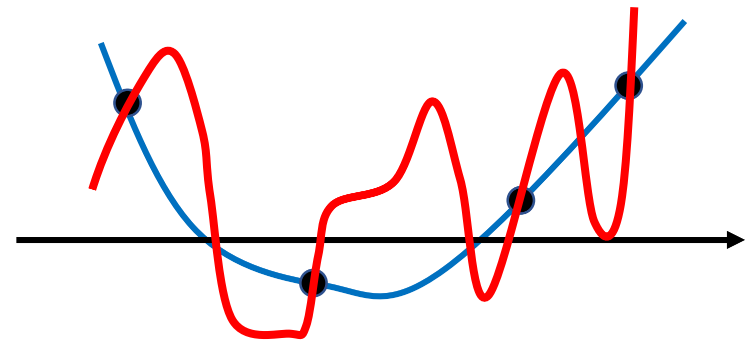
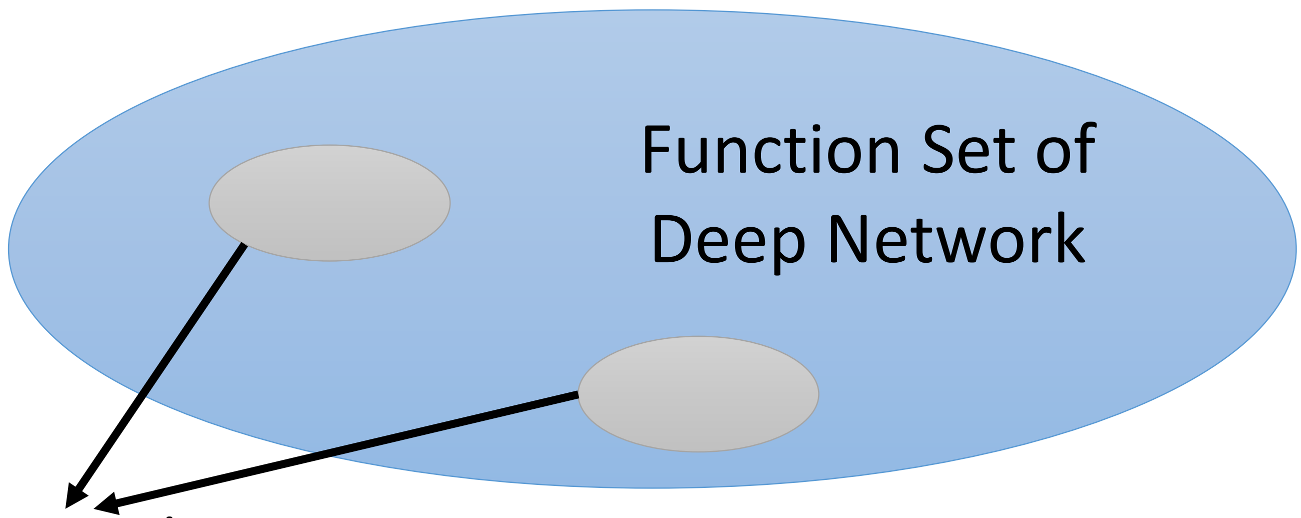
Indicator of Generalization

Introduction





Training zero is zero

我們需要一些indicator來告訴我們哪些是有助於training的

- ➢ If many global optimums can zero training errors, which one can obtain generalized results?
- ➢ Use the indicator to find solution that generalizes well.

兩個知名的inidcator

- ➢ ***Sharpness*** and ***Sensitivity***

Brute-force Memorization ?

- Real labels v.s. random labels

random label real label

First layer of CIFAR-10

https://arxiv.org/pdf/1706.05394.pdf

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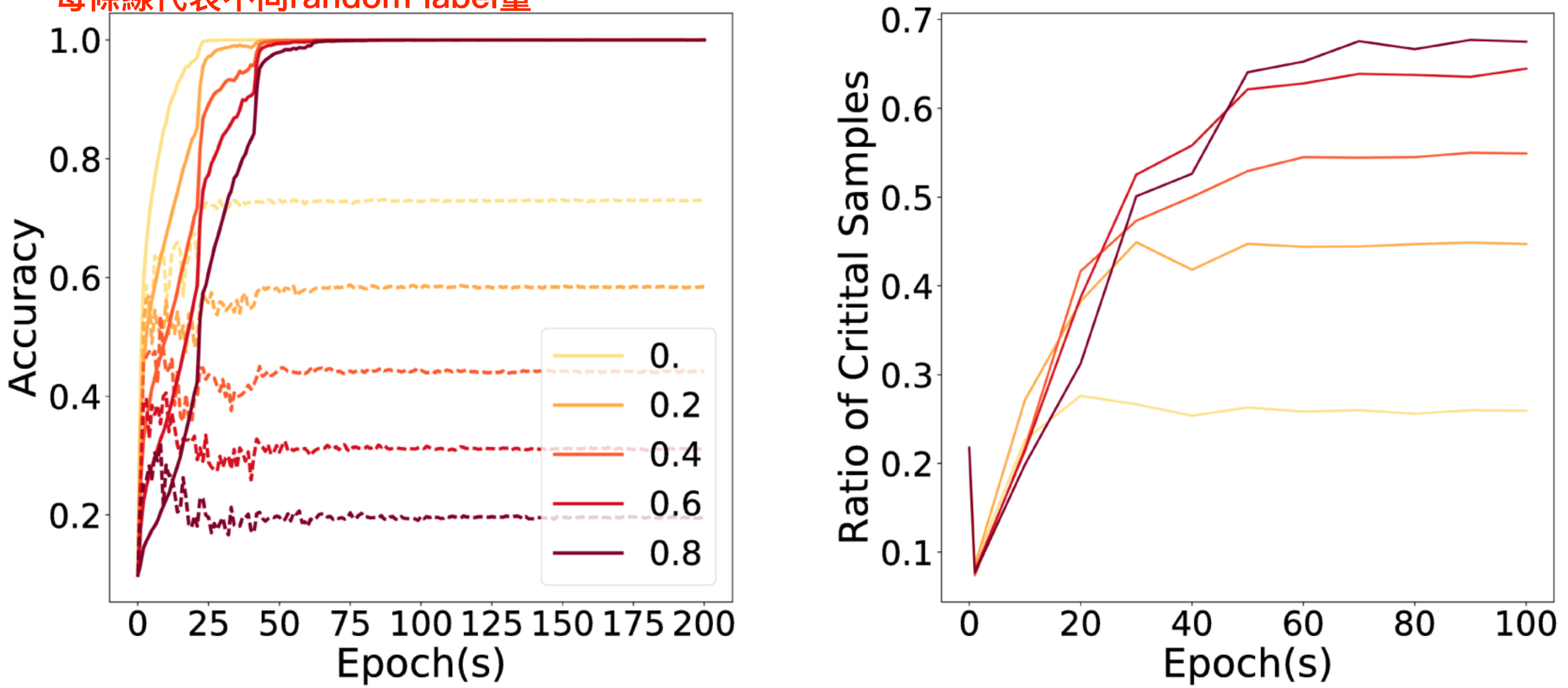
Brute-force Memorization ?

