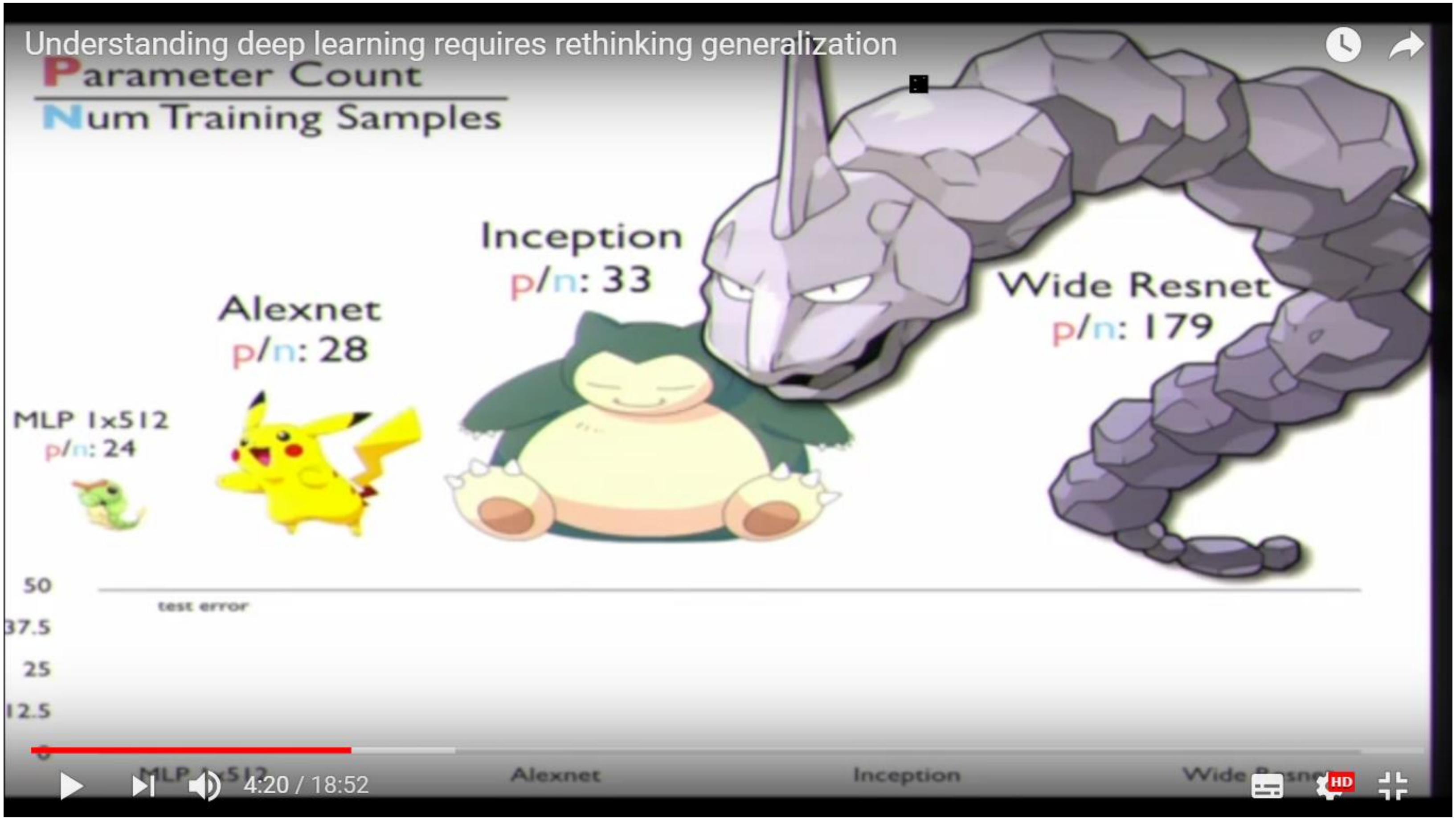
Generalization Ability

We use very large network today



Source of image: https://www.youtube.com/watch?v=kCj51pTQPKI

機器學習基石
https://youtu.be/XxPB9GlJEUk

Generalization Gap

No matter the data distribution

With probability $1-\delta$

$$E_{train} \leq E_{test} \leq E_{train} + \Omega(R, M, \delta)$$

Smaller δ, larger Ω

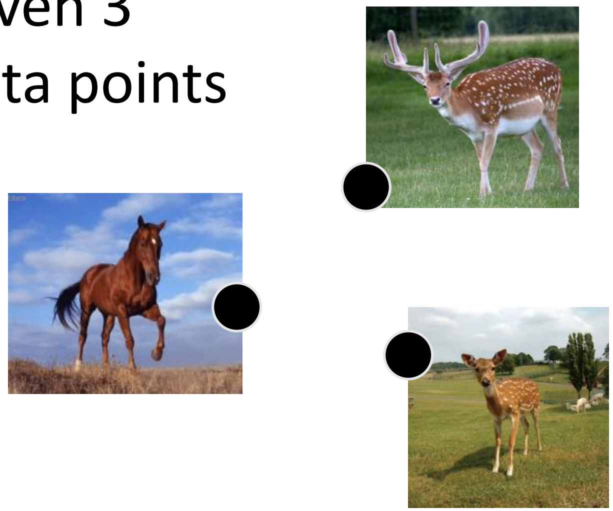
R is the number of training data → Larger R, smaller Ω

M is the "capacity" of your model → Larger M, larger Ω

("size" of the function set)

How to measure the "capacity"? VC dimension (d_{VC})

Given 3
data points



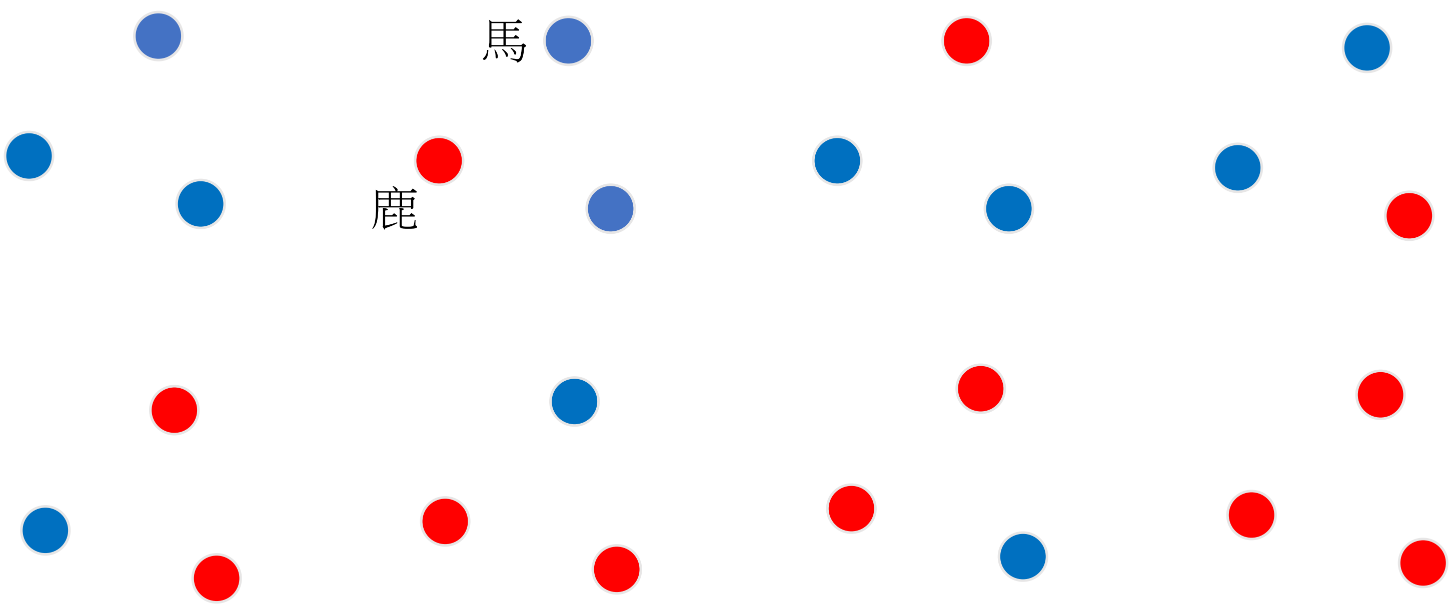
Random label (故意亂教)

Model M can always achieve 0% error rate

(亂教 Model M 都學得會)

VC dimension (d_{VC}) of Model M $\geq$ 3

e.g. linear model

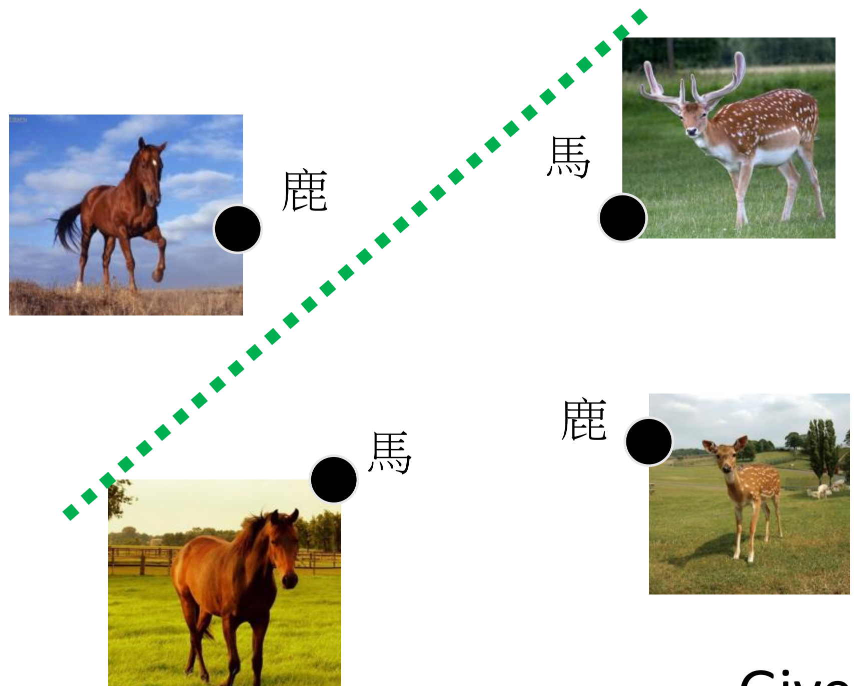


Random label (故意亂教)

There are some cases linear model can not learn.

