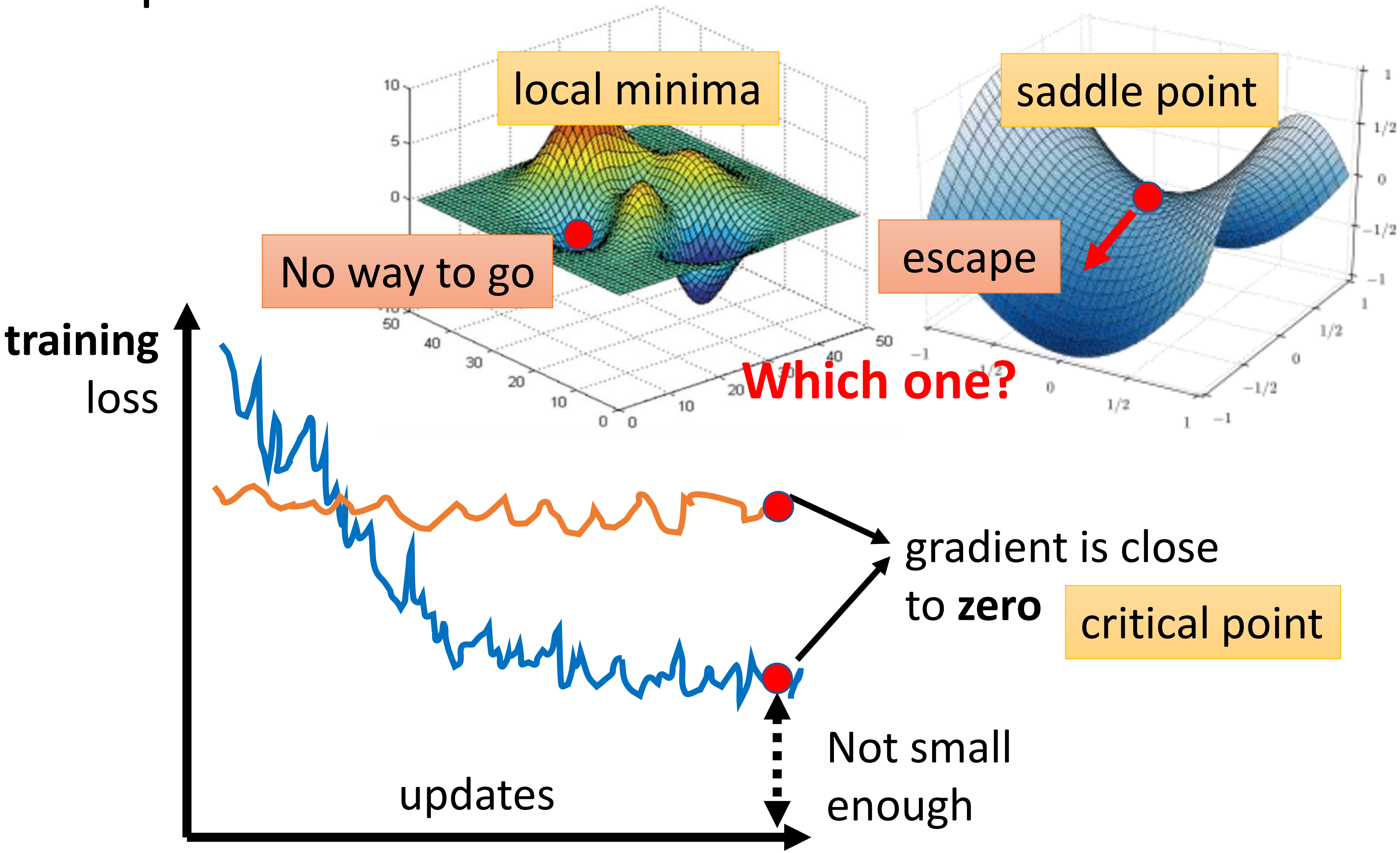
When gradient is small …

Hung-yi Lee 李宏毅

Optimization Fails because ……



Warning of Math

Tayler Series Approximation

$L(\boldsymbol{\theta})$ around $\boldsymbol{\theta} = \boldsymbol{\theta}'$ can be approximated below

$$L(\boldsymbol{\theta}) \approx L(\boldsymbol{\theta}') + \boxed{(\boldsymbol{\theta} - \boldsymbol{\theta}')^T \boldsymbol{g}} + \boxed{\frac{1}{2}(\boldsymbol{\theta} - \boldsymbol{\theta}')^T H (\boldsymbol{\theta} - \boldsymbol{\theta}')}$$

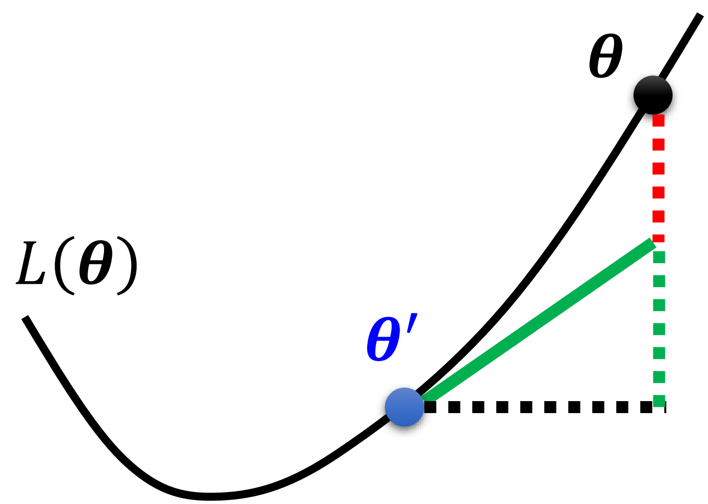
L在theta'附近做展開
若gradient不為零，則只需要朝gradient之反方向做update
即可使loss降低

Gradient $\boldsymbol{g}$ is a ***vector***

$$\boldsymbol{g} = \nabla L(\boldsymbol{\theta}') \qquad \boldsymbol{g}_i = \frac{\partial L(\boldsymbol{\theta}')}{\partial \boldsymbol{\theta}_i}$$

Hessian H is a ***matrix***

$$H_{ij} = \frac{\partial^2}{\partial \boldsymbol{\theta}_i \partial \boldsymbol{\theta}_j} L(\boldsymbol{\theta}')$$



Source of image:http://www.offconvex.org/2016/03/22/saddlepoints/

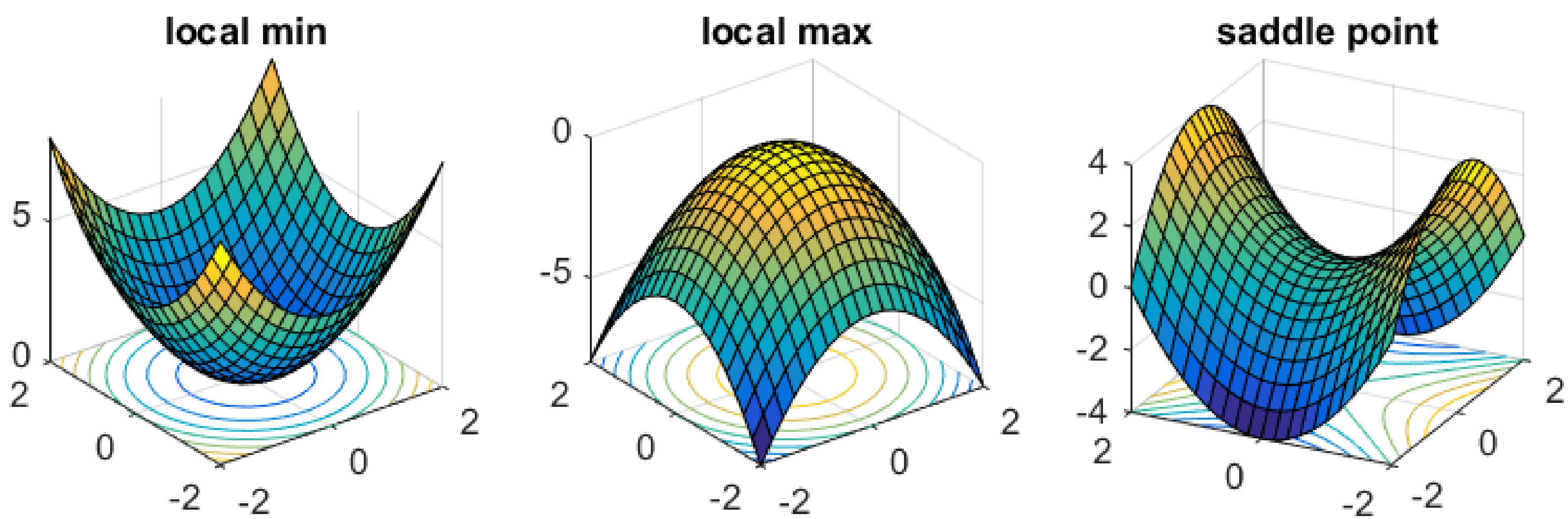
Hessian

$L(\boldsymbol{\theta})$ around $\boldsymbol{\theta} = \boldsymbol{\theta}'$ can be approximated below

$$L(\boldsymbol{\theta}) \approx L(\boldsymbol{\theta}') + \boxed{\cancel{(\boldsymbol{\theta} - \boldsymbol{\theta}')^T \boldsymbol{g}}} + \boxed{\frac{1}{2}(\boldsymbol{\theta} - \boldsymbol{\theta}')^T H (\boldsymbol{\theta} - \boldsymbol{\theta}')}$$

At critical point

telling the properties of critical points



Hessian

At critical point:

$$\boldsymbol{v}^T H \boldsymbol{v}$$

$$L(\boldsymbol{\theta}) \approx L(\boldsymbol{\theta}') + \boxed{\frac{1}{2}(\boldsymbol{\theta} - \boldsymbol{\theta}')^T H (\boldsymbol{\theta} - \boldsymbol{\theta}')}$$

For all $\boldsymbol{v}$

$\boldsymbol{v}^T H \boldsymbol{v} > 0$ ➡ Around $\boldsymbol{\theta}'$: $L(\boldsymbol{\theta}) > L(\boldsymbol{\theta}')$ ➡ **Local minima**

= H is positive definite = All eigen values are positive. ⬆

For all $\boldsymbol{v}$

$\boldsymbol{v}^T H \boldsymbol{v} < 0$ ➡ Around $\boldsymbol{\theta}'$: $L(\boldsymbol{\theta}) < L(\boldsymbol{\theta}')$ ➡ **Local maxima**

