

# 梯度下降與反向傳播

## Gradient Descend and Back Propagation

2025/6/17

PRESENTED BY AI Foundation

CREATED FOR

**INNOLUX**

# 梯度下降與反向傳播

## Gradient Descend and Back Propagation

1 梯度下降

2 反向傳播

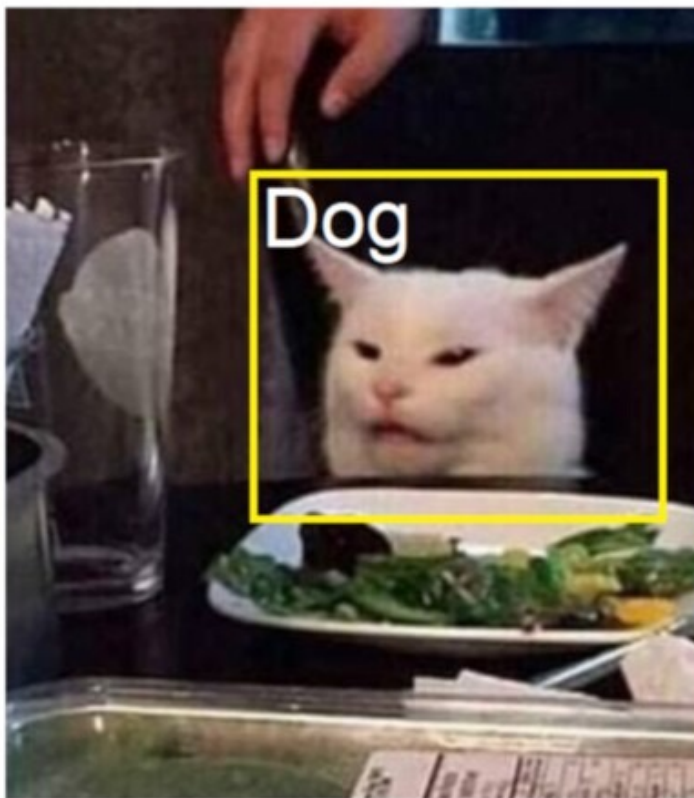


# 梯度下降

Media saying AI will  
take over the world



My Neural Network



AI will take over soon

# 何為「學習」？

$$y = 5$$

$$5 - 1.5 = 3.5$$

$$5 - 6.5 = -1.5$$

$$5 - 4.5 = 0.5$$

$$x = 2$$

$$b = 0.5$$

你的答案  
太小了

你的答案  
太大了

你的答案  
有點小

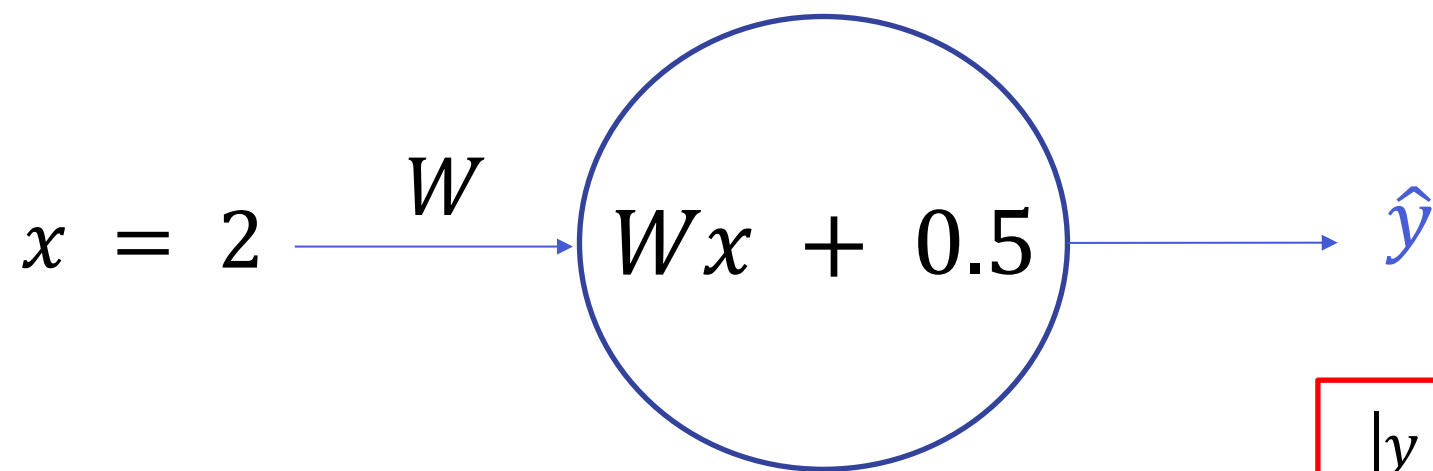
$$Wx + b = y$$
$$2 \quad 0.5$$

$$W = 0.5$$
$$y = 1.5$$

$$W = 3$$
$$y = 6.5$$

$$W = 2$$
$$y = 4.5$$

# 何為「學習」？



$$|y - \hat{y}| \text{ Loss}$$

$$W = 0.5$$

$$\hat{y} = 1.5 \quad \xleftrightarrow{3.5} \quad y = 5$$

$$W = 3$$

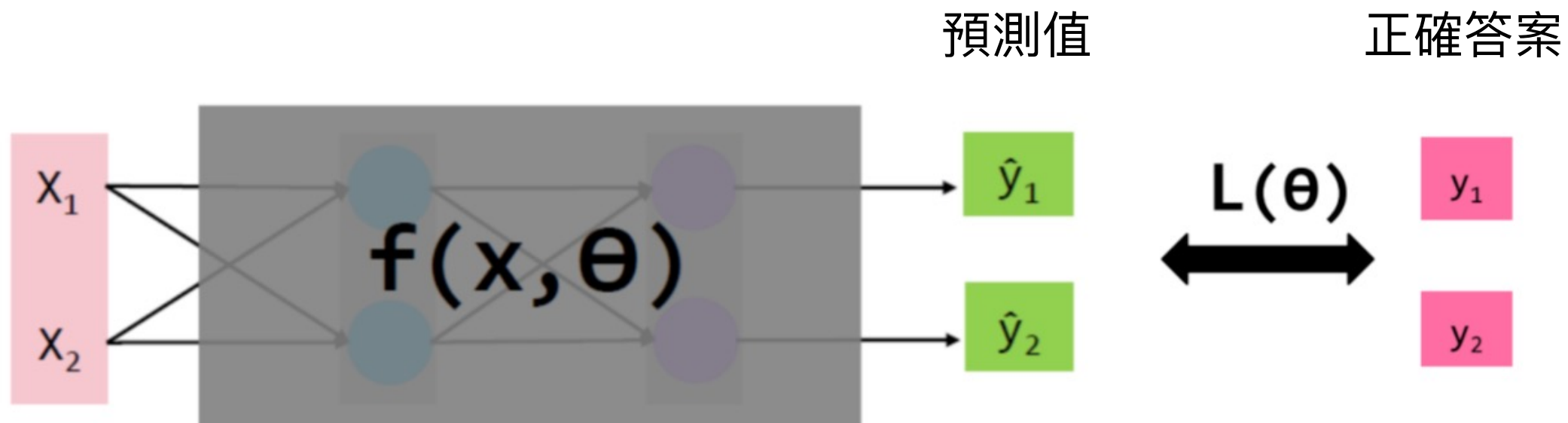
$$\hat{y} = 6.5 \quad \xleftrightarrow{1.5} \quad y = 5$$

$$W = 2$$

$$\hat{y} = 4.5 \quad \xleftrightarrow{0.5} \quad y = 5$$

# 梯度下降 Gradient Descent

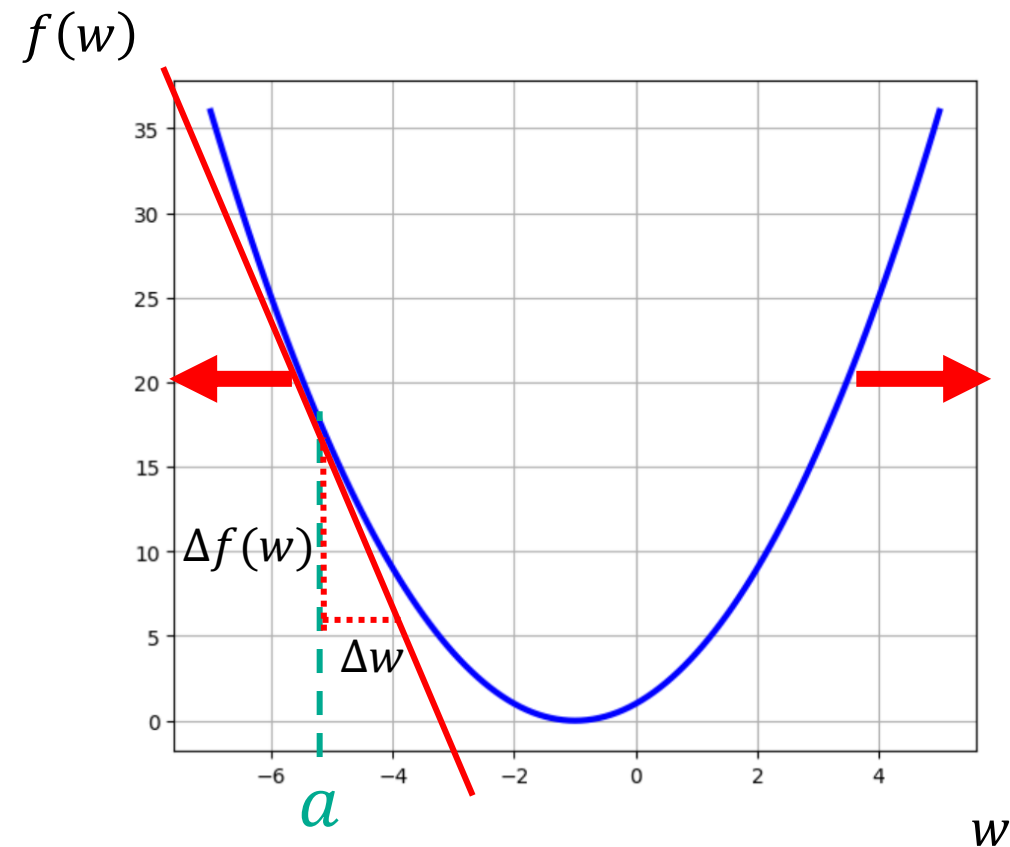
目標： $\theta^* = \operatorname{argmin}_{\theta} L(\theta)$   $L$  為損失函數，  
 $\theta = \{w, b\}$  為模型參數



