \left( \frac{1}{2} \left[ 1 + k \log \left( 1 + \frac{\|w\|_2^2}{k\sigma^2} \right) \right] + \log \left( \frac{n}{\delta} \right) + 2 \log(6n + 3k) \right)}$$

$$\leq \left( 1 - \frac{1}{\sqrt{n}} \right) \max_{\|\epsilon\|_2 \leq \rho} L_S(w + \epsilon) + \frac{1}{\sqrt{n}} + \sqrt{\frac{1}{4(n-1)} \left( 1 + k \log \left( 1 + \frac{\|w\|_2^2}{k\sigma^2} \right) + 2 \log \left( \frac{n}{\delta} \right) + 4 \log(6n + 3k) \right)}$$

$$\leq \max_{\|\epsilon\|_2 \leq \rho} L_S(w + \epsilon) + \sqrt{\frac{1}{4(n-1)} \left( 1 + k \log \left( 1 + \frac{\|w\|_2^2}{\rho^2} \left( 1 + \sqrt{\frac{2 \ln(n)}{k}} \right)^2 \right) + 2 \log \left( \frac{n}{\delta} \right) + 4 \log(6n + 3k) \right)}$$

SAM optimizer

# Framing into min-max optimization problem

$$\min_w \max_{\|\epsilon\|_2 \leq \rho} L_S(w + \epsilon) + \sqrt{\frac{1 + k \log \left( 1 + \frac{\|w\|_2^2}{\rho^2} \left( 1 + \sqrt{\frac{2 \ln(n)}{k}} \right)^2 \right) + 2 \log \left( \frac{n}{\delta} \right) + 4 \log(6n + 3k)}{4(n-1)}}$$

$$= \min_w \max_{\|\epsilon\|_2 \leq \rho} L_S(w + \epsilon) + h \left( \frac{\|w\|_2^2}{\rho^2} \right) \approx \min_w \max_{\|\epsilon\|_p \leq \rho} L_S(w + \epsilon) + \lambda \|w\|_2^2$$

$$= \min_w \max_{\|\epsilon\|_p \leq \rho} L_S(w + \epsilon) - L_S(w) + L_S(w) + \lambda \|w\|_2^2$$

Sharpness

Training Loss

Regularizer

How quickly the training loss can be increased by moving from  $w$  to a nearby parameter value

# Solving min-max optimization problem

1.  $\max_{\|\epsilon\|_p \leq \rho} L_S(w + \epsilon)$

$$\epsilon^*(w) = \arg \max_{\|\epsilon\|_p \leq \rho} L_S(w + \epsilon) \approx \arg \max_{\|\epsilon\|_p \leq \rho} L_S(w) + \epsilon^T \nabla_w L_S(w) = \arg \max_{\|\epsilon\|_p \leq \rho} \epsilon^T \nabla_w L_S(w)$$

$$\approx \rho \frac{\text{sign}(\nabla_w L_S(w)) |\nabla_w L_S(w)|^{\frac{q}{p}}}{(\|\nabla_w L_S(w)\|_q)^{\frac{q}{p}}} \quad (:= \hat{\epsilon}(w)) \quad \text{where} \quad \frac{1}{p} + \frac{1}{q} = 1$$

If  $p = 2$ , then  $\|\hat{\epsilon}(w)\|_2 = \rho$  and  $\hat{\epsilon}(w) = \rho \nabla_w L_S(w) / \|\nabla_w L_S(w)\|_2$



# Solving min-max optimization problem

2.  $\min_w L_S(w + \hat{\epsilon}(w))$

$$\begin{aligned}\nabla_w L_S(w_t + \hat{\epsilon}(w_t)) &= \frac{d(w + \hat{\epsilon}(w))}{dw} \nabla_w L_S(w) \Big|_{w_t + \hat{\epsilon}(w_t)} \\ &= \nabla_w L_S(w) \Big|_{w_t + \hat{\epsilon}(w_t)} + \cancel{\frac{d\hat{\epsilon}(w)}{dw} \nabla_w L_S(w) \Big|_{w_t + \hat{\epsilon}(w_t)}} \\ &\approx \nabla_w L_S(w) \Big|_{w_t + \hat{\epsilon}(w_t)}\end{aligned}$$