= H is negative definite = All eigen values are negative. ⬆

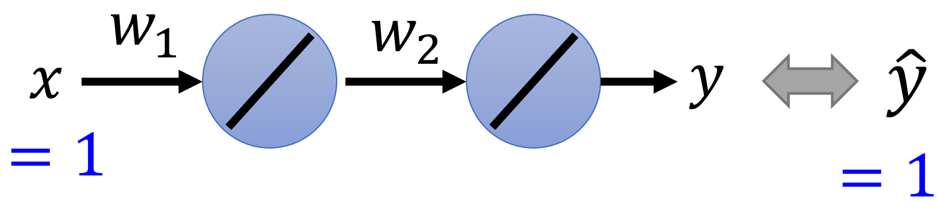
Sometimes $\boldsymbol{v}^T H \boldsymbol{v} > 0$, sometimes $\boldsymbol{v}^T H \boldsymbol{v} < 0$ ➡ **Saddle point**

Some eigen values are positive, and some are negative. ⬆

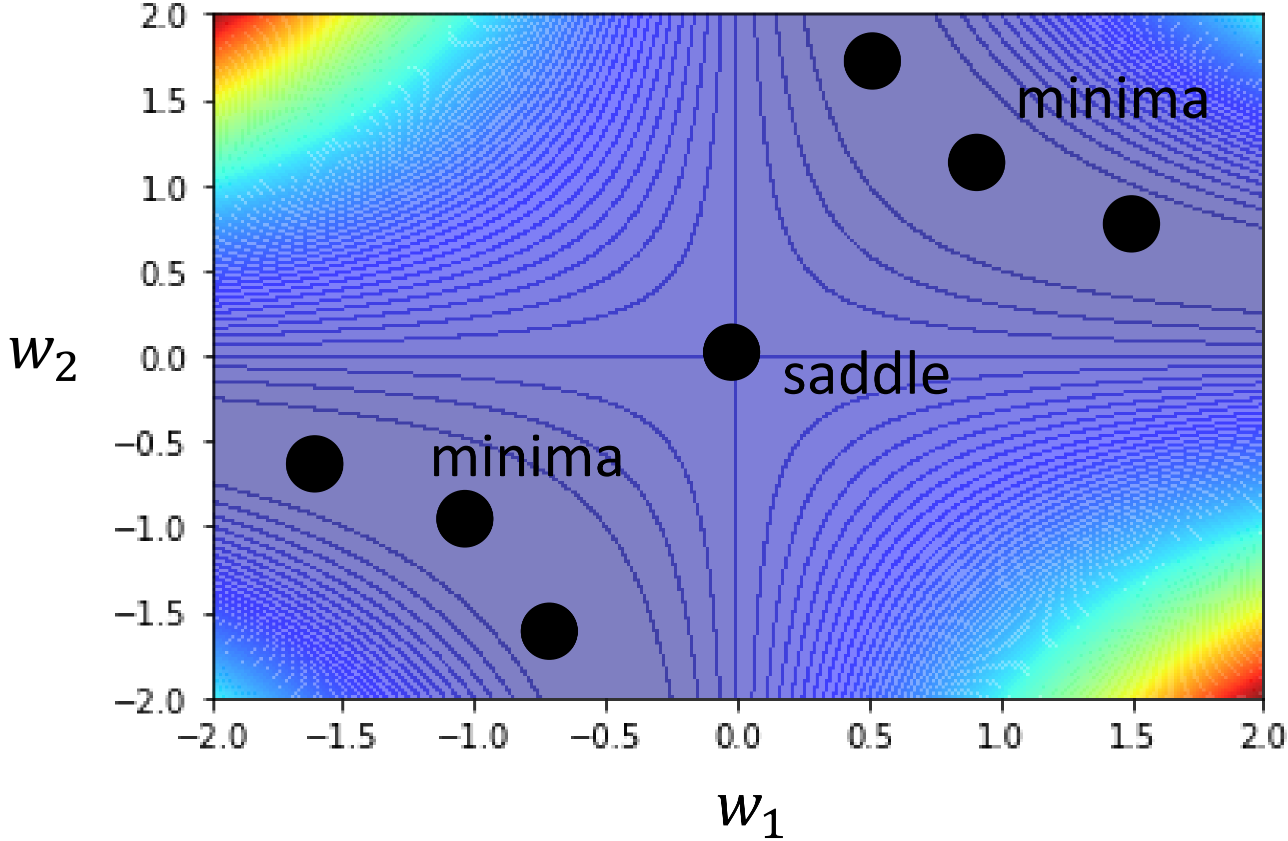
Example

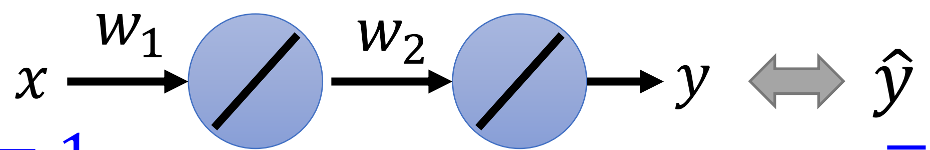
只有一筆training data: (1, 1)

$$y = w_1 w_2 x$$

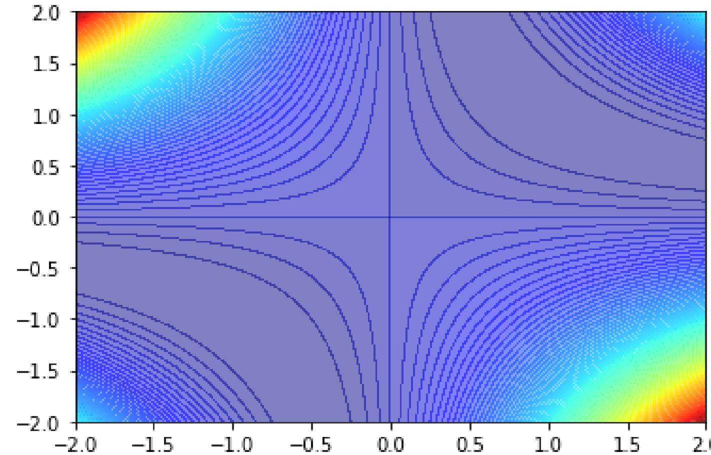


Error Surface





$= 1$ $\qquad = 1$



$$L = (\hat{y} - w_1 w_2 x)^2 = (1 - w_1 w_2)^2$$

$$\boxed{\frac{\partial L}{\partial w_1}} = 2(1 - w_1 w_2)(-w_2) \quad = 0$$

$$\boxed{\frac{\partial L}{\partial w_2}} = 2(1 - w_1 w_2)(-w_1) \quad = 0$$

$\boldsymbol{g}$

Critical point: $w_1 = 0, w_2 = 0$

$$H = \begin{bmatrix} 0 & -2 \\ -2 & 0 \end{bmatrix} \quad \lambda_1 = 2, \lambda_2 = -2$$

<u>Saddle point</u>

H

$$\boxed{\frac{\partial^2 L}{\partial {w_1}^2}} = 2(-w_2)(-w_2) \quad = 0 \qquad \boxed{\frac{\partial^2 L}{\partial w_1 \partial w_2}} = -2 + 4 w_1 w_2 \quad = -2$$

$$\boxed{\frac{\partial^2 L}{\partial w_2 \partial w_1}} = -2 + 4 w_1 w_2 \quad = -2 \qquad \boxed{\frac{\partial^2 L}{\partial {w_2}^2}} = 2(-w_1)(-w_1) \quad = 0$$

Don't afraid of saddle point?

當在saddle point時，gradient為零
但可以使用eigen value為負之eigen vector去update參數
亦可以降低loss

$$\boldsymbol{v}^T H \boldsymbol{v}$$

At critical point: $L(\boldsymbol{\theta}) \approx L(\boldsymbol{\theta}') + \boxed{\frac{1}{2}(\boldsymbol{\theta} - \boldsymbol{\theta}')^T H (\boldsymbol{\theta} - \boldsymbol{\theta}')}$

Sometimes $\boldsymbol{v}^T H \boldsymbol{v} > 0$, sometimes $\boldsymbol{v}^T H \boldsymbol{v} < 0$ ➡ Saddle point

H may tell us parameter update direction!

$\boldsymbol{u}$ is an eigen vector of H

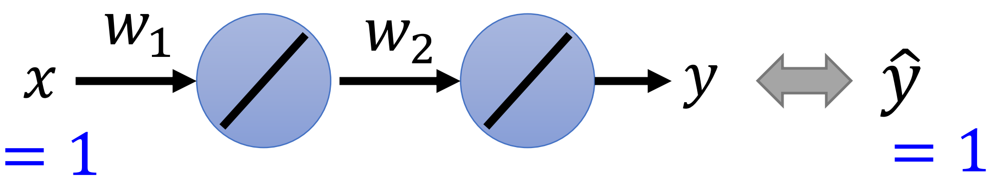
λ is the eigen value of $\boldsymbol{u}$

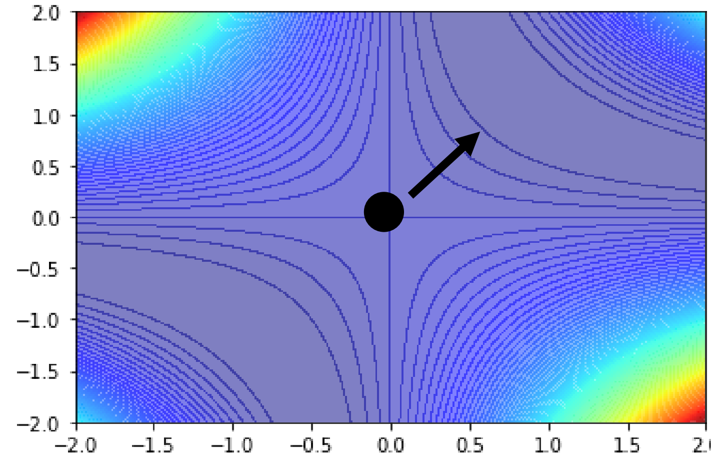
$\lambda < 0$

➡ $\underbrace{\boldsymbol{u}^T H \boldsymbol{u}}_{< 0} = \boldsymbol{u}^T (\lambda \boldsymbol{u}) = \underbrace{\lambda \|\boldsymbol{u}\|^2}_{< 0}$

$$L(\boldsymbol{\theta}) \approx L(\boldsymbol{\theta}') + \frac{1}{2}(\overbrace{\boldsymbol{\theta} - \boldsymbol{\theta}'}^{\boldsymbol{u}})^T H (\overbrace{\boldsymbol{\theta} - \boldsymbol{\theta}'}^{\boldsymbol{u}})$$ ➡ $L(\boldsymbol{\theta}) < L(\boldsymbol{\theta}')$