# 梯度 Gradient

假設有一個函數  $f(w)$ ，  
梯度就是  $f(w)$  在  $w = a$  的切線斜率。

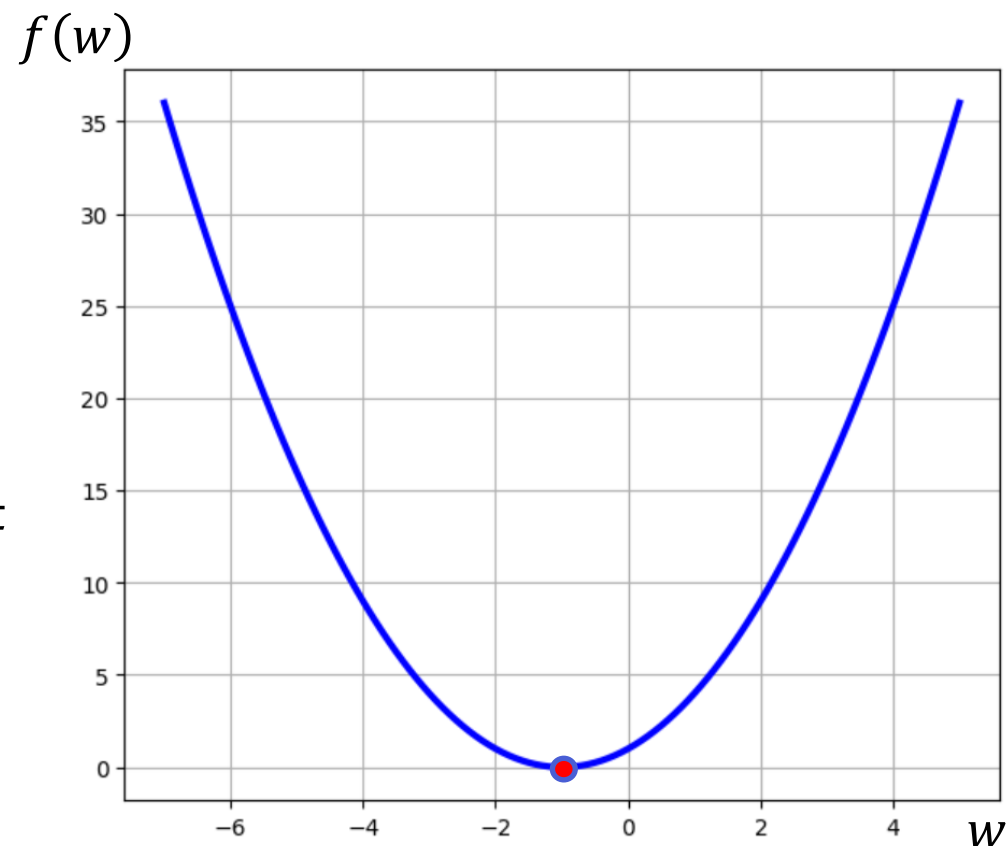
- 正負號會決定函數在  $w = a$  的增長方向。
- 其數值就是在這個方向上的增長變化量。





# 梯度 Gradient

- 假設給定的函數是： $f(w) = w^2 + 2w + 1$
- 先對 $f(w)$ 進行微分，找出 $f(x)$ 的導數
$$f'(w) = \frac{df(w)}{dw} = 2w + 2 = 2(w + 1)$$
- 梯度為 0 的時候會出現極值
- 當 $w = -1$ 時， $f(w)$ 出現極小值（實際上這樣就是公式解，並不適用在神經網路的參數更新上）



# 梯度下降 Gradient Descent

$$\text{Loss } L(W) = f(W) = W^2 + 2W + 1$$
$$\nabla L(W) = f'(W) = 2(W + 1)$$

包含學習率調整的參數更新公式：

$$W^{t+1} = W^t - \eta \cdot \nabla L(W^t)$$

1. 初始化  $W^t = -6$  ,  $\text{Loss} = L(-6) = 25$

2. 將  $W^t$  代入梯度函數得到梯度

$$\nabla L(-6) = f'(-6) = -10$$

3. 用梯度更新  $W^{t+1} = W^t - \eta \cdot \nabla L(W^t)$

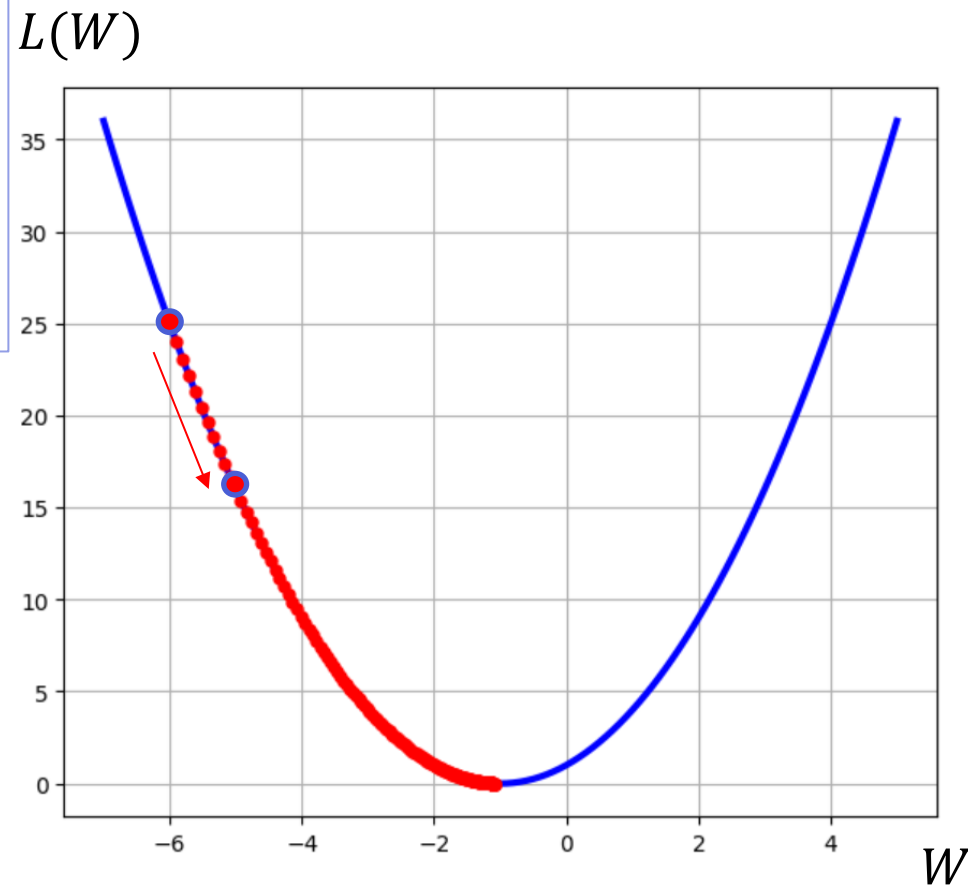
$$W^{t+1} = -6 - 0.1(-10) = -5$$

4. 將  $W^{t+1}$  代入梯度函數得到新的梯度

$$\nabla L(-5) = f'(-5) = -8$$

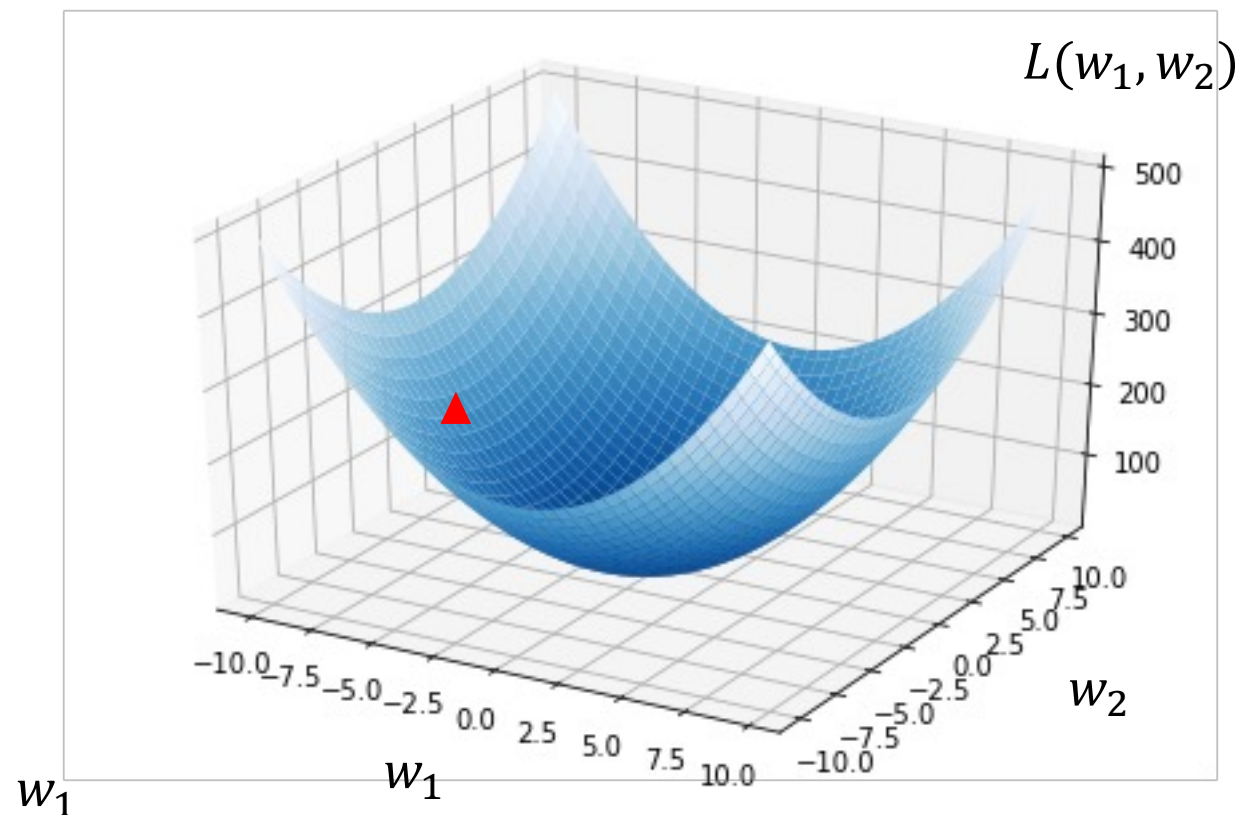
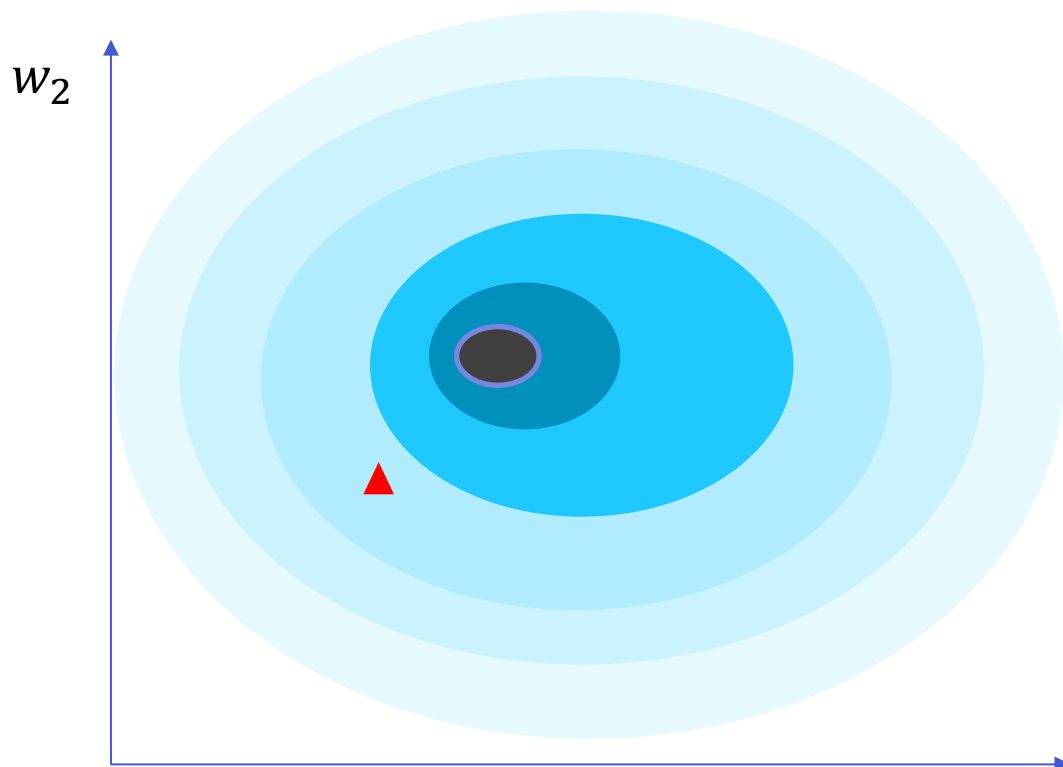
5. 再次用梯度更新  $W^{t+1} \rightarrow W^{t+2}$

