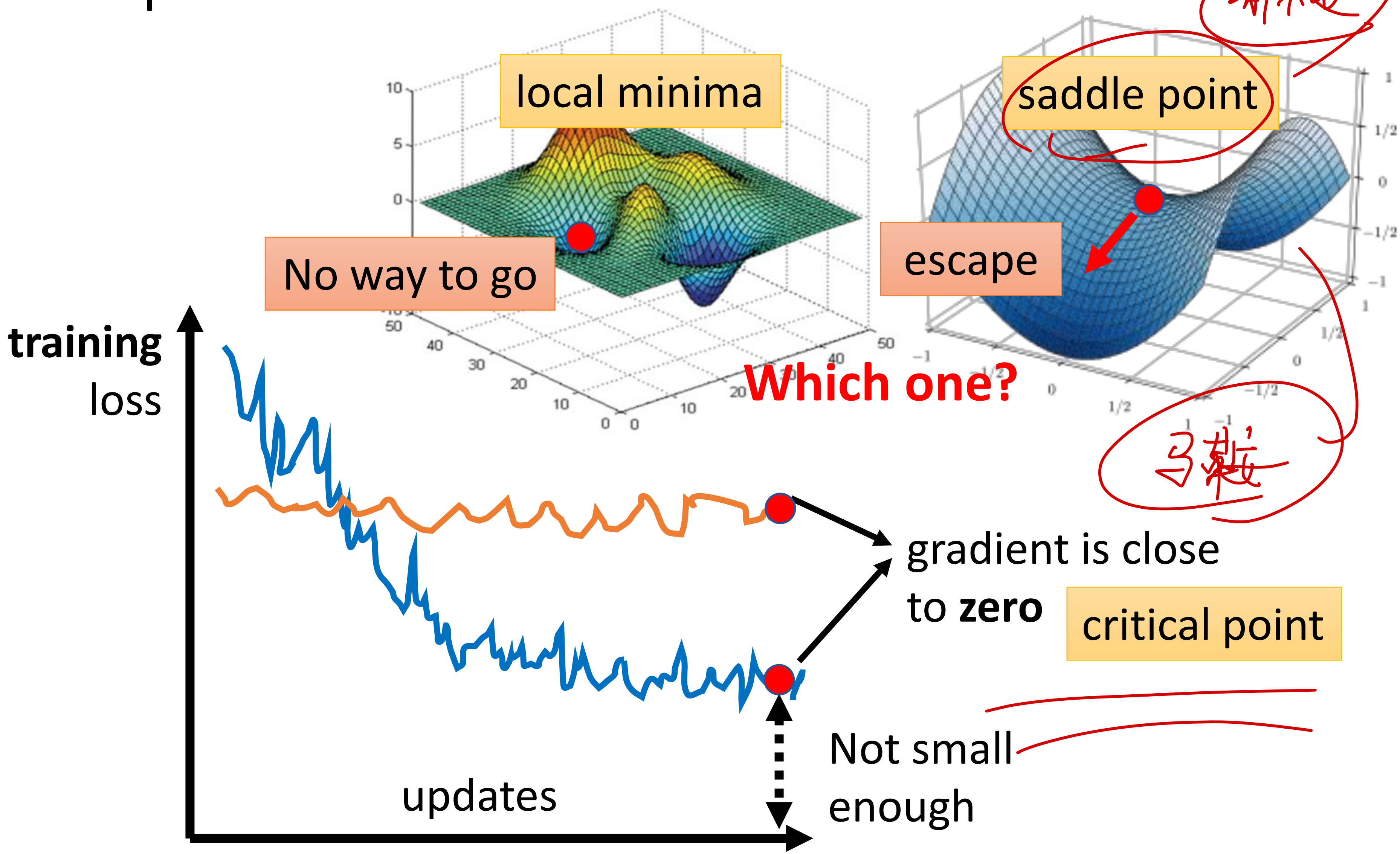
# When gradient is small …

Hung-yi Lee 李宏毅

# Optimization Fails because ……

都不是



# Warning of Math

# Tayler Series Approximation

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

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

附近点

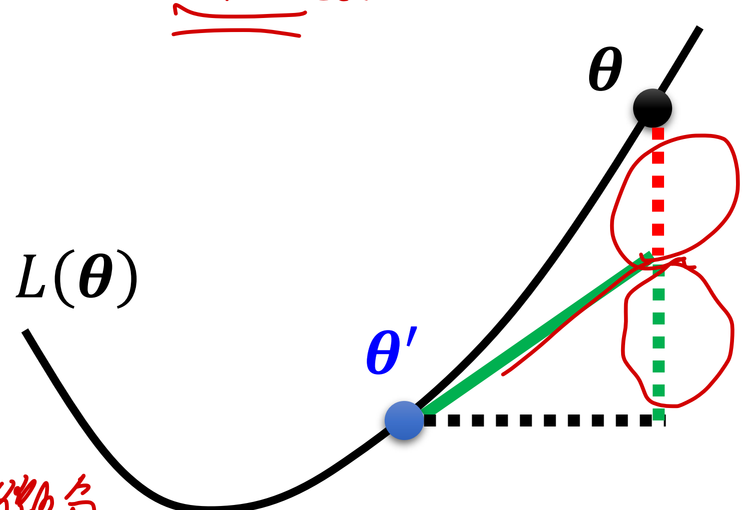
**Gradient** $\boldsymbol{g}$ is a ***vector***

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

**Hessian** $H$ is a ***matrix***

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

两次微分



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

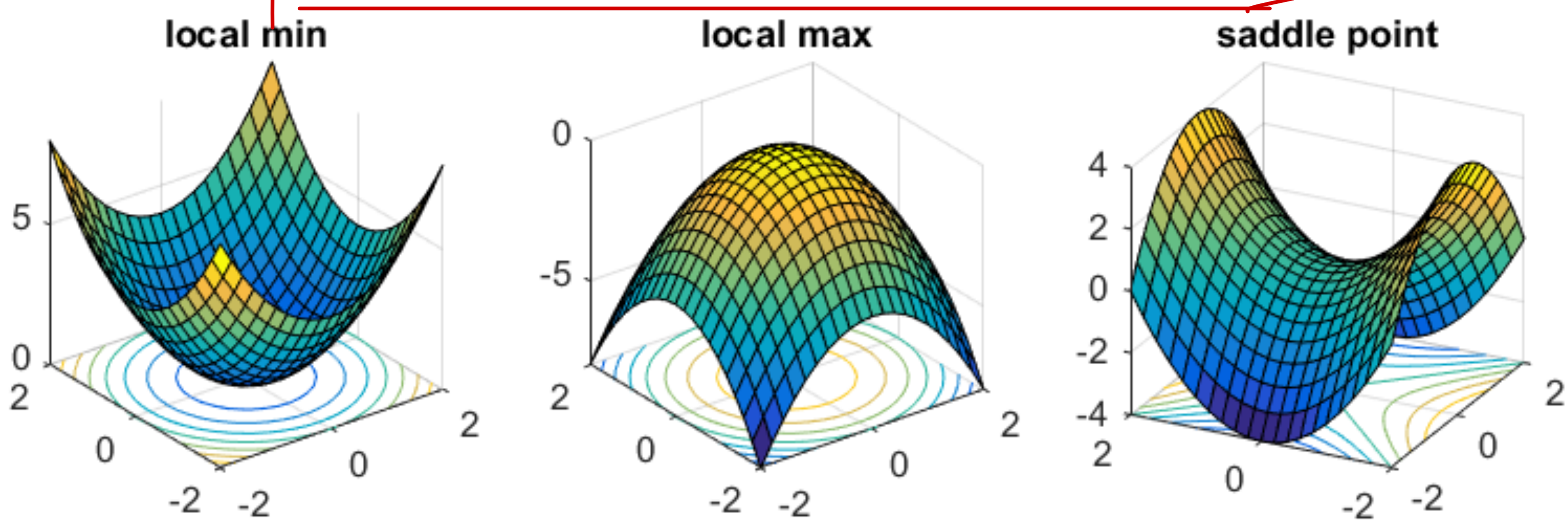
# Hessian

$L(\boldsymbol{\theta})$ 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**

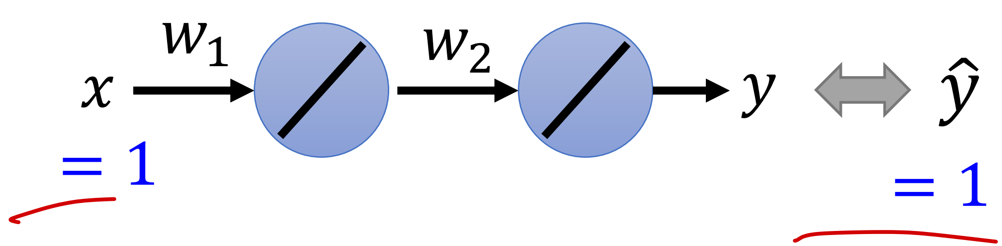
= $H$ is negative definite = All eigen values are negative. ⬆