$\boldsymbol{\theta} - \boldsymbol{\theta}' = \boldsymbol{u}$ $\quad$ $\boldsymbol{\theta} = \boldsymbol{\theta}' + \boldsymbol{u}$ $\quad$ Decrease L





$$L = (\hat{y} - w_1 w_2 x)^2 \;= (1 - w_1 w_2)^2$$

$$\frac{\partial L}{\partial w_1} = 2(1 - w_1 w_2)(-w_2)$$

$$\frac{\partial L}{\partial w_2} = 2(1 - w_1 w_2)(-w_1)$$

Critical point: $w_1 = 0, w_2 = 0$

$$H = \begin{bmatrix} 0 & -2 \\ -2 & 0 \end{bmatrix} \quad \lambda_1 = 2, \lambda_2 = -2$$

Saddle point

$\lambda_2 = -2$ Has eigenvector $\boldsymbol{u} = \begin{bmatrix} 1 \\ 1 \end{bmatrix}$

Update the parameter along the direction of $\boldsymbol{u}$

You can escape the saddle point and decrease the loss.

(this method is seldom used in practice)

End of Warning

Saddle Point v.s. Local Minima

- A.D. 1543

來源《三體Ⅲ·死神永生》

Saddle Point v.s. Local Minima

- The Magician Diorena（魔法師狄奧倫娜）

From 3 dimensional space, it is sealed.

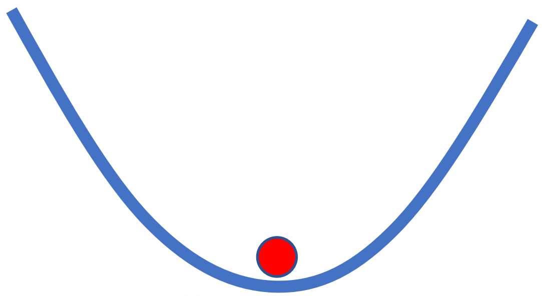
It is not in higher dimensions.

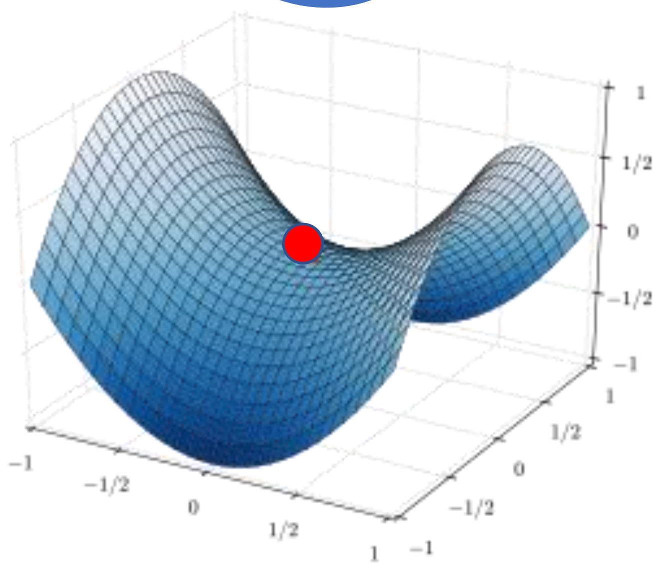
Source of image: https://read01.com/mz2DBPE.html#.YECz22gzbIU

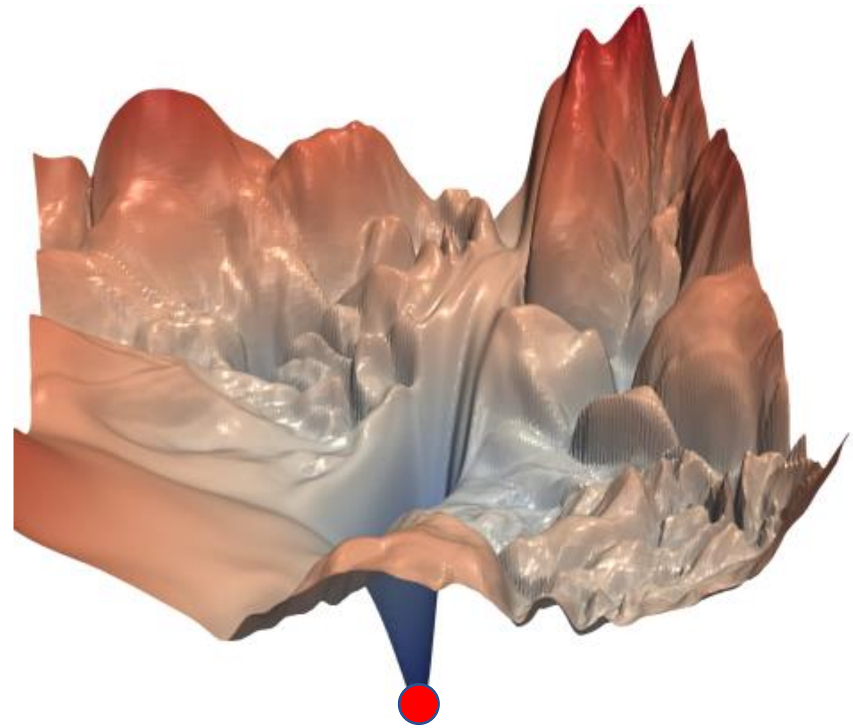
Source of image: https://arxiv.org/abs/1712.09913

Saddle Point v.s. Local Minima

在低維度看起來是local minima的時候，
在高維度中其實有可能只是個saddle point





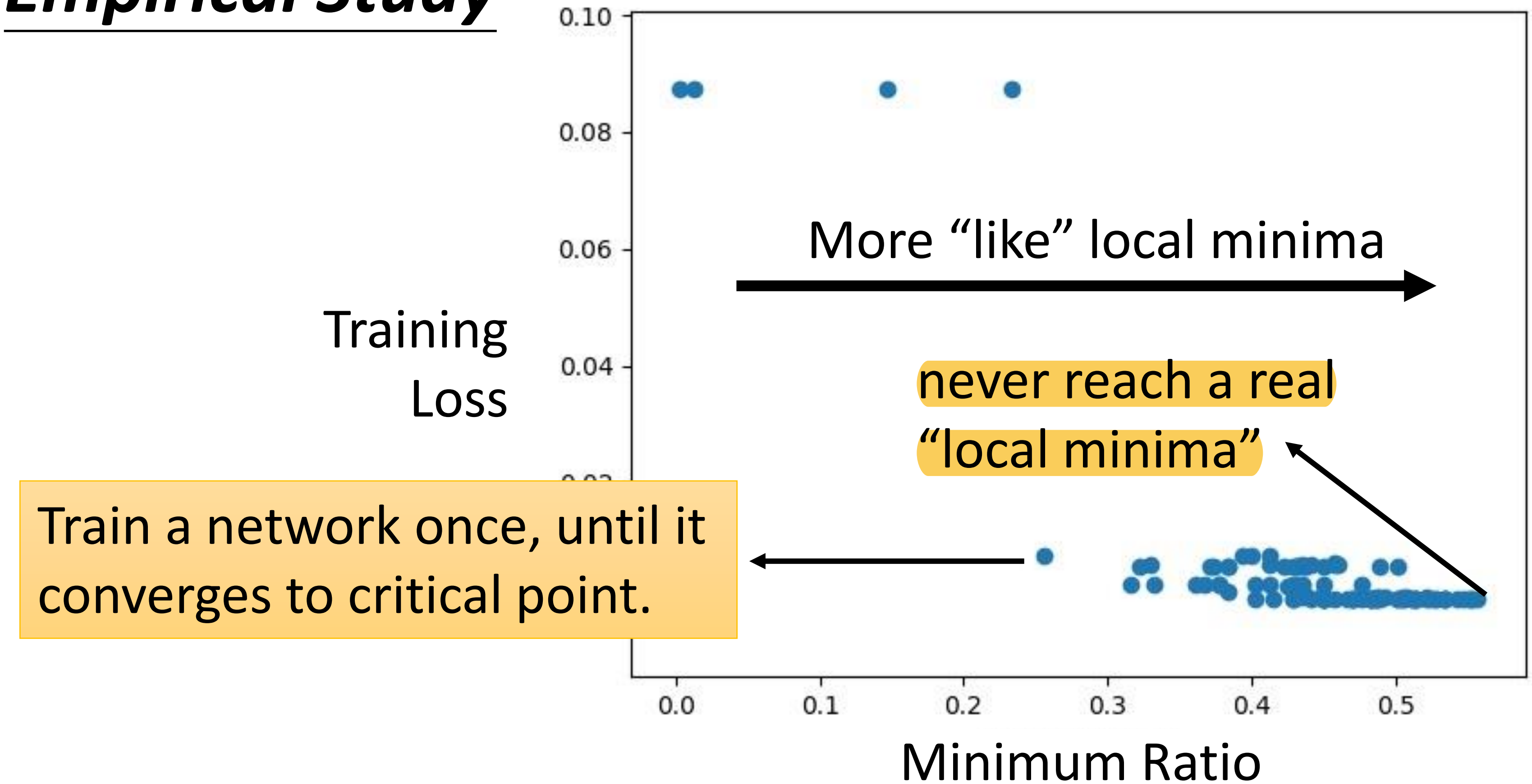


Saddle point in higher dimension?

有許多實驗支持這個假說

When you have lots of parameters, perhaps local minima is rare?