$$W^{t+2} = -5 - 0.1(-8) = -4.2$$



# 梯度下降 Gradient Descent

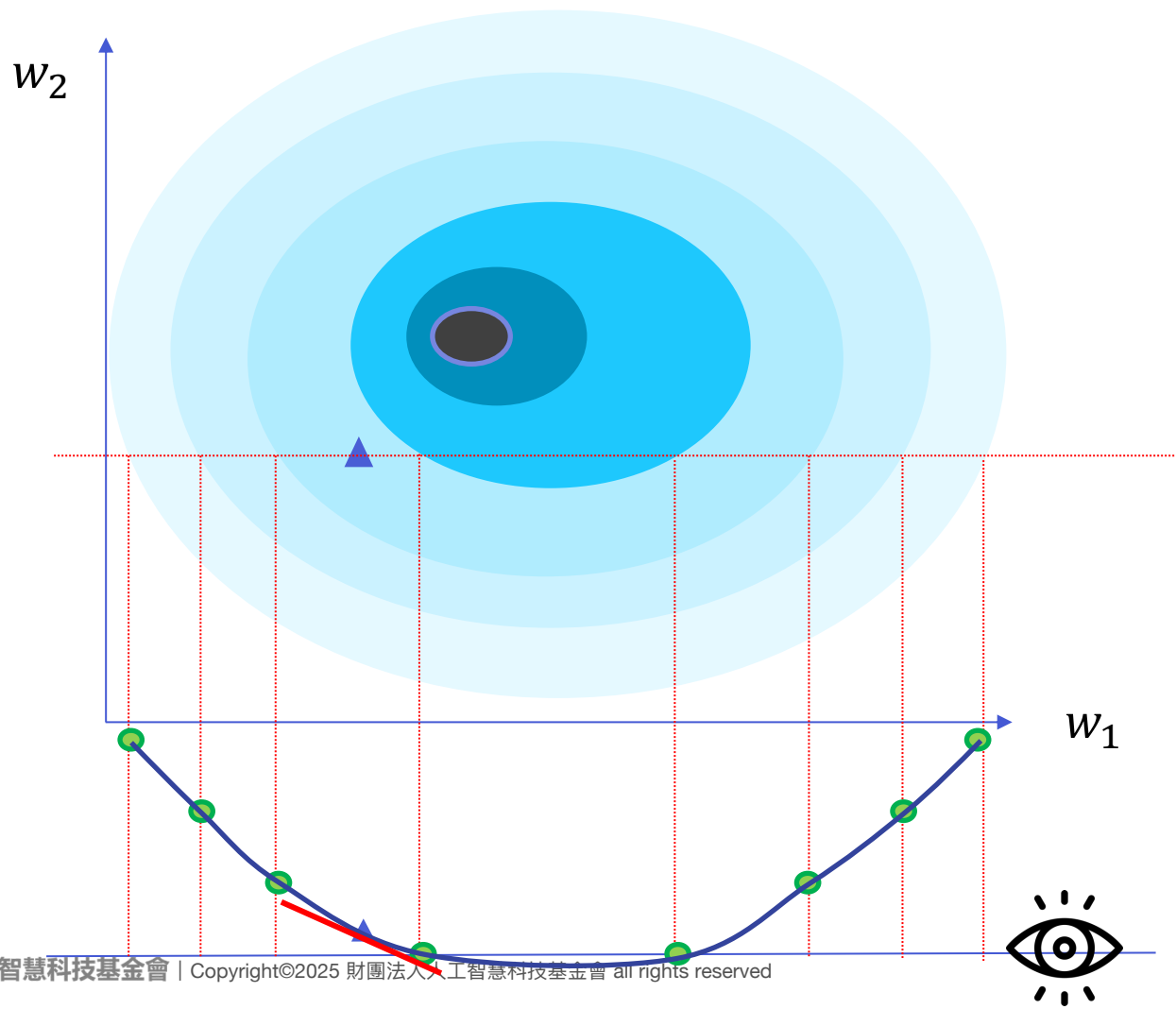
畫成等高線圖，越中心  $L(w_1, w_2)$  越低，▲為一組初始的數值



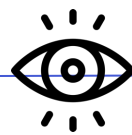
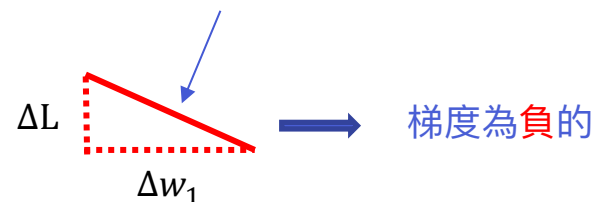
擴展到參數有兩個的狀況下，此時需要求取不同方向的變化量以得到梯度