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

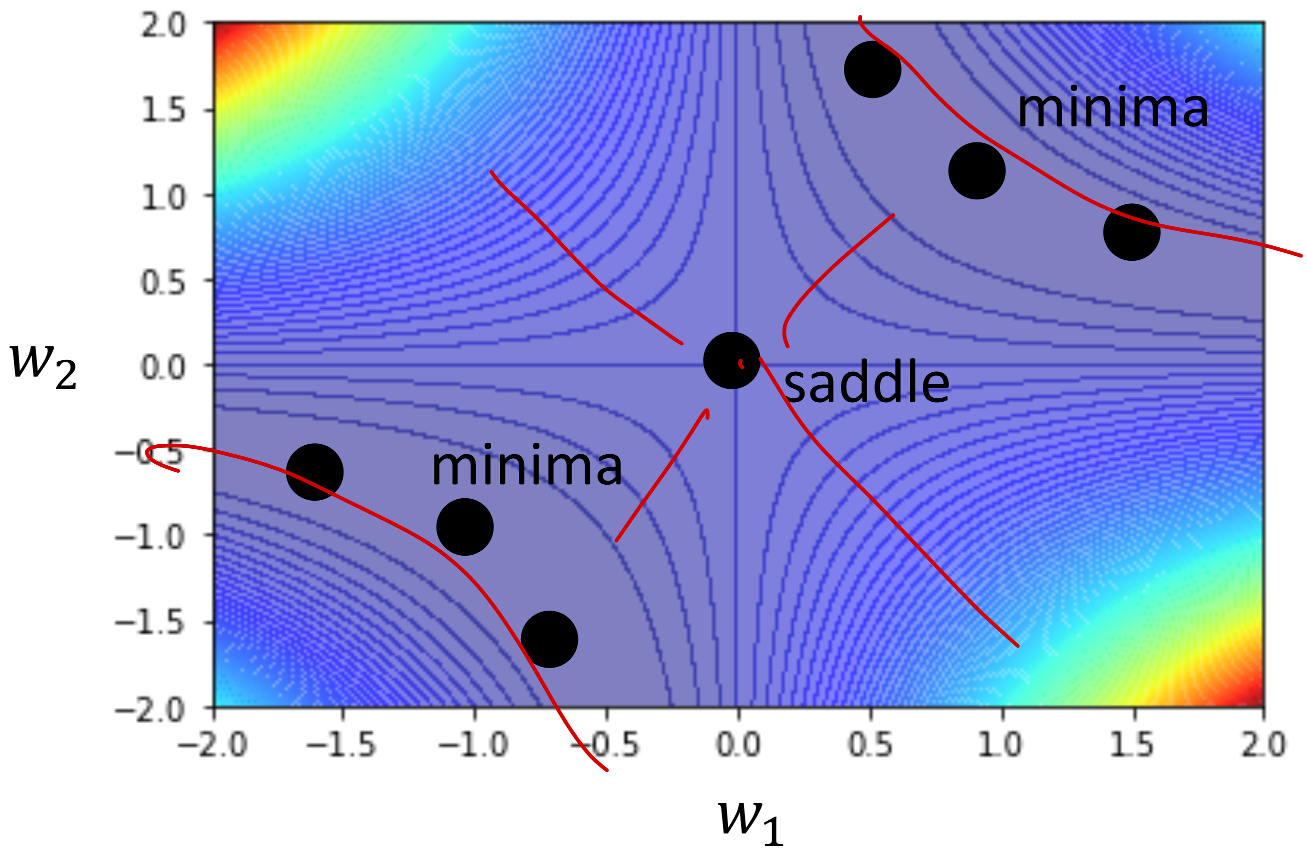
Some eigen values are positive, and some are negative. ⬆

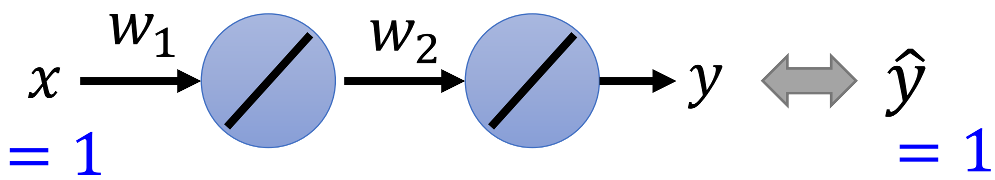
# ***Example***

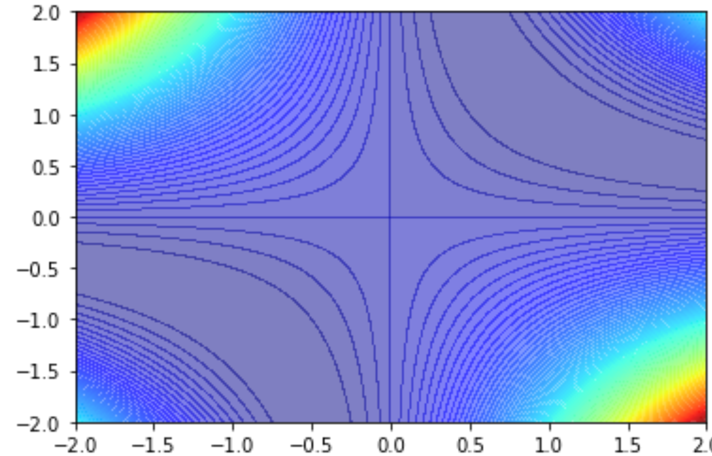
$$y = w_1 w_2 x$$




*Error Surface*






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

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

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

$g$

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

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

**Saddle point**

$H$

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

$$\frac{\partial^2 L}{\partial w_1 \partial w_2} = -2 + 4 w_1 w_2 \quad = -2$$

$$\frac{\partial^2 L}{\partial w_2 \partial w_1} = -2 + 4 w_1 w_2 \quad = -2$$

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

# *Don't afraid of saddle point?*

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

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 $H$

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

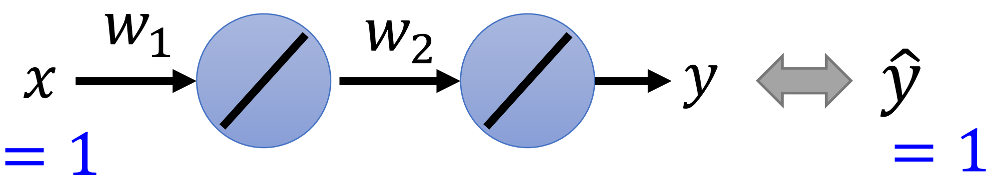
$\lambda < 0$

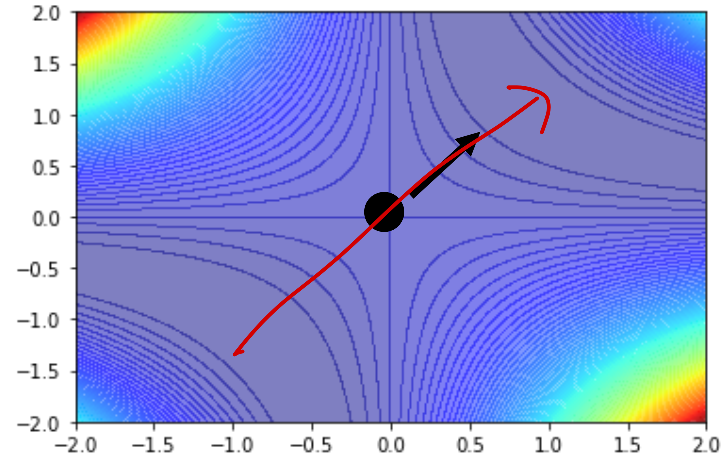
➡ $\boldsymbol{u}^T H \boldsymbol{u} = \boldsymbol{u}^T (\lambda \boldsymbol{u}) = \lambda \|\boldsymbol{u}\|^2$

$< 0$ $\quad$ $< 0$

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

$\boldsymbol{\theta} - \boldsymbol{\theta}' = \boldsymbol{u}$ $\qquad$ $\boldsymbol{\theta} = \boldsymbol{\theta}' + \boldsymbol{u}$ $\qquad$ 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（魔法師狄奥倫娜）

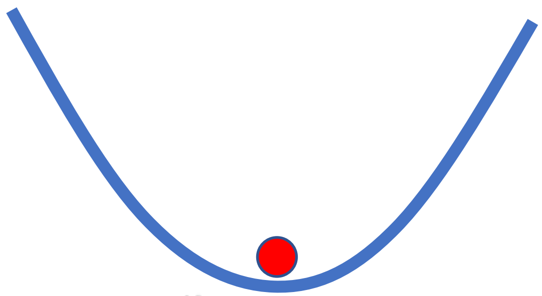
From 3 dimensional space, it is sealed.