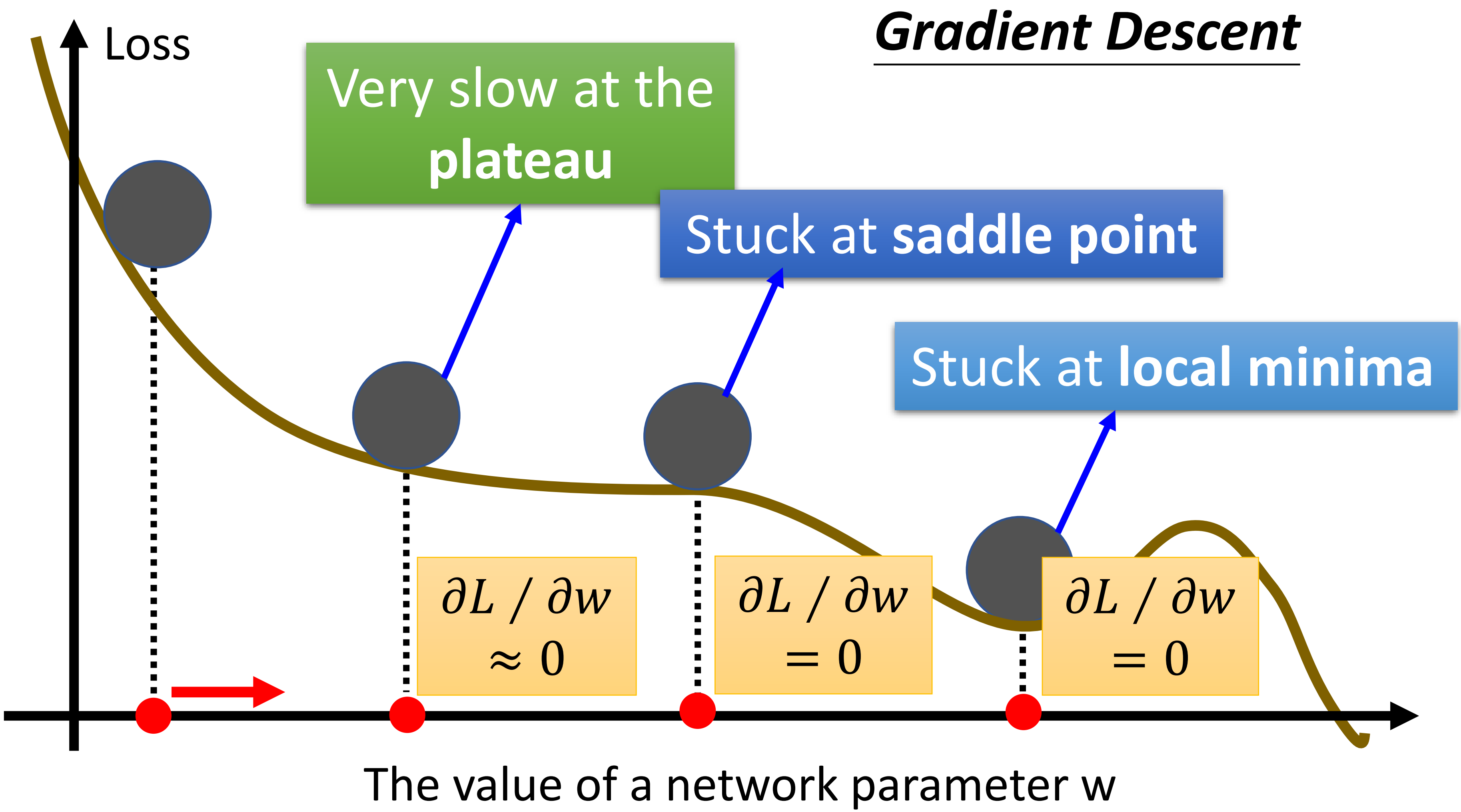
Empirical Study



$$\text{Minimum ratio} = \frac{\text{Number of } \textbf{Positive} \text{ Eigen values}}{\text{Number of Eigen values}}$$

Source:https://docs.google.com/presentation/d/1siUFXARYRpNiMeSRwgFbt7mZVjkMPhR5od09w0Z8xaU/edit#slide=id.g31470fd33a_0_33

Small Gradient ...



Tips for training:
Batch and Momentum

Batch

Review: Optimization with Batch

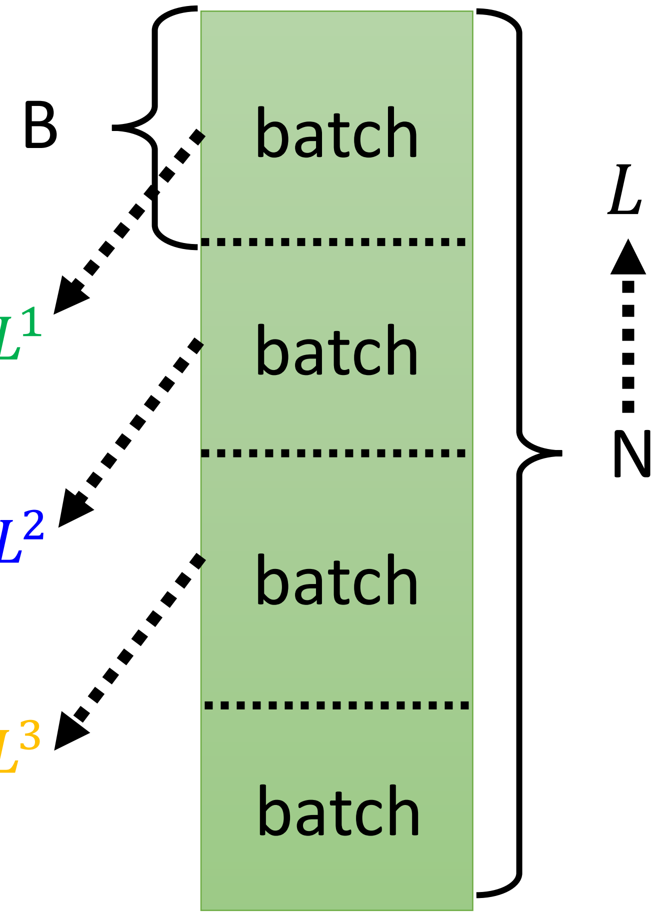
$$\boldsymbol{\theta}^* = arg\min_{\boldsymbol{\theta}} L$$

- (Randomly) Pick initial values $\boldsymbol{\theta}^0$
- Compute gradient $\boldsymbol{g^0} = \nabla L^1(\boldsymbol{\theta}^0)$ L^1

  update $\boldsymbol{\theta}^1 \leftarrow \boldsymbol{\theta}^0 - \eta \boldsymbol{g^0}$
- Compute gradient $\boldsymbol{g^1} = \nabla L^2(\boldsymbol{\theta}^1)$ L^2

  update $\boldsymbol{\theta}^2 \leftarrow \boldsymbol{\theta}^1 - \eta \boldsymbol{g^1}$
- Compute gradient $\boldsymbol{g^3} = \nabla L^3(\boldsymbol{\theta}^2)$ L^3

  update $\boldsymbol{\theta}^3 \leftarrow \boldsymbol{\theta}^2 - \eta \boldsymbol{g^3}$



1 **epoch** = see all the batches once → **Shuffle** after each epoch

Small Batch v.s. Large Batch

Consider 20 examples (N=20)

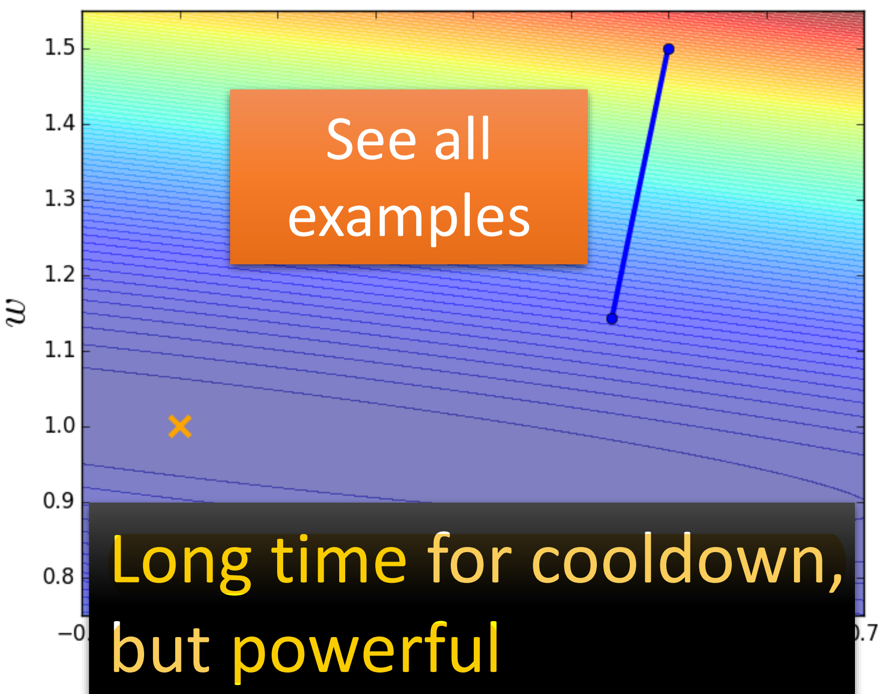
Batch size = N (Full batch)

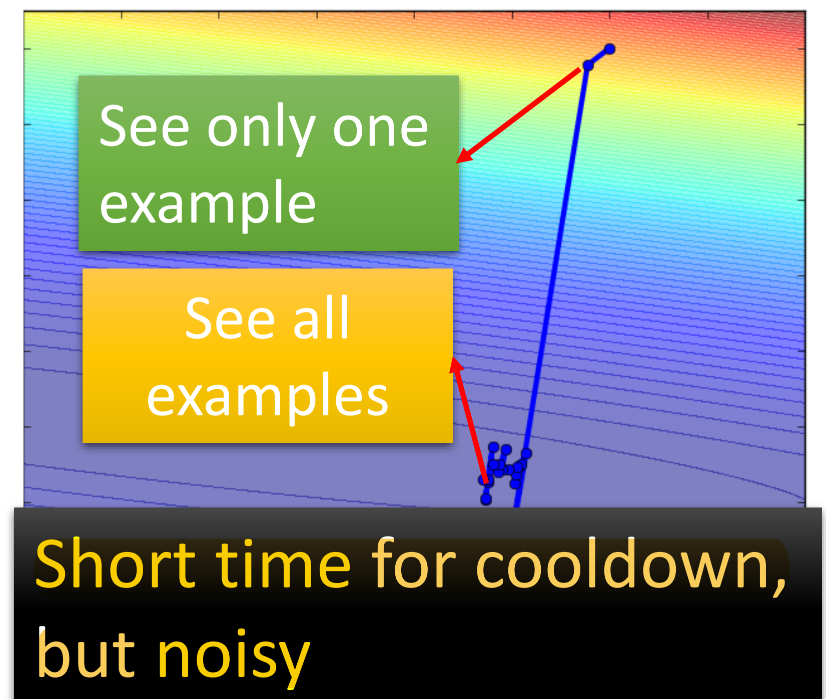
Update after seeing all the 20 examples

Batch size = 1

Update for each example

Update 20 times in an epoch





若使用平行運算，可以解決計算時間久之問題

oldest slides: http://speech.ee.ntu.edu.tw/~tlkagk/courses/MLDS_2015_2/Lecture/DNN%20(v4).pdf
old slides: http://speech.ee.ntu.edu.tw/~tlkagk/courses/ML_2017/Lecture/Keras.pdf