# 梯度下降 Gradient Descent

畫成等高線圖，越中心  $L(w_1, w_2)$  越低，▲為一組初始的數值

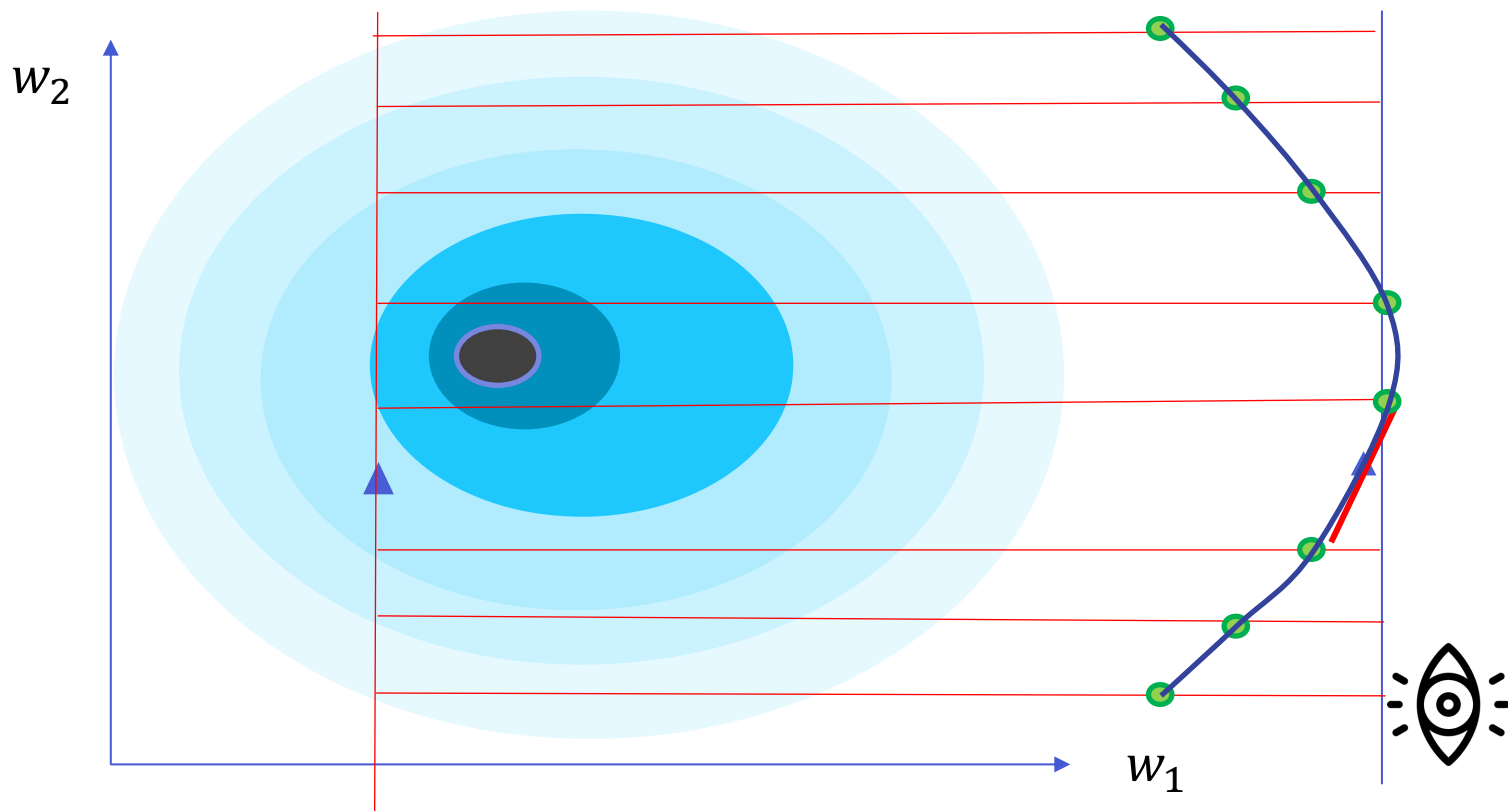


此處▲的梯度： $\frac{\partial L(w_1, w_2)}{\partial w_1}$

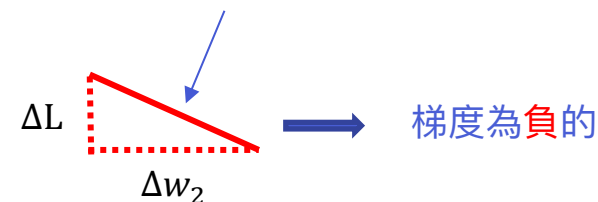


# 梯度下降 Gradient Descent

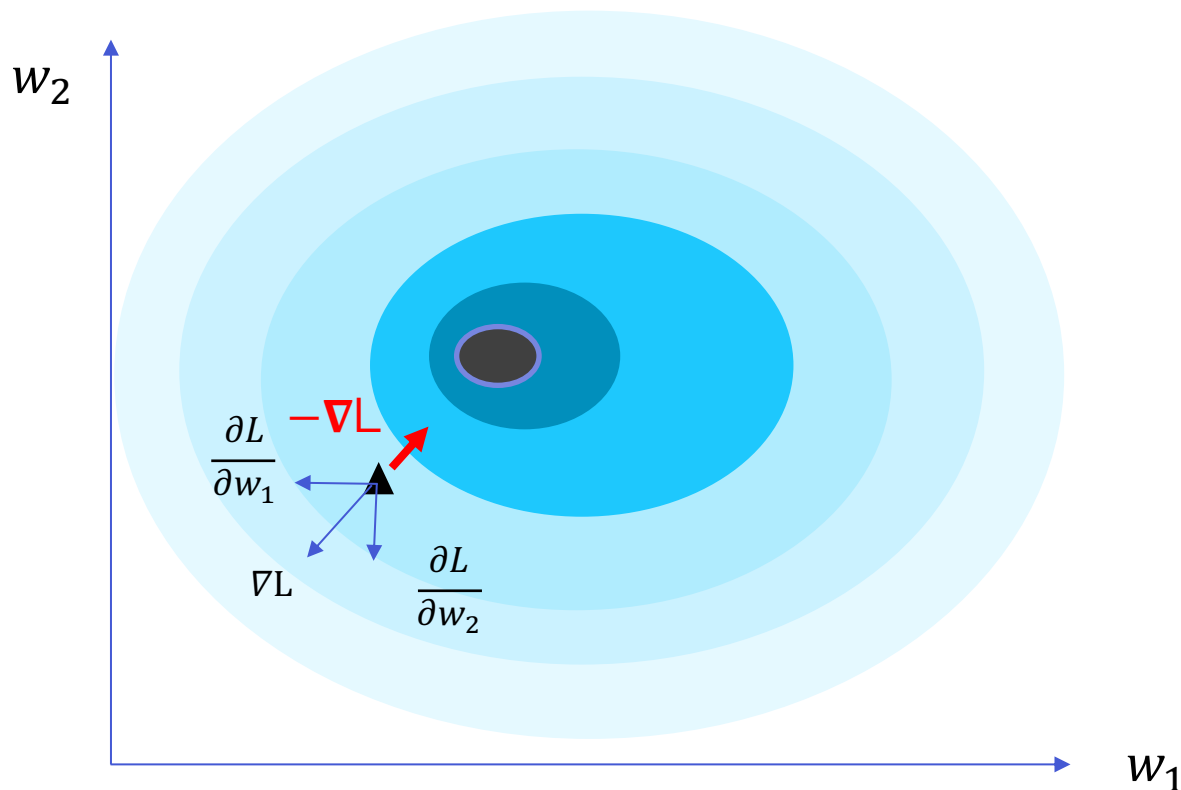
畫成等高線圖，越中心  $L(w_1, w_2)$  越低，▲為一組初始的數值



此處 ▲ 的梯度： $\frac{\partial L(w_1, w_2)}{\partial w_2}$



# 梯度下降 Gradient Descent



▲ 的梯度方向為： $\overrightarrow{\nabla L} = \overrightarrow{\frac{\partial L}{\partial w_1}} + \overrightarrow{\frac{\partial L}{\partial w_2}}$

⇒ ▲ 下一次位置為  $\blacktriangle^{t+1} = \blacktriangle^t - \eta \nabla L$

註：由於參數更新的目標是要Loss越來越小，因此更新方向是梯度的反方向  $-\nabla L$

# 梯度下降 Gradient Descent

目標： $\theta^* = \operatorname{argmin}_{\theta} L(\theta)$

$L$ : 損失函數,  
 $\theta = \{w, b\}$ : 參數

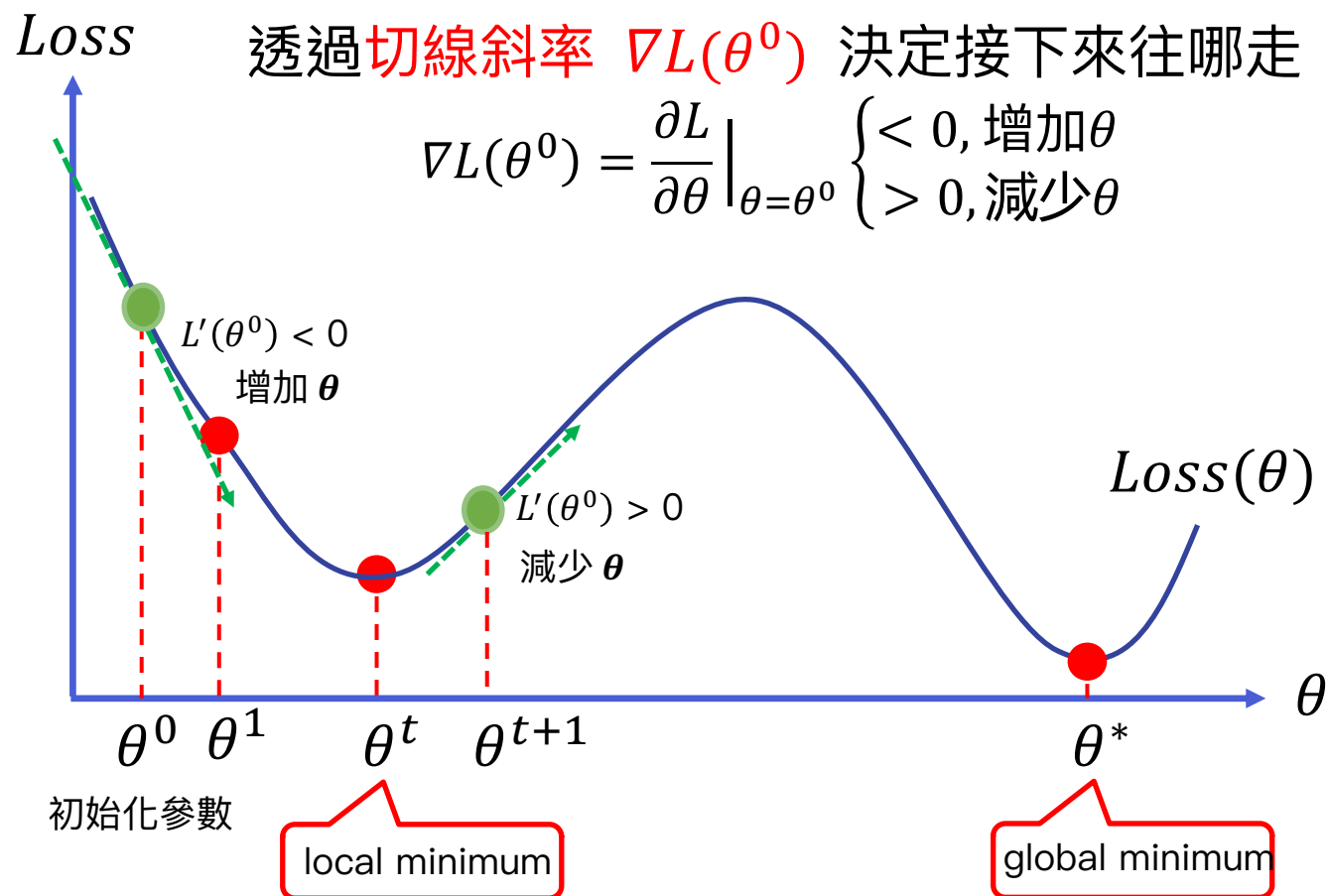
1. 隨機初始化參數 $\theta^0$
2. 計算 $L'(\theta^0)$ 決定方向
3. 訂定 $\eta$ 學習率