- Simple pattern first, then memorize exception

雖然最後train出來都可以達到1.0acc，但是其實是不同的network

每條線代表不同random label量

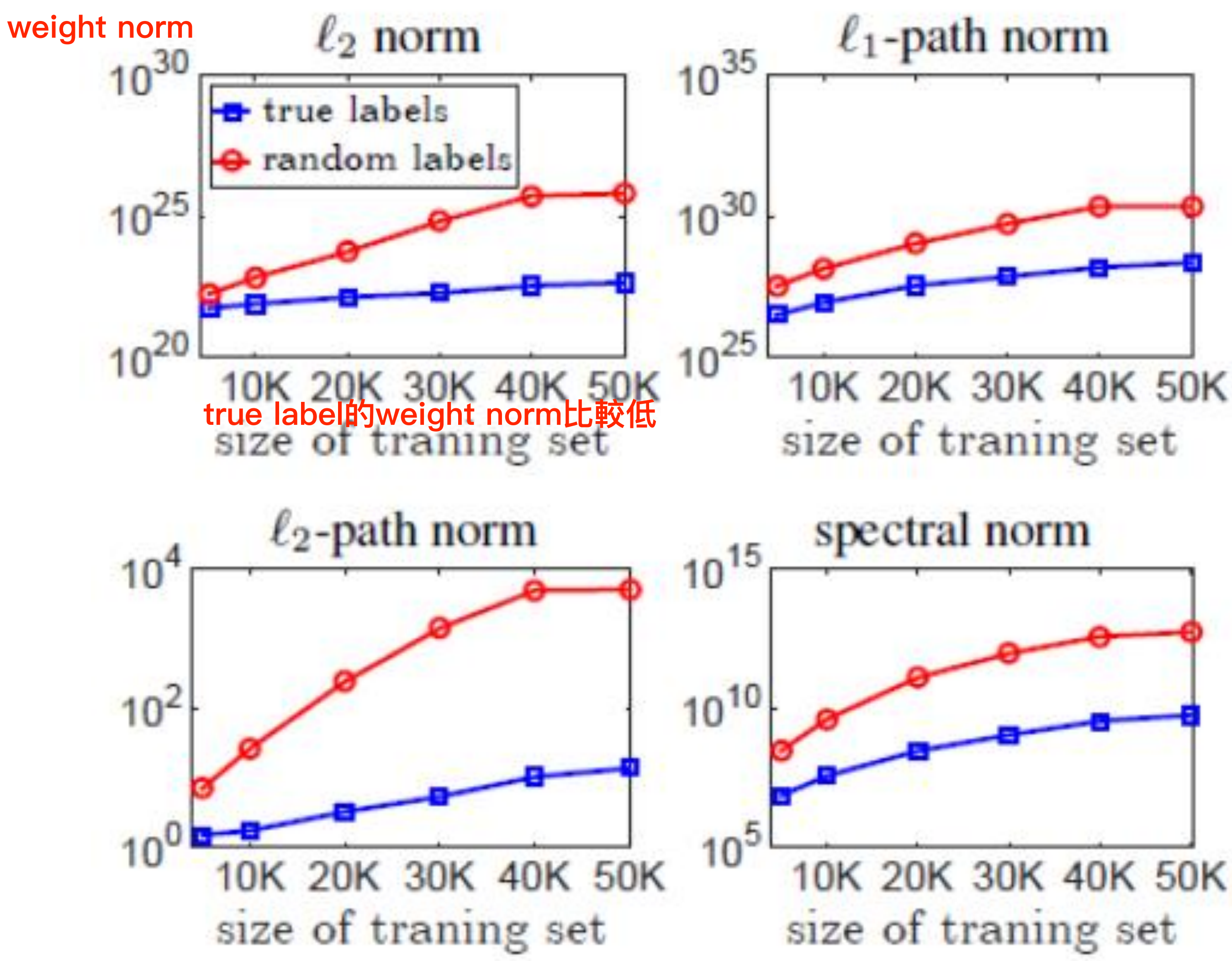


(b) Noise added on classification labels.

他將label　data做PCA後呈現，如果發現這個point周圍擁有許多不同的label，

表示他可能加入一點noise就會產生不同結果，意味著這是saddle point

Brute-force Memorization ?



Sensitivity

Google Deepmind

Jacobian Matrix

$$y = f(x) \qquad x = \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} \qquad y = \begin{bmatrix} y_1 \\ y_2 \end{bmatrix}$$

$$\frac{\partial y}{\partial x} =$$

分別拿x1/x2/x3對y1/y2做偏微分

size of y

size of x

Example

$$\begin{bmatrix} x_1 + x_2 x_3 \\ 2x_3 \end{bmatrix} = f\left(\begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix}\right) \qquad \frac{\partial y}{\partial x} = \begin{bmatrix} 1 & x3 & x2 \\ 0 & 0 & 2 \end{bmatrix}$$

Sensitivity

要有data以及network才可以算sensitivity

透過sensitivity，我們可以計算這筆test data對整個network的變化影響多大，越大表示越容易判斷錯誤

- Given a network f, the sensitivity of a data point x is the Frobenius norm of the Jacobian

$$y = f(x) \qquad \frac{\partial y}{\partial x} = \begin{bmatrix} \partial y_1/\partial x_1 & \partial y_1/\partial x_2 & \partial y_1/\partial x_3 \\ \partial y_2/\partial x_1 & \partial y_2/\partial x_2 & \partial y_2/\partial x_3 \end{bmatrix}$$

$$\text{Sensitivity of x} = \sqrt{\sum_i \sum_j \left(\frac{\partial y_j}{\partial x_i}\right)^2}$$

By the sensitivity of a test data x, we can predict the performance.

Without label

input一個少量的變化對我們的輸出有什麼樣的影響
（x有一點變化的時候對結果y有什麼樣的變化）

It is not surprise that sensitivity is related to generalization.

Regularization is kind of minimzing sensitivity.