(來亂的，所以學不會)

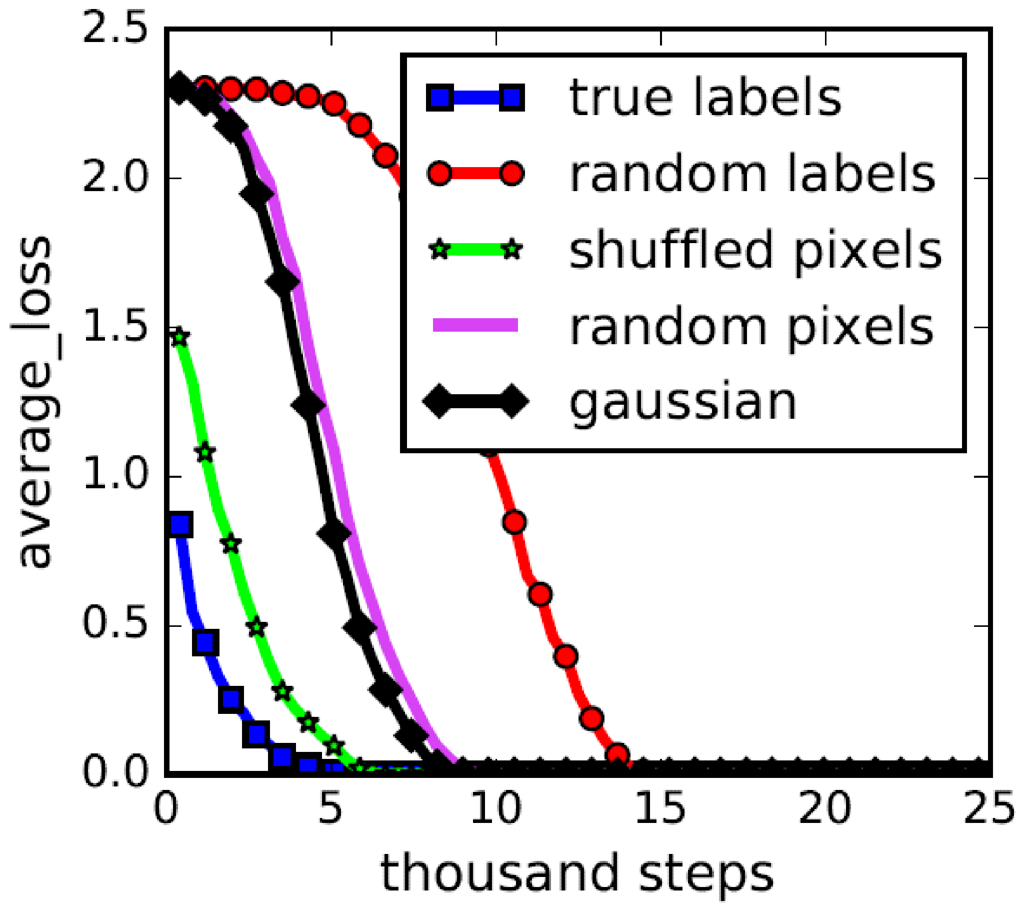
VC dimension (d_{VC}) of Linear Model < 4



Given 4 data points

What is the capacity of deep models?

Inception model on the CIFAR10



Chiyuan Zhang, Samy Bengio, Moritz Hardt, Benjamin Recht, Oriol Vinyals, "Understanding deep learning requires rethinking generalization", ICLR 2017

Overparameterized Network?

No matter the data distribution

With probability $1-\delta$

$$E_{test} \leq E_{train} + \Omega(R, M, \delta)$$

Smaller δ, larger Ω

R is the number of training data → Larger R, smaller Ω

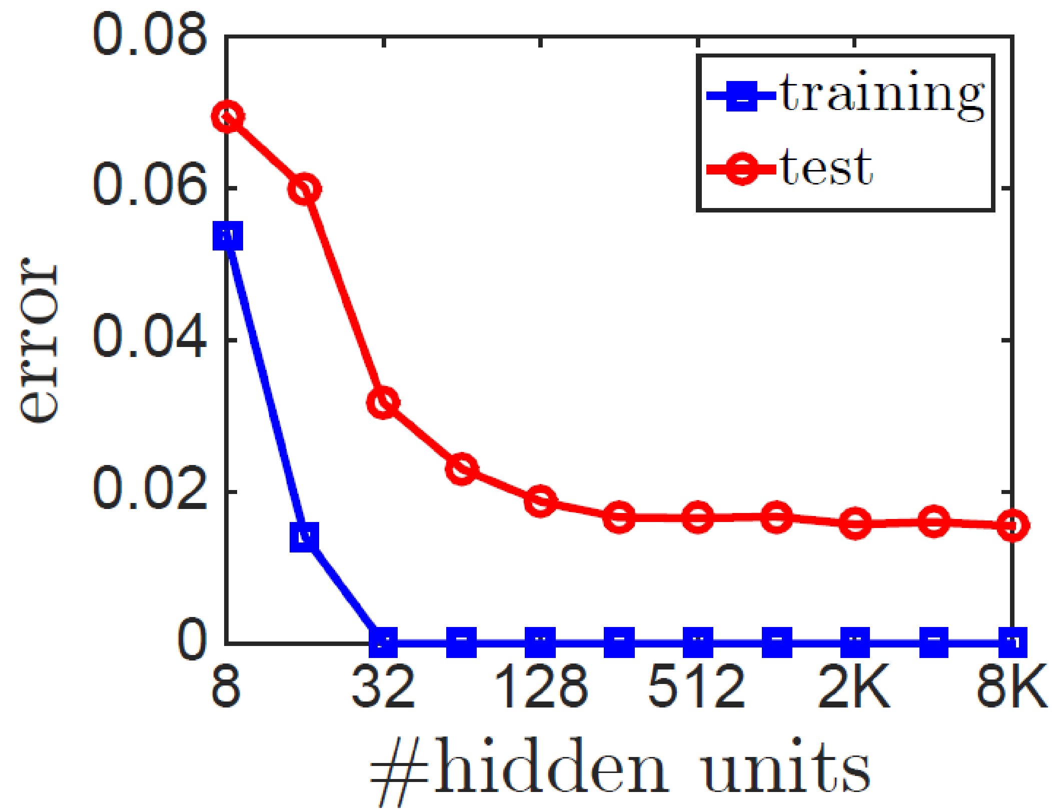
M is the "capacity" of your model → Larger M, larger Ω

("size" of the function set)

If two models have the same E_{train} → Select the one with smaller capacity

Demo

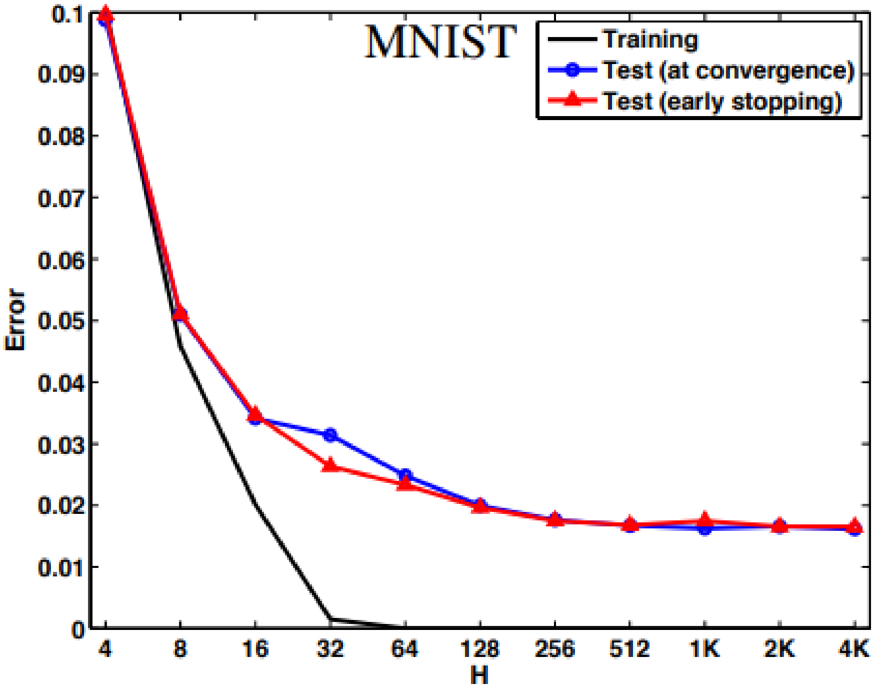
Overparameterized Network?

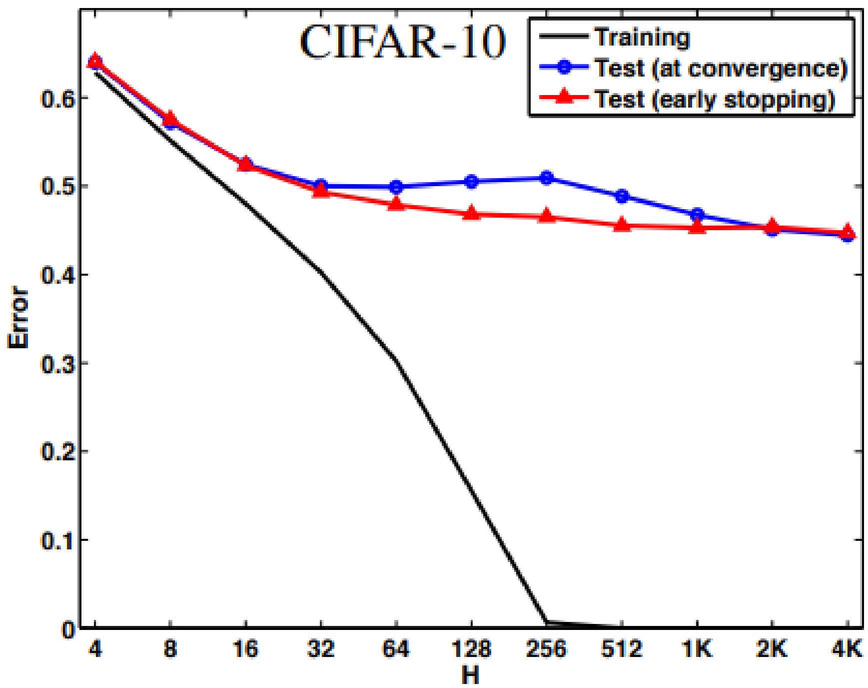


MNIST

https://arxiv.org/abs/1706.08947

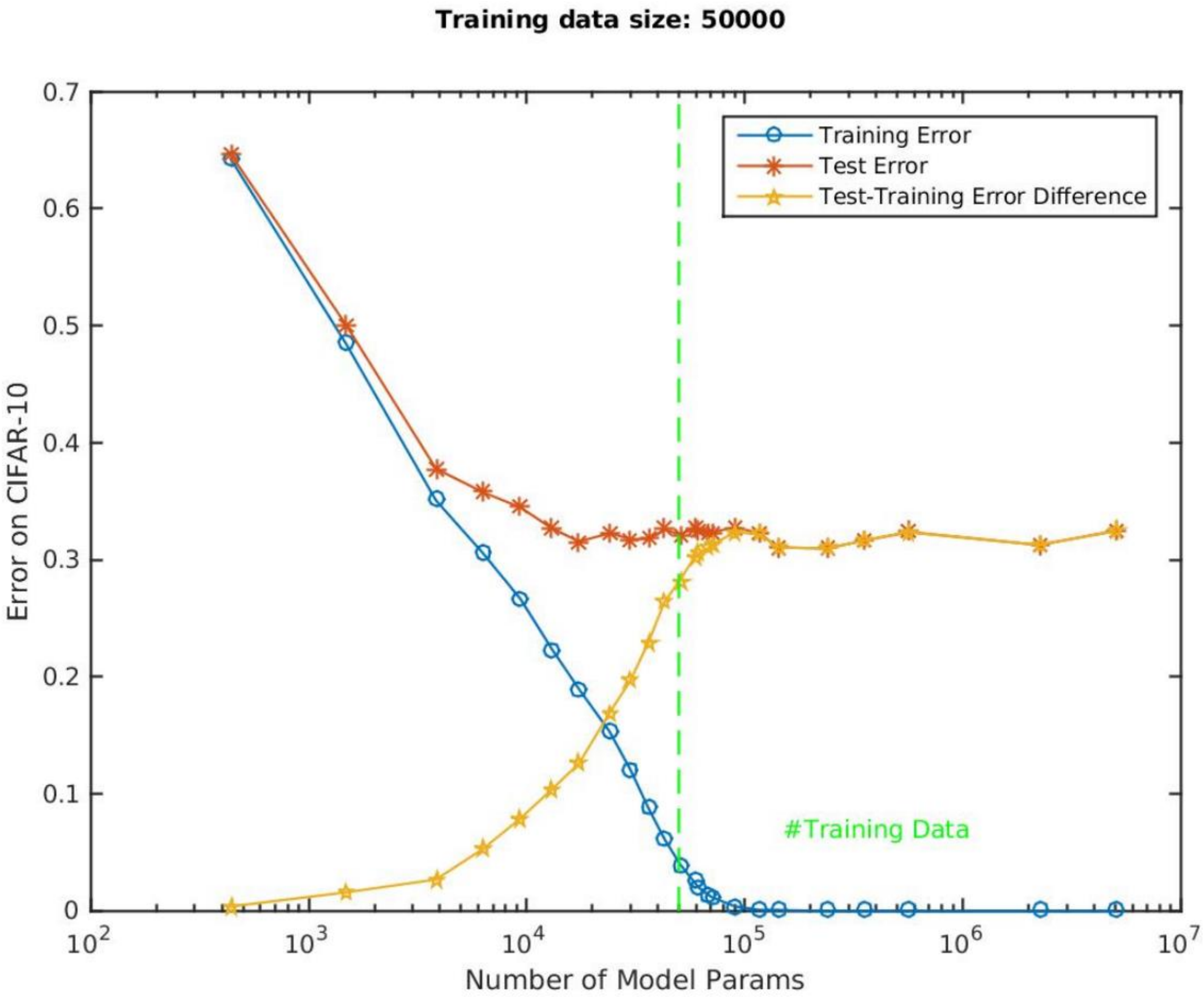
Overparameterized Network?