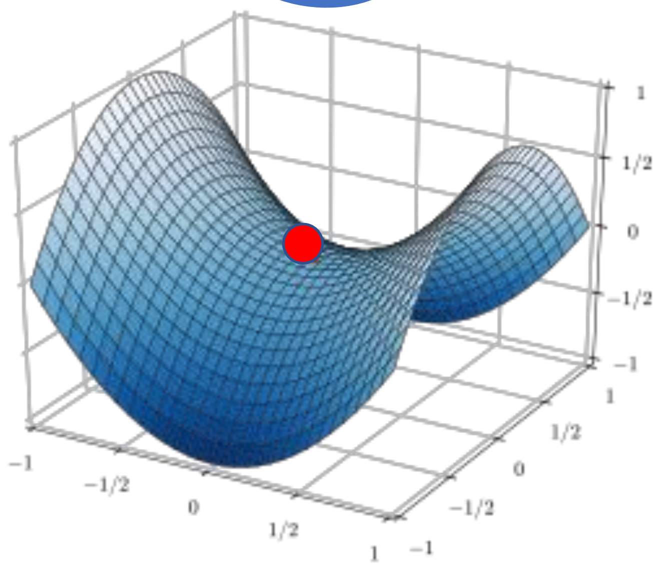
It is not in higher dimensions.

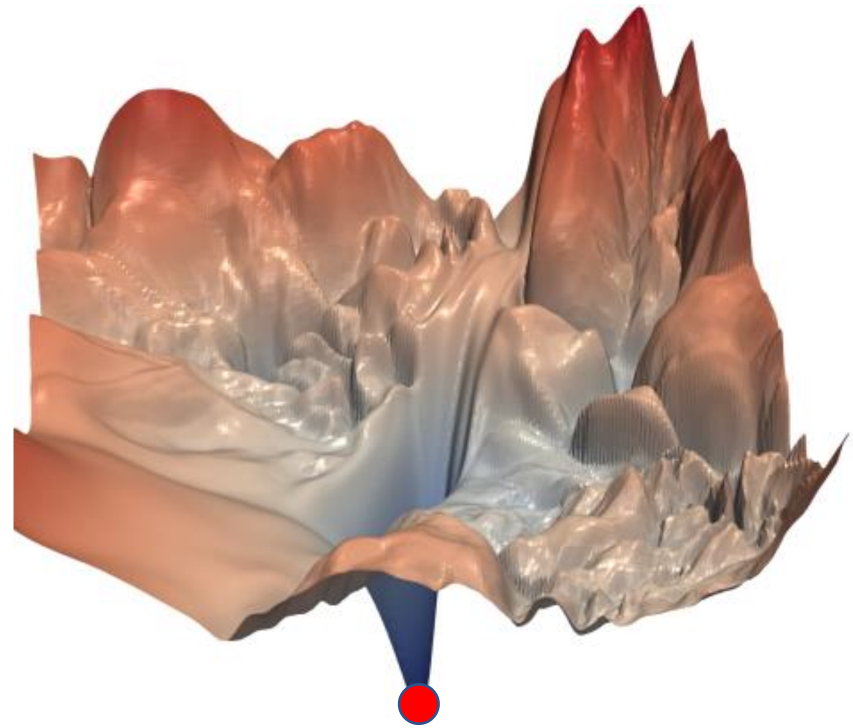
Source of image: https://read01.com/mz2DBPE.html#.YECz22gzbIU

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

# Saddle Point v.s. Local Minima



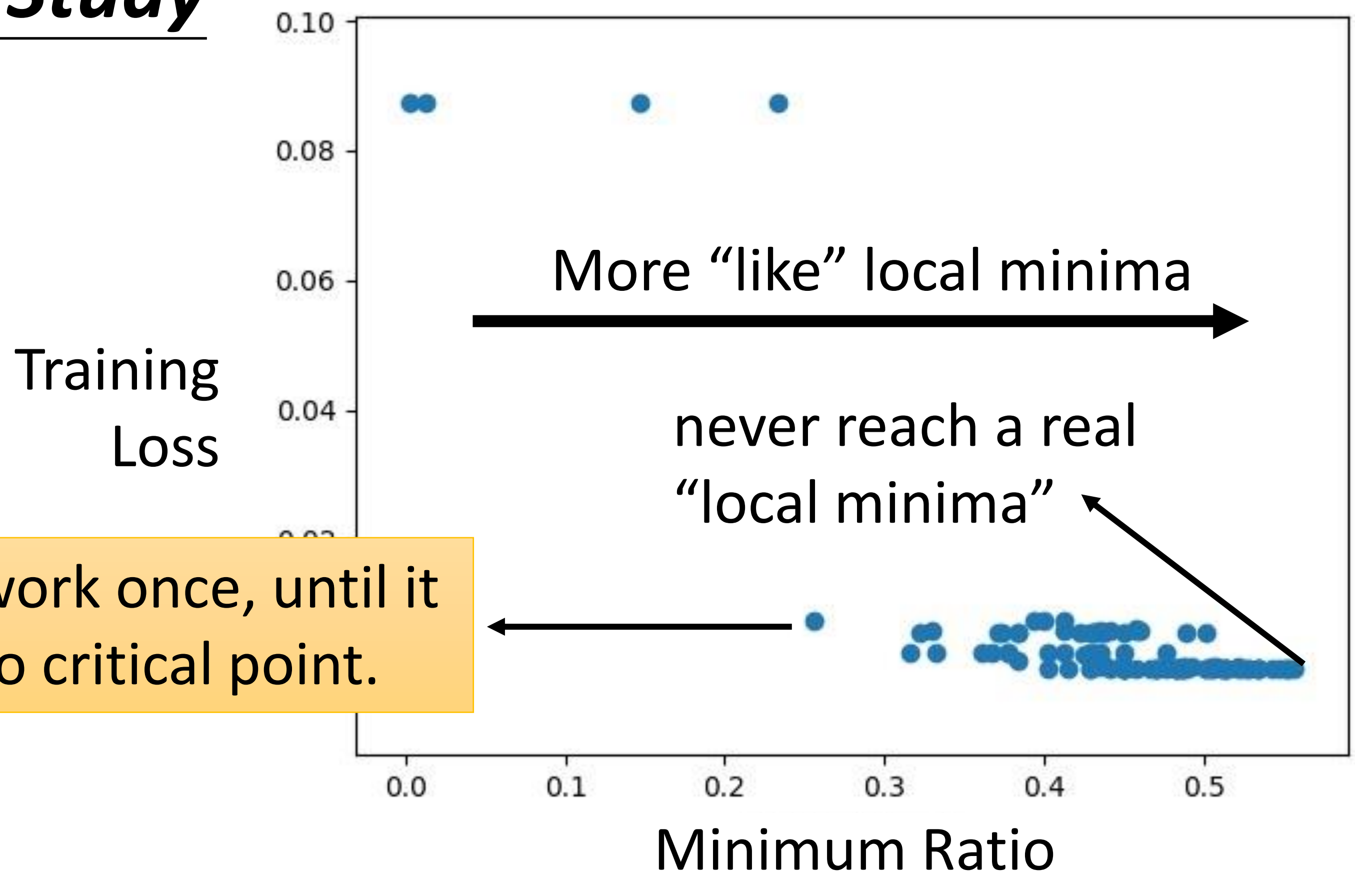


Saddle point in higher dimension?

