Sharpness-Aware Minimization

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Modern Optimization Methods

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SAM in a few words

SAM is an optimization algorithm that:

- Minimizes loss value **AND** sharpness
- Is efficient and easy to implement
- Strongly improves generalization (SOTA on Imagenet, CIFAR, SVHN, and others)
- Robust to label noise

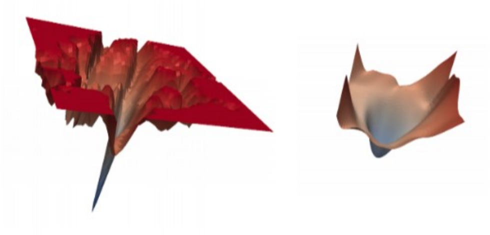


Figure: (left) A sharp minimum to which a ResNet trained with SGD converged. (right) A wide minimum to which the same ResNet trained with SAM converged.

SAM in a few words

- Is more interpretable

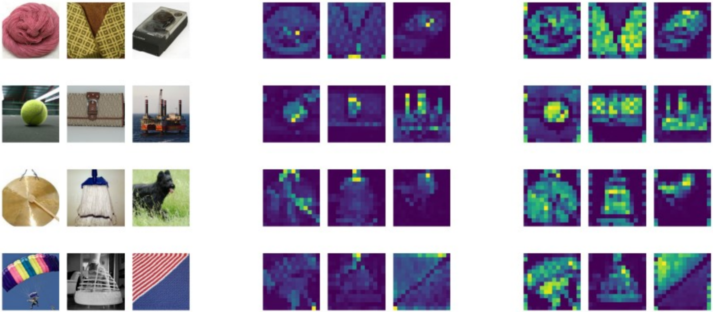


Figure 3: Raw images (**Left**) and attention maps of ViT-S/16 with (**Right**) and without (**Middle**) sharpness-aware optimization.

SOTA for today

Task	Dataset	Model	Metric Name	Metric Value	Global Rank	Uses Extra Training Data	Result	Benchmark
Fine-Grained Image Classification	Birdsnap	EffNet-L2 (SAM)	Accuracy	90.07%	# 1	✓		Compare
Image Classification	CIFAR-10	PyramidNet (SAM)	Percentage correct	98.6	# 28	✓		Compare
Image Classification	CIFAR-100	PyramidNet (SAM)	Percentage correct	89.7	# 28	✓		Compare
Image Classification	CIFAR-100	EffNet-L2 (SAM)	Percentage correct	96.08	# 1	✓		Compare
Image Classification	Fashion-MNIST	Shake-Shake (SAM)	Percentage error	3.59	# 2	×		Compare
			Accuracy	96.41	# 3	×		Compare
Fine-Grained Image Classification	FGVC Aircraft	EffNet-L2 (SAM)	Top-1 Error Rate	4.82	# 1	✓		Compare
Image Classification	Flowers-102	EffNet-L2 (SAM)	Accuracy	99.65%	# 4	✓		Compare
Fine-Grained Image Classification	Food-101	EffNet-L2 (SAM)	Accuracy	96.18	# 1	✓		Compare

SOTA for today

Image Classification	ImageNet	ResNet-152 (SAM)	Top 1 Accuracy	81.6%	# 440	×		Compare
			Top 5 Accuracy	95.65	# 107	×		Compare
Image Classification	ImageNet	EfficientNet-L2-475 (SAM)	Top 1 Accuracy	88.61%	# 32	✓		Compare
			Number of params	480M	# 775	✓		Compare
			Hardware Burden	None	# 1	✓		Compare
			Operations per network pass	None	# 1	✓		Compare
Fine-Grained Image Classification	Oxford-IIIT Pet Dataset	EffNet-L2 (SAM)	Top-1 Error Rate	2.90%	# 1	✓		Compare
			Accuracy	97.10%	# 1	✓		Compare
Fine-Grained Image Classification	Stanford Cars	EffNet-L2 (SAM)	Accuracy	95.96%	# 4	✓		Compare
Image Classification	SVHN	WRN28-10 (SAM)	Percentage error	0.99	# 1	×		Compare

Neural Network training

- Training dataset $\mathcal{S} \triangleq \cup_{i=1}^{n}\{(\boldsymbol{x}_i, \boldsymbol{y}_i)\}$ drawn i.i.d. from distribution $\mathscr{D}$
- Neural network with weights $\boldsymbol{w} \in \mathcal{W} \subseteq \mathbb{R}^d$;
- Per-data-point loss function $l : \mathcal{W} \times \mathcal{X} \times \mathcal{Y} \to \mathbb{R}_+$,
- Training loss $L_S(\boldsymbol{w}) \triangleq \frac{1}{n}\sum_{i=1}^{n} l(\boldsymbol{w}, \boldsymbol{x}_i, \boldsymbol{y}_i)$ which approximates $L_{\mathscr{D}}(\boldsymbol{w}) \triangleq \mathbb{E}_{(\boldsymbol{x},\boldsymbol{y})\sim D}[l(\boldsymbol{w}, \boldsymbol{x}, \boldsymbol{y})]$.