希望network的weight越接近0越好，這樣output的值也會比較小，sensitivity也會比較小

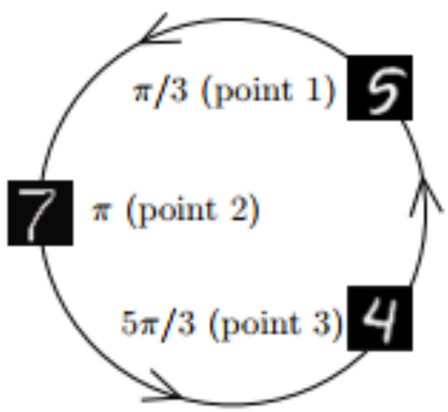
Sensitivity – Emprical Results

- Sensitivity on and off the training data manifold

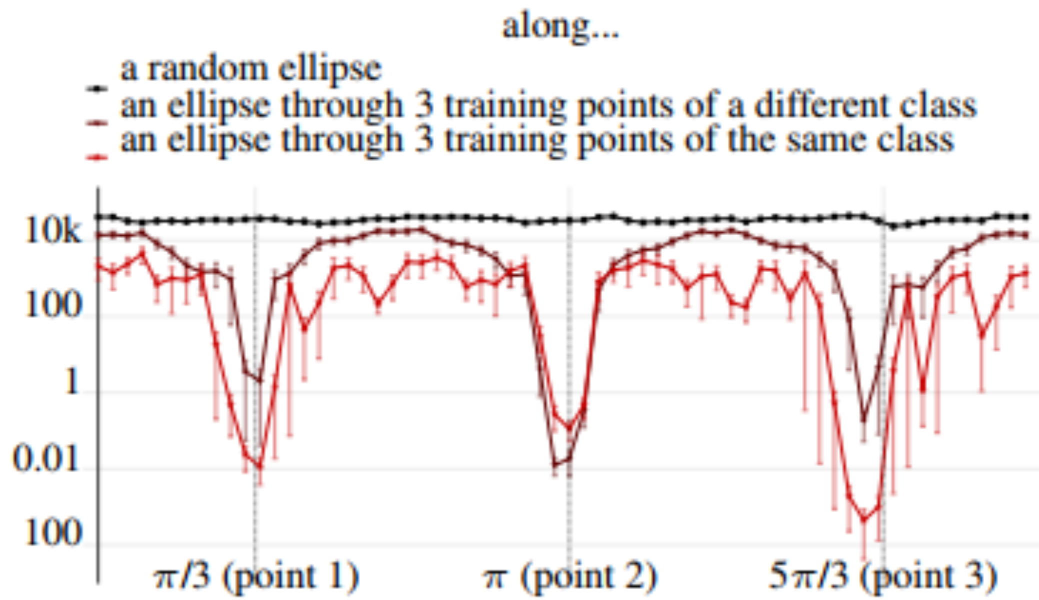
training data出現的地方sensitivity會變得比較小

Trajectory

每個點都是彼此的interpolation



Mean Jacobian norm

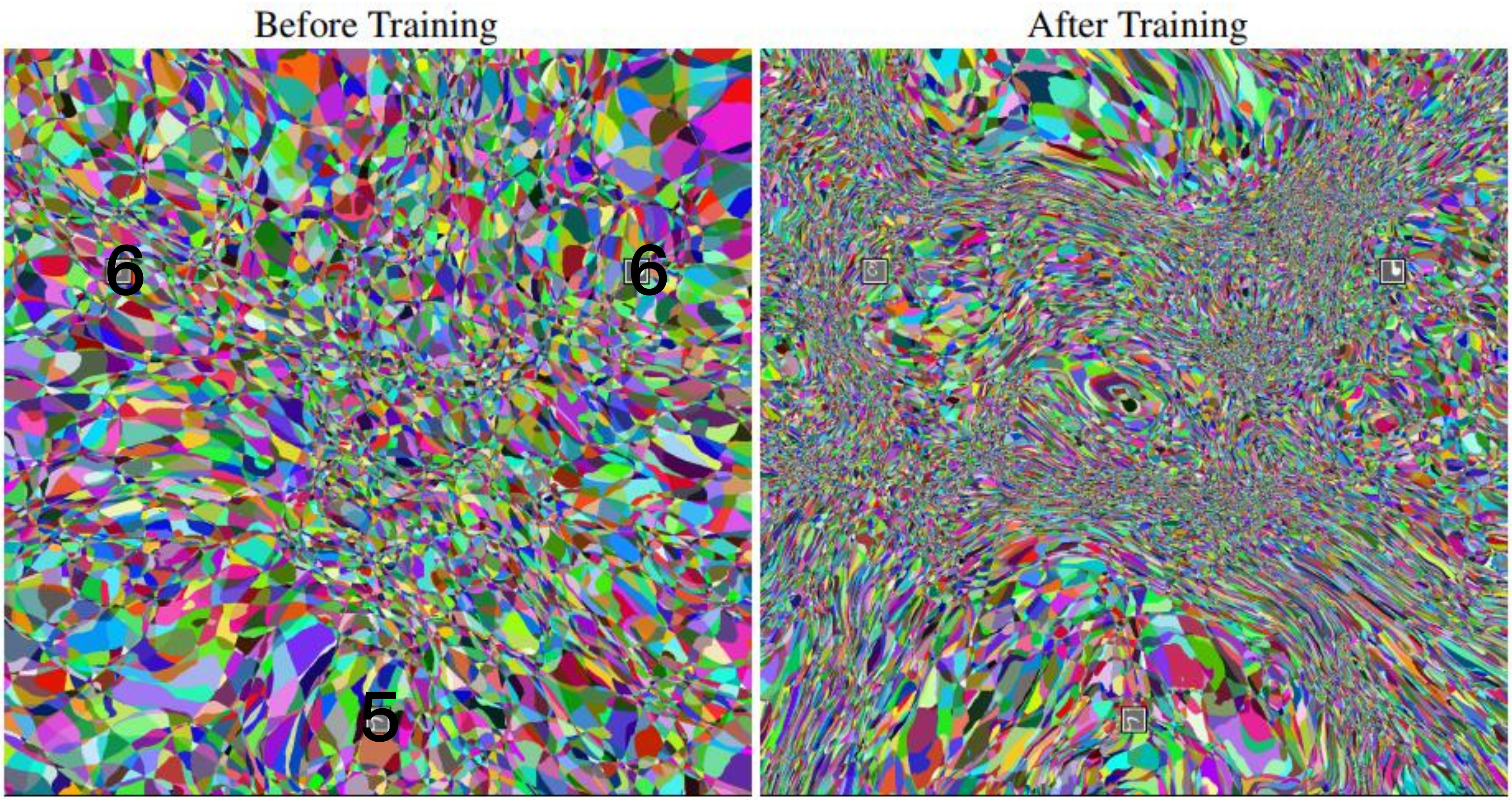