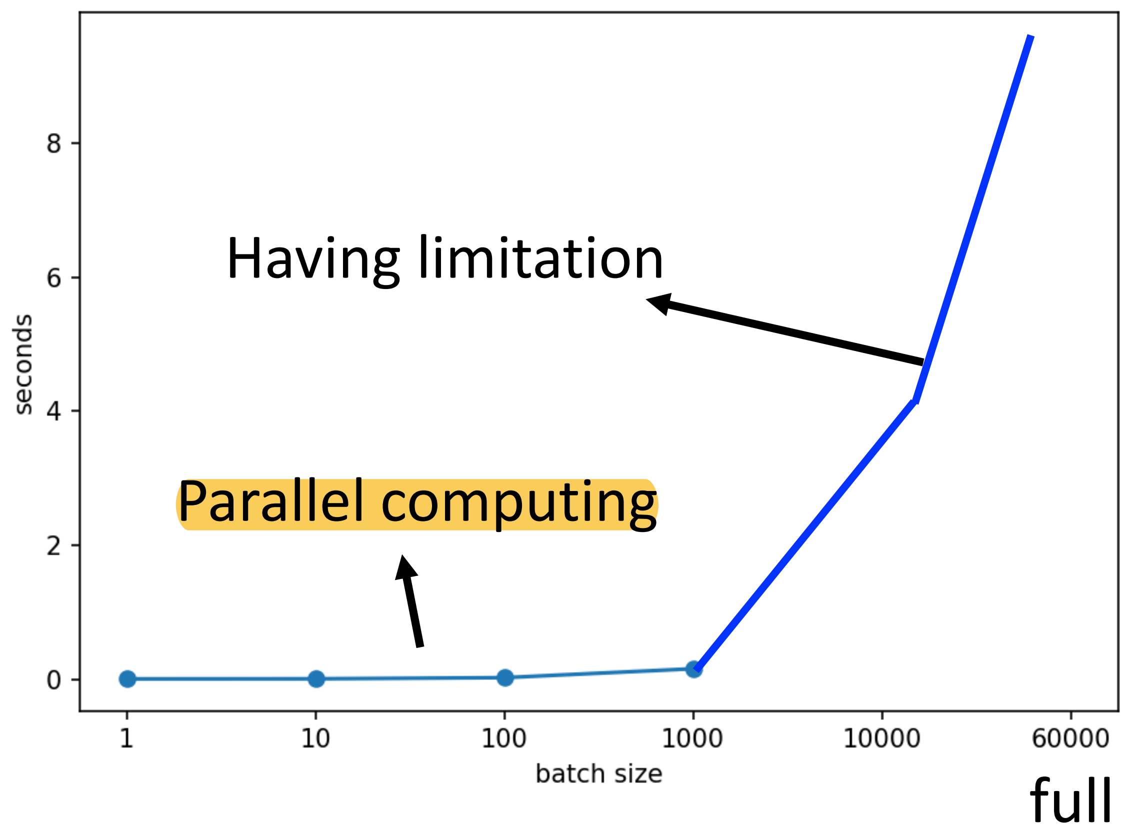
Small Batch v.s. Large Batch

- Larger batch size does **not** require longer time to compute gradient (unless batch size is too large)

Time for each update

MNIST: digit classification

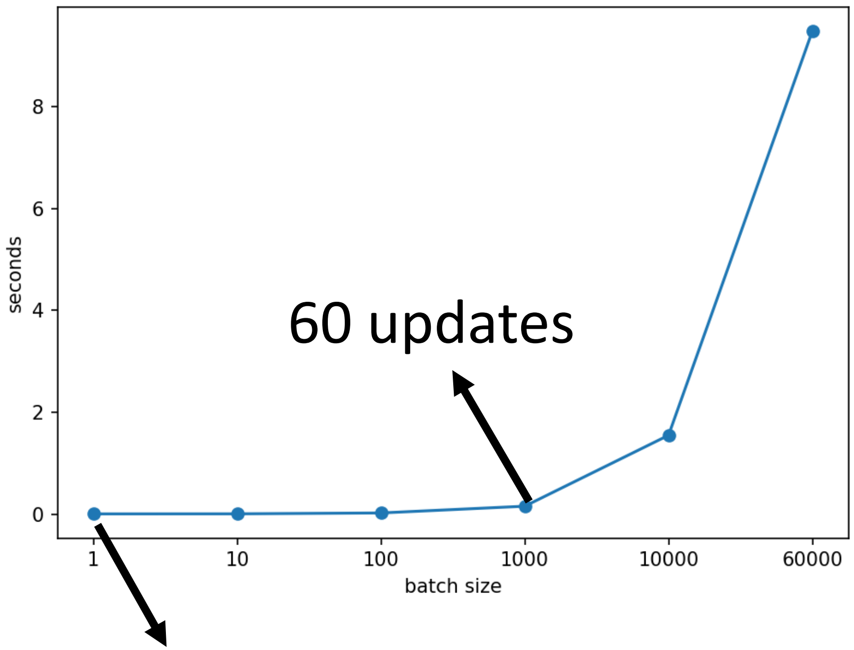
Tesla V100 GPU



Small Batch v.s. Large Batch

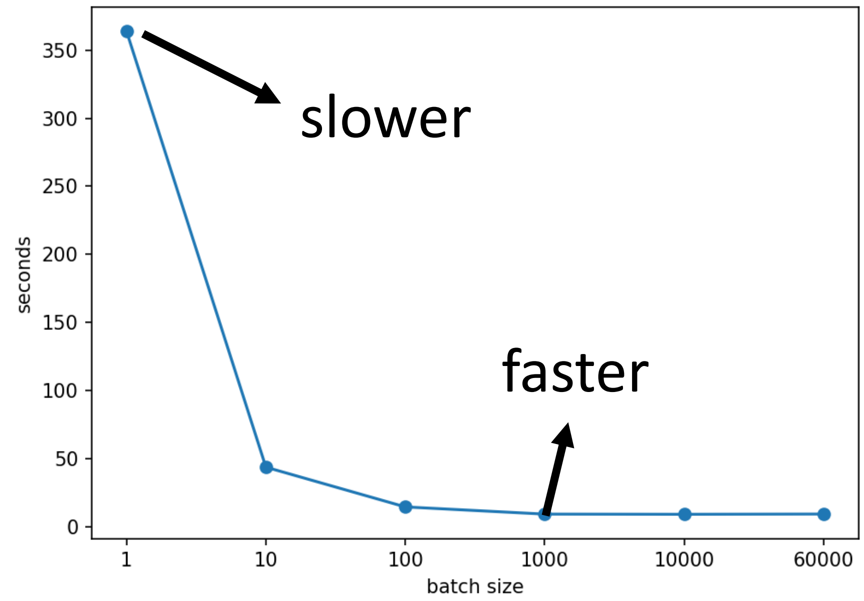
- Smaller batch requires longer time for one epoch (longer time for seeing all data once)

Time for one **update**



60000 updates in one epoch

Time for one **epoch**

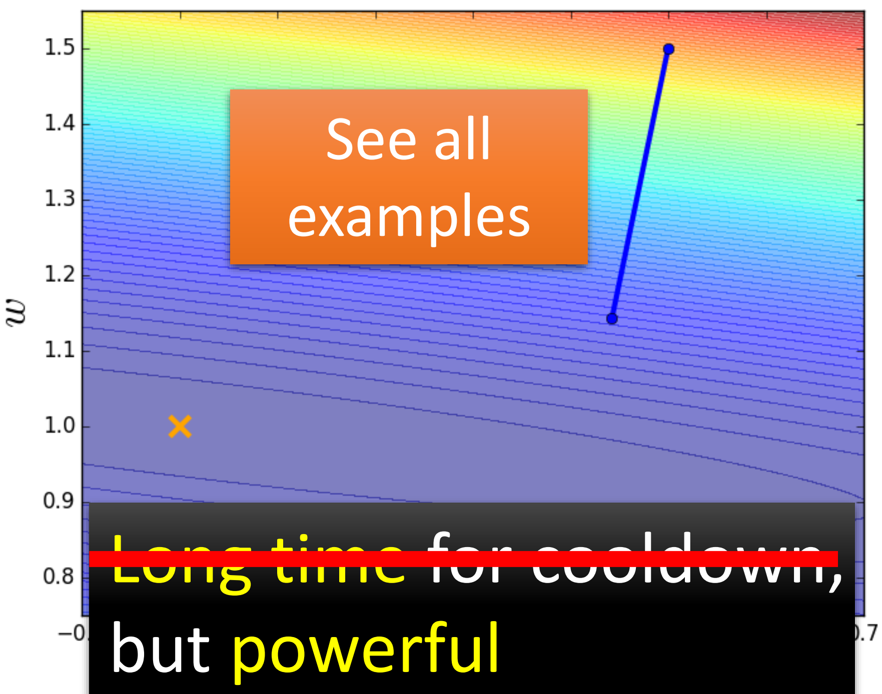


Small Batch v.s. Large Batch

Consider 20 examples (N=20)

Batch size = N (Full Batch)