$$\theta^{t+1} = \theta^t + \eta \cdot (-\nabla L(\theta^t))$$

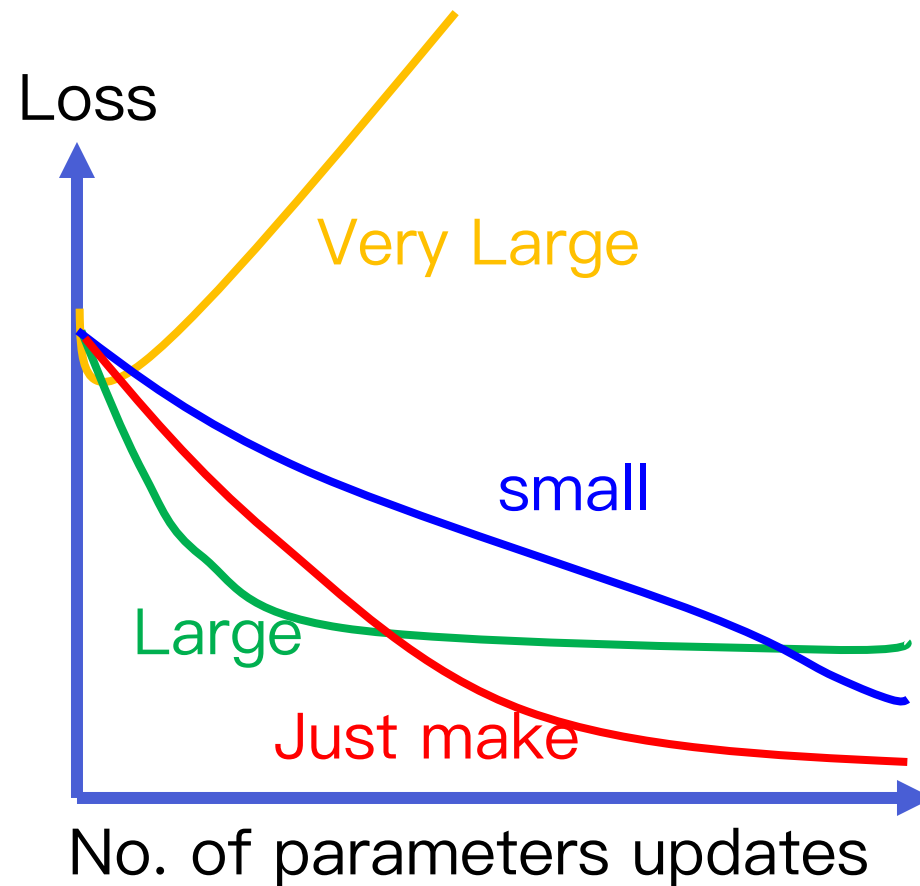
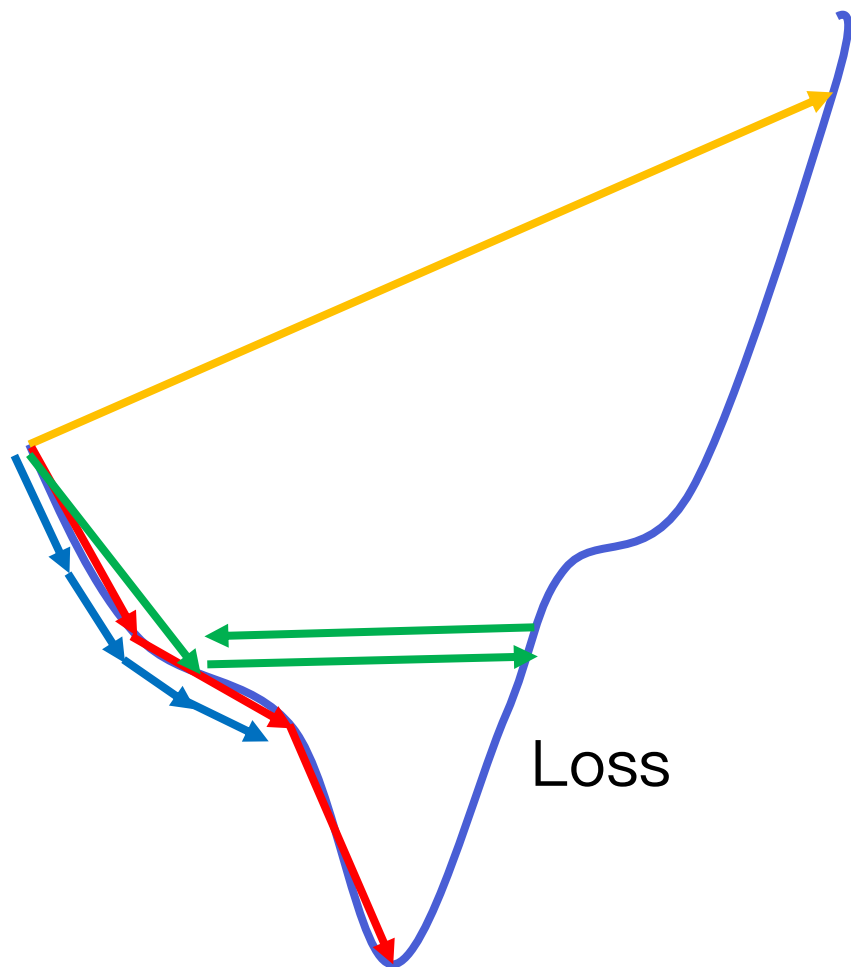
$$\nabla L(\theta) = \frac{\partial L}{\partial \theta} = \begin{bmatrix} \frac{\partial L}{\partial w} \\ \frac{\partial L}{\partial b} \end{bmatrix}$$

透過切線斜率  $\nabla L(\theta^0)$  決定接下來往哪走：

$$\nabla L(\theta^0) = \frac{\partial L}{\partial \theta} \Big|_{\theta=\theta^0} \begin{cases} < 0, \text{增加}\theta \\ > 0, \text{減少}\theta \end{cases}$$



# 學習率 Learning rate





# 影響參數更新因素

## 梯度下降 Gradient Descent

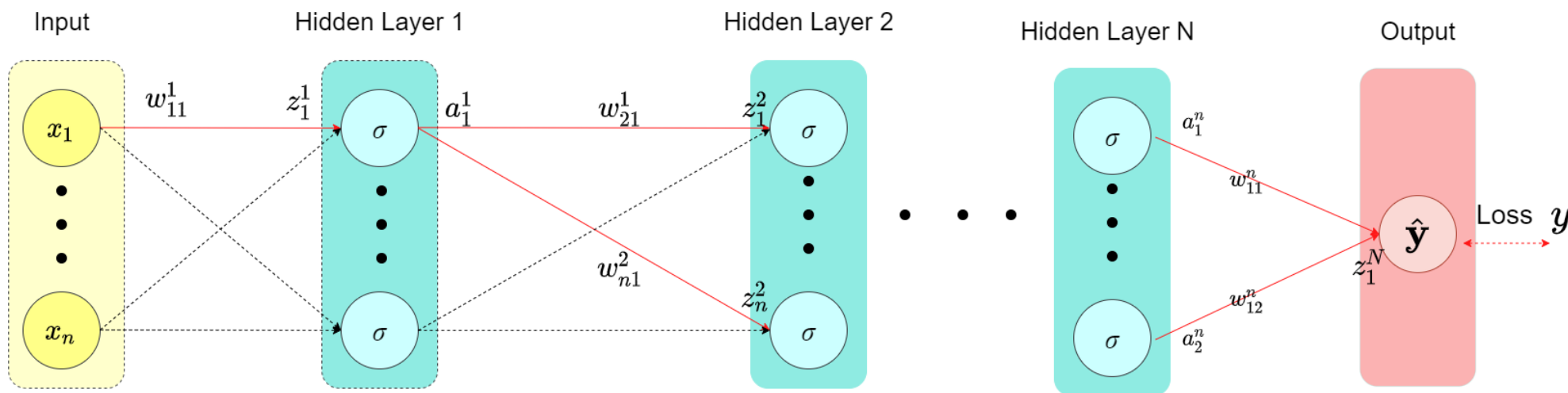
$$\theta^{t+1} = \theta^t - \eta \cdot \nabla L(\theta^t)$$

$$L(\theta) = \frac{1}{n} \sum_{i=1}^n (y_i - \hat{y}_i)^2$$

$$\hat{y} = \sigma(W^T X + b)$$

1. 受 學習率  $\eta$  影響
2. 受 損失函數  $L(\theta)$  影響
3. 受 參數初始化  $\theta^0 = \{w, b\}$  影響
4. 受 樣本數量  $n$  影響
5. 受 激勵函數  $\sigma$  影響

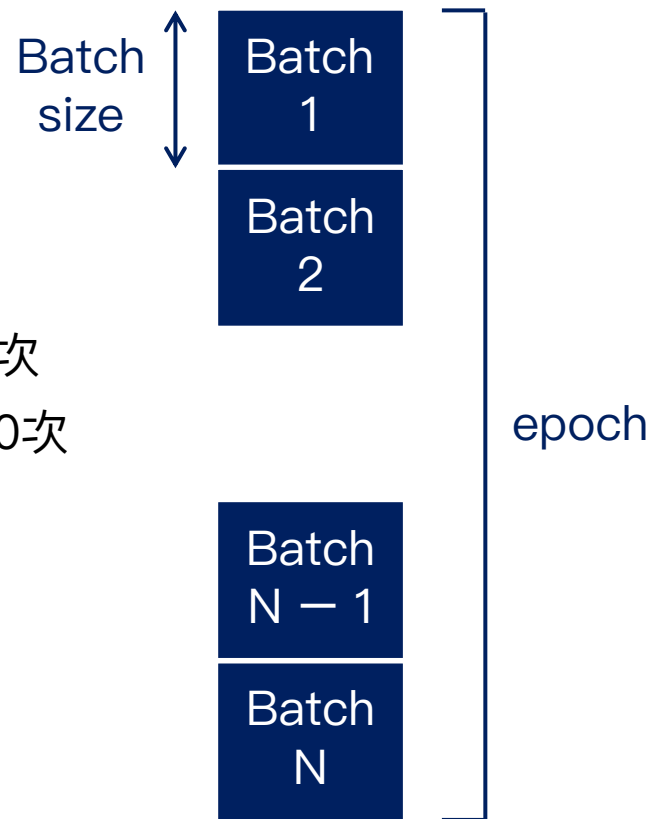
# 梯度下降的缺點



- 梯度下降看完全部的資料集（即1個epoch）才更新一次，收斂速度很慢，有辦法加速嗎？  
→ 使用「Mini-Batch」來解決
- 梯度下降法不保證找到全域最佳解，該怎麼解決？  
→ 利用「動量 Momentum」的概念，來突破區域最小值

# Mini-batch & Epoch

- 1個epoch = 一輪的訓練 = 模型看完整個訓練資料集1次
- Mini-batch：把所有的資料拆分成多份
  - 假設資料集有一1000筆資料
  - Batch-size設定為100，則可以拆分成10份 → 1個 epoch內會更新10次
  - Batch-size設定為10，則可以拆分成100份 → 1個 epoch內會更新100次
- 如何設定 Batch size
  - 常見的設定值 2 的次方：8、16、32、64、128、256 .....
  - 太小 → 無法善用 GPU 平行運算的優勢
  - 太大 → 塞不進 GPU 記憶體