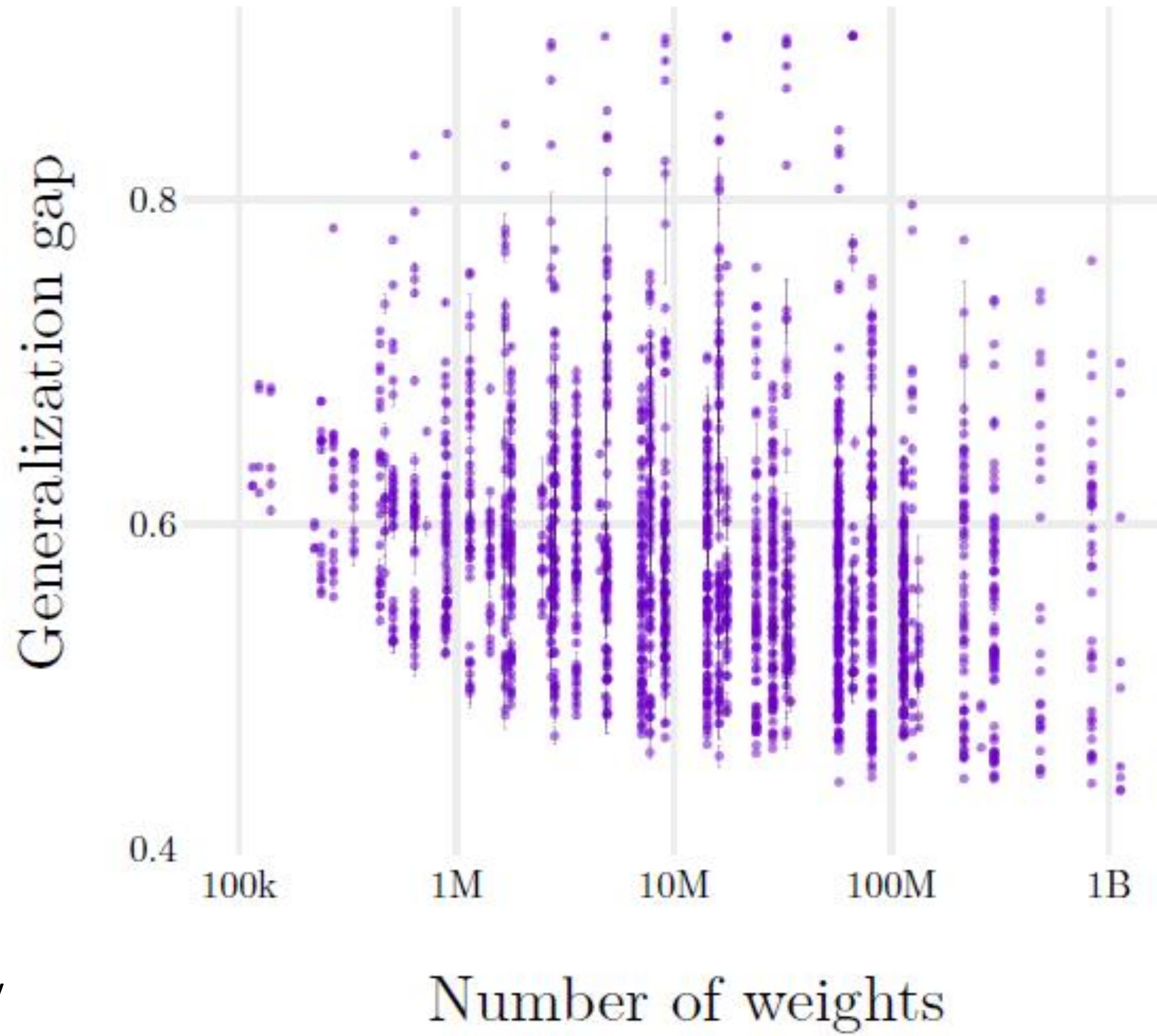


https://arxiv.org/pdf/1412.6614.pdf

Overparameterized Network?

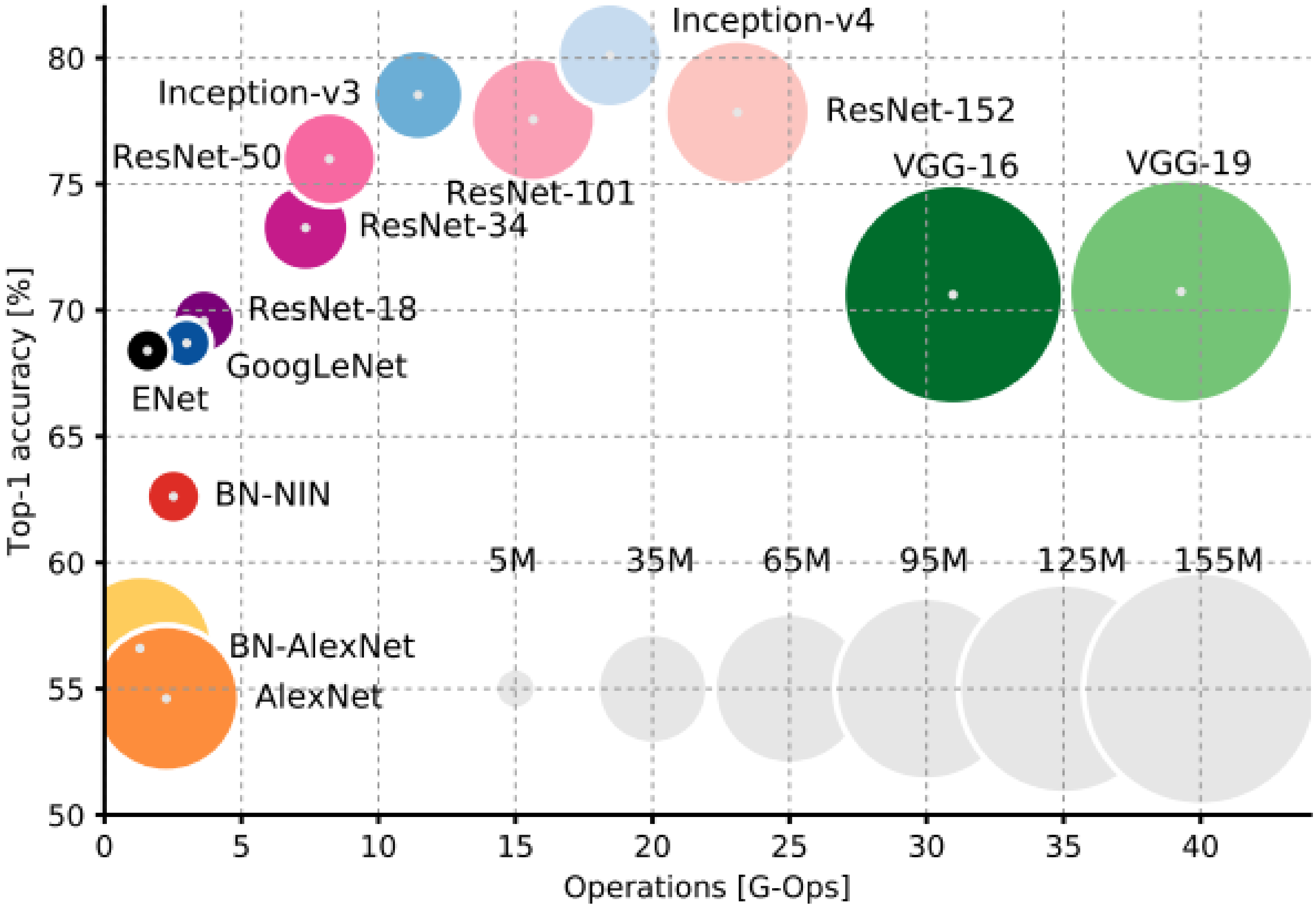


https://arxiv.org/abs/1801.00173



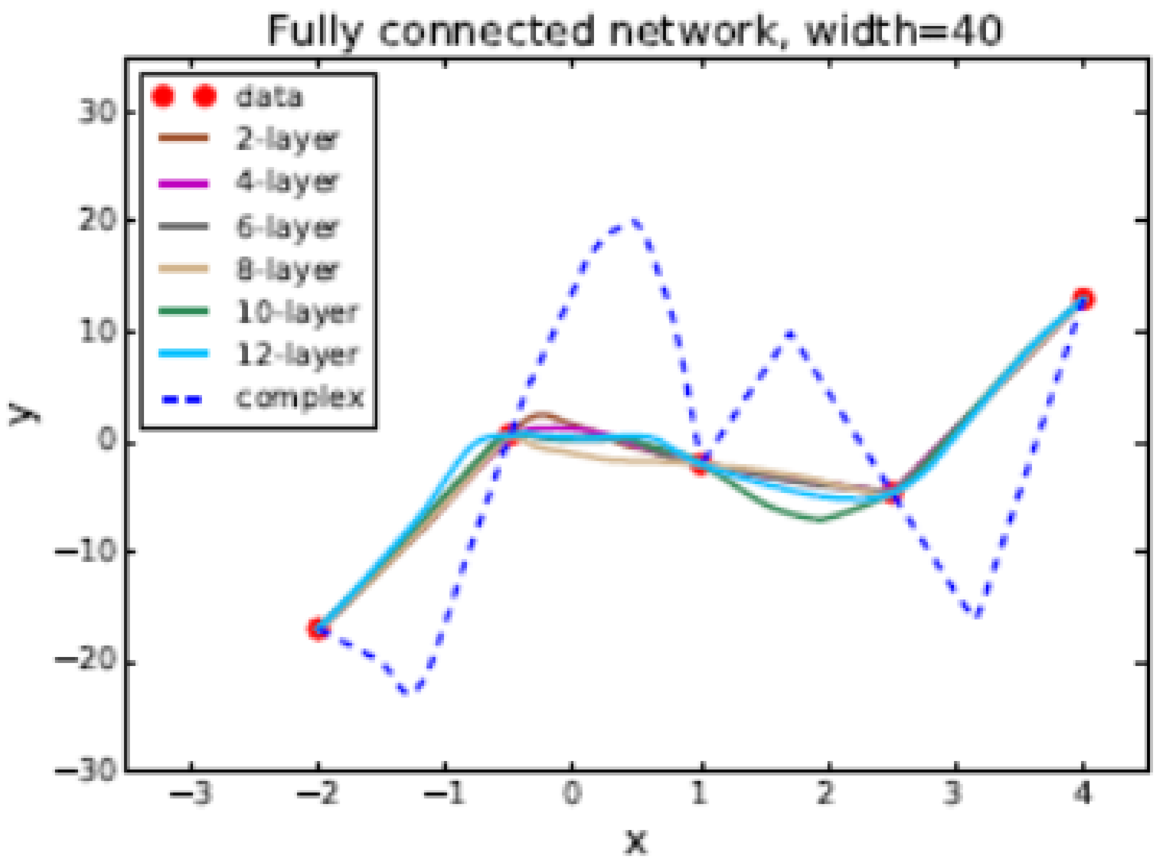
CIFIR-10, 100%
training accuracy

https://arxiv.org/pdf/1802.08760.pdf



https://arxiv.org/abs/1605.07678

Network regularizes itself?