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

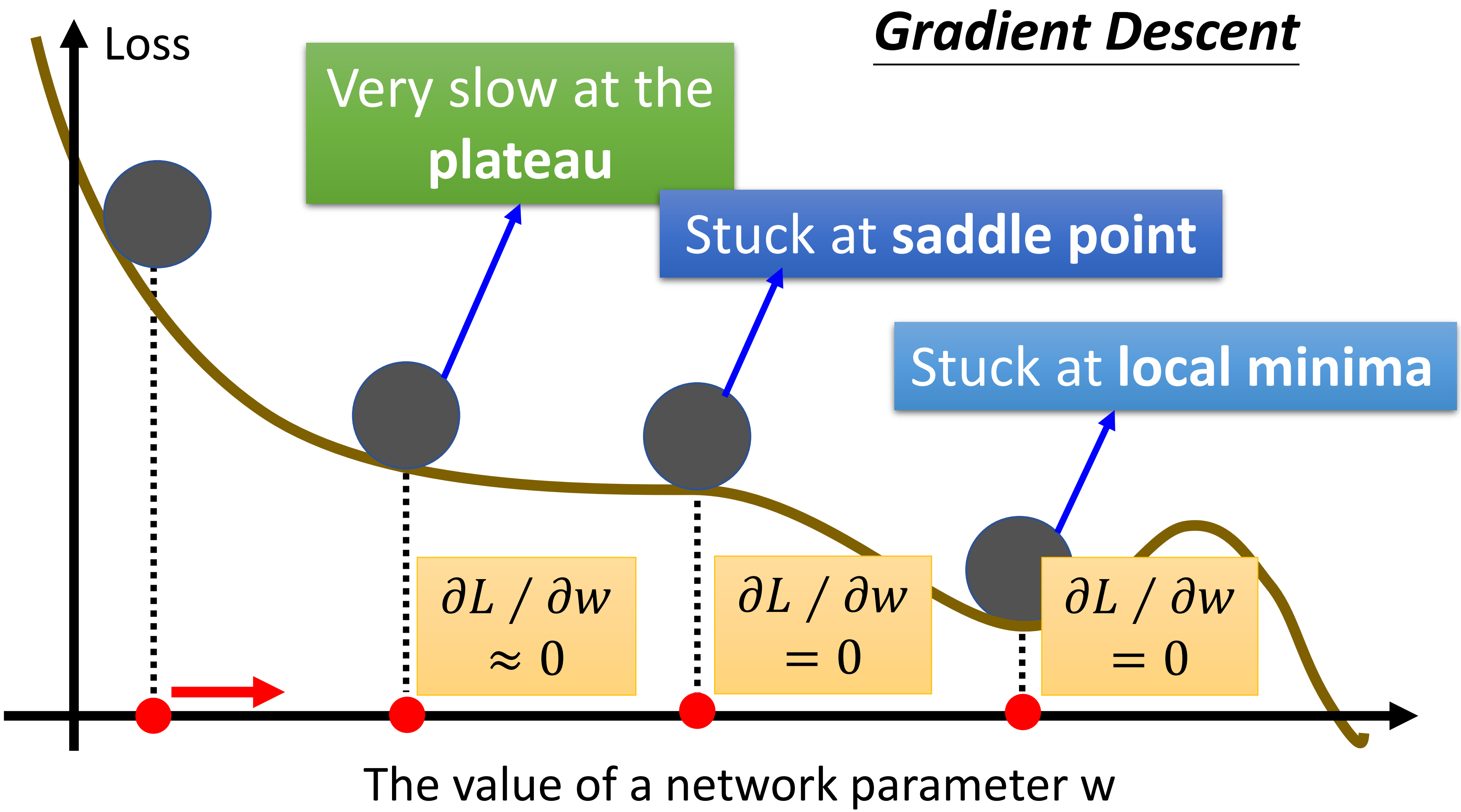
# ***Empirical Study***




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

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

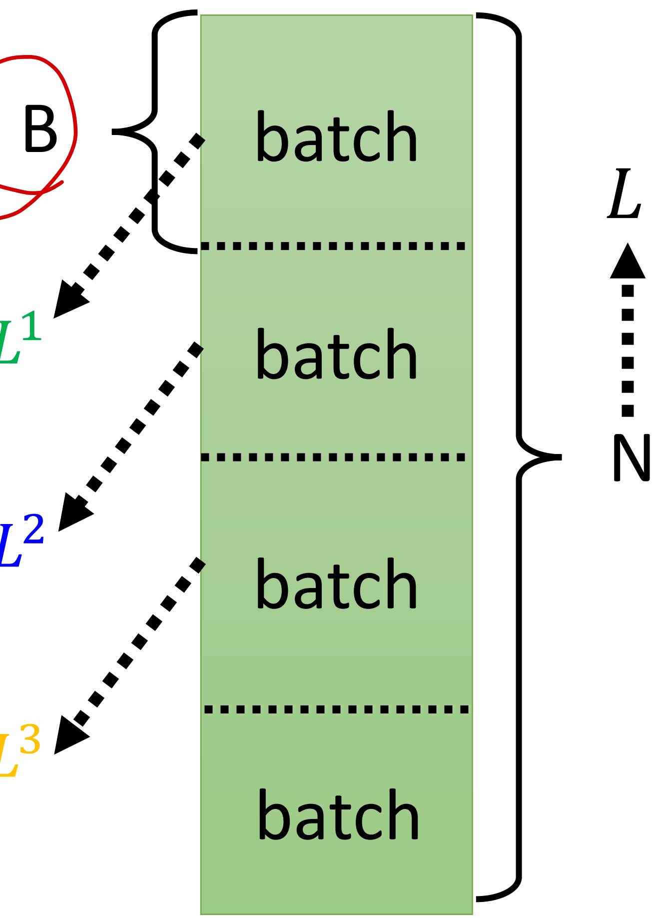
$$\boldsymbol{\theta}^* = arg\min_{\boldsymbol{\theta}} L$$

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

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

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

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



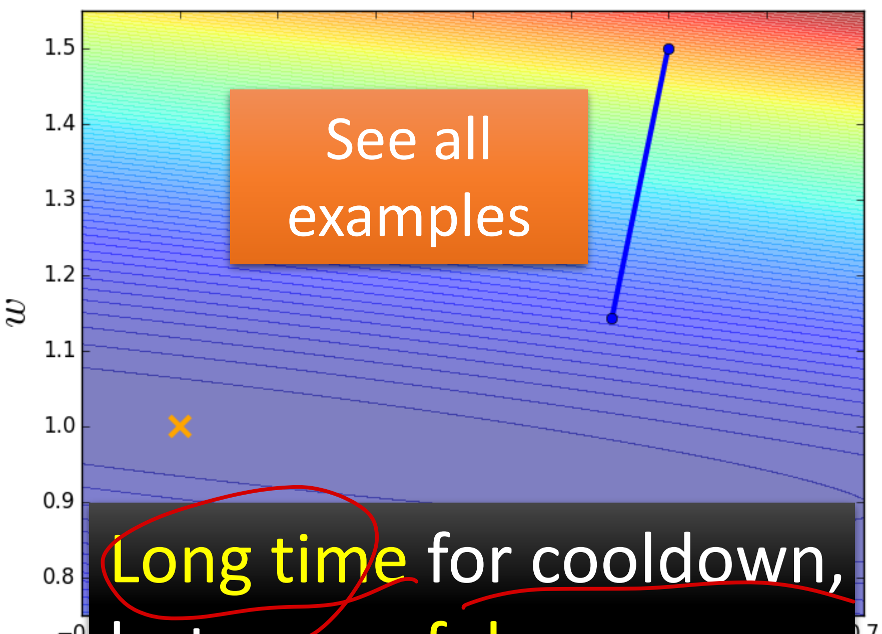

1 **epoch** = see all the batches once ➡ **Shuffle** after each epoch

# Small Batch v.s. Large Batch

Consider 20 examples (N=20)