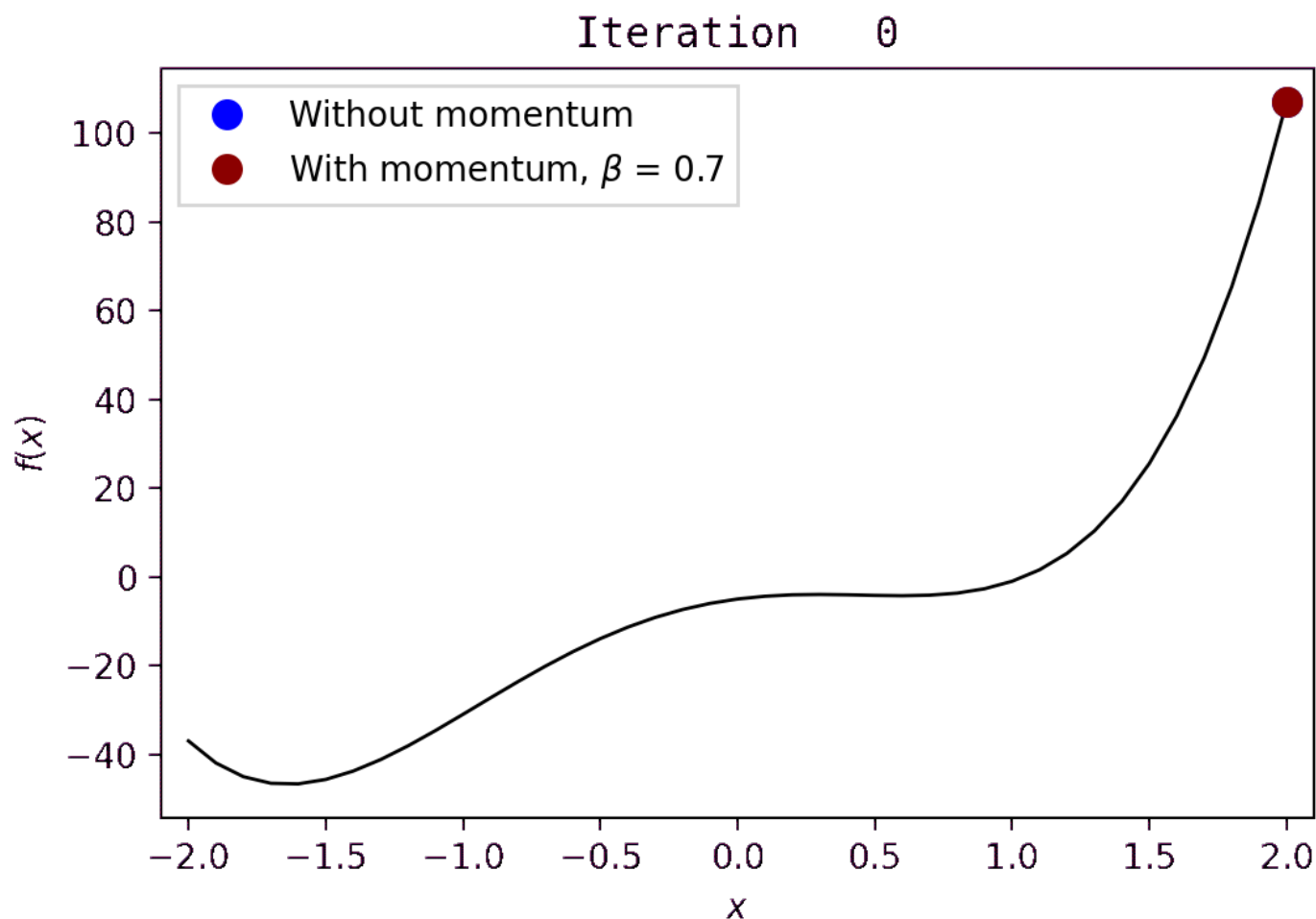


# 不同樣本數量的梯度下降法

- 用 一個 epoch 來求梯度 → 稱為 (Batch) Gradient Descent, (B)GD
- 用 一筆資料 來求梯度 → 稱為 Stochastic Gradient Descent, SGD
- 用 一個 Mini-batch 來求梯度 → 稱為 Mini-batch Gradient Descent



# 動量 Momentum



SGD :

$$\theta^{t+1} = \theta^t - \eta(\nabla L(\theta^t))$$

SGD + momentum :

$$v^t = \begin{cases} \eta \nabla L(\theta^t), & t = 0 \\ \beta v^{t-1} + \eta(\nabla L(\theta^t)), & t \geq 1 \end{cases}$$

$$\theta^{t+1} = \theta^t - v^t$$

$\beta$  為動量項係數，一般設為 0.9。

# AdaGrad

- 在前面的優化中，有一個超參數一直都是固定值，但它也是極為重要的數值，那就是 **Learning rate**。
- 我們應該要試著讓此超參也隨著梯度去改變。當梯度趨近於最小值時，Learning rate也跟著變小。
- $\epsilon$  為平滑值，加上  $\epsilon$  的原因是為了不讓分母為0
- $n$  為前面所有梯度值的平方和，利用前面學習的梯度值 **平方和** 來調整 Learning rate

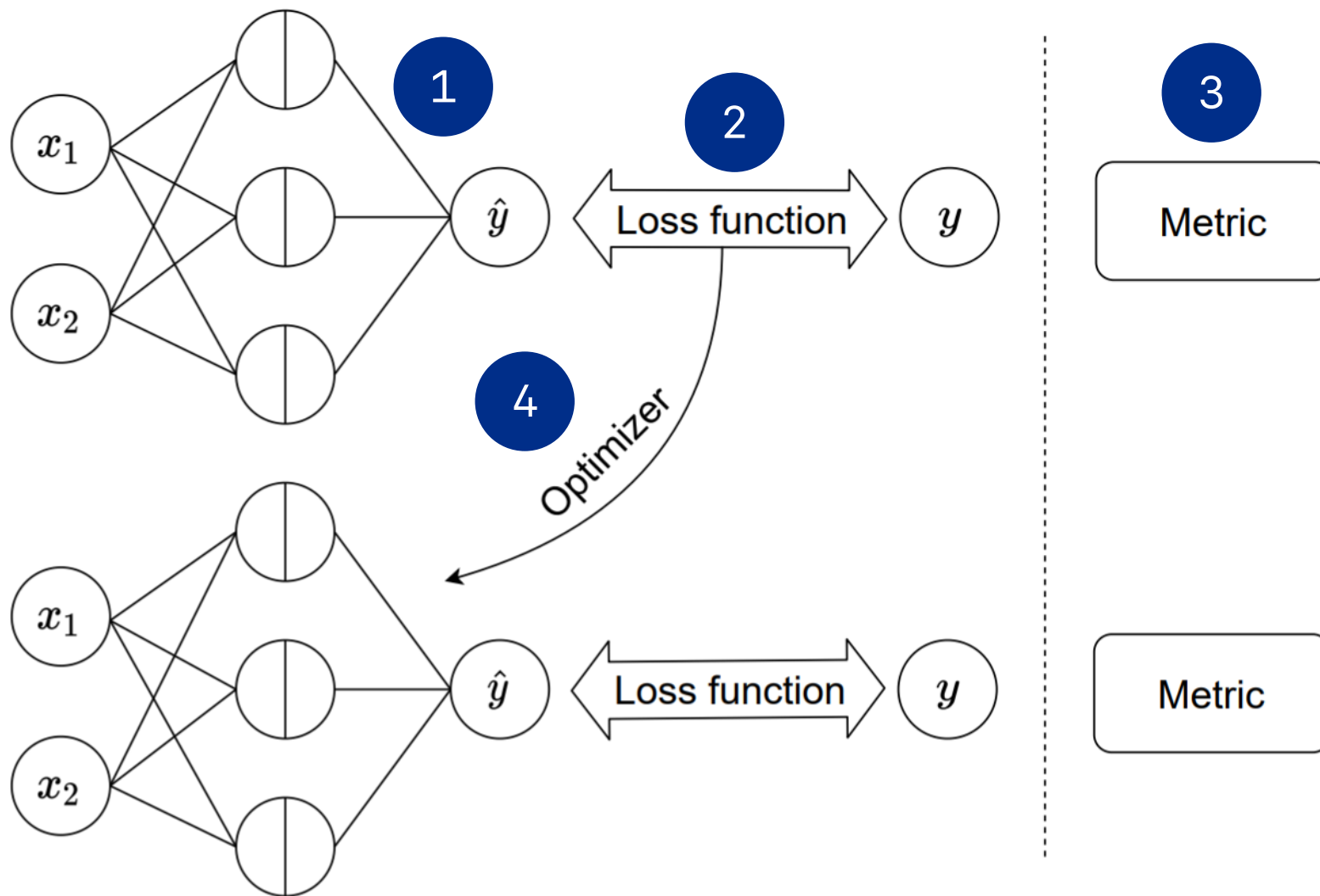
$$W \leftarrow W - \eta \frac{1}{\sqrt{n + \epsilon}} \frac{\partial L}{\partial W}$$

$$n = \sum_{r=1}^t \left( \frac{\partial L_r}{\partial W_r} \right)^2$$

$$W \leftarrow W - \eta \frac{1}{\sqrt{\sum_{r=1}^t \left( \frac{\partial L_r}{\partial W_r} \right)^2 + \epsilon}} \frac{\partial L}{\partial W}$$