- Train the network to get $\boldsymbol{w}$ having low population loss $L_{\mathscr{D}}(\boldsymbol{w})$.

Not all minima created are equal

Training a neural network with different optimization strategies (for example, change batch size), we get:

- Perfect fit on the training set.
- Training loss approaching zero.
- But very different test accuracy.

Table: Train and test accuracy for a convolutional network trained on CIFAR10, for different batch sizes (reproducing an experiment from [SMN+16])

batch size	train accuracy	test accuracy	train loss
1	100.0 (100.0 - 100.0)	77.2 (77.7 - 76.4)	0.00 (0.00 - 0.00)
8	100.0 (100.0 - 100.0)	76.5 (76.7 - 75.9)	0.00 (0.00 - 0.00)
256	100.0 (100.0 - 100.0)	63.2 (63.4 - 61.3)	0.00 (0.00 - 0.00)
2048	100.0 (100.0 - 99.8)	60.2 (60.6 - 58.6)	0.00 (0.02 - 0.00)

Conclusion: Some global minima generalize better than others

Main theorem

Theorem

For any $\rho > 0$, with high probability over training set $\mathcal{S}$ generated from distribution $\mathscr{D}$,

$$L_{\mathscr{D}}(\boldsymbol{w}) \leq \max_{\|\epsilon\|_2 \leq \rho} L_{\mathcal{S}}(\boldsymbol{w} + \epsilon) + h(\|\boldsymbol{w}\|_2^2 / \rho^2),$$

where $h : \mathbb{R}^+ \to \mathbb{R}^+$ is a strictly increasing function (under some technical conditions on $L_{\mathscr{D}}(\boldsymbol{w})$).

Simplifying lower bound

Re-arranging the terms to make the sharpness term more explicit:

$$[\max_{\|\epsilon\|_2 \leq \rho} L_{\mathcal{S}}(\boldsymbol{w}+\epsilon) - L_{\mathcal{S}}(\boldsymbol{w})] + L_{\mathcal{S}}(\boldsymbol{w}) + h(\|\boldsymbol{w}\|_2^2/\rho^2).$$

The expression of h heavily depends on the proof method, we substitute the second term with $\lambda\|\boldsymbol{w}\|_2^2$ for standard L2 regularization.

This gives us the SAM objective:

$$\min_{\boldsymbol{w}} L_{\mathcal{S}}^{SAM}(\boldsymbol{w}) + \lambda||\boldsymbol{w}||_2^2 \qquad \text{where} \qquad L_{\mathcal{S}}^{SAM}(\boldsymbol{w}) \triangleq \max_{||\epsilon||_p \leq \rho} L_S(\boldsymbol{w}+\epsilon),$$

Solving min-max problem

Do a first order approximation of the objective:

$$\epsilon^*(\boldsymbol{w}) \triangleq \arg\max_{\|\epsilon\|_p \le \rho} L_{\mathcal{S}}(\boldsymbol{w}+\epsilon) \approx \arg\max_{\|\epsilon\|_p \le \rho} L_{\mathcal{S}}(\boldsymbol{w}) + \epsilon^T \nabla_{\boldsymbol{w}} L_{\mathcal{S}}(\boldsymbol{w})$$
$$= \arg\max_{\|\epsilon\|_p \le \rho} \epsilon^T \nabla_{\boldsymbol{w}} L_{\mathcal{S}}(\boldsymbol{w}).$$

Well known solution to the dual norm problem:

$$\hat{\epsilon}(\boldsymbol{w}) = \rho \,\text{sign}\left(\nabla_{\boldsymbol{w}} L_{\mathcal{S}}(\boldsymbol{w})\right) |\nabla_{\boldsymbol{w}} L_{\mathcal{S}}(\boldsymbol{w})|^{q-1} / \left(\|\nabla_{\boldsymbol{w}} L_{\mathcal{S}}(\boldsymbol{w})\|_q^q \right)^{1/p} \quad (2)$$

Computing the SAM gradient

$$\nabla_{\boldsymbol{w}} L_{\mathcal{S}}^{SAM}(\boldsymbol{w}) \approx \nabla_{\boldsymbol{w}} L_{\mathcal{S}}(\boldsymbol{w}+\hat{\epsilon}(\boldsymbol{w})) = \frac{d(\boldsymbol{w}+\hat{\epsilon}(\boldsymbol{w}))}{d\boldsymbol{w}} \nabla_{\boldsymbol{w}} L_{\mathcal{S}}(\boldsymbol{w})|_{\boldsymbol{w}+\hat{\epsilon}(w)}$$
$$= \nabla_{\boldsymbol{w}} L_{\mathcal{S}}(\boldsymbol{w})|_{\boldsymbol{w}+\hat{\epsilon}(\boldsymbol{w})} + \frac{d\hat{\epsilon}(\boldsymbol{w})}{d\boldsymbol{w}} \nabla_{\boldsymbol{w}} L_{\mathcal{S}}(\boldsymbol{w})|_{\boldsymbol{w}+\hat{\epsilon}(\boldsymbol{w})}.$$

The algorithm

Input: Training set $\mathcal{S} \triangleq \cup_{i=1}^{n}\{(\boldsymbol{x}_i, \boldsymbol{y}_i)\}$, Loss function $l : \mathcal{W} \times \mathcal{X} \times \mathcal{Y} \to \mathbb{R}_+$, Batch size b, Step size $\eta > 0$, Neighborhood size $\rho > 0$.