Hessian computation

By Stochastic Gradient Descent (SGD),  $w_{t+1} = w_t - \eta \nabla_w L_S(w) \Big|_{w_t + \hat{\epsilon}(w_t)}$

Experiment

# Image classification

Model	Augmentation	CIFAR-10		CIFAR-100	
		SAM	SGD	SAM	SGD
WRN-28-10 (200 epochs)	Basic	<b>2.7<math>\pm</math>0.1</b>	3.5 $\pm$ 0.1	<b>16.5<math>\pm</math>0.2</b>	18.8 $\pm$ 0.2
WRN-28-10 (200 epochs)	Cutout	<b>2.3<math>\pm</math>0.1</b>	2.6 $\pm$ 0.1	<b>14.9<math>\pm</math>0.2</b>	16.9 $\pm$ 0.1
WRN-28-10 (200 epochs)	AA	<b>2.1<math>\pm</math>&lt;0.1</b>	2.3 $\pm$ 0.1	<b>13.6<math>\pm</math>0.2</b>	15.8 $\pm$ 0.2
WRN-28-10 (1800 epochs)	Basic	<b>2.4<math>\pm</math>0.1</b>	3.5 $\pm$ 0.1	<b>16.3<math>\pm</math>0.2</b>	19.1 $\pm$ 0.1
WRN-28-10 (1800 epochs)	Cutout	<b>2.1<math>\pm</math>0.1</b>	2.7 $\pm$ 0.1	<b>14.0<math>\pm</math>0.1</b>	17.4 $\pm$ 0.1
WRN-28-10 (1800 epochs)	AA	<b>1.6<math>\pm</math>0.1</b>	2.2 $\pm$ <0.1	<b>12.8<math>\pm</math>0.2</b>	16.1 $\pm$ 0.2
Shake-Shake (26 2x96d)	Basic	<b>2.3<math>\pm</math>&lt;0.1</b>	2.7 $\pm$ 0.1	<b>15.1<math>\pm</math>0.1</b>	17.0 $\pm$ 0.1
Shake-Shake (26 2x96d)	Cutout	<b>2.0<math>\pm</math>&lt;0.1</b>	2.3 $\pm$ 0.1	<b>14.2<math>\pm</math>0.2</b>	15.7 $\pm$ 0.2
Shake-Shake (26 2x96d)	AA	<b>1.6<math>\pm</math>&lt;0.1</b>	1.9 $\pm$ 0.1	<b>12.8<math>\pm</math>0.1</b>	14.1 $\pm$ 0.2
PyramidNet	Basic	<b>2.7<math>\pm</math>0.1</b>	4.0 $\pm$ 0.1	<b>14.6<math>\pm</math>0.4</b>	19.7 $\pm$ 0.3
PyramidNet	Cutout	<b>1.9<math>\pm</math>0.1</b>	2.5 $\pm$ 0.1	<b>12.6<math>\pm</math>0.2</b>	16.4 $\pm$ 0.1
PyramidNet	AA	<b>1.6<math>\pm</math>0.1</b>	1.9 $\pm$ 0.1	<b>11.6<math>\pm</math>0.1</b>	14.6 $\pm$ 0.1
PyramidNet+ShakeDrop	Basic	<b>2.1<math>\pm</math>0.1</b>	2.5 $\pm$ 0.1	<b>13.3<math>\pm</math>0.2</b>	14.5 $\pm$ 0.1
PyramidNet+ShakeDrop	Cutout	<b>1.6<math>\pm</math>&lt;0.1</b>	1.9 $\pm$ 0.1	<b>11.3<math>\pm</math>0.1</b>	11.8 $\pm$ 0.2
PyramidNet+ShakeDrop	AA	<b>1.4<math>\pm</math>&lt;0.1</b>	1.6 $\pm$ <0.1	<b>10.3<math>\pm</math>0.1</b>	10.6 $\pm$ 0.1