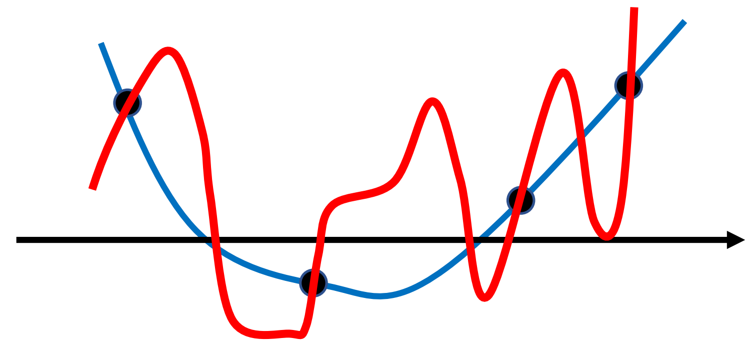
https://arxiv.org/pdf/1706.10239.pdf

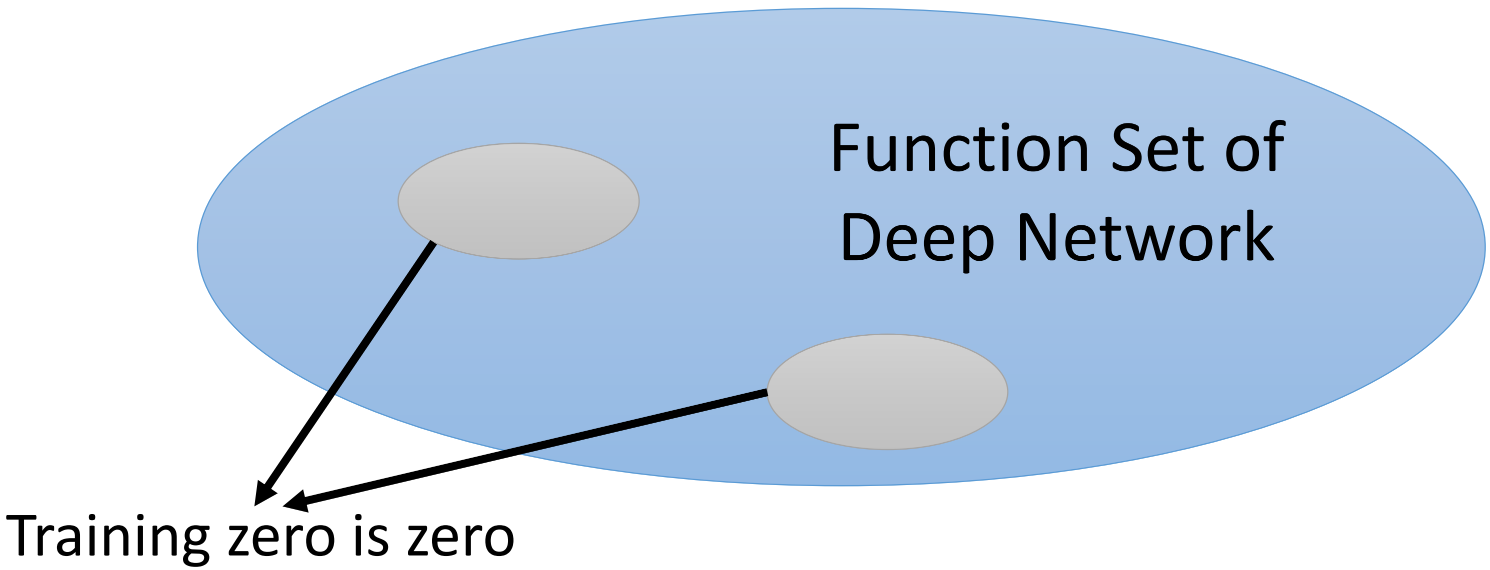
Concluding Remarks

- The capacity of deep model is large.
- However, it does not overfit!
- The reason is not clear yet.

Indicator of Generalization

Introduction





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

Brute-force Memorization ?

- Real labels v.s. random labels

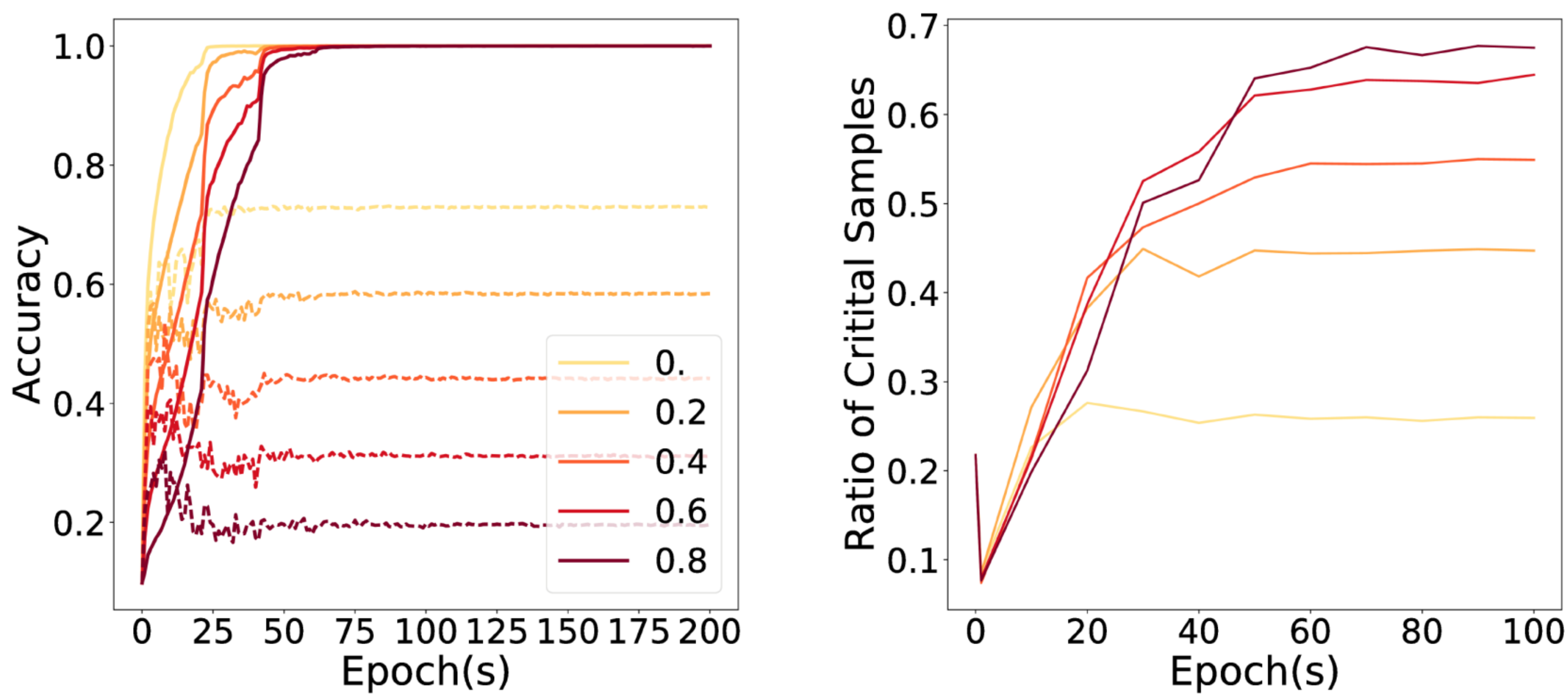
First layer of CIFAR-10

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

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

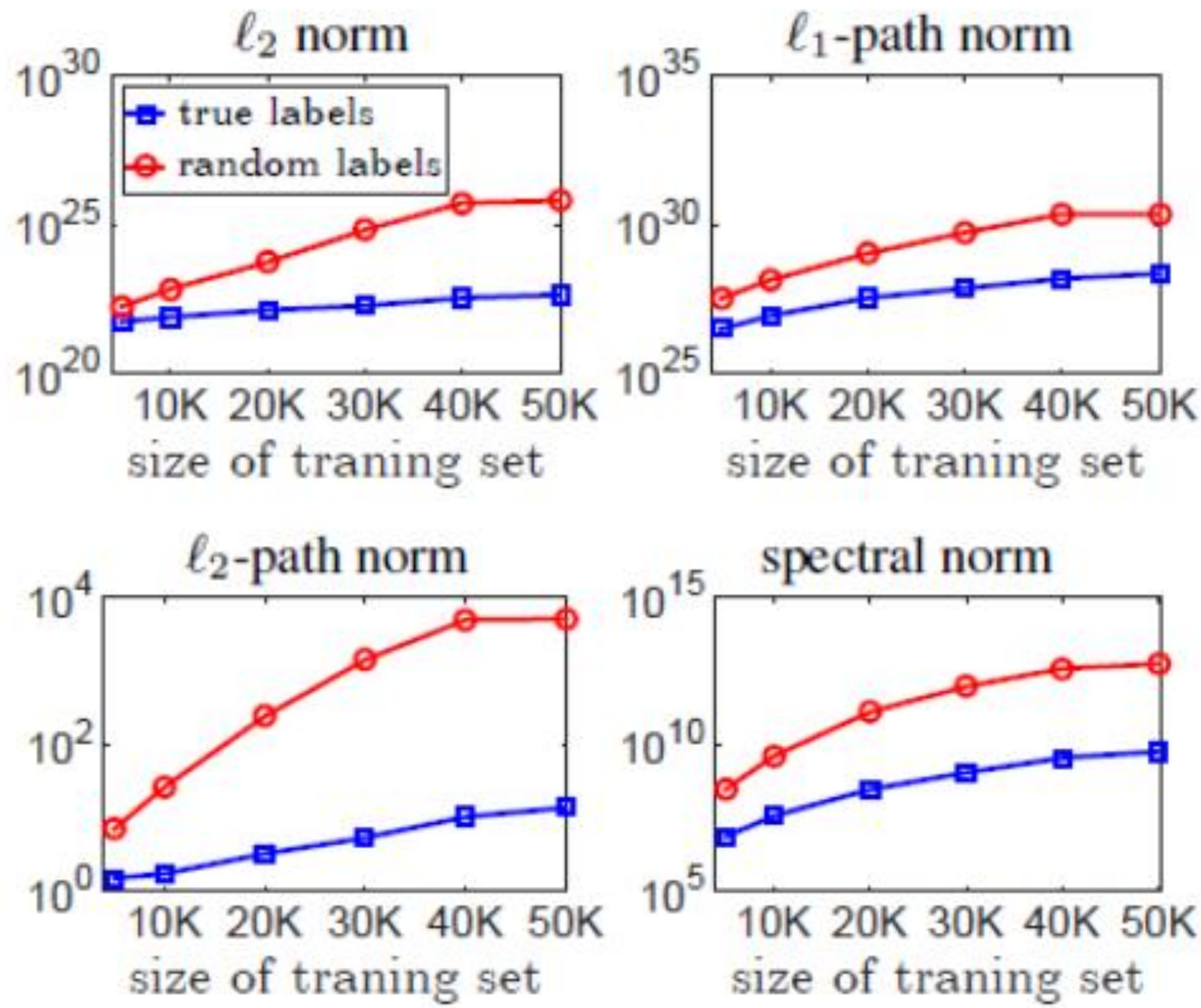
Brute-force Memorization ?