**Batch size = N (Full batch)**

Update after seeing all the 20 examples

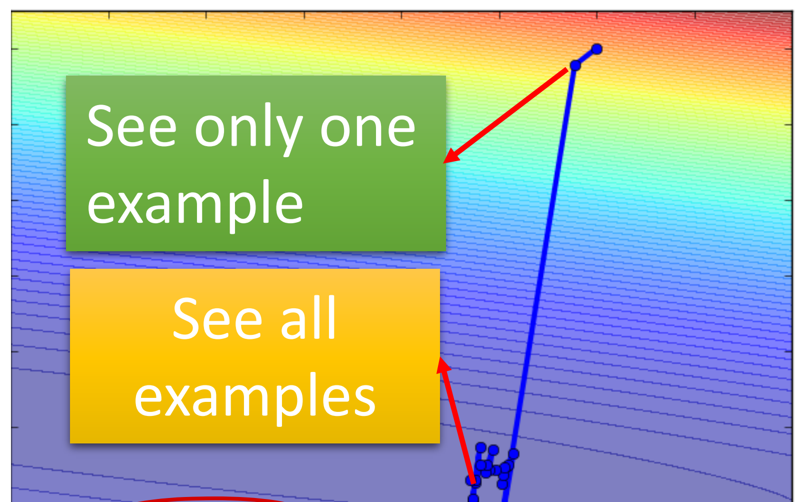



Long time for cooldown, but powerful

**Batch size = 1**

Update for each example

Update 20 times in an epoch




Short time for cooldown, but noisy

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

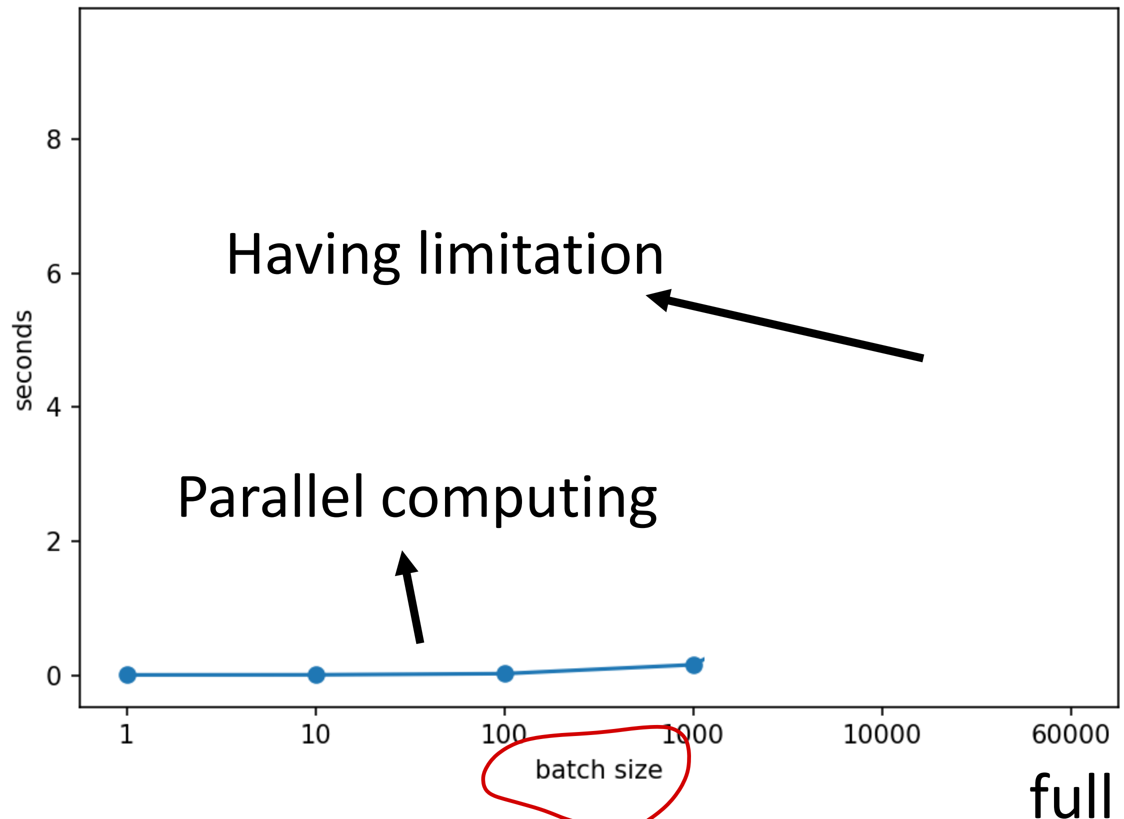
# Small Batch v.s. Large Batch

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

**Time for each update**

MNIST: digit classification

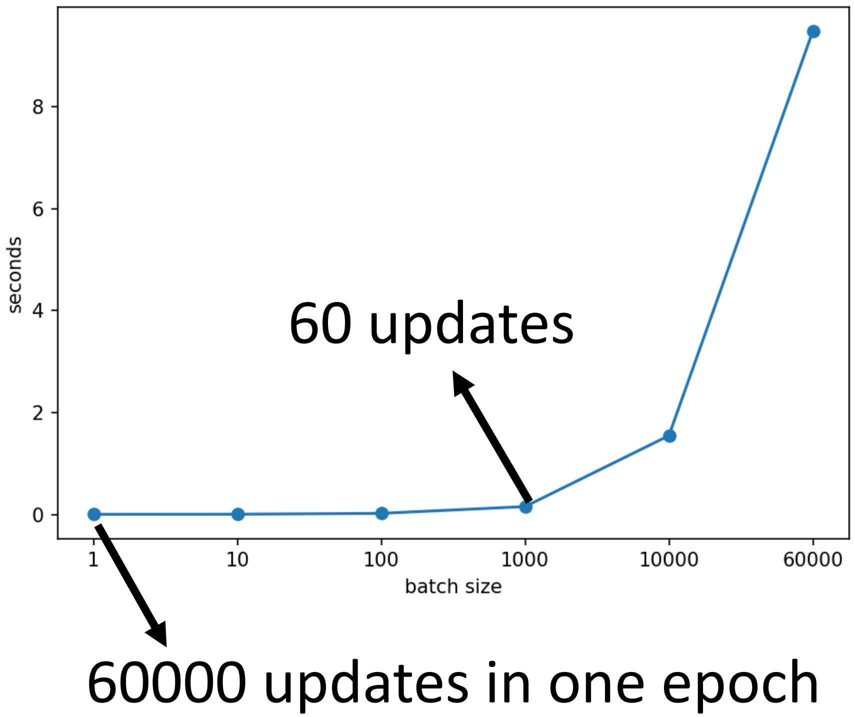
**Tesla V100 GPU**



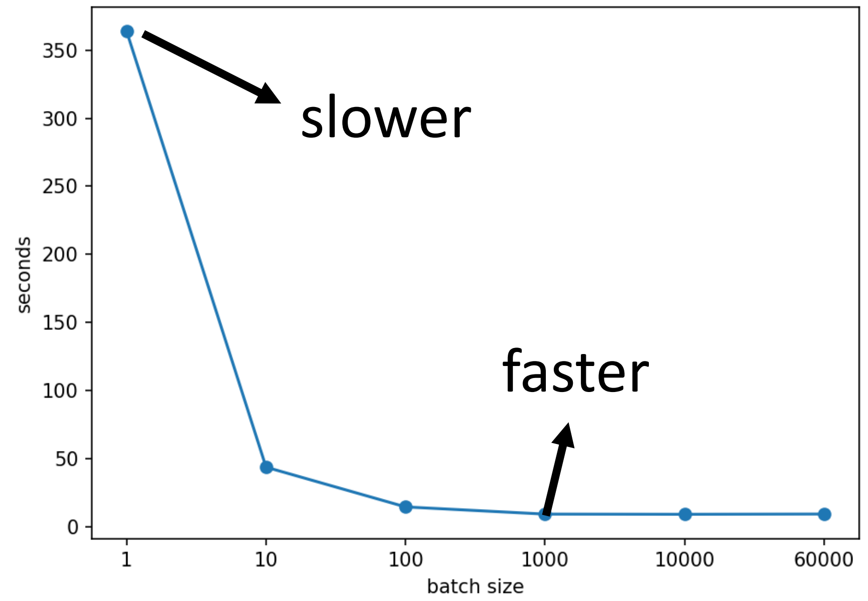
# Small Batch v.s. Large Batch

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

Time for one **update**




Time for one **epoch**



# Small Batch v.s. Large Batch

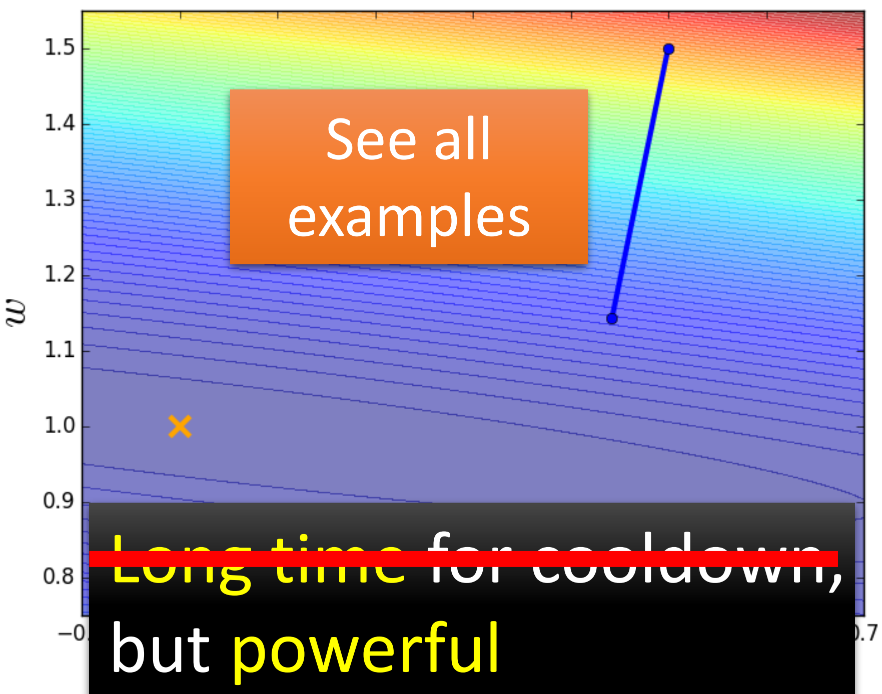
Consider 20 examples (N=20)