Comparison of SAM and SGD for the test error rate on **CIFAR-{10, 100}**  
 (Similar trend is observed on **SVHN** and **Fashion-MNIST**)

# Image classification

Model	Epoch	SAM		Standard Training (No SAM)	
		Top-1	Top-5	Top-1	Top-5
ResNet-50	100	<b>22.5</b> $\pm 0.1$	6.28 $\pm 0.08$	22.9 $\pm 0.1$	6.62 $\pm 0.11$
	200	<b>21.4</b> $\pm 0.1$	5.82 $\pm 0.03$	22.3 $\pm 0.1$	6.37 $\pm 0.04$
	400	<b>20.9</b> $\pm 0.1$	5.51 $\pm 0.03$	22.3 $\pm 0.1$	6.40 $\pm 0.06$
ResNet-101	100	<b>20.2</b> $\pm 0.1$	5.12 $\pm 0.03$	21.2 $\pm 0.1$	5.66 $\pm 0.05$
	200	<b>19.4</b> $\pm 0.1$	4.76 $\pm 0.03$	20.9 $\pm 0.1$	5.66 $\pm 0.04$
	400	<b>19.0</b> $\pm <0.01$	4.65 $\pm 0.05$	22.3 $\pm 0.1$	6.41 $\pm 0.06$
ResNet-152	100	<b>19.2</b> $\pm <0.01$	4.69 $\pm 0.04$	20.4 $\pm <0.0$	5.39 $\pm 0.06$
	200	<b>18.5</b> $\pm 0.1$	4.37 $\pm 0.03$	20.3 $\pm 0.2$	5.39 $\pm 0.07$
	400	<b>18.4</b> $\pm <0.01$	4.35 $\pm 0.04$	20.9 $\pm <0.0$	5.84 $\pm 0.07$

Comparison of SAM and SGD for the test error rate on ImageNet

# Finetuning the pretrained model

Pretrained on ImageNet



Pretrained on ImageNet and unlabeled JFT



Dataset	EffNet-b7 + SAM	EffNet-b7	Prev. SOTA (ImageNet only)	EffNet-L2 + SAM	EffNet-L2	Prev. SOTA
FGVC_Aircraft	<b>6.80</b> $\pm 0.06$	8.15 $\pm 0.08$	<b>5.3</b> (TBMSL-Net)	<b>4.82</b> $\pm 0.08$	5.80 $\pm 0.1$	5.3 (TBMSL-Net)
Flowers	<b>0.63</b> $\pm 0.02$	1.16 $\pm 0.05$	0.7 (BiT-M)	<b>0.35</b> $\pm 0.01$	0.40 $\pm 0.02$	0.37 (EffNet)
Oxford_IIT_Pets	<b>3.97</b> $\pm 0.04$	4.24 $\pm 0.09$	4.1 (Gpipe)	<b>2.90</b> $\pm 0.04$	3.08 $\pm 0.04$	4.1 (Gpipe)
Stanford_Cars	5.18 $\pm 0.02$	5.94 $\pm 0.06$	<b>5.0</b> (TBMSL-Net)	4.04 $\pm 0.03$	4.93 $\pm 0.04$	<b>3.8</b> (DAT)
CIFAR-10	<b>0.88</b> $\pm 0.02$	0.95 $\pm 0.03$	1 (Gpipe)	<b>0.30</b> $\pm 0.01$	0.34 $\pm 0.02$	0.63 (BiT-L)
CIFAR-100	<b>7.44</b> $\pm 0.06$	7.68 $\pm 0.06$	7.83 (BiT-M)	<b>3.92</b> $\pm 0.06$	4.07 $\pm 0.08$	6.49 (BiT-L)
Birdsnap	<b>13.64</b> $\pm 0.15$	14.30 $\pm 0.18$	15.7 (EffNet)	<b>9.93</b> $\pm 0.15$	10.31 $\pm 0.15$	14.5 (DAT)
Food101	7.02 $\pm 0.02$	7.17 $\pm 0.03$	7.0 (Gpipe)	<b>3.82</b> $\pm 0.01$	3.97 $\pm 0.03$	4.7 (DAT)
ImageNet	<b>15.14</b> $\pm 0.03$	15.3	<b>14.2</b> (KDforAA)	<b>11.39</b> $\pm 0.02$	11.8	11.45 (ViT)