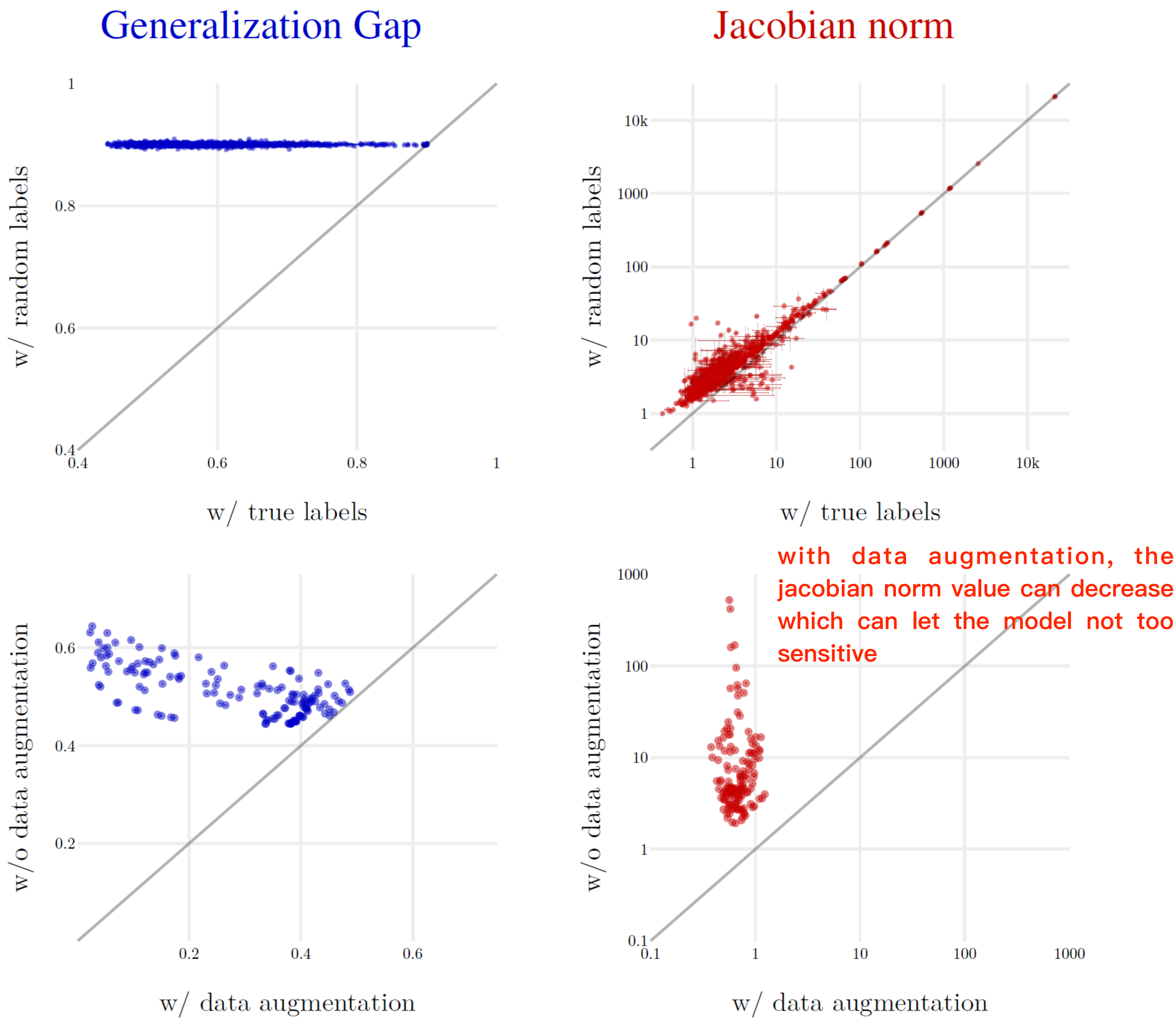
sample每個點所計算的jacobian norm

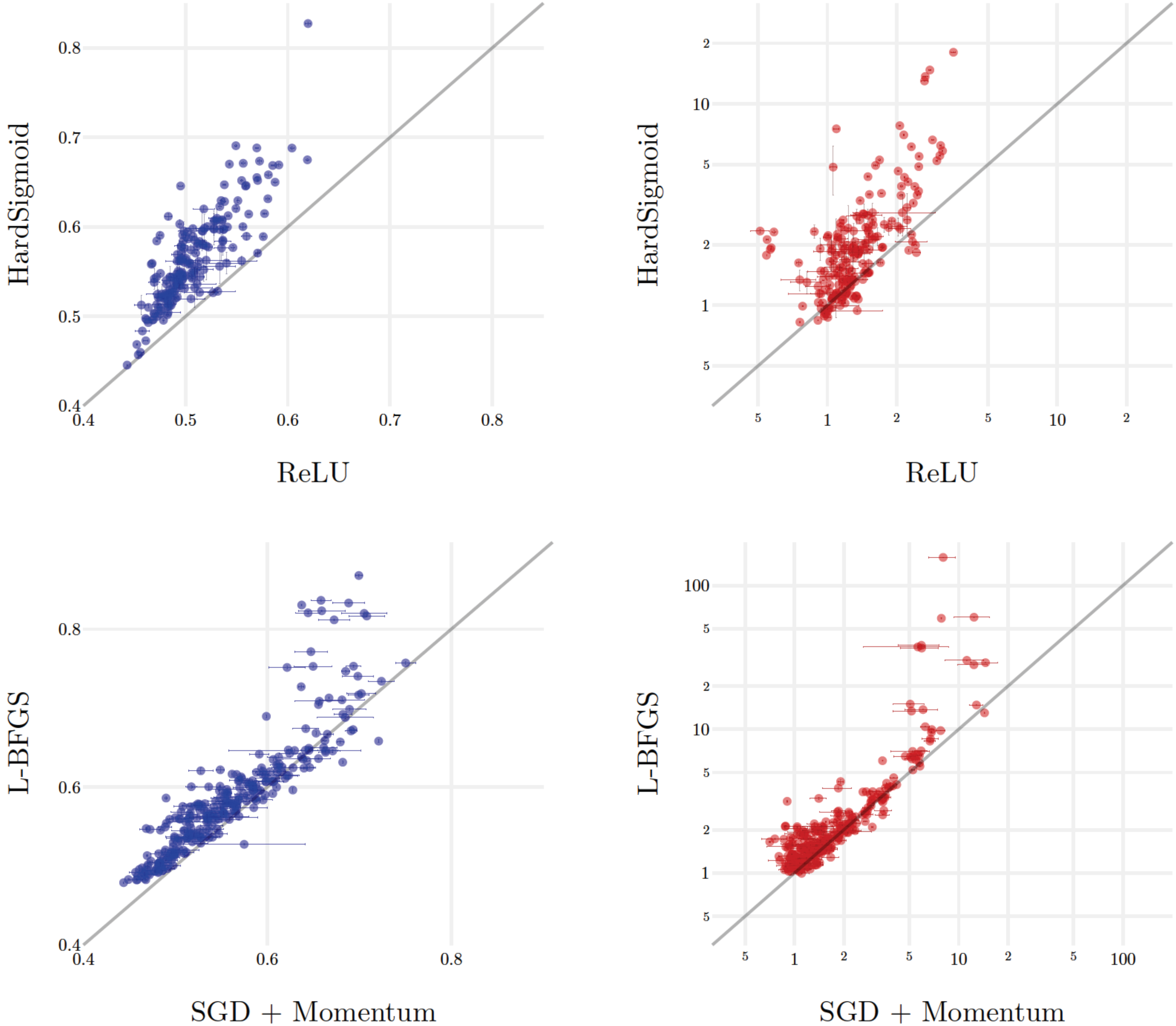
Sensitivity – Emprical Results

有數字的地方relu的piece比較大，也就是sensitivity比較低

- Sensitivity on and off the training data manifold

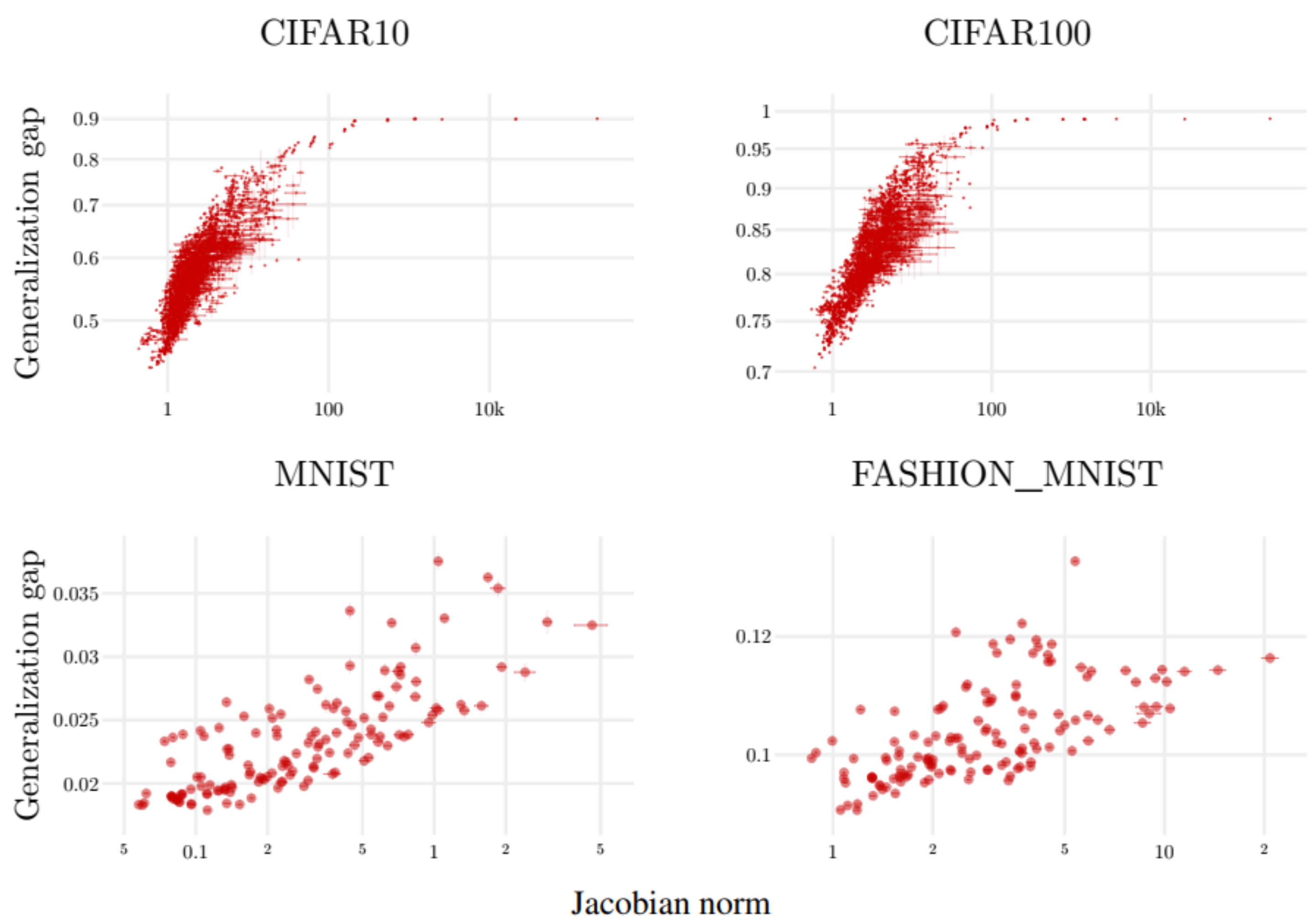



Generalization Gap
Jacobian norm
w/ random labels
w/ true labels
w/o data augmentation