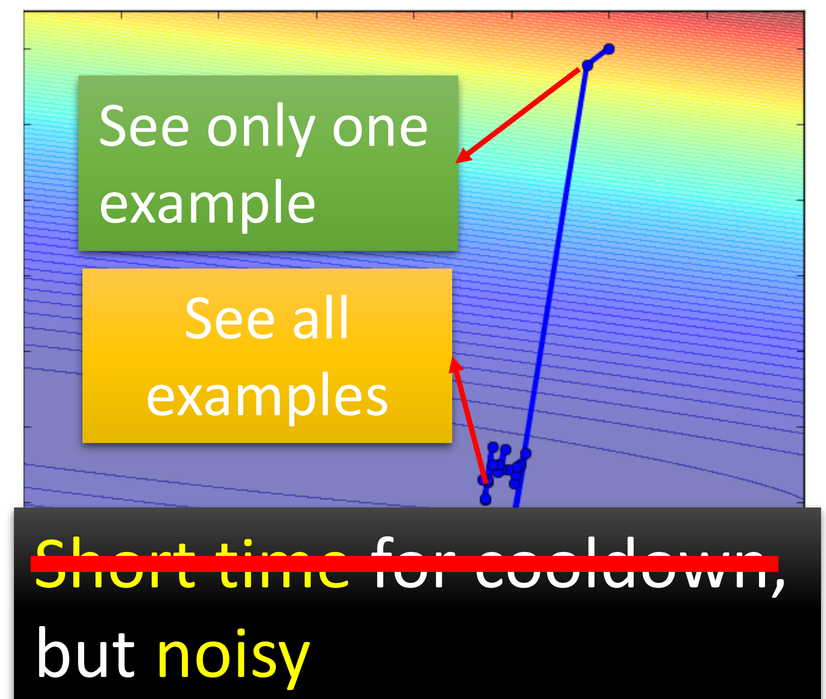
**Batch size = N (Full Batch)** time $\approx$ **Batch size = 1**

Update after seeing all the 20 examples

Update for each example

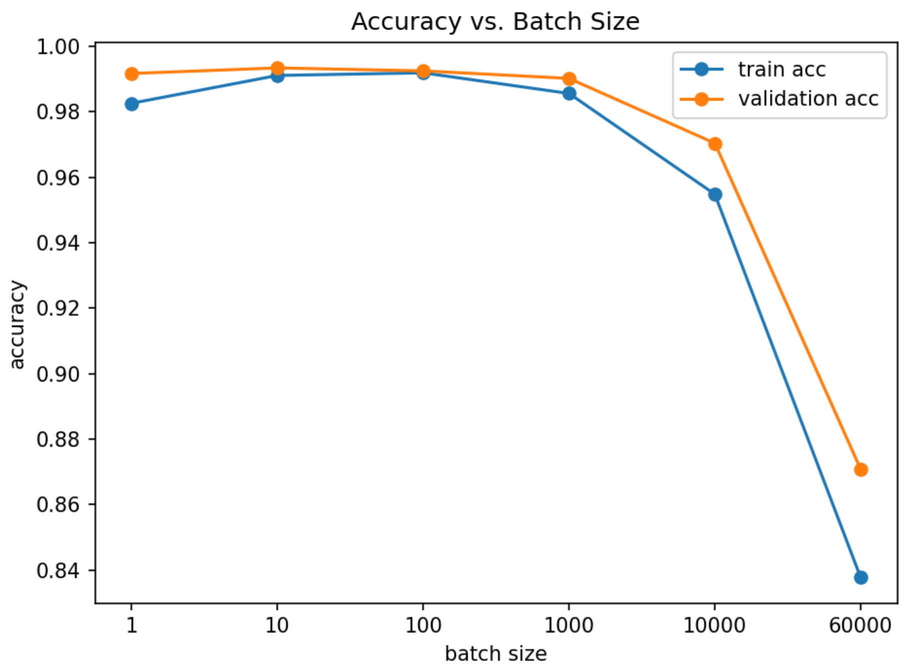
Update 20 times in an epoch



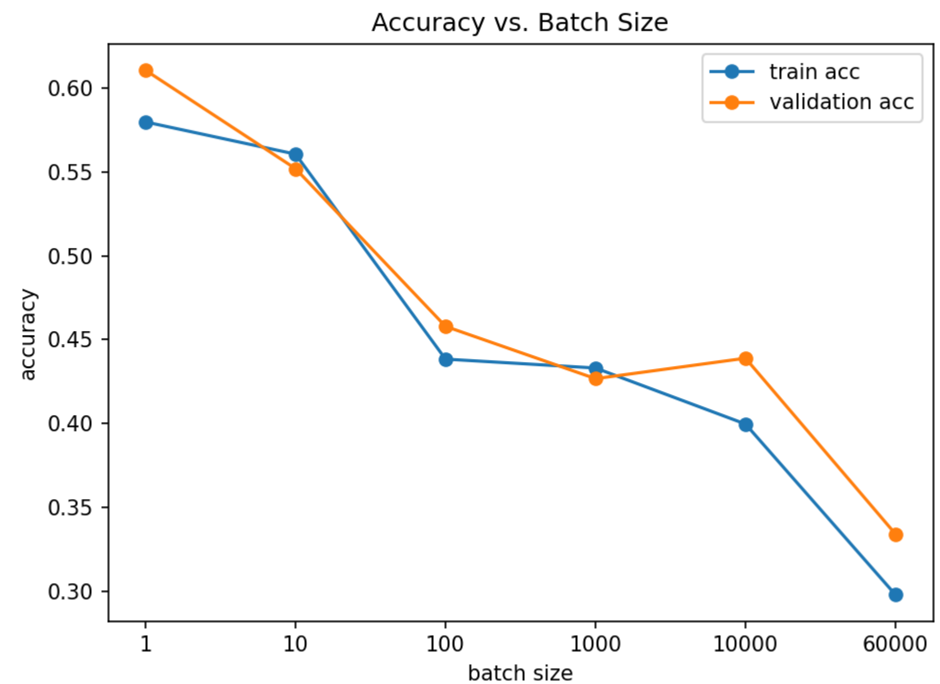



# Small Batch v.s. Large Batch

## ***MNIST***



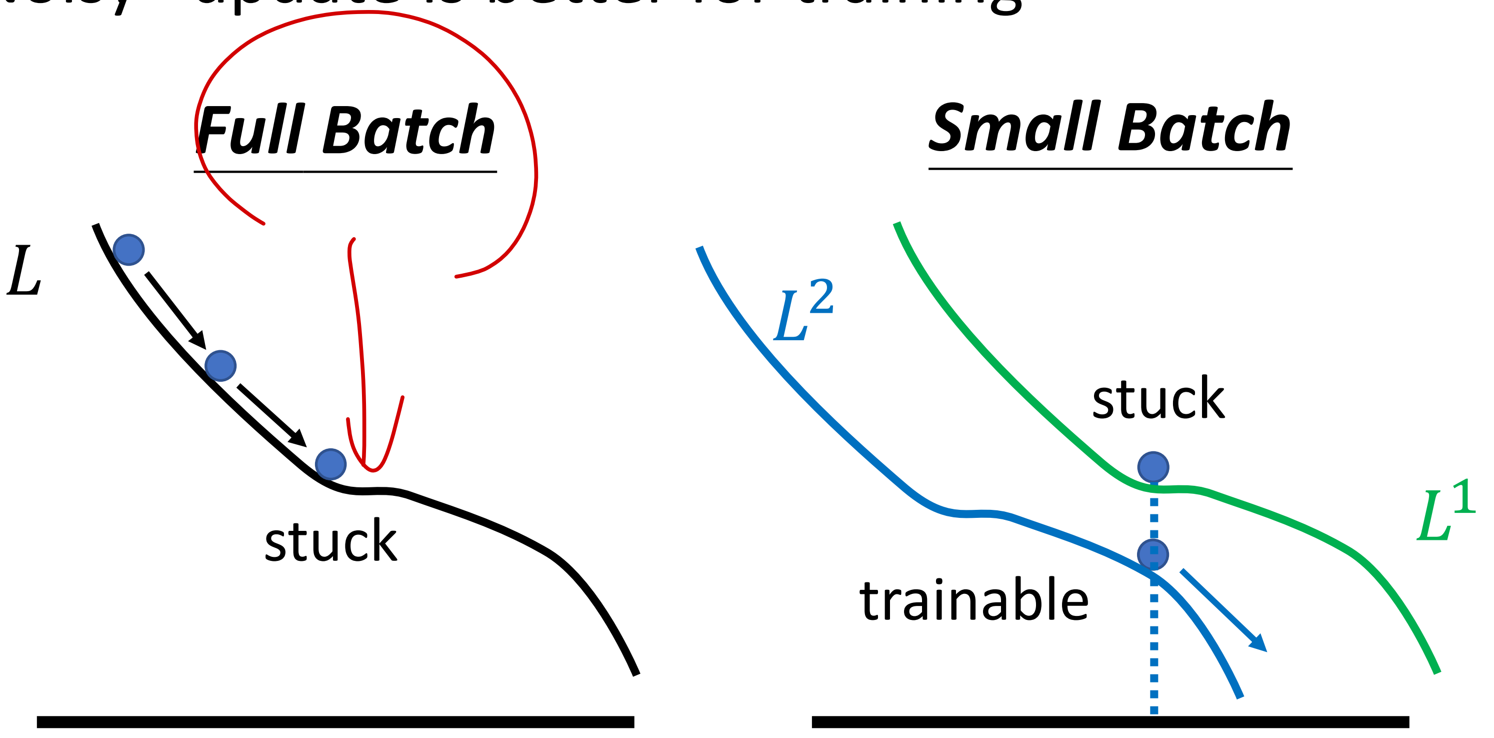

## ***CIFAR-10***




- Smaller batch size has better performance 大组
- 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



# Small Batch v.s. Large Batch

- Small batch is better on testing data?