Top-1 error rates for finetuning EffNet-b7 or EffNet-L2 to various target datasets

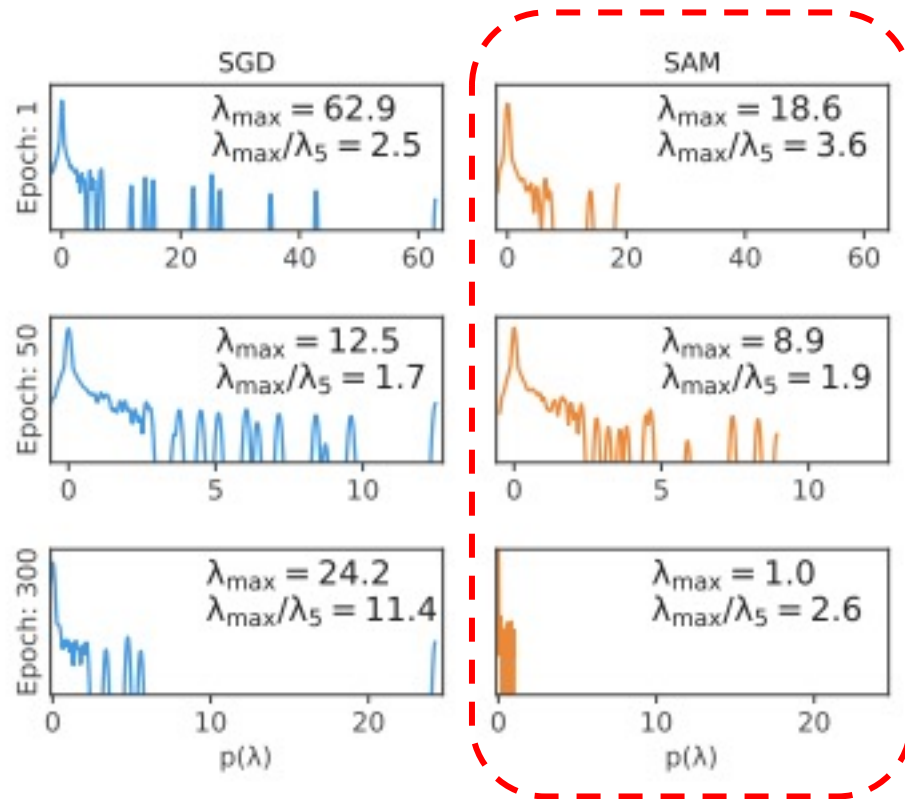
# Robustness to label noise

Method	Noise rate (%)			
	20	40	60	80
Sanchez et al. (2019)	94.0	92.8	90.3	74.1
Zhang & Sabuncu (2018)	89.7	87.6	82.7	67.9
Lee et al. (2019)	87.1	81.8	75.4	-
Chen et al. (2019)	89.7	-	-	52.3
Huang et al. (2019)	92.6	90.3	43.4	-
MentorNet (2017)	92.0	91.2	74.2	60.0
Mixup (2017)	94.0	91.5	86.8	76.9
MentorMix (2019)	<b>95.6</b>	<b>94.2</b>	91.3	<b>81.0</b>
SGD	84.8	68.8	48.2	26.2
Mixup	93.0	90.0	83.8	70.2
Bootstrap + Mixup	93.3	92.0	87.6	72.0
SAM	95.1	93.4	90.5	77.9
Bootstrap + SAM	95.4	94.2	91.8	79.9