w/ data augmentation
with data augmentation, the jacobian norm value can decrease which can let the model not too sensitive



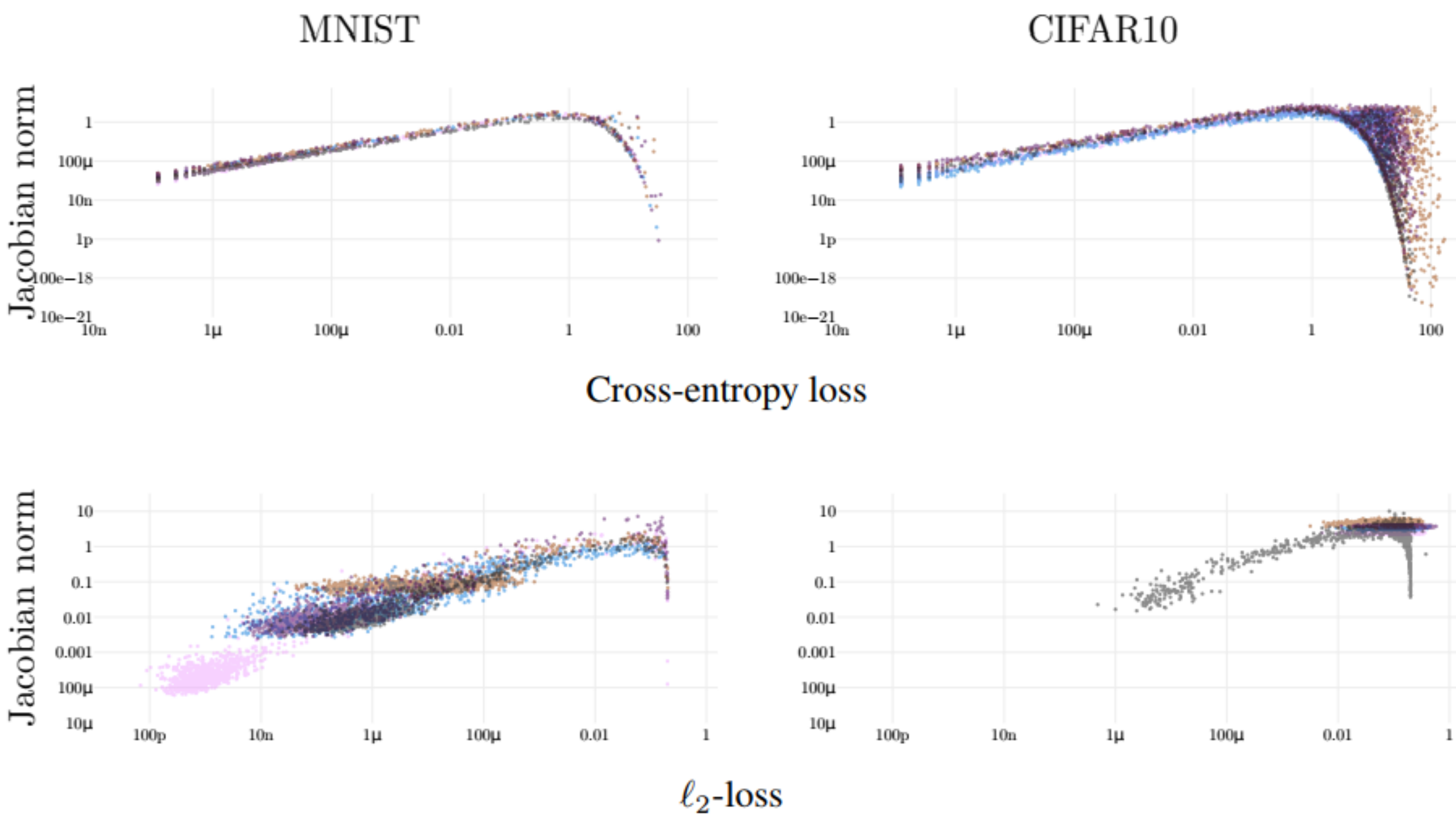
HardSigmoid
0.8
0.7
0.6
0.5
0.4
0.4
0.5
0.6
0.7
0.8
ReLU
HardSigmoid
2
10
5
2
1
5
5
1
2
5
10
2
ReLU
L-BFGS
0.8
0.6
0.4
0.4
0.6
0.8
SGD + Momentum
L-BFGS
100
5
2
10
5
2
1
5
5
1
2
5
10
2
5
100
SGD + Momentum