- Simple pattern first, then memorize exception



(b) Noise added on classification labels.

Brute-force Memorization ?



Sensitivity

Jacobian Matrix

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

$$\frac{\partial y}{\partial x} = \underbrace{\left.\phantom{\begin{matrix} \quad\quad\quad\quad\quad\quad\quad\quad\quad\quad \\ \\ \\ \end{matrix}}\right\}\text{size of y}}_{\text{size of x}}$$

Example

$$\begin{bmatrix} x_1 + x_2 x_3 \\ 2x_3 \end{bmatrix} = f\left(\begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix}\right) \qquad \frac{\partial y}{\partial x} = \begin{bmatrix} \quad\quad\quad\quad\quad\quad \end{bmatrix}$$

Sensitivity

- 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.

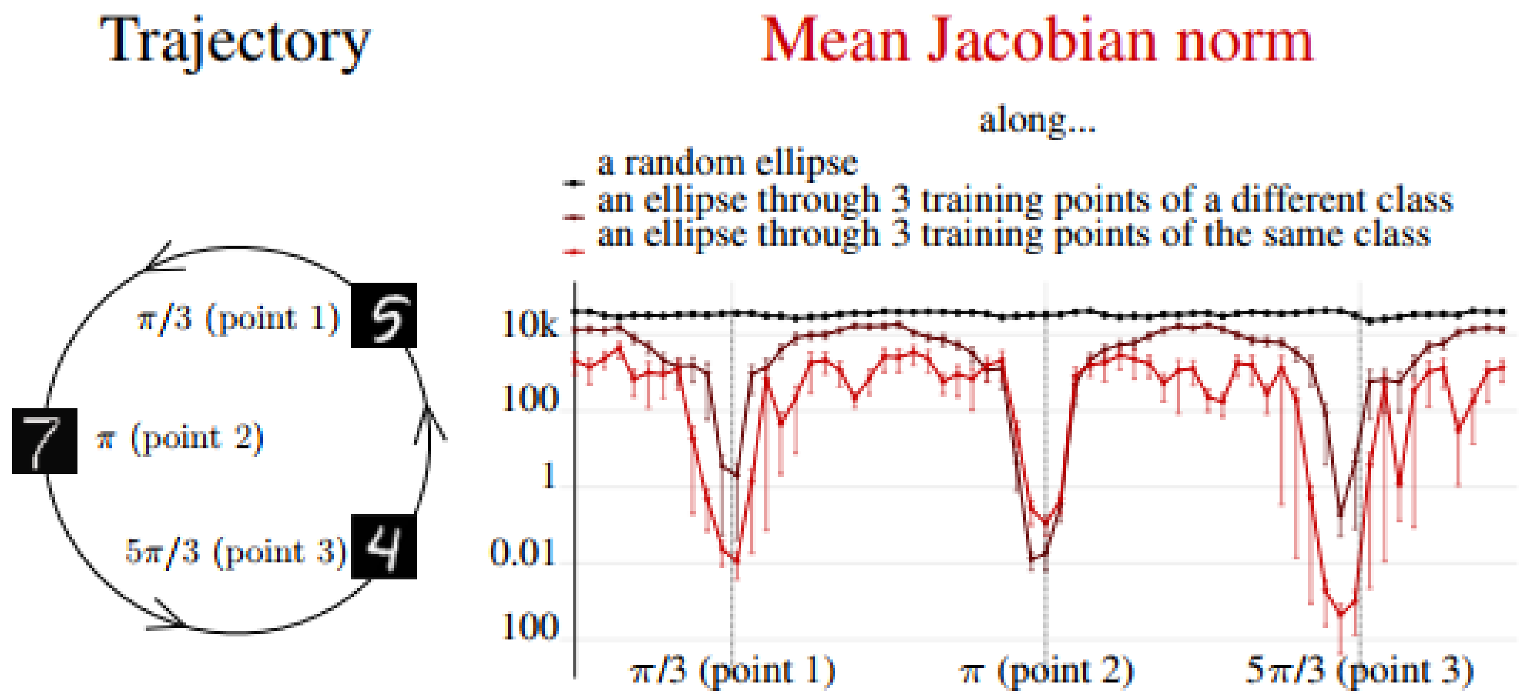
Without label

It is not surprise that sensitivity is related to generalization.

Regularization is kind of minimzing sensitivity.

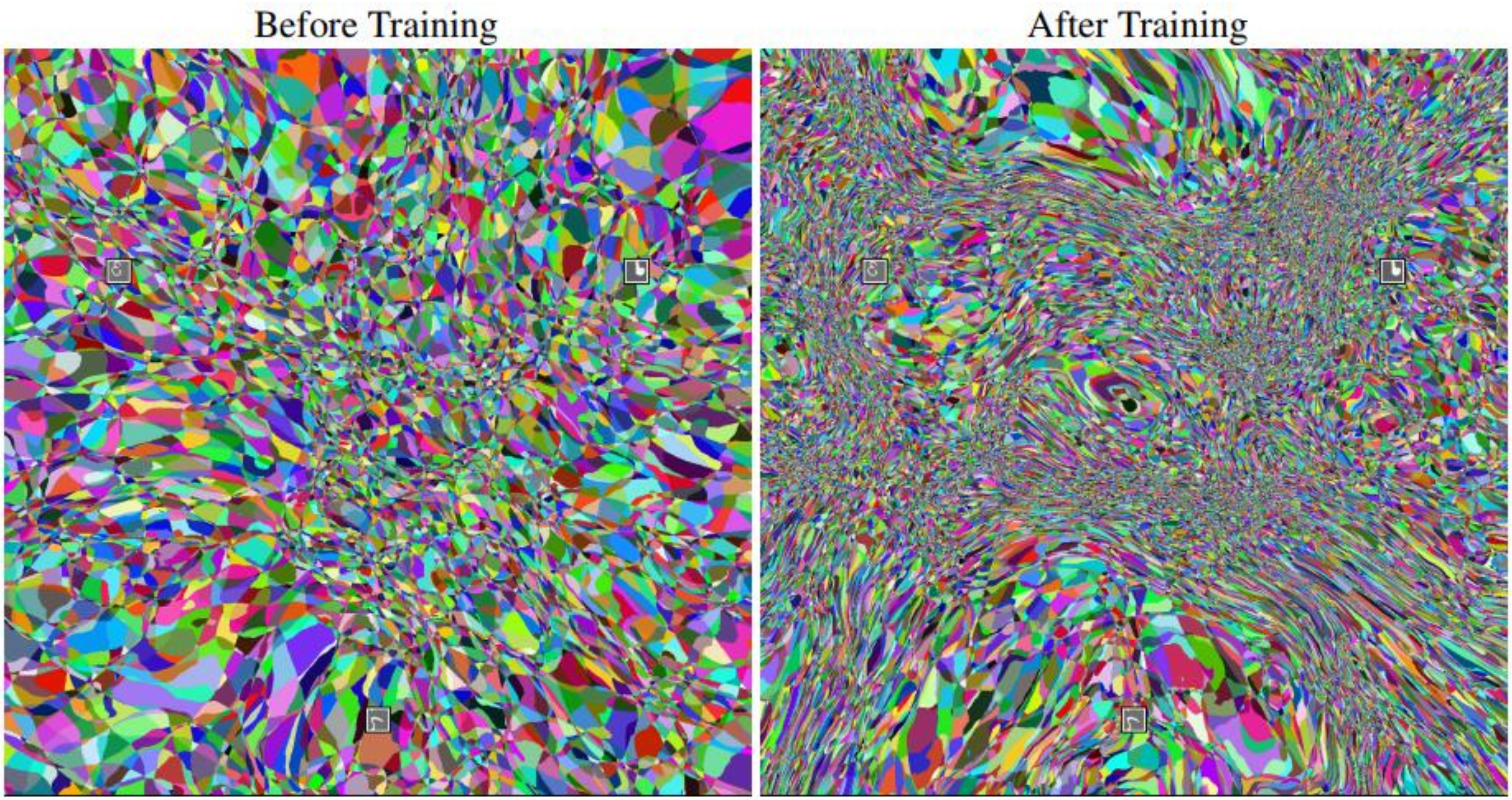
Sensitivity – Emprical Results

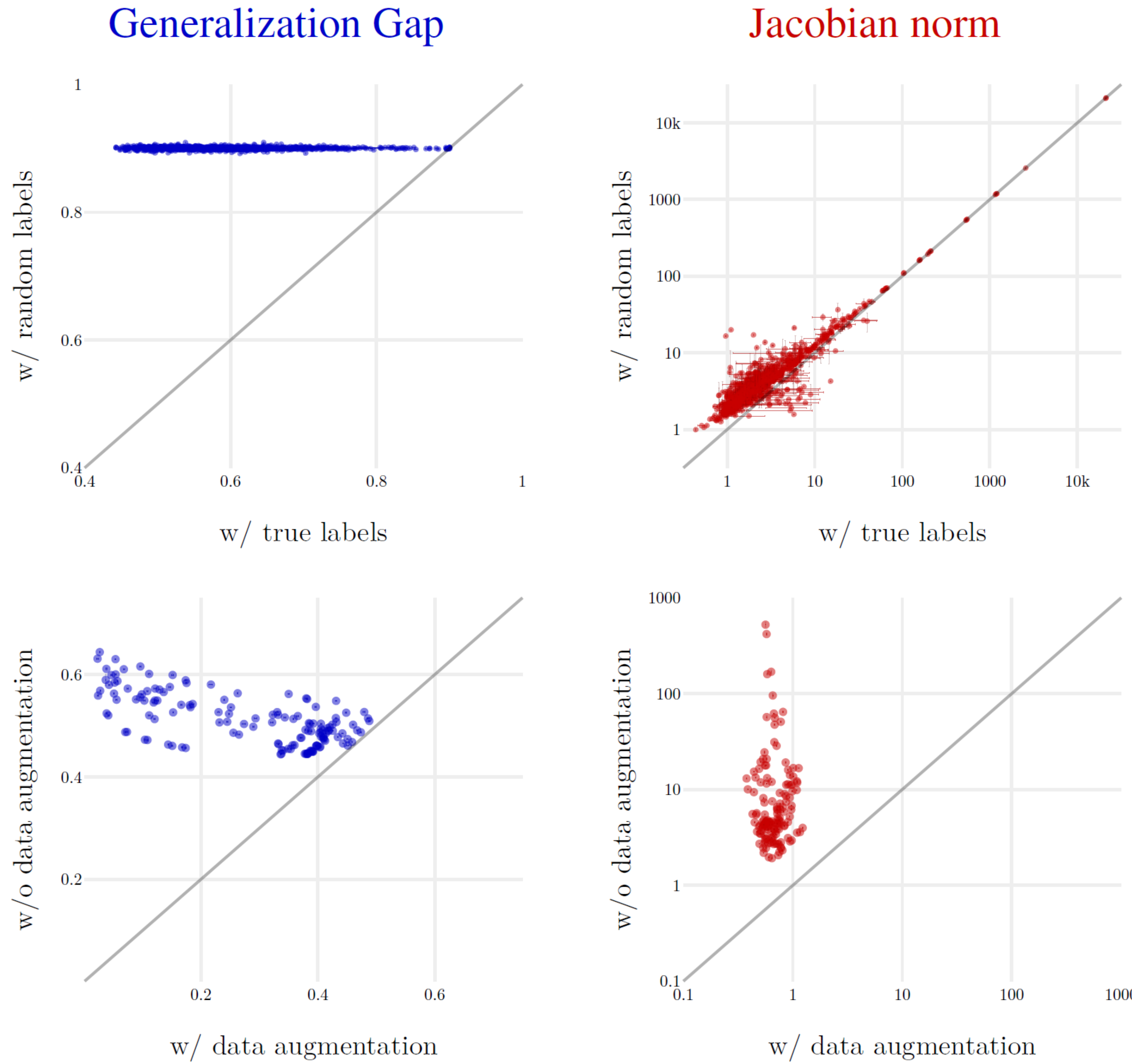
- Sensitivity on and off the training data manifold