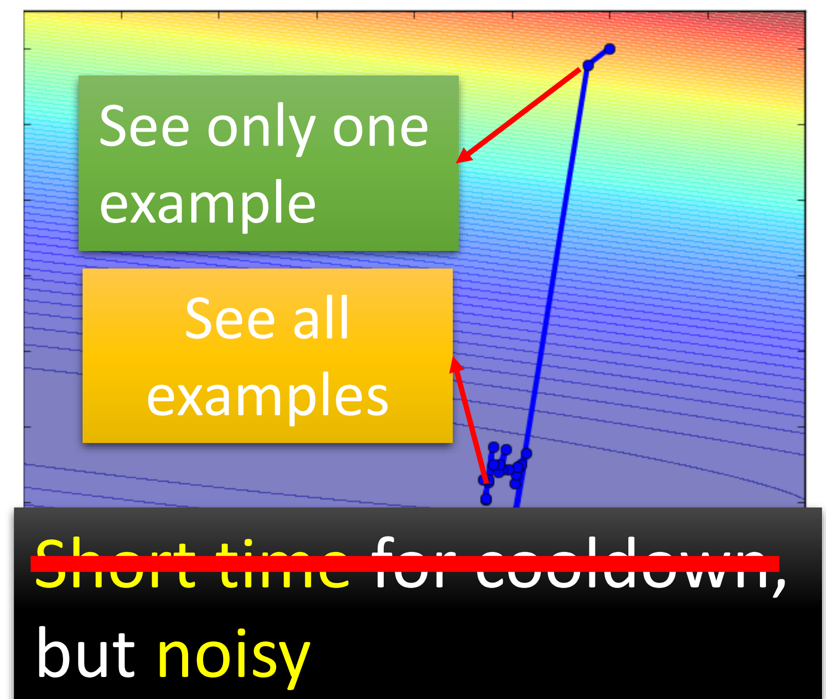
Update after seeing all the 20 examples



Batch size = 1

Update for each example

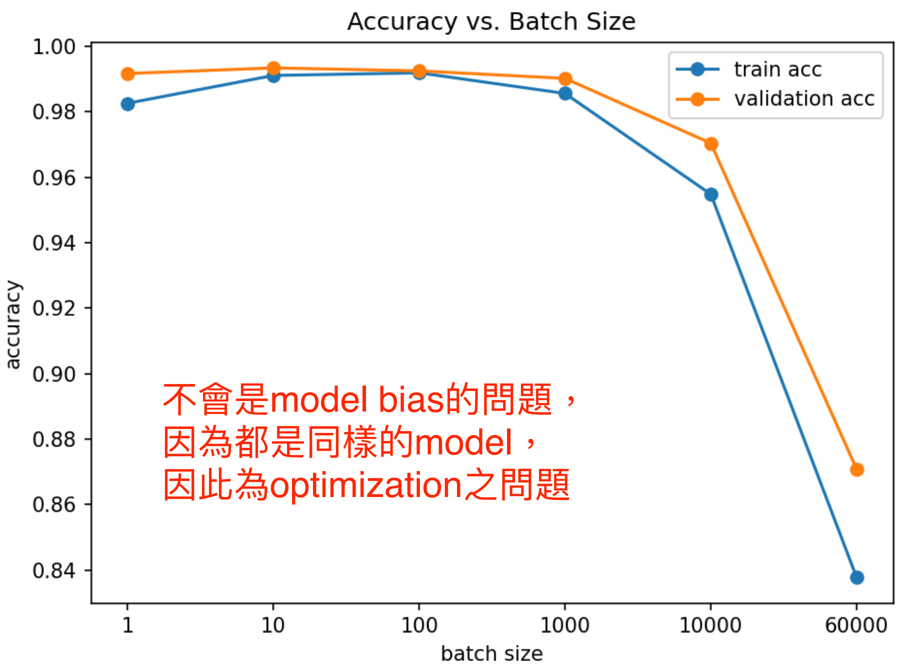
Update 20 times in an epoch



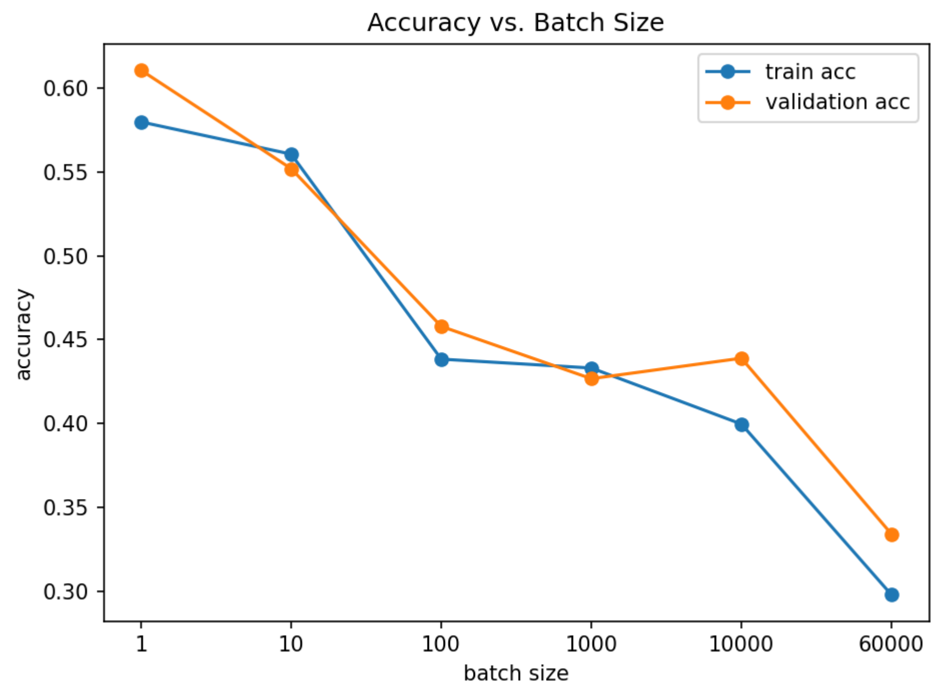
however, noisy can help update

Small Batch v.s. Large Batch

MNIST



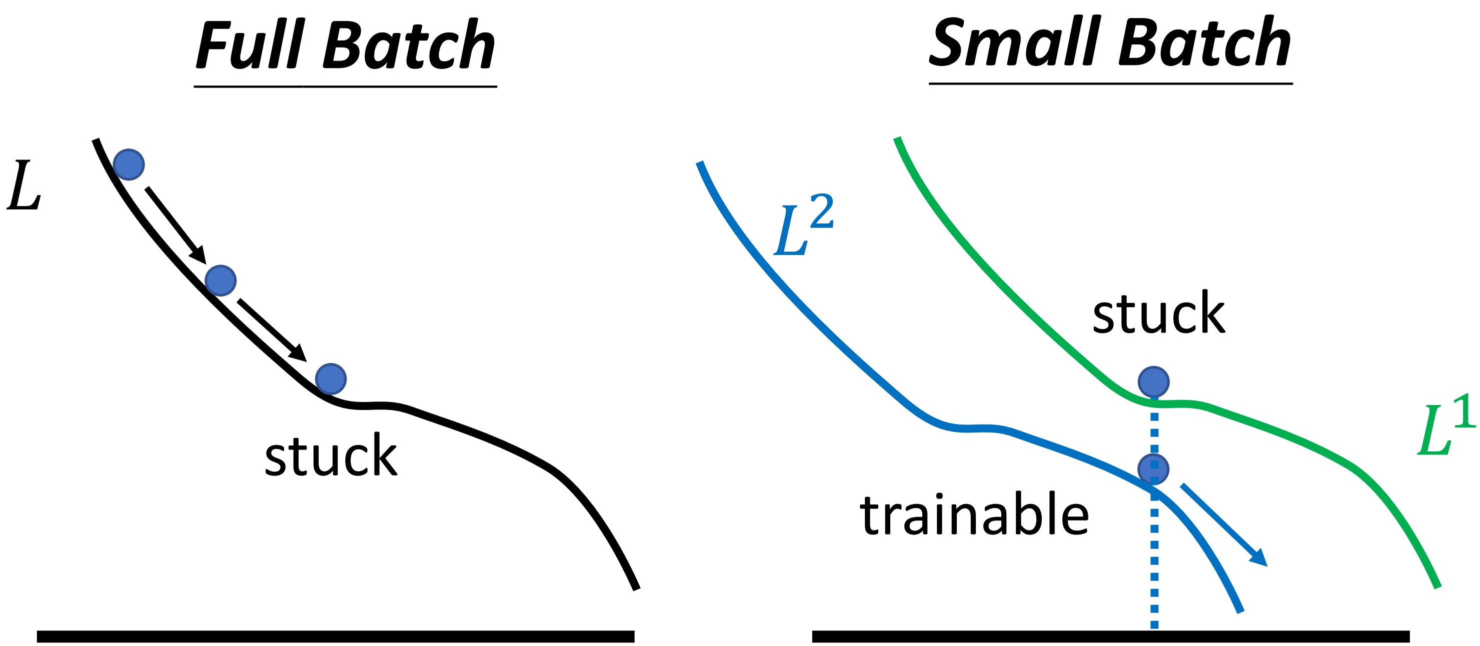
CIFAR-10



- Smaller batch size has better performance
- What's wrong with large batch size?   Optimization Fails

Small Batch v.s. Large Batch

- Smaller batch size has better performance
- “Noisy” update is better for training



On Large-Batch Training for Deep Learning: Generalization Gap and Sharp Minima
https://arxiv.org/abs/1609.04836

Small Batch v.s. Large Batch

有個實驗指出
若想盡辦法將big batch之training accuracy調至與small batch之training accuracy一樣好
但在testing上，顯示出small batch之testing accuracy會比較好

- Small batch is better on testing data?