Sensitivity v.s. Generalization



Sensitivity v.s. Generalization

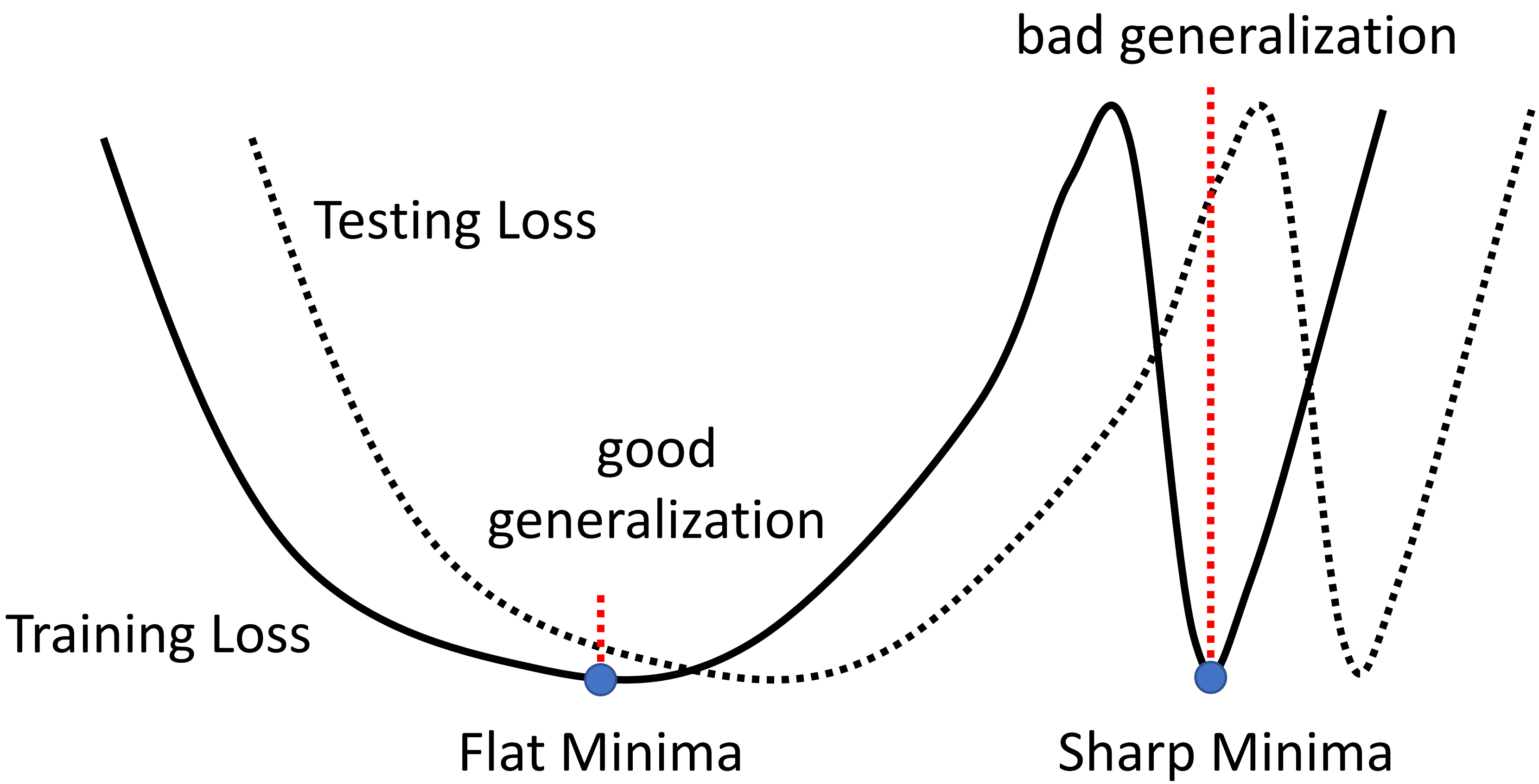
- individual points



Sharpness

Sharp Minima v.s Flat Minima

可能testing set的distribution與training set是有誤差的

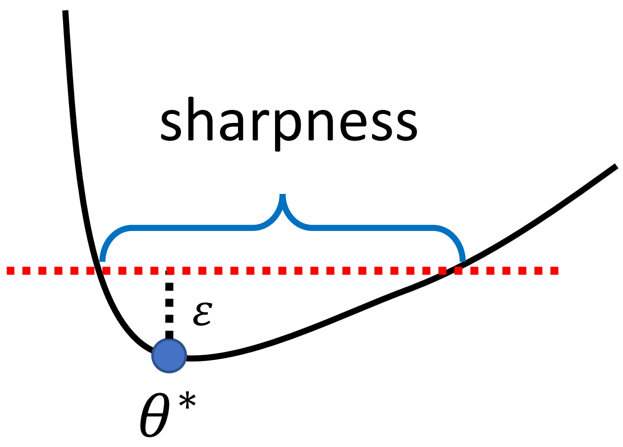


flat minima比較能夠對應testing set distribution的mismatch

Explain self regularization?