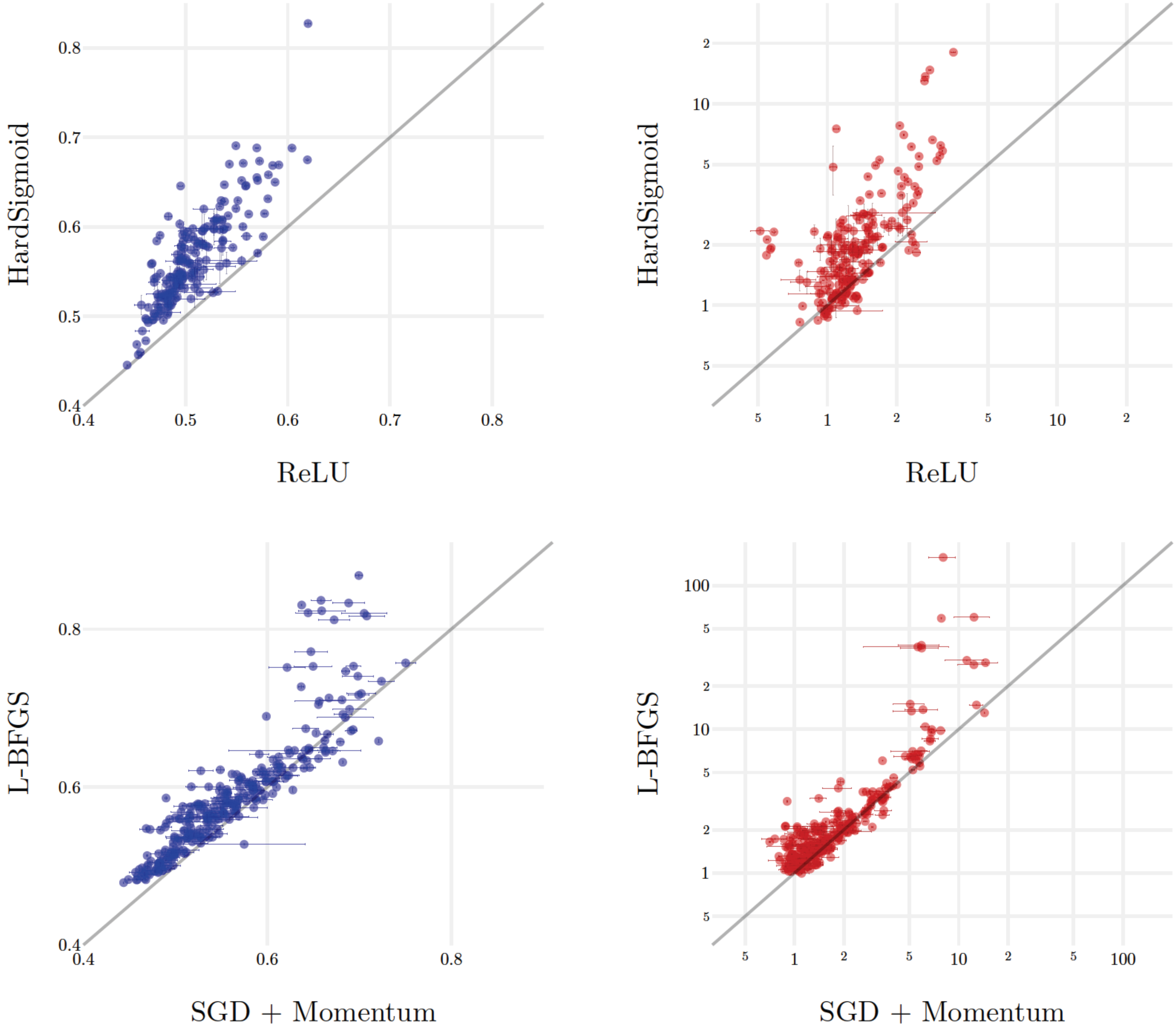


Sensitivity – Emprical Results

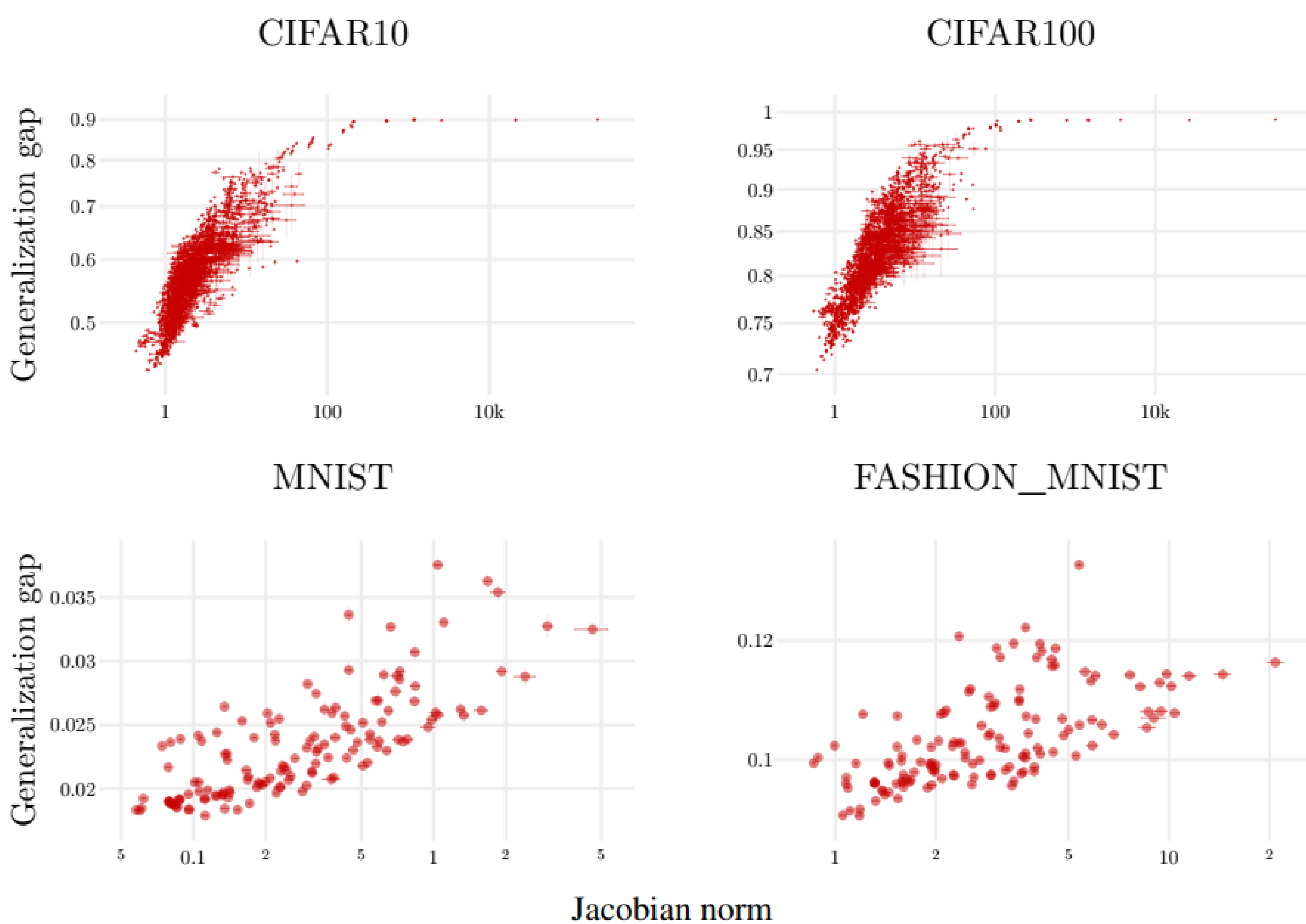
- Sensitivity on and off the training data manifold




Generalization Gap
Jacobian norm
w/ random labels
w/ true labels
w/o data augmentation
w/ data augmentation
0.4
0.6
0.8
1
1
10
100
1000
10k
0.2
0.1

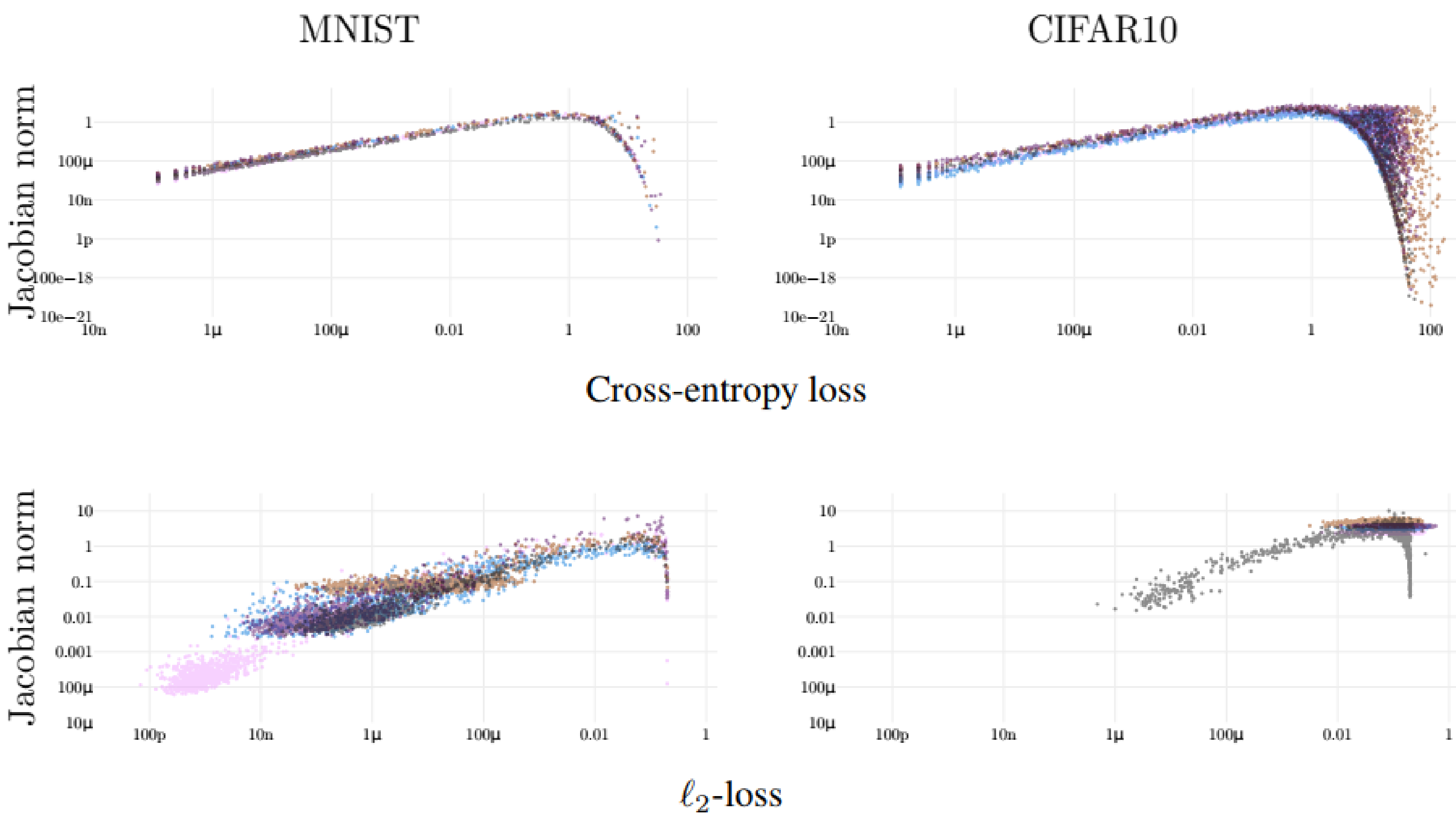

HardSigmoid
ReLU
HardSigmoid
ReLU
L-BFGS
SGD + Momentum
L-BFGS
SGD + Momentum
0.4
0.5
0.6
0.7
0.8
1
2
5
10
100