small batch size
large batch size
SB = 256

LB =

0.1 x data set

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

testing 明顯差於training，
即為overfitting

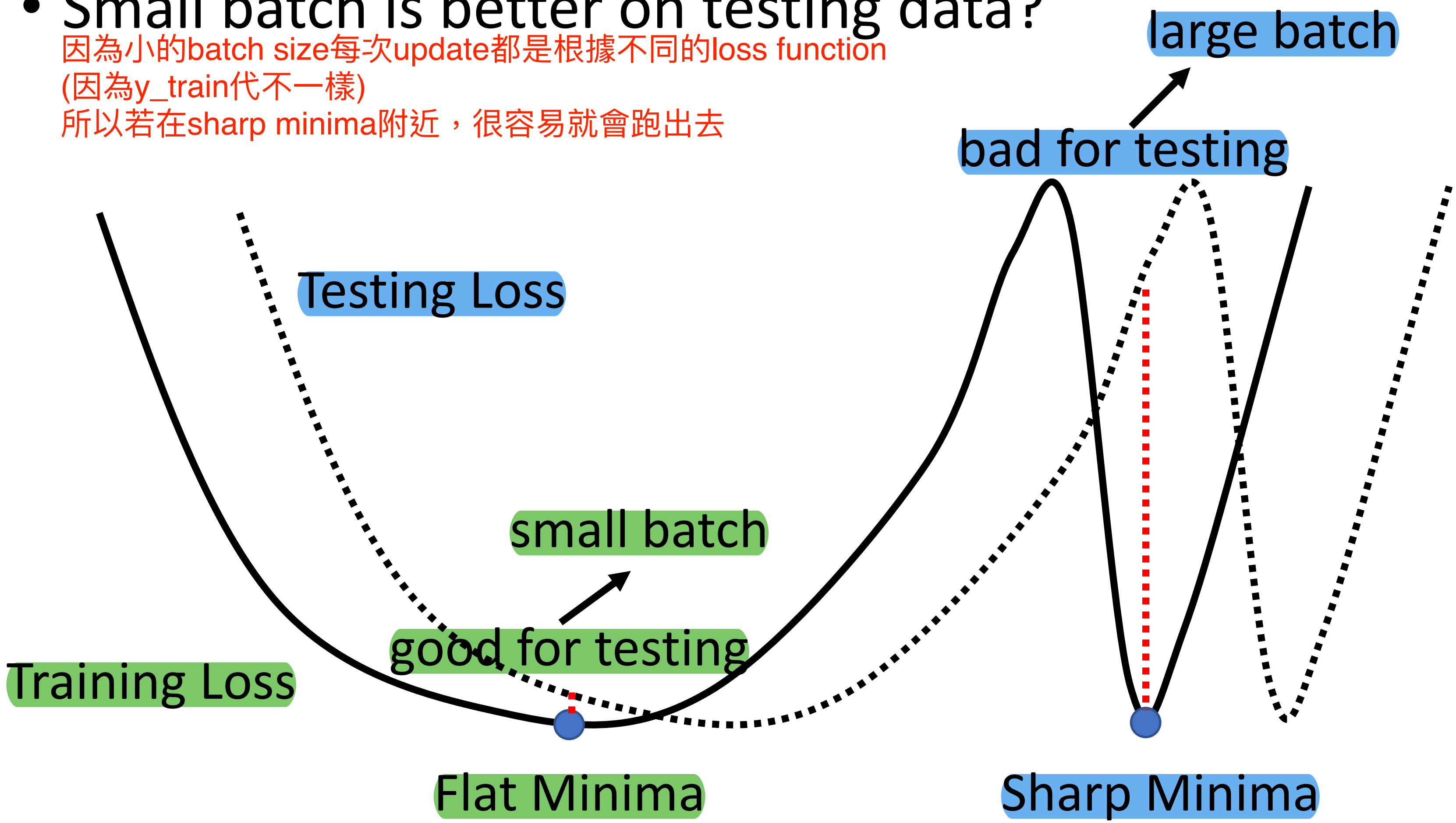
	Training Accuracy		Testing Accuracy	
Name	SB	LB	SB	LB
F_1	$99.66\% \pm 0.05\%$	$99.92\% \pm 0.01\%$	$98.03\% \pm 0.07\%$	$97.81\% \pm 0.07\%$
F_2	$99.99\% \pm 0.03\%$	$98.35\% \pm 2.08\%$	$64.02\% \pm 0.2\%$	$59.45\% \pm 1.05\%$
C_1	$99.89\% \pm 0.02\%$	$99.66\% \pm 0.2\%$	$80.04\% \pm 0.12\%$	$77.26\% \pm 0.42\%$
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	$99.10\% \pm 1.23\%$	$99.57\% \pm 1.84\%$	$63.08\% \pm 0.5\%$	$57.81\% \pm 0.17\%$

Small Batch v.s. Large Batch

大家普遍相信
小的batch size會讓參數走到flat minima
大的batch size會讓參數走到sharp minima

- Small batch is better on testing data?

因為小的batch size每次update都是根據不同的loss function
(因為y_train代不一樣)
所以若在sharp minima附近，很容易就會跑出去



Small Batch v.s. Large Batch

	Small	Large
Speed for one update (no parallel)	Faster	Slower
Speed for one update (with parallel)	Same	Same (not too large)
Time for one epoch	Slower	Faster
Gradient	Noisy	Stable
Optimization	Better	Worse
Generalization	Better	Worse

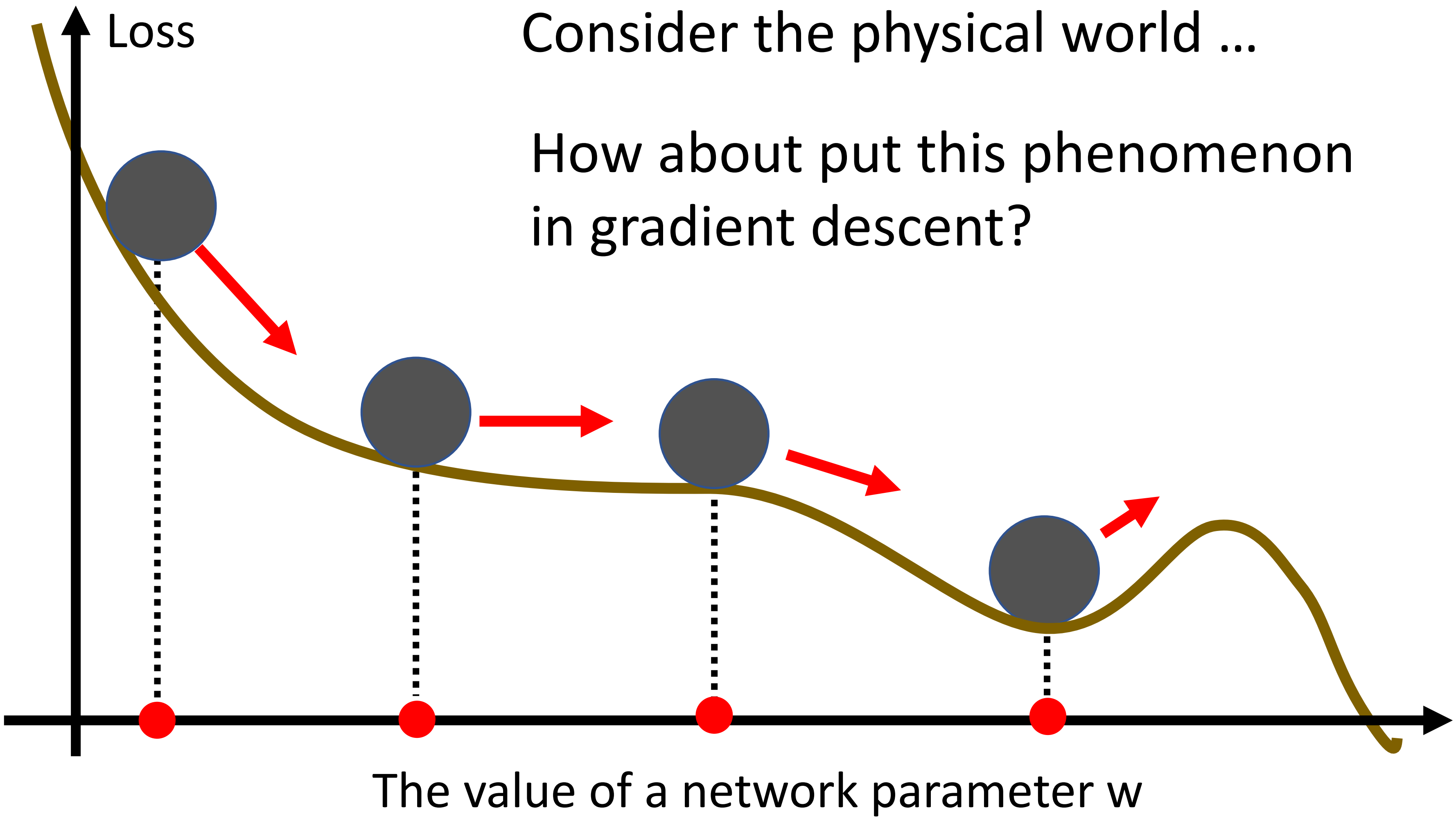
Batch size is a hyperparameter you have to decide.

Have both fish and bear's paws?

- Large Batch Optimization for Deep Learning: Training BERT in 76 minutes (https://arxiv.org/abs/1904.00962)
- Extremely Large Minibatch SGD: Training ResNet-50 on ImageNet in 15 Minutes (https://arxiv.org/abs/1711.04325)
- Stochastic Weight Averaging in Parallel: Large-Batch Training That Generalizes Well (https://arxiv.org/abs/2001.02312)
- Large Batch Training of Convolutional Networks (https://arxiv.org/abs/1708.03888)
- Accurate, large minibatch sgd: Training imagenet in 1 hour (https://arxiv.org/abs/1706.02677)

Momentum

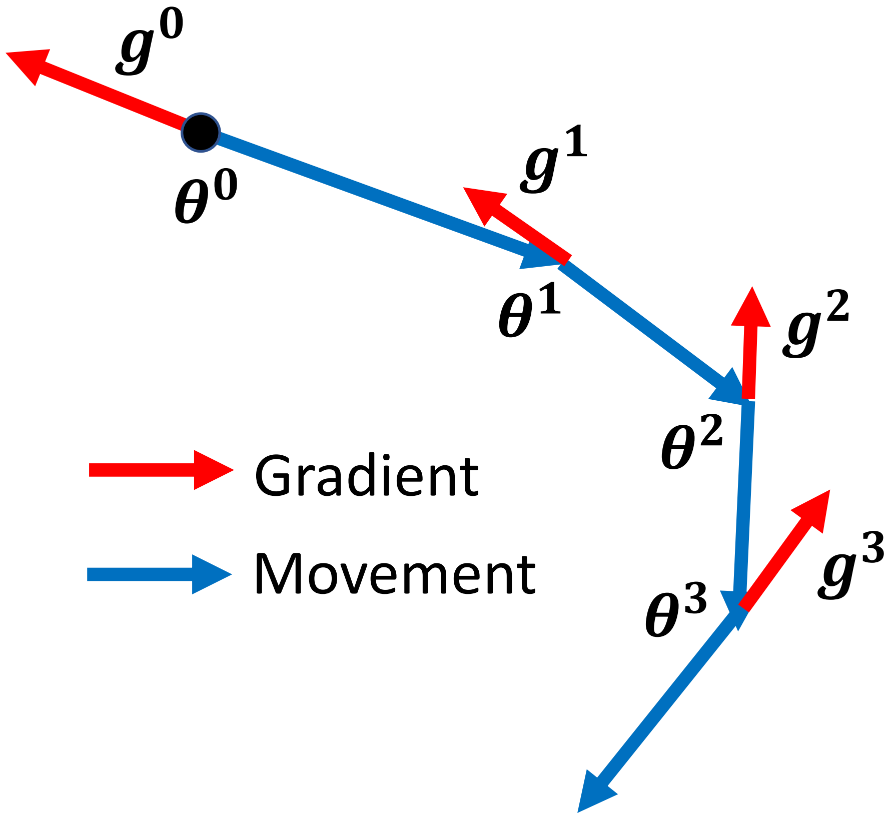
Small Gradient …



Consider the physical world …

How about put this phenomenon in gradient descent?