Test accuracy on clean test dataset while trained with noisy labels

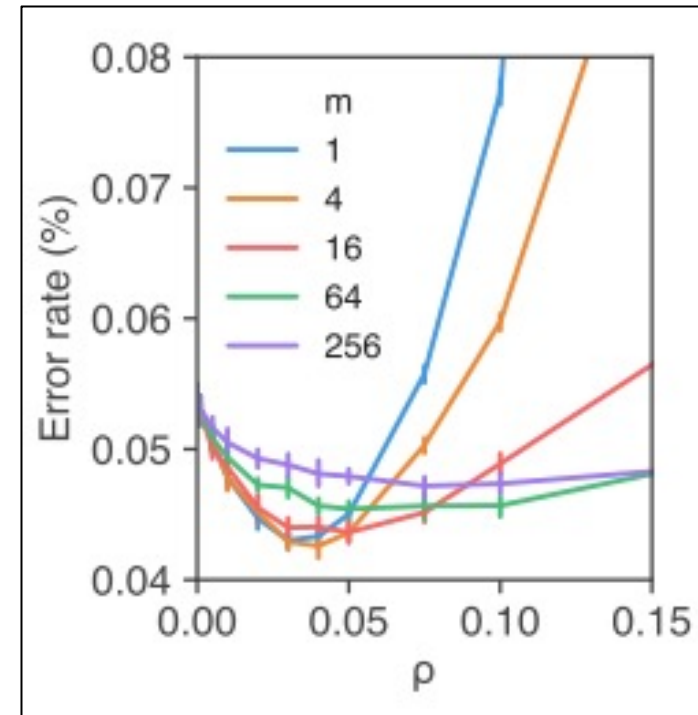


# Sharpness and Generalization



Evolution of Hessian spectrum along epoch

- SGD : to sharp minima
- SAM : to flat minima



Effect of batch size( $m$ ) to test error rate

- Small batch training leads to flat minima
- Model gets less robustness to hyperparameter  $\rho$

Critique

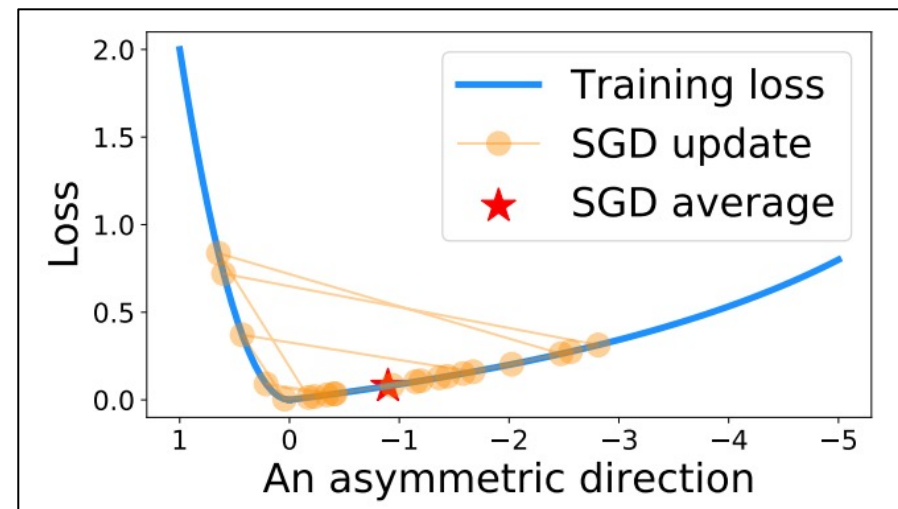
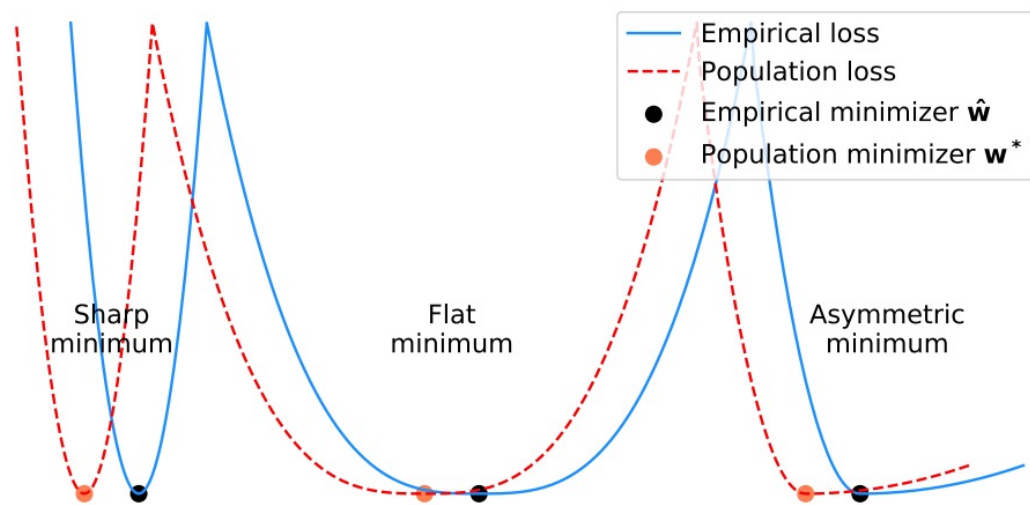