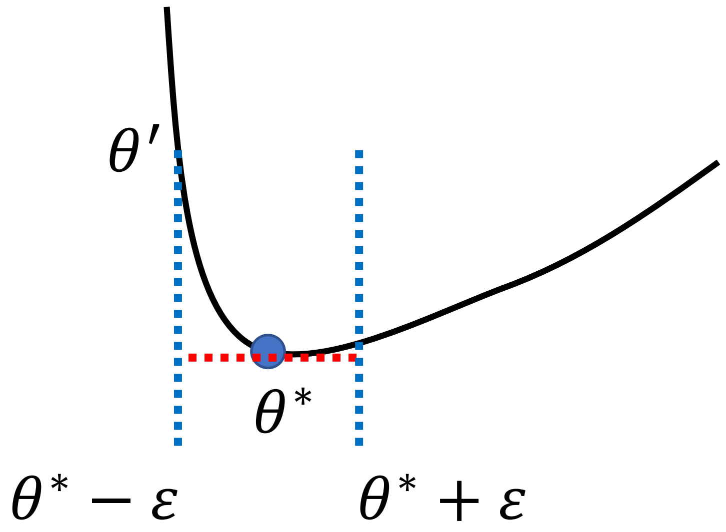
Definition of Sharpness

Definition 1



Definition 2

$$\text{Sharpness} = L(\theta') - L(\theta^*)$$



Batch Size

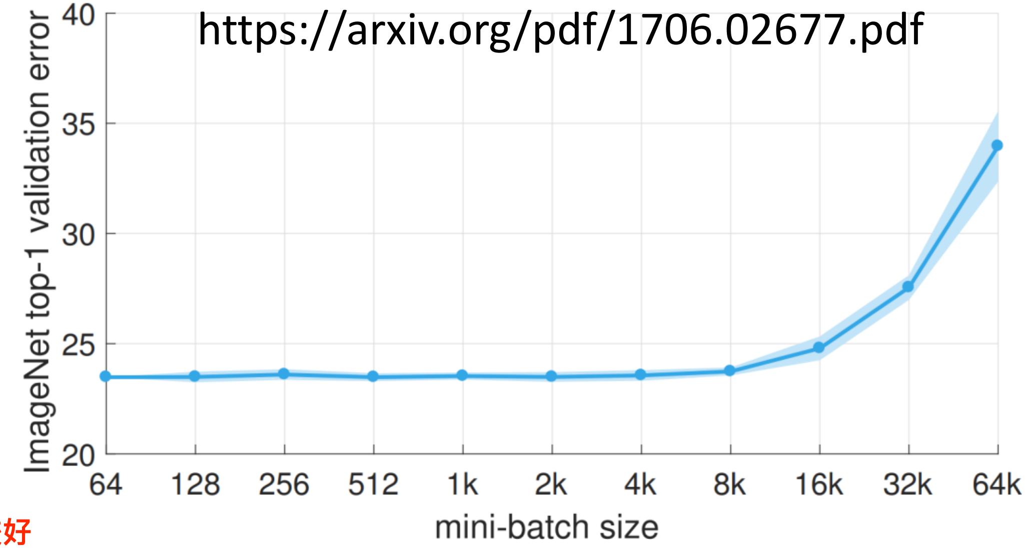
batch size跟sharpness是有關係的

一般來說batch_size越大 validation error越大

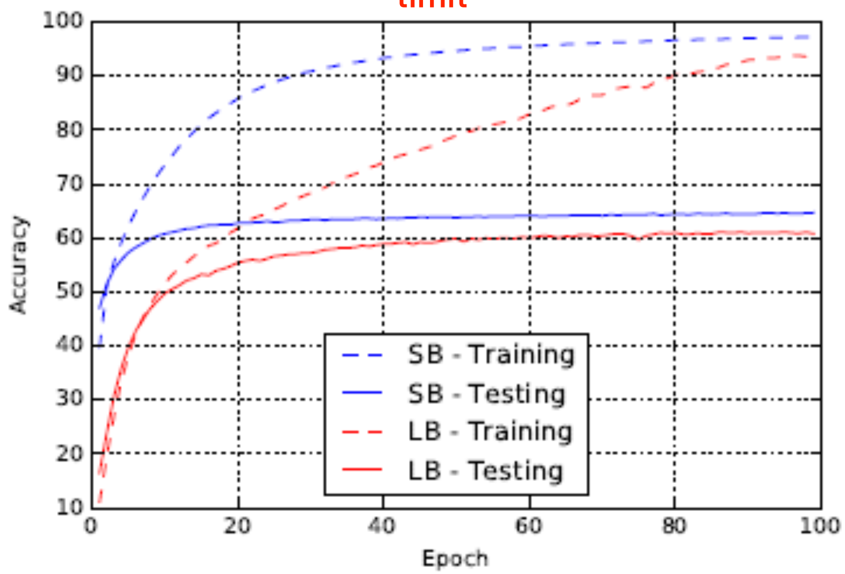
batch_size變化對testing acc有影響
如果epoch夠多 training acc都可以接近

small batch size對於model的generalization能力比較好

https://arxiv.org/pdf/1706.02677.pdf

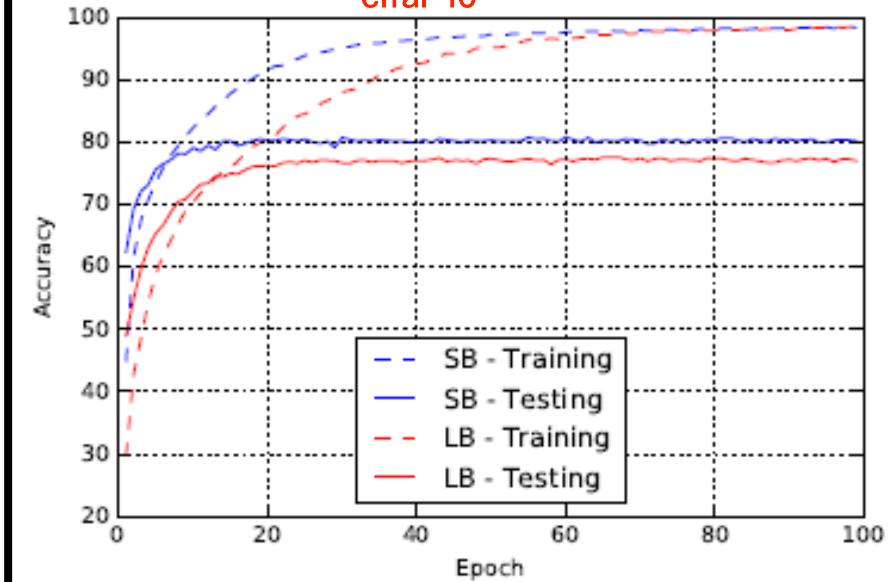


timit



(a) Network F_2

cifar 10



(b) Network C_1

Batch Size v.s. Sharpness

Name	Network Type	Data set
F_1	Fully Connected	MNIST (LeCun et al., 1998a)
F_2	Fully Connected	TIMIT (Garofolo et al., 1993)
C_1	(Shallow) Convolutional	CIFAR-10 (Krizhevsky & Hinton, 2009)
C_2	(Deep) Convolutional	CIFAR-10
C_3	(Shallow) Convolutional	CIFAR-100 (Krizhevsky & Hinton, 2009)
C_4	(Deep) Convolutional	CIFAR-100

	Training Accuracy		Testing Accuracy	
Name	SB	LB	SB	LB
F_1	$99.66\% \pm 0.05\%$	$99.92\% \pm 0.01\%$	$98.03\% \pm 0.07\%$	$97.81\% \pm 0.07\%$
F_2	$99.99\% \pm 0.03\%$	$98.35\% \pm 2.08\%$	$64.02\% \pm 0.2\%$	$59.45\% \pm 1.05\%$
C_1	$99.89\% \pm 0.02\%$	$99.66\% \pm 0.2\%$	$80.04\% \pm 0.12\%$	$77.26\% \pm 0.42\%$
C_2	$99.99\% \pm 0.04\%$	$99.99\% \pm 0.01\%$	$89.24\% \pm 0.12\%$	$87.26\% \pm 0.07\%$
C_3	$99.56\% \pm 0.44\%$	$99.88\% \pm 0.30\%$	$49.58\% \pm 0.39\%$	$46.45\% \pm 0.43\%$
C_4	$99.10\% \pm 1.23\%$	$99.57\% \pm 1.84\%$	$63.08\% \pm 0.5\%$	$57.81\% \pm 0.17\%$