Sensitivity v.s. Generalization



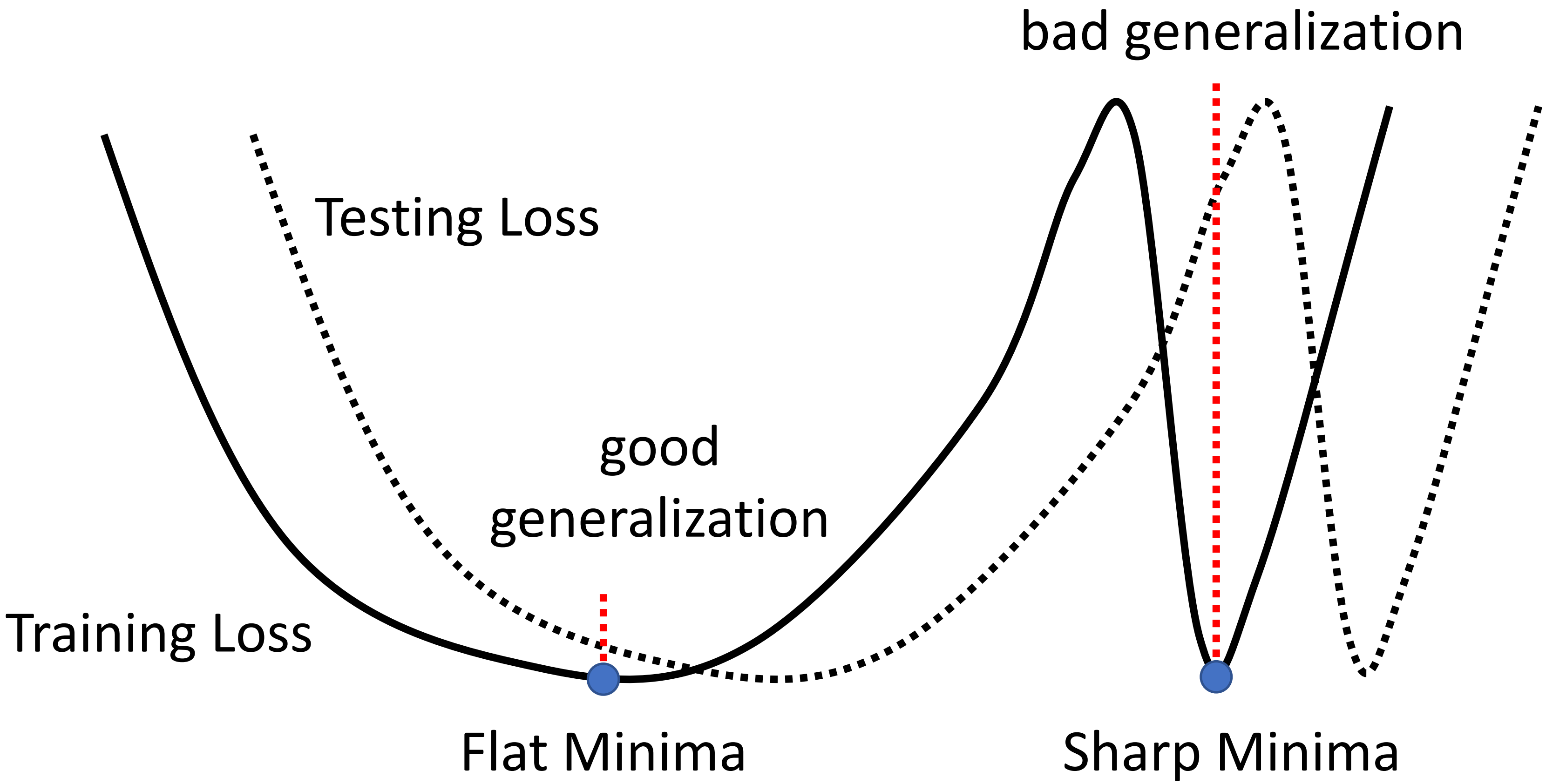
Sensitivity v.s. Generalization

- individual points



Sharpness

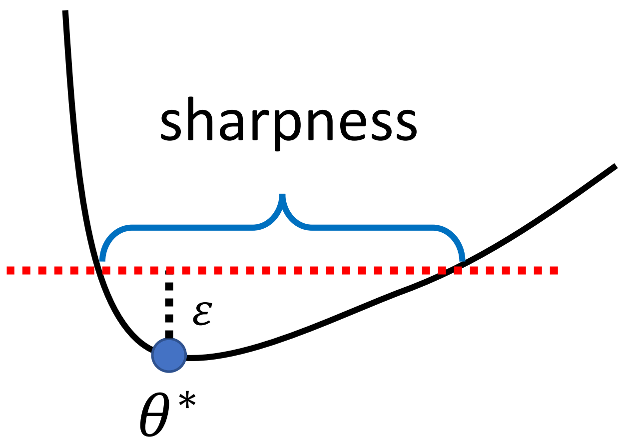
Sharp Minima v.s Flat Minima



Explain self regularization?

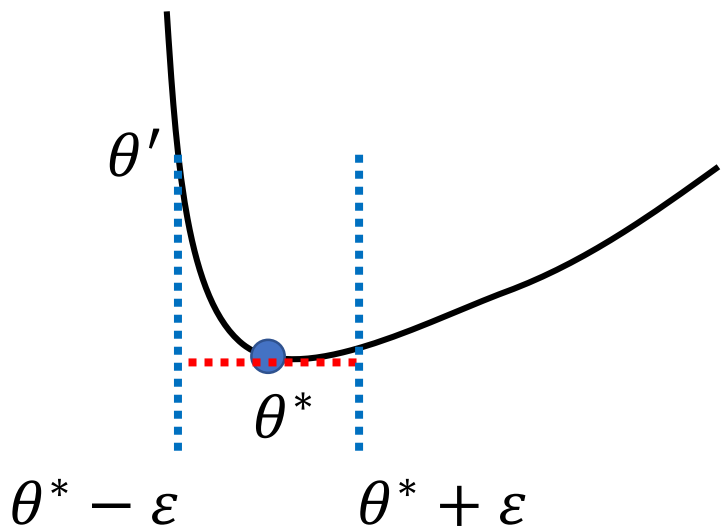
Definition of Sharpness

Definition 1



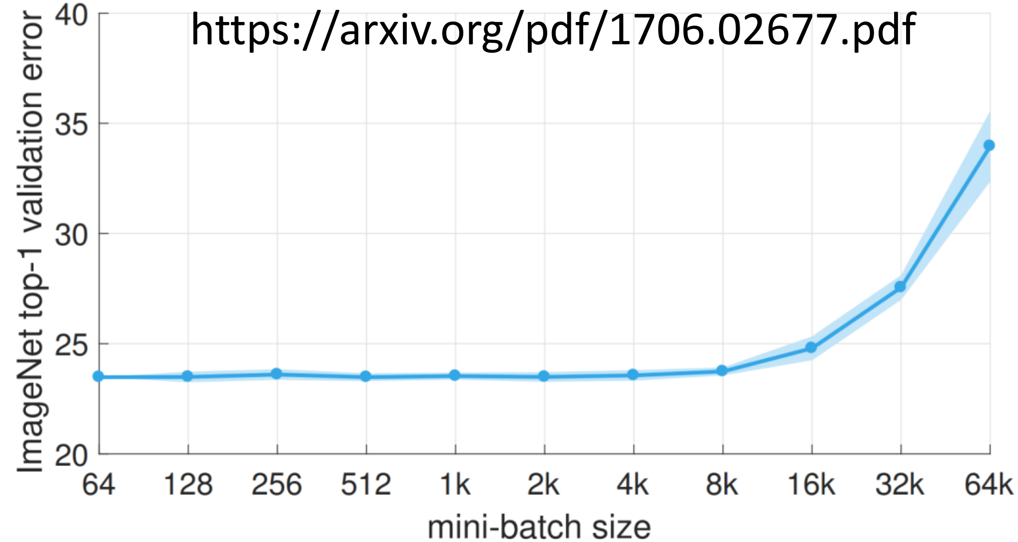
Definition 2

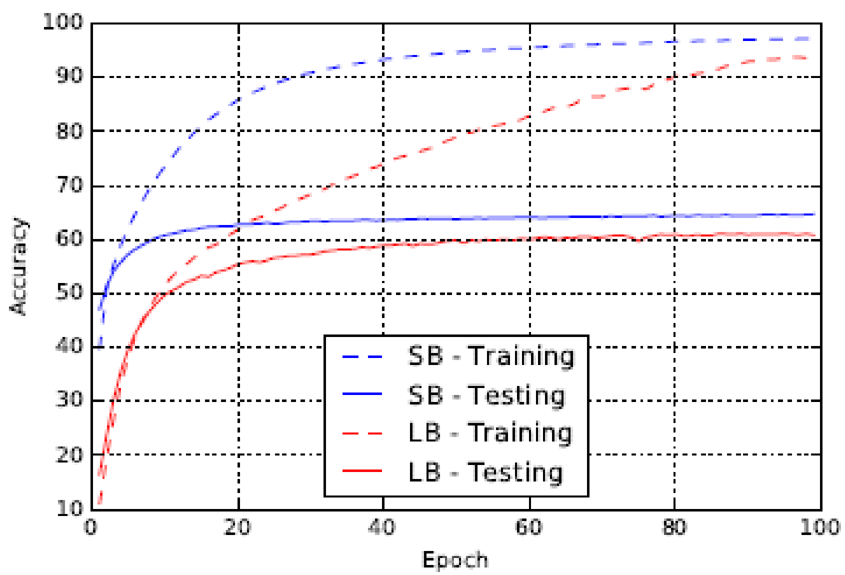
$$\text{Sharpness} = L(\theta') - L(\theta^*)$$