# In-between sharpness and flatness?

Known to be in sharp minima



By sampling the loss function in a neighborhood of **LB solutions**, we observe that it rises steeply only along a small dimensional subspace (e.g. 5% of the whole space); on most other directions, the function is relatively flat

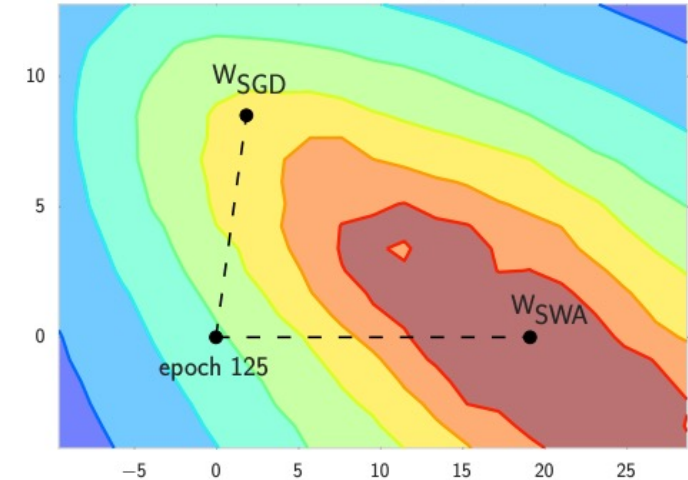
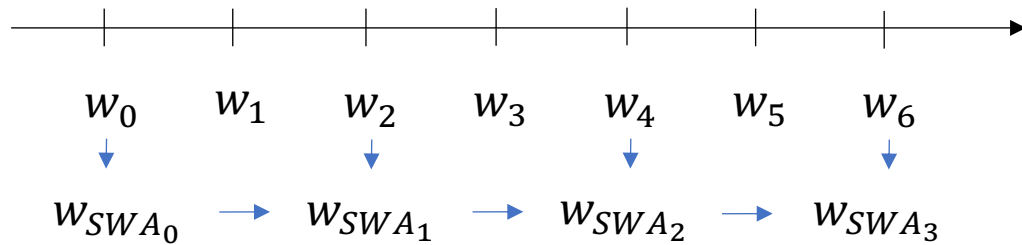