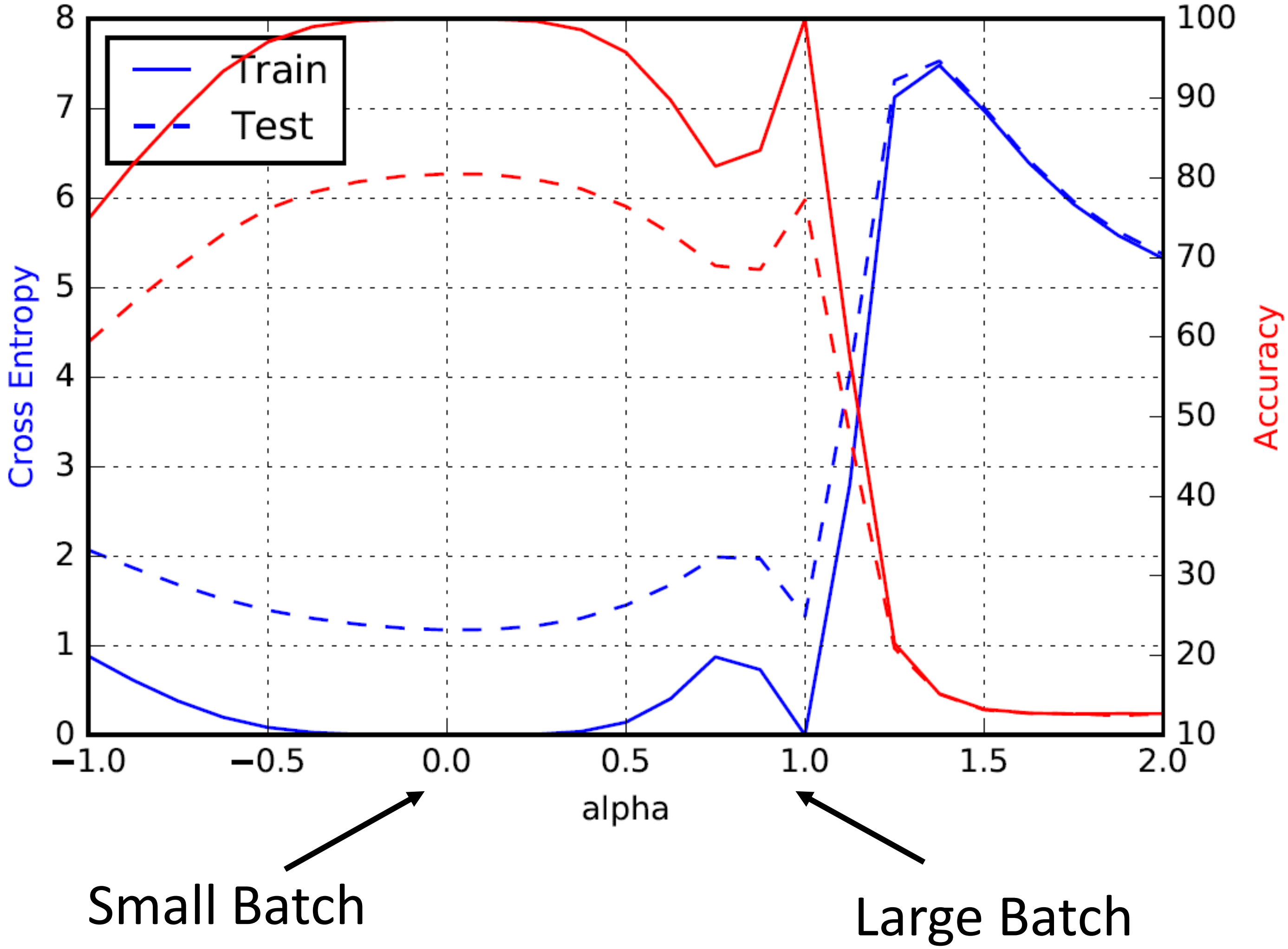
	$\epsilon = 10^{-3}$		$\epsilon = 5 \cdot 10^{-4}$	
	SB	LB	SB	LB
F_1	1.23 ± 0.83	205.14 ± 69.52	0.61 ± 0.27	42.90 ± 17.14
F_2	1.39 ± 0.02	310.64 ± 38.46	0.90 ± 0.05	93.15 ± 6.81
C_1	28.58 ± 3.13	707.23 ± 43.04	7.08 ± 0.88	227.31 ± 23.23
C_2	8.68 ± 1.32	925.32 ± 38.29	2.07 ± 0.86	175.31 ± 18.28
C_3	29.85 ± 5.98	258.75 ± 8.96	8.56 ± 0.99	105.11 ± 13.22
C_4	12.83 ± 3.84	421.84 ± 36.97	4.07 ± 0.87	109.35 ± 16.57

SB = 256

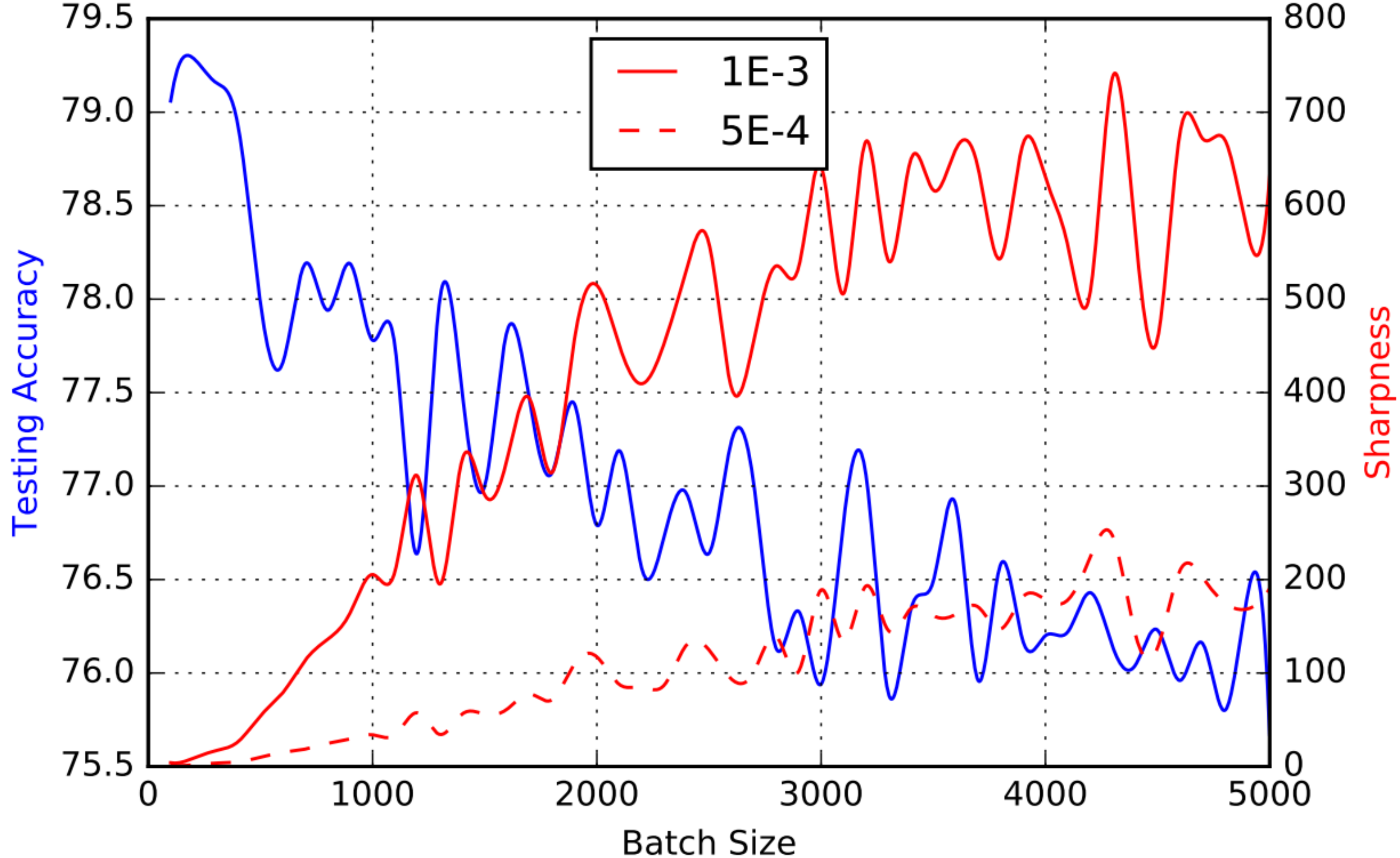
LB = 0.1 x data set

Batch Size v.s. Sharpness

ian good fellow



Batch Size v.s. Sharpness



Concluding Remarks

Summary

- Good generalization are associated with sensitivity
- Good generalization are associated with flatness (?)
- Understaning the indicator for generalization helps us develop algorithm in the future

知道什麼樣的network可以對generalization有幫助，就把他加入net

Reference

分析有沒有overfitting的差別

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