SB = 256

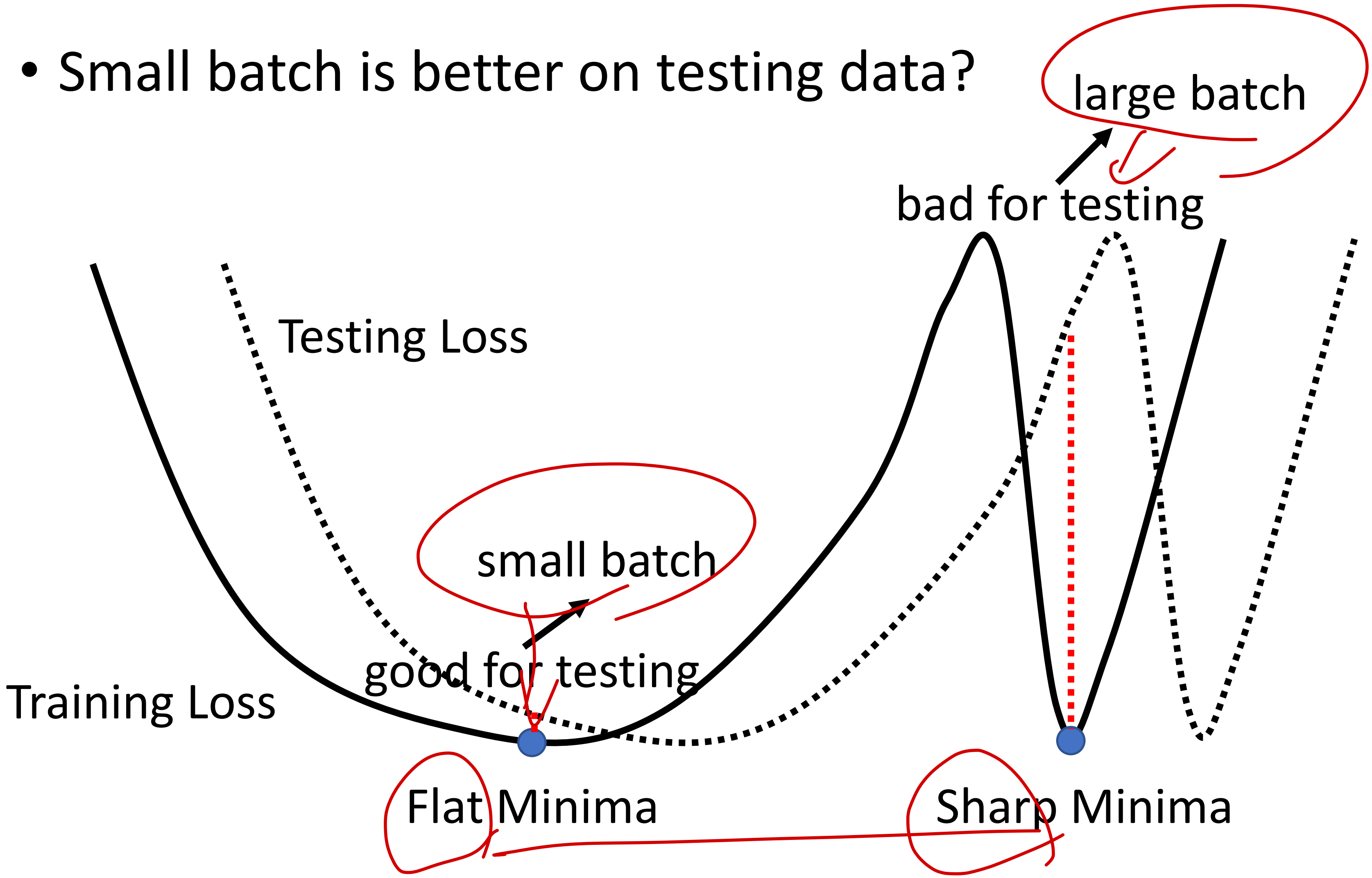
LB = 0.1 x data set

| 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 |

| | 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

- Small batch is better on testing data?



# 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 WIN |
| Gradient | Noisy | Stable |
| Optimization | Better WIN | Worse |
| Generalization | Better WIN | Worse |

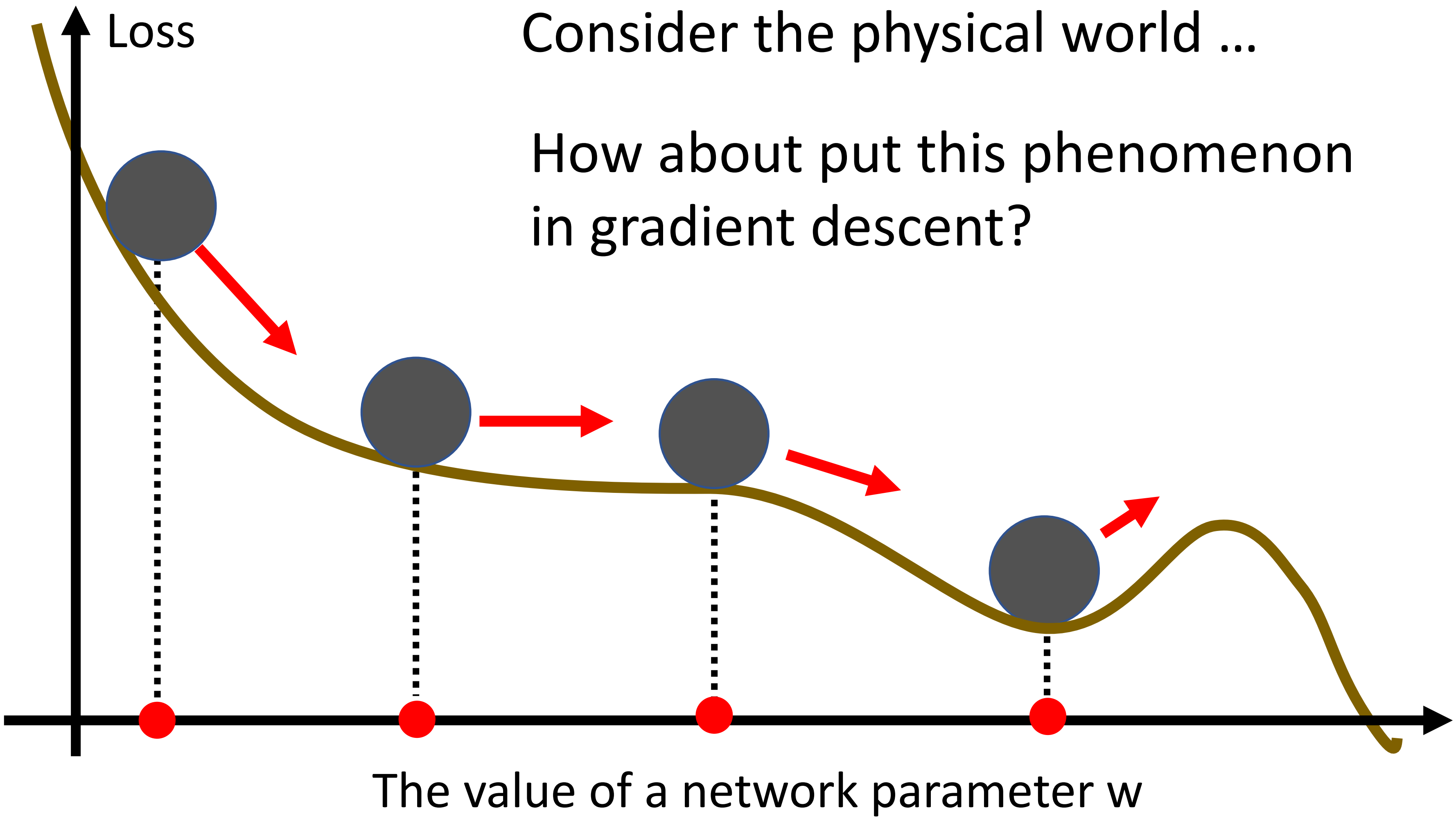
Batch size is a hyperparameter you have to decide.