Notion of **sharpness** and **flatness** may be oversimplification

Averaging SGD trajectory leads to flat side

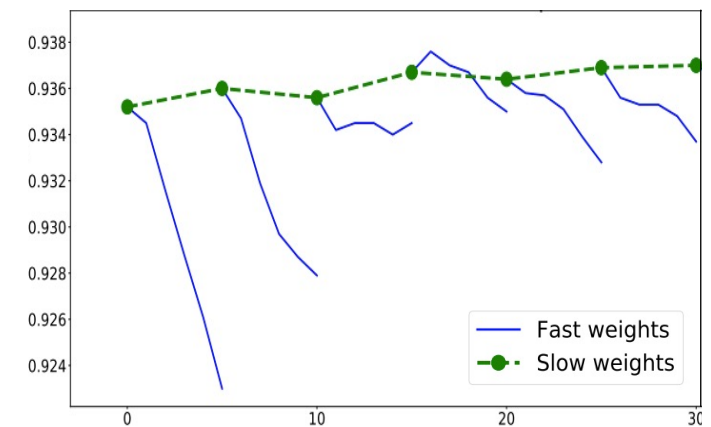
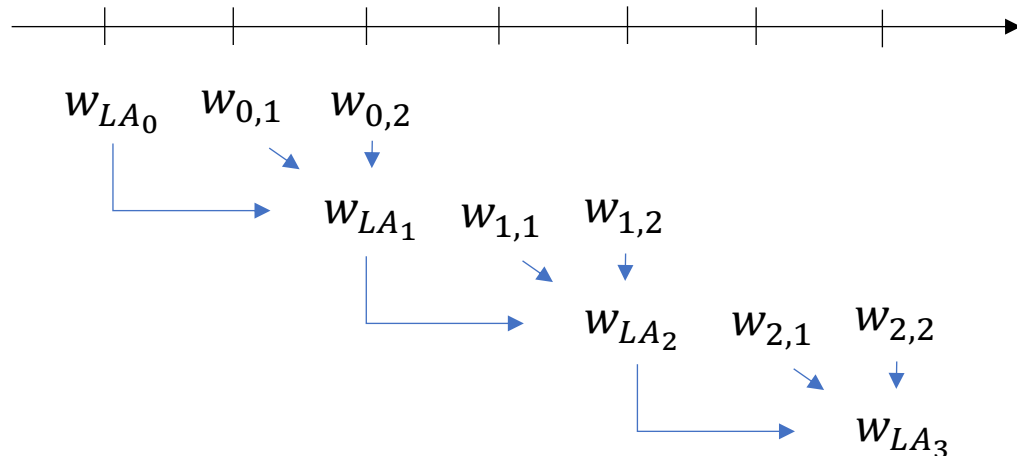
# How to free the choice of batch size?

## Stochastic Weight Averaging (SWA), UAI 2018



Contour plot of test loss surface

## Look ahead(LA), NeurIPS 2019



Test accuracy along epoch

Izmailov, Pavel, et al. "Averaging weights leads to wider optima and better generalization.", UAI 2018.

Zhang, Michael R., et al. "Lookahead optimizer: k steps forward, 1 step back.", NeurIPS, 2019.

Thank you for your attention

# Appendix

# Learning algorithm w/ PAC-bayes bound

1. Fix a probability  $\delta > 0$  and a distribution  $P = \mathcal{N}(\mu_P, \sigma_P^2 I)$
2. Collect an i.i.d. dataset  $S$  of size  $n$
3. Compute the optimal distribution  $Q = \mathcal{N}(\mu_Q, \sigma_Q^2 I)$  that minimizes

$$\mathbb{E}_{w \sim Q}[L_S(w)] + \sqrt{\frac{1}{2(n-1)} \left( KL(Q|P) + \ln\left(\frac{n}{\delta}\right) \right)}$$

4. Return the randomized classifier given by  $Q$

\* *Closed form expression of KL divergence* :  $KL(Q|P) = \frac{1}{2} \left[ \frac{k\sigma_Q^2 + \|\mu_P - \mu_Q\|_2^2}{\sigma_P^2} - k + k \ln\left(\frac{\sigma_P^2}{\sigma_Q^2}\right) \right]$

# How can we set the prior $P$ in advance?

- Predefine values for  $\sigma_P^2$  and pick the best one in that set
- Set  $\delta_j = \frac{6\delta}{\pi^2 j^2}$  and  $\sigma_P^2 \in T := \left\{ c \exp\left(\frac{1-j}{k}\right) \mid j \in \mathbb{N} \right\}$

Let  $A_j$  is an event s.t.  $\mathbb{E}[Z] > \bar{Z} + g(\delta_j)$  where  $\Pr(A_j) < \delta_j$

Then,  $\Pr(\cup_{j \in \mathbb{N}} A_j) < \sum_{j \in \mathbb{N}} \delta_j = \frac{6\delta}{\pi^2} \sum_{j \in \mathbb{N}} \frac{1}{j^2} = \delta$

$\therefore$  With probability  $1 - \delta$ , PAC-bayes bound holds for all  $\sigma_P^2 \in T$