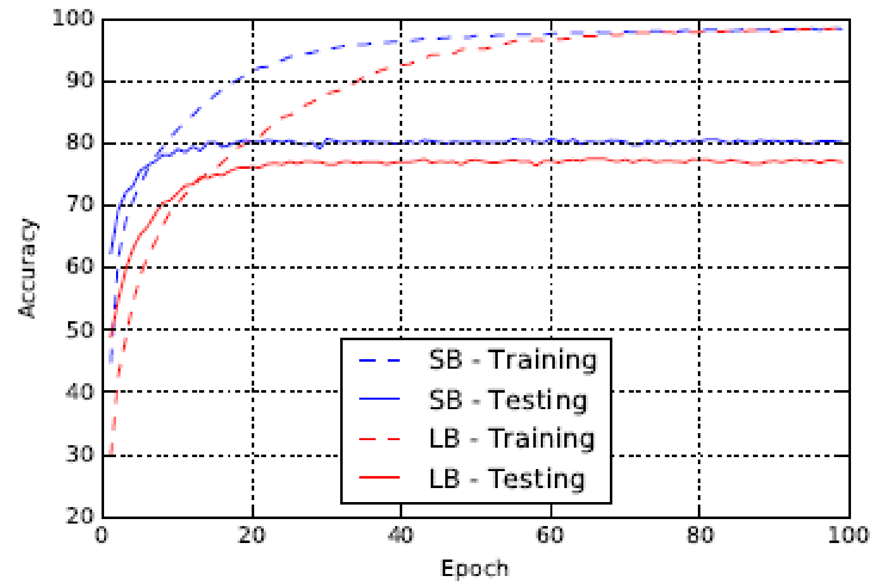
Batch Size

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





(a) Network F_2



(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

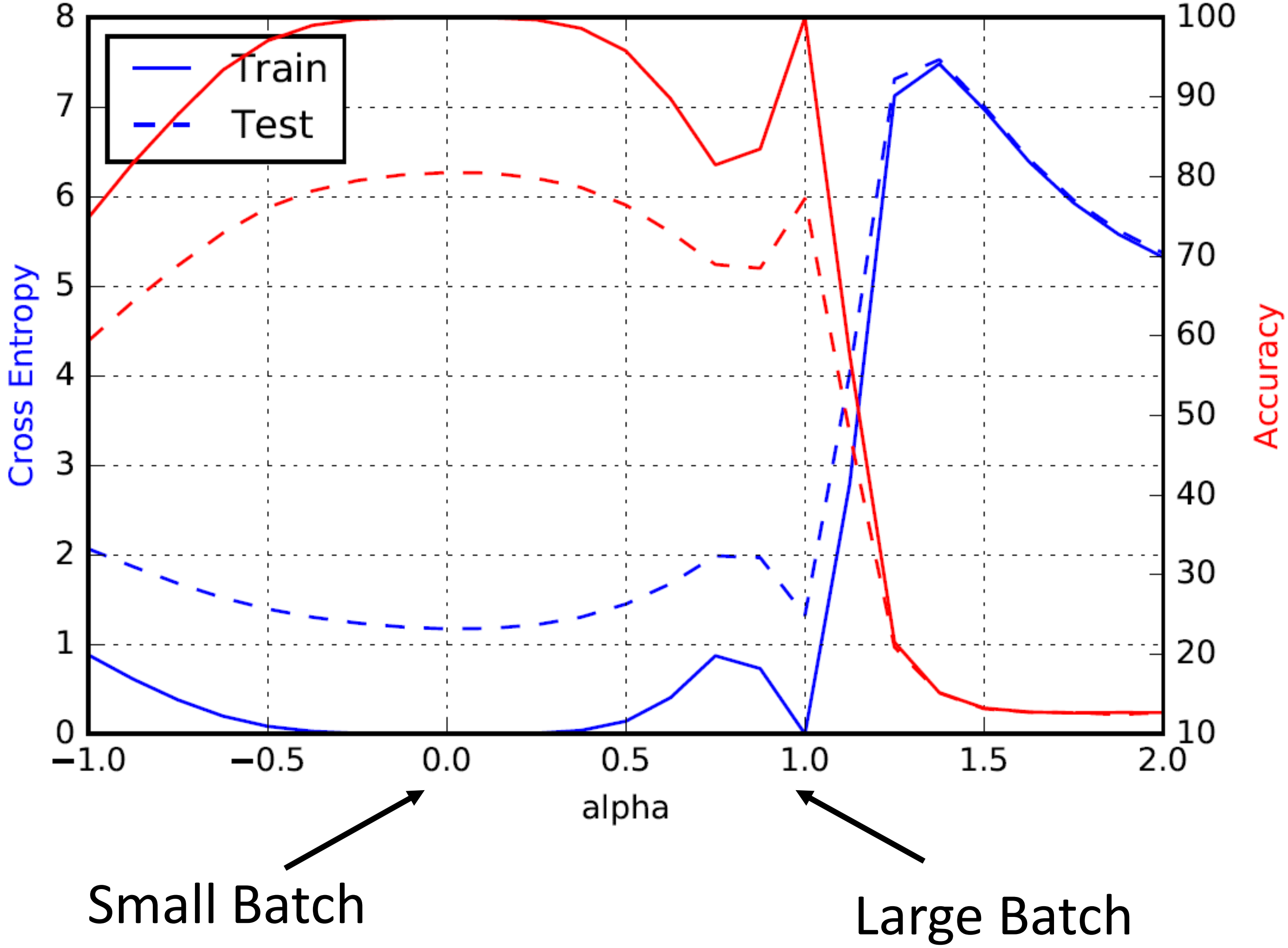
	Training Accuracy		Testing Accuracy	
Name	SB	LB	SB	LB
F_1	$99.66\% \pm 0.05\%$	$99.92\% \pm 0.01\%$	$98.03\% \pm 0.07\%$	$97.81\% \pm 0.07\%$
F_2	$99.99\% \pm 0.03\%$	$98.35\% \pm 2.08\%$	$64.02\% \pm 0.2\%$	$59.45\% \pm 1.05\%$
C_1	$99.89\% \pm 0.02\%$	$99.66\% \pm 0.2\%$	$80.04\% \pm 0.12\%$	$77.26\% \pm 0.42\%$
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

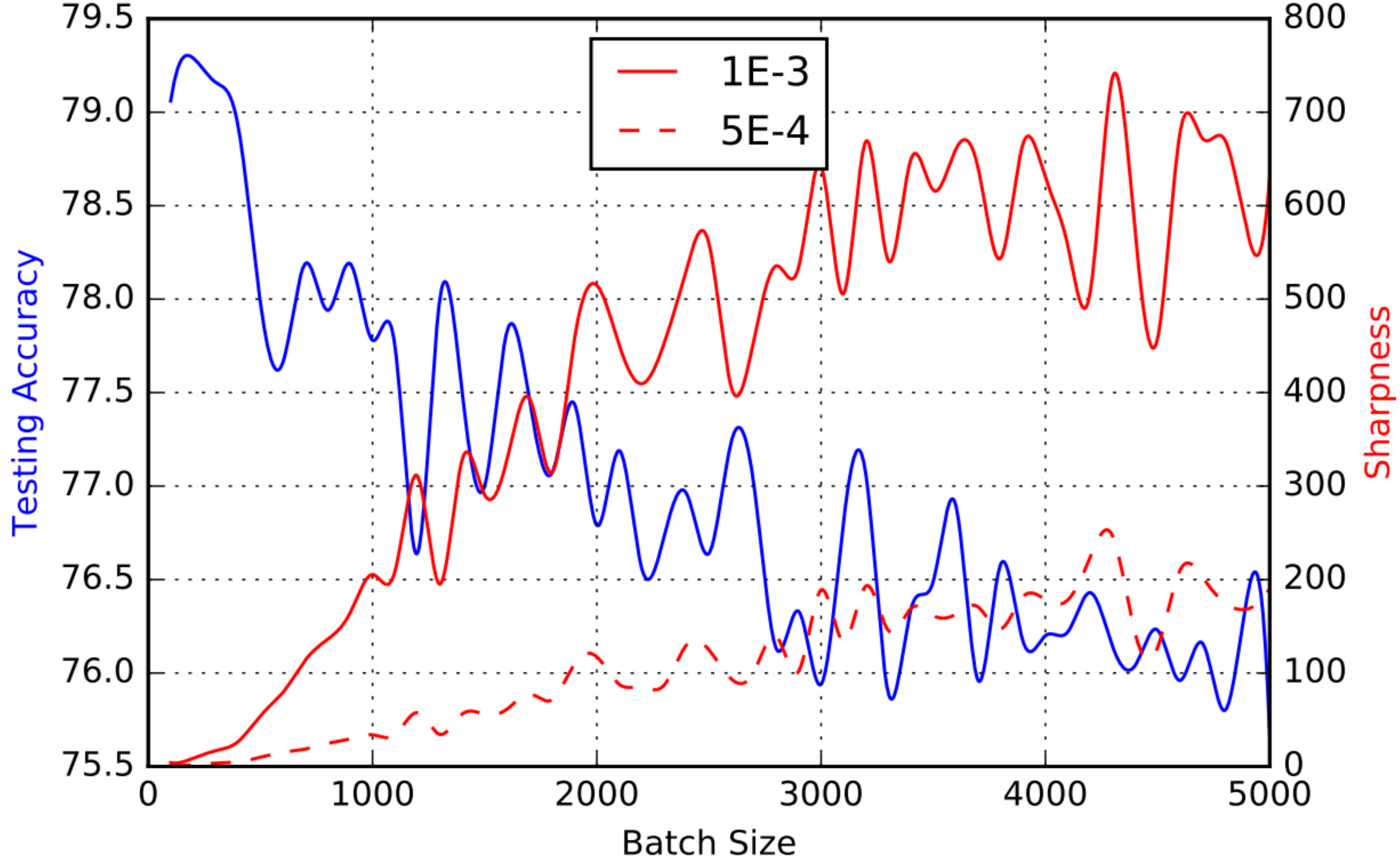
SB = 256

LB = 0.1 x data set

Batch Size v.s. Sharpness



Batch Size v.s. Sharpness



Concluding Remarks

Summary

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

感謝 張景程 同學發現投影片上的錯字

Reference

- Devansh Arpit, Stanisław Jastrzębski, Nicolas Ballas, David Krueger, Emmanuel Bengio, Maxinder S. Kanwal, Tegan Maharaj, Asja Fischer, Aaron Courville, Yoshua Bengio, Simon Lacoste-Julien, “A Closer Look at Memorization in Deep Networks”, ICML, 2017
- Nitish Shirish Keskar, Dheevatsa Mudigere, Jorge Nocedal, Mikhail Smelyanskiy, Ping Tak Peter Tang, “On Large-Batch Training for Deep Learning: Generalization Gap and Sharp Minima”, ICLR, 2017
- Pratik Chaudhari, Anna Choromanska, Stefano Soatto, Yann LeCun, Carlo Baldassi, Christian Borgs, Jennifer Chayes, Levent Sagun, Riccardo Zecchina, "Entropy-SGD: Biasing Gradient Descent Into Wide Valleys", ICLR, 2017
- Behnam Neyshabur, Srinadh Bhojanapalli, David McAllester, Nathan Srebro, Exploring Generalization in Deep Learning, NIPS, 2017
- Laurent Dinh, Razvan Pascanu, Samy Bengio, Yoshua Bengio, Sharp Minima Can Generalize For Deep Nets, PMLR, 2017
- Roman Novak, Yasaman Bahri, Daniel A. Abolafia, Jeffrey Pennington, Jascha Sohl-Dickstein, Sensitivity and Generalization in Neural Networks: an Empirical Study, ICLR, 2018