Output: Model trained with SAM

Initialize weights $\boldsymbol{w}_0$, $t = 0$;

while *not converged* **do**

  Sample batch $\mathcal{B} = \{(\boldsymbol{x}_1, \boldsymbol{y}_1), ...(\boldsymbol{x}_b, \boldsymbol{y}_b)\}$;

  $\delta(\boldsymbol{w}) = \nabla_{\boldsymbol{w}} L_{\mathcal{B}}(\boldsymbol{w})$;

  $\hat{\epsilon} = \frac{\delta(\boldsymbol{w}_t)}{\|\delta(\boldsymbol{w}_t)\|}$;

  $\boldsymbol{w}_{\mathrm{adv}} = \boldsymbol{w}_t + \hat{\epsilon}$;

  $\boldsymbol{g} = \delta(\boldsymbol{w}_{\mathrm{adv}})$;

  $\boldsymbol{w}_{t+1} = \boldsymbol{w}_t - \eta \boldsymbol{g}$;

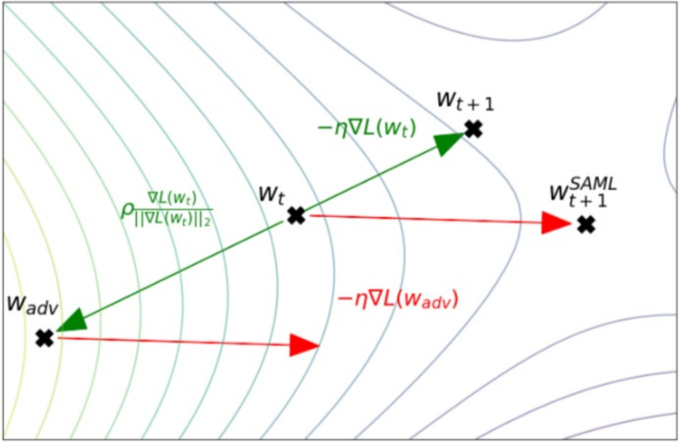
  $t = t + 1$;

end

return $\boldsymbol{w}_t$

The algorithm

Figure: One update of SAM against one update of plain gradient descent.



Robustness to corrupted labels

Method	Noise rate (%)			
	20	40	60	80
[SOA+19]	94.0	92.8	90.3	74.1
[ZS18]	89.7	87.6	82.7	67.9
[LYL+19]	87.1	81.8	75.4	-
[CLCZ19]	89.7	-	-	52.3
[HQJZ19]	92.6	90.3	43.4	-
MentorNet [JZL+17]	92.0	91.2	74.2	60.0
Mixup [ZCDLP17]	94.0	91.5	86.8	76.9
MentorMix [JHLY19]	**95.6**	**94.2**	91.3	**81.0**
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

Table: Test accuracy on the clean test set for models trained on CIFAR-10 with noisy labels. Lower block is our implementation, upper block gives scores

Multiple Columns

Heading

1. Statement
2. Explanation
3. Example

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Obtained results

Table: Test error rates for ResNet trained on CIFAR-10, with and without SAM.

CIFAR-10	Epoch	top-1	top-k
No SAM	100	15.34	0.91
No SAM	200	12.94	0.89
No SAM	400	11.24	**0.8**
SAM	100	**14.5**	**0.7**
SAM	200	**12.48**	**0.55**
SAM	400	**11.07**	1.08

Obtained results

Table: Test error rates for ResNet trained on CIFAR-100, with and without SAM.

CIFAR-100	Epoch	top-1	top-k
No SAM	100	89.93	66.33
No SAM	200	90.19	66.19
No SAM	400	**48.98**	**20.6**
SAM	100	**57.6**	**25.5**
SAM	200	**55.25**	**24.93**
SAM	400	78.09	43.27

FGSM (Fast Gradient Sign Method)

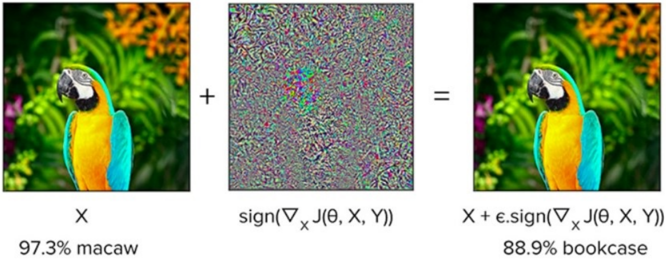

Figure 1: The Fast Gradient Sign Method (FGSM) for adversarial image generation

$$\hat{\epsilon}(\boldsymbol{w}) = \rho \ \mathrm{sign}\left(\nabla_{\boldsymbol{w}} L_{\mathcal{S}}(\boldsymbol{w})\right)$$

References

Pierre Foret, Ariel Kleiner, Hossein Mobahi, 2021
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The End