# 模型訓練流程

第 1 次訓練

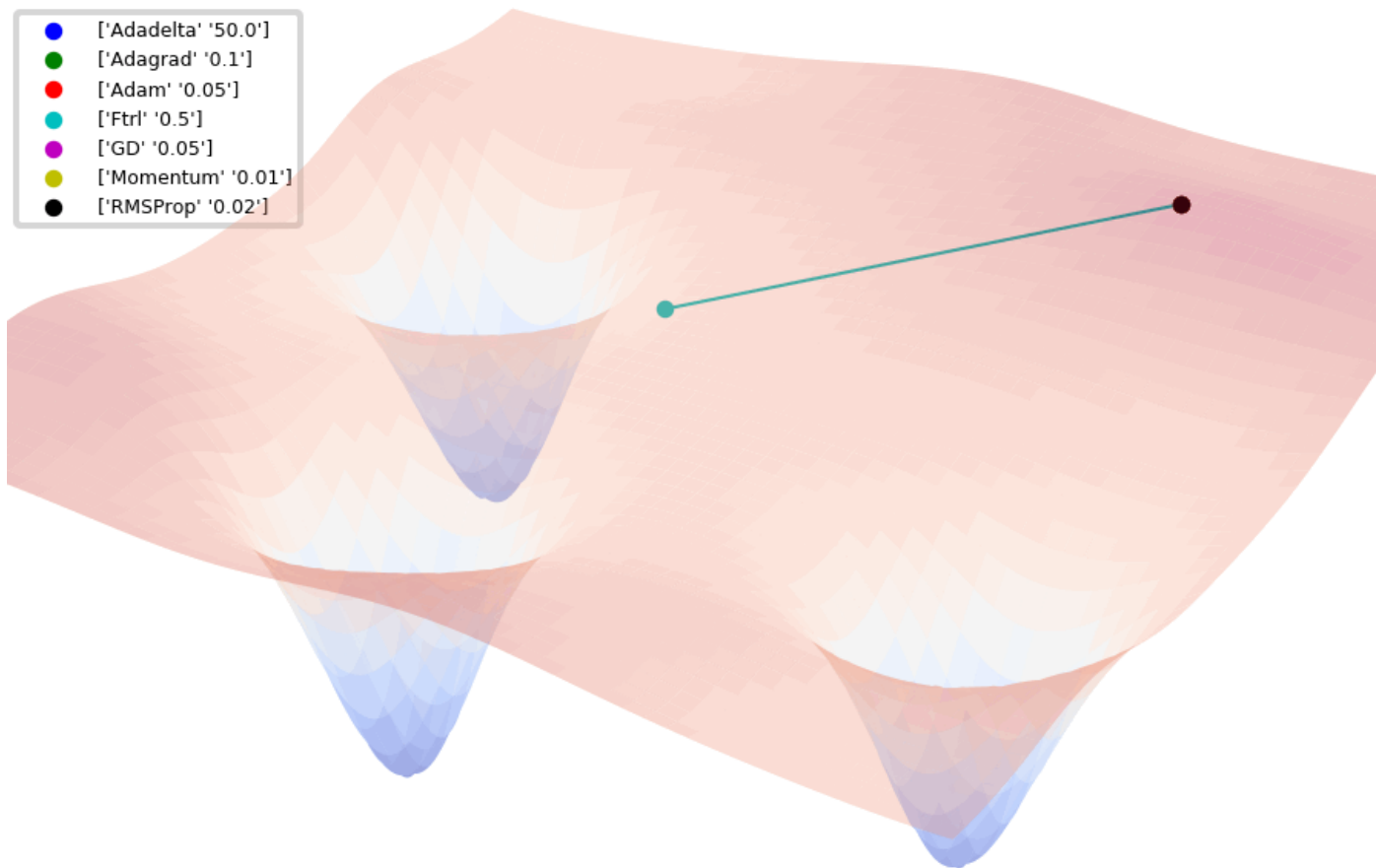


第 2 次訓練



# 最佳化器 Optimizer

- SGD
- Adagrad
- Adadelata
- Adam
- Adamax
- Nadam
- RMSprop
- Ftrl



Back propagation

# 反向傳播

# 反向傳播 Back propagation

## 反向傳播

將誤差訊號反向傳播回去，測試並調整不同神經元傳遞



直到錯誤率最低，機器就成功學會如何辨識一隻貓了

A yellow rectangular warning sign with a black border. The top section has a black background with a yellow exclamation mark inside a triangle on the left and the word "WARNING" in yellow capital letters on the right. The bottom section has a yellow background with the words "MATH" and "AHEAD" in large, bold, black capital letters.

**! WARNING**

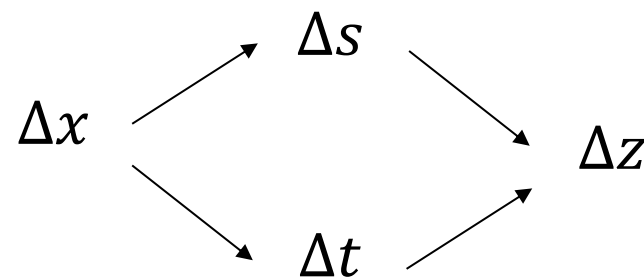
**MATH  
AHEAD**

# 反向傳播使用到的微積分：連鎖律

- $y = f(x)$      $z = g(y)$
- $z = g(f(x)) = (g \circ f)(x)$
- 如果給  $x$  變化，會影響到  $y$ ， $y$  會影響到  $z$
- 此時  $z$  對  $x$  的微分

$$\nabla_Z = \frac{dz}{dx} = \frac{dz}{dy} \frac{dy}{dx}$$

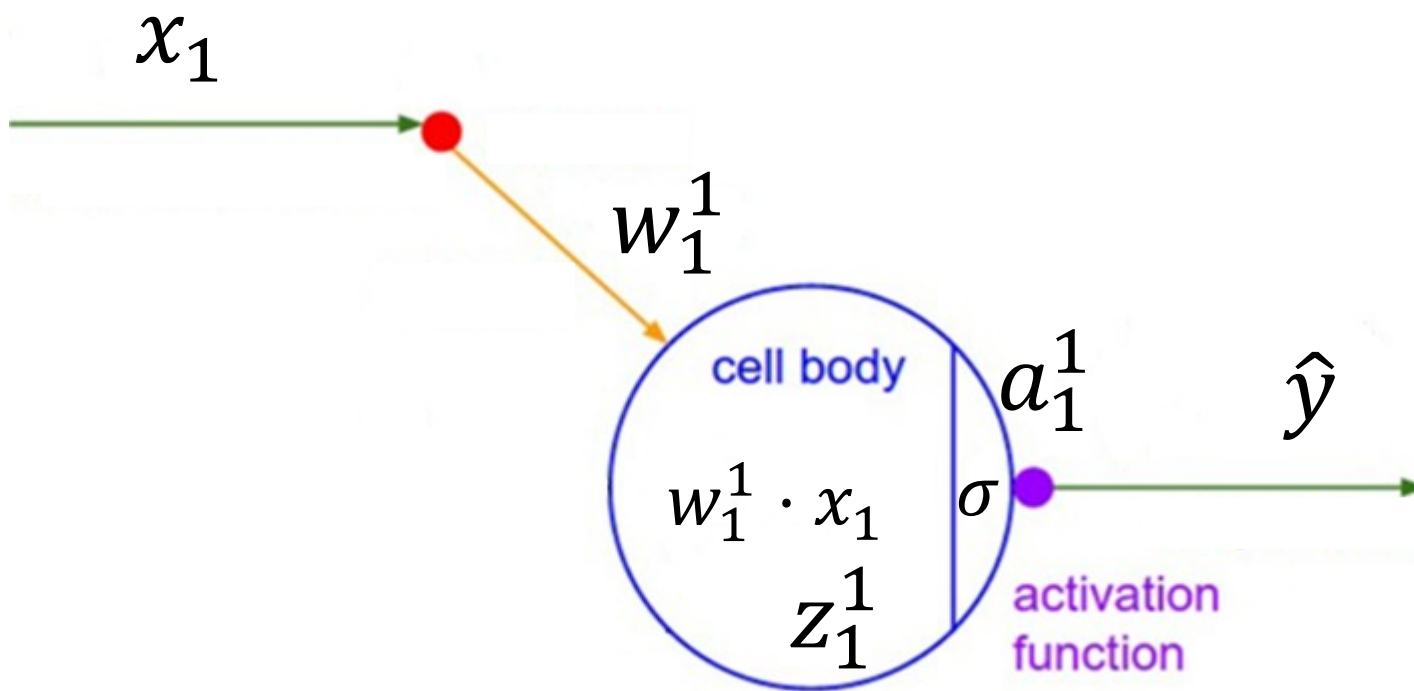
- $s = g(x)$ ,  $t = h(x)$ ,  $z = f(s, t)$



- 此時  $z$  對  $x$  的微分

$$\nabla_Z = \frac{dz}{dx} = \frac{\partial z}{\partial s} \frac{ds}{dx} + \frac{\partial z}{\partial t} \frac{dt}{dx}$$

# 反向傳播 Back propagation



$$z_1^1 = w_1^1 \cdot x_1$$

$$a_1^1 = \sigma(z_1^1)$$

$$\hat{y} = a_1^1$$

$$L = \text{loss}(\hat{y}, y)$$

$$\widehat{w}_1^1 = w_1^1 + \eta \cdot \left(-\frac{\partial L}{\partial w_1^1}\right)$$

# 反向傳播 Back propagation

$$\widehat{w}_1^1 = w_1^1 - \eta \cdot \left( \frac{\partial L}{\partial w_1^1} \right)$$

根據連鎖律

$$\frac{\partial L}{\partial w_1^1} = \frac{\partial L}{\partial \hat{y}} \frac{\partial \hat{y}}{\partial a_1^1} \frac{\partial a_1^1}{\partial z_1^1} \frac{\partial z_1^1}{\partial w_1^1}$$

$$L = \text{loss}(\hat{y}, y)$$

$$\hat{y} = a_1^1 = \sigma(z_1^1)$$

$$z_1^1 = w_1^1 \cdot x_1$$

**Chain rule:**

- $y = f(x), z = g(y), z = g(f(x)) = (g \circ f)(x)$

$$(g \circ f)'(x) = \frac{dg}{dx} = \frac{dg}{df} \frac{df}{dx}$$

- $z = f(x, y)$ , where  $x = g(t), y = h(t)$

$$\frac{df}{dt} = \frac{\partial f}{\partial g} \frac{dg}{dt} + \frac{\partial f}{\partial h} \frac{dh}{dt}$$

# 反向傳播 Back propagation

根據連鎖律

$$\frac{\partial L}{\partial w_1^1} = \frac{\partial L}{\partial \hat{y}} \frac{\partial \hat{y}}{\partial a_1^1} \frac{\partial a_1^1}{\partial z_1^1} \frac{\partial z_1^1}{\partial w_1^1} = \frac{\partial}{\partial \hat{y}} \overset{L}{\boxed{\frac{1}{2n} (\hat{y} - y)^2}} \frac{\partial}{\partial a_1^1} \overset{\hat{y}}{\boxed{a_1^1}} \frac{\partial}{\partial z_1^1} \overset{a_1^1}{\boxed{\sigma(z_1^1)}} \frac{\partial}{\partial w_1^1} \overset{z_1^1}{\boxed{(w_1^1 \cdot x_1)}}$$