(Vanilla) Gradient Descent



Starting at $\boldsymbol{\theta}^0$

Compute gradient $\boldsymbol{g}^0$

Move to $\boldsymbol{\theta}^1 = \boldsymbol{\theta}^0 - \eta \boldsymbol{g}^0$

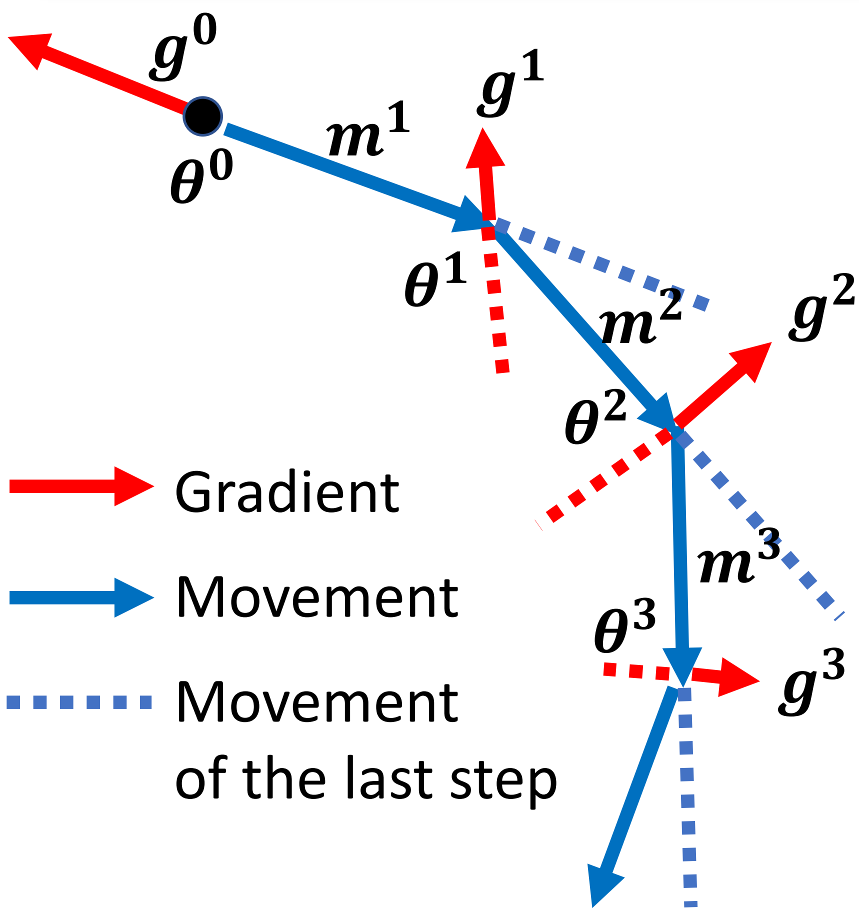
Compute gradient $\boldsymbol{g}^1$

Move to $\boldsymbol{\theta}^2 = \boldsymbol{\theta}^1 - \eta \boldsymbol{g}^1$

⋮

Gradient Descent + Momentum

Movement: **movement of last step** minus **gradient** at present



Starting at $\boldsymbol{\theta}^0$

Movement $\boldsymbol{m}^0 = \mathbf{0}$

Compute gradient $\boldsymbol{g}^0$

Movement $\boldsymbol{m}^1 = \lambda \boldsymbol{m}^0 - \eta \boldsymbol{g}^0$

Move to $\boldsymbol{\theta}^1 = \boldsymbol{\theta}^0 + \boldsymbol{m}^1$

Compute gradient $\boldsymbol{g}^1$

Movement $\boldsymbol{m}^2 = \lambda \boldsymbol{m}^1 - \eta \boldsymbol{g}^1$

Move to $\boldsymbol{\theta}^2 = \boldsymbol{\theta}^1 + \boldsymbol{m}^2$

Movement not just based on gradient, but previous movement.

Gradient Descent + Momentum

Movement: **movement of last step** minus **gradient** at present

$\boldsymbol{m}^i$ is the weighted sum of all the previous gradient: $\boldsymbol{g}^0, \boldsymbol{g}^1, \ldots, \boldsymbol{g}^{i-1}$

$$\boldsymbol{m}^0 = \boldsymbol{0}$$

$$\boldsymbol{m}^1 = -\eta \boldsymbol{g}^0$$

$$\boldsymbol{m}^2 = -\lambda\eta \boldsymbol{g}^0 - \eta \boldsymbol{g}^1$$

$$\vdots$$

Starting at $\boldsymbol{\theta}^0$

Movement $\boldsymbol{m}^0 = \boldsymbol{0}$

Compute gradient $\boldsymbol{g}^0$

Movement $\boldsymbol{m}^1 = \lambda \boldsymbol{m}^0 - \eta \boldsymbol{g}^0$

Move to $\boldsymbol{\theta}^1 = \boldsymbol{\theta}^0 + \boldsymbol{m}^1$

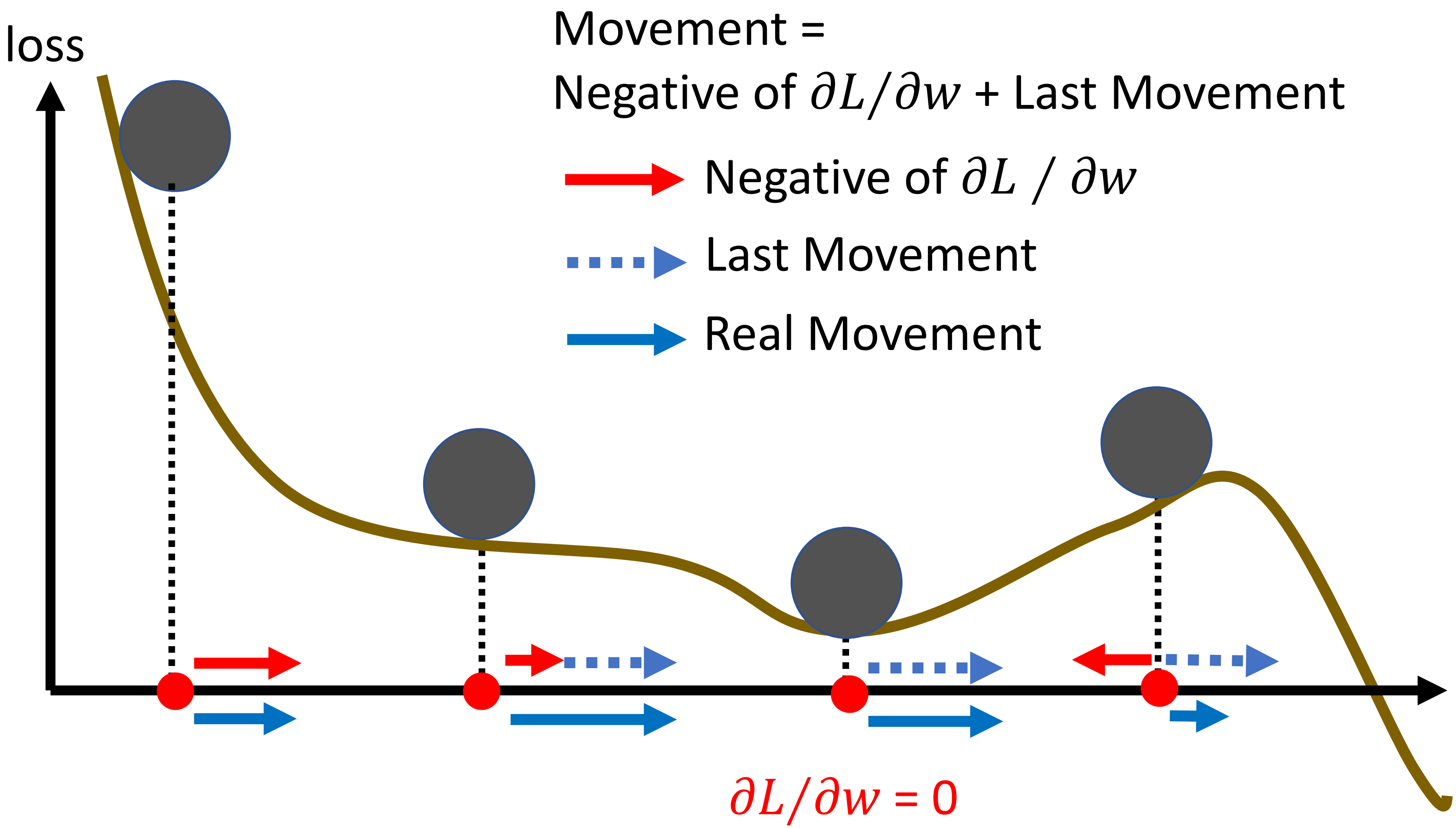
Compute gradient $\boldsymbol{g}^1$

Movement $\boldsymbol{m}^2 = \lambda \boldsymbol{m}^1 - \eta \boldsymbol{g}^1$

Move to $\boldsymbol{\theta}^2 = \boldsymbol{\theta}^1 + \boldsymbol{m}^2$

Movement not just based on gradient, but previous movement.

Gradient Descent + Momentum



Concluding Remarks

- Critical points have zero gradients.
- Critical points can be either saddle points or local minima.
  - Can be determined by the Hessian matrix.
  - It is possible to escape saddle points along the direction of eigenvectors of the Hessian matrix.
  - Local minima may be rare.
- Smaller batch size and momentum help escape critical points.

Acknowledgement

- 感謝作業二助教團隊(陳宣叡、施貽仁、孟妍李威緒)幫忙跑實驗以及蒐集資料