# 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 …

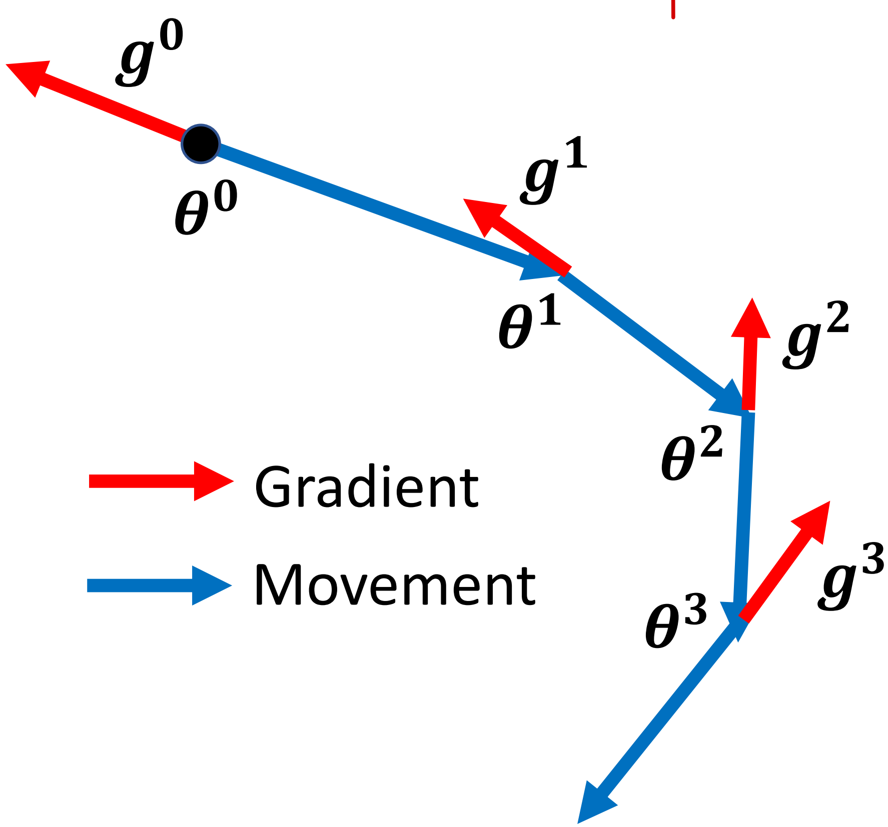



Consider the physical world …

How about put this phenomenon in gradient descent?

# (Vanilla) Gradient Descent

一般(简单)




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 $\boldsymbol{m}^0 = \mathbf{0}$ 前一步

Compute gradient $\boldsymbol{g}^0$

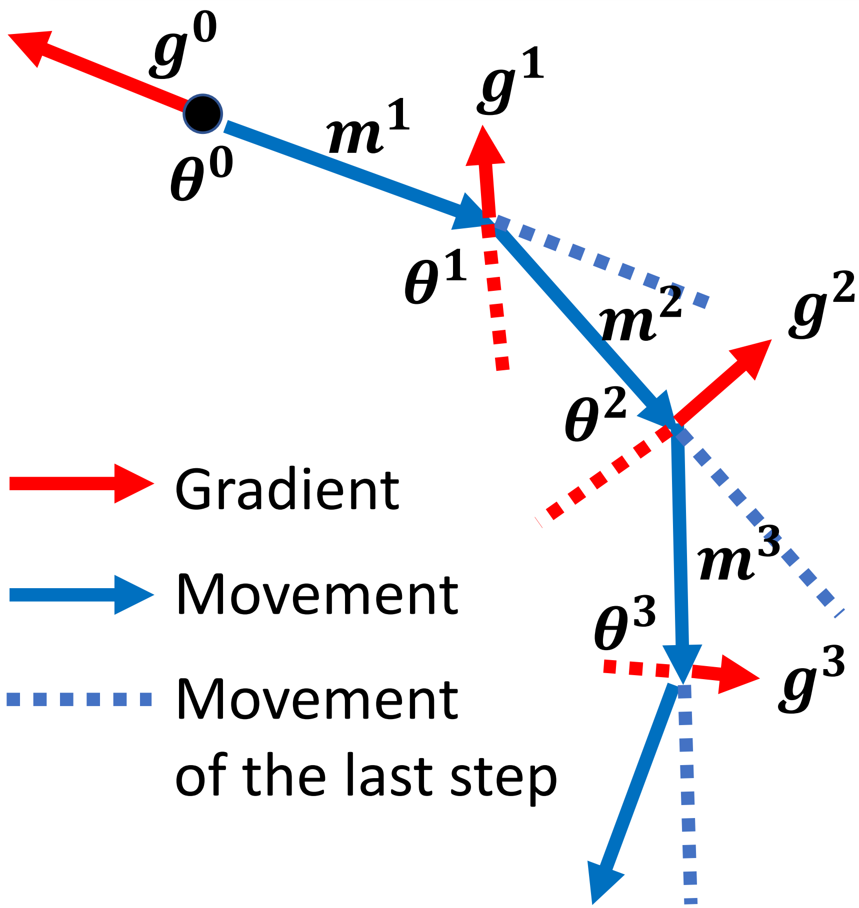
Movement $\boldsymbol{m}^1 = \lambda \boldsymbol{m}^0 - \eta \boldsymbol{g}^0$

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

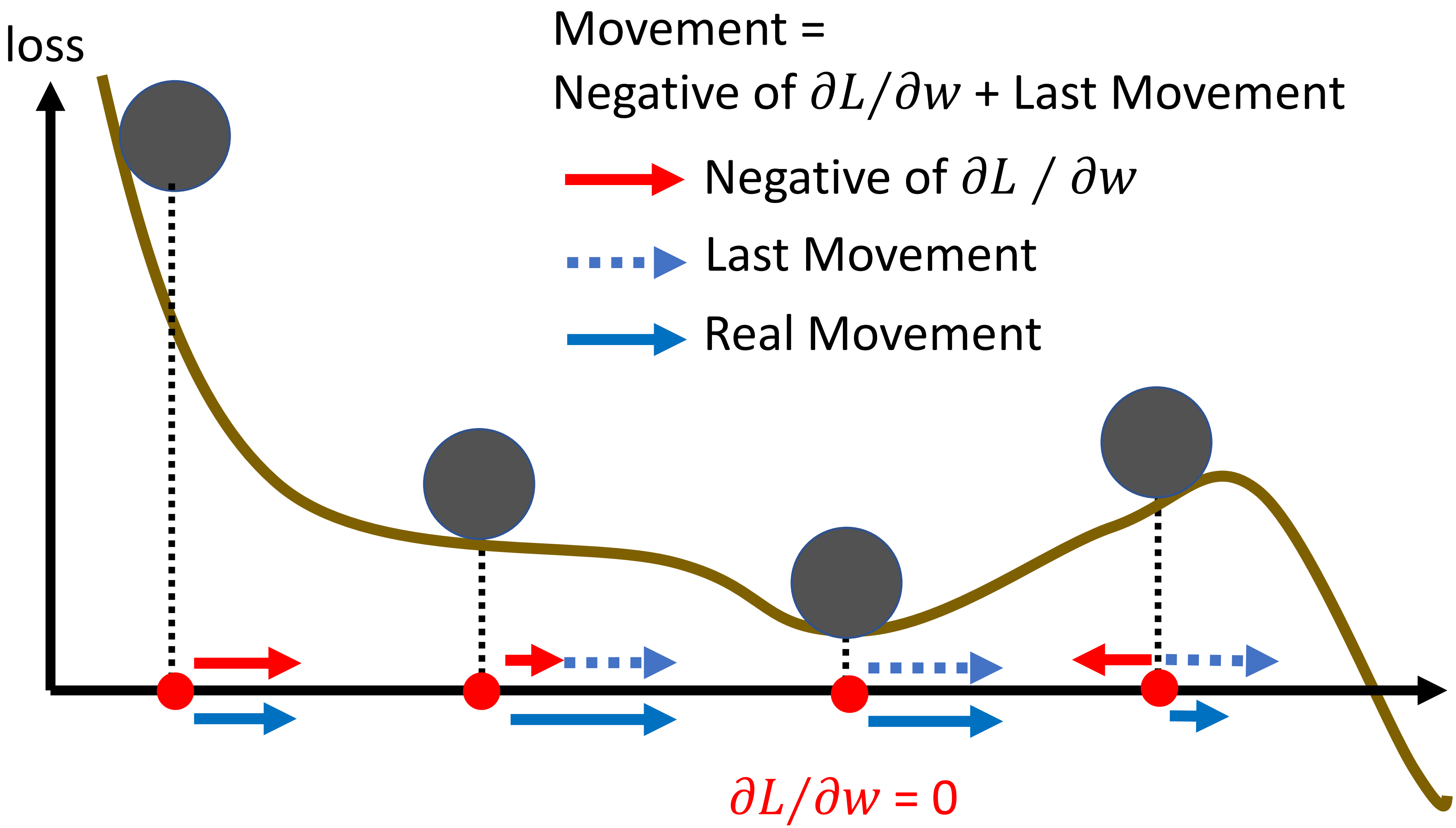
Compute gradient $\boldsymbol{g}^1$

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