損失函數 MSE

$$L = \frac{1}{2n} (\hat{y} - y)^2$$

$$L' = \frac{1}{n} (\hat{y} - y)$$

激勵函數 Sigmoid

$$\sigma(z) = \frac{1}{1 + e^{-z}}$$

$$\sigma'(z) = \frac{1}{1 + e^{-z}} \frac{e^{-z}}{1 + e^{-z}}$$

$$= \sigma(z)(1 - \sigma(z))$$



# 反向傳播 Back propagation

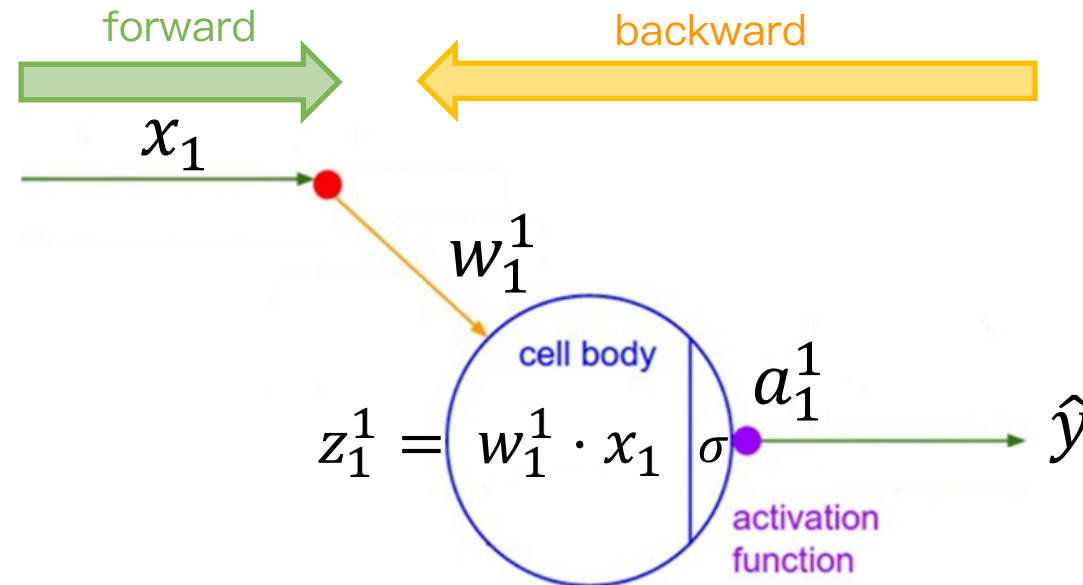
$$\frac{\partial L}{\partial w_1^1} = \underbrace{\frac{\partial L}{\partial \hat{y}} \cdot \frac{\partial \hat{y}}{\partial a_1^1} \cdot \frac{\partial a_1^1}{\partial z_1^1}}_{\text{backward}} \cdot \underbrace{\frac{\partial z_1^1}{\partial w_1^1}}_{\text{forward}} = \frac{1}{n} (\hat{y} - y) \cdot 1 \cdot \sigma(z_1^1)(1 - \sigma(z_1^1)) \cdot x_1$$

$$z_1^1 = w_1^1 \cdot x_1$$

$$\hat{y} = a_1^1 = \sigma(z_1^1)$$

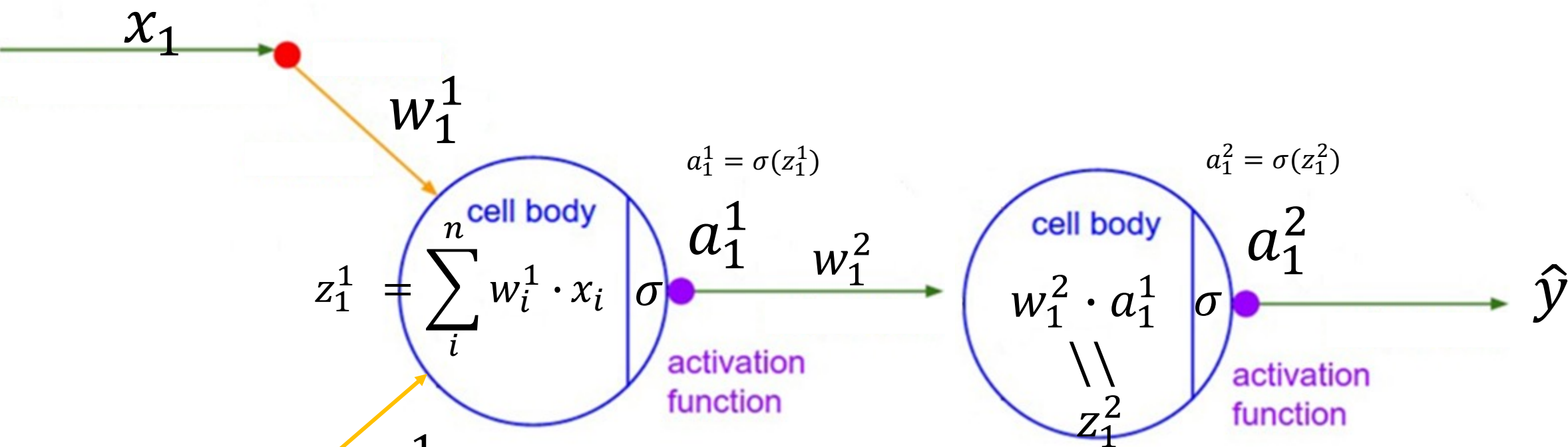
$$L = \text{loss}(\hat{y}, y)$$

$$\widehat{w}_1^1 = w_1^1 + \eta \cdot \left(-\frac{\partial L}{\partial w_1^1}\right)$$

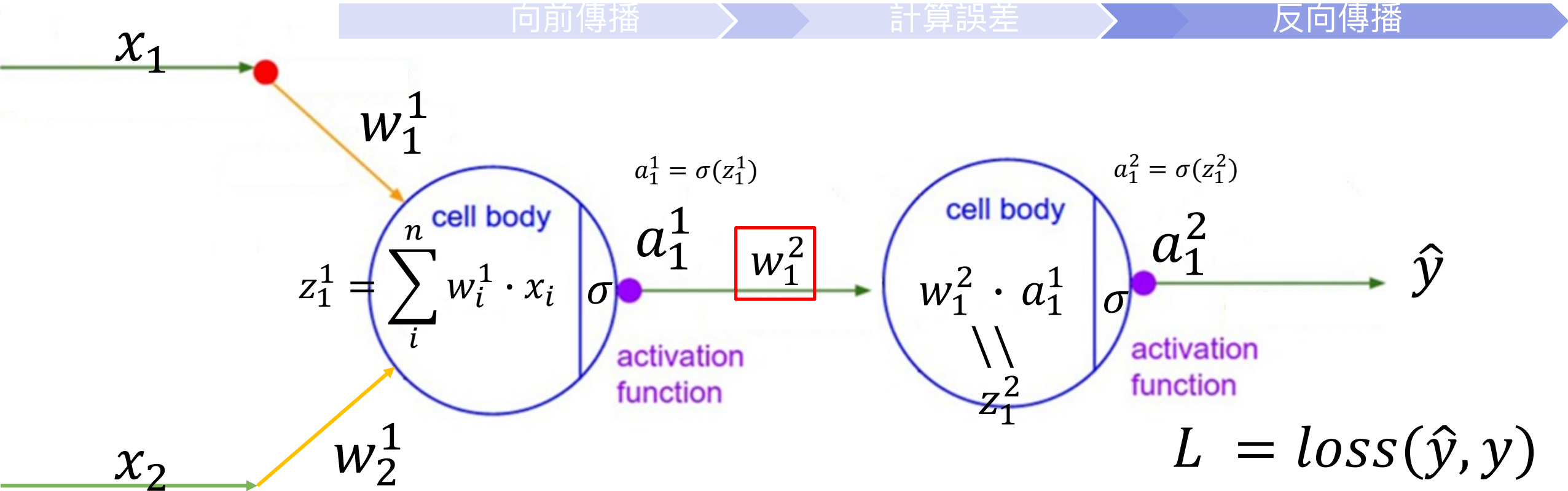


# 反向傳播 Back propagation

從單層神經元延伸到多層神經元



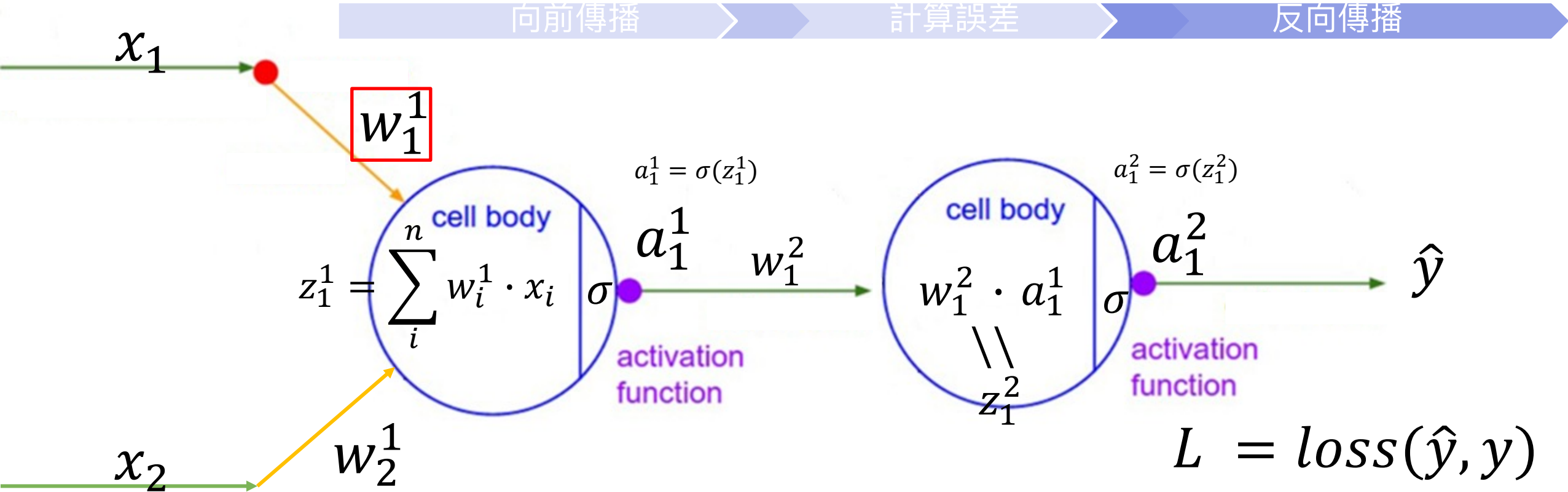
$$L = \text{loss}(\hat{y}, y)$$



$$\widehat{w_1^2} = w_1^2 - \eta \cdot \frac{\partial L}{\partial w_1^2}$$

$$\frac{\partial L}{\partial w_1^2} = \frac{\partial L}{\partial \hat{y}} \frac{\partial \hat{y}}{\partial a_1^2} \frac{\partial a_1^2}{\partial z_1^2} \frac{\partial z_1^2}{\partial w_1^2}$$

$$\widehat{w_1^2} = w_1^2 - \eta \cdot \frac{1}{n} (\hat{y} - y) \cdot \sigma(z_1^1) (1 - \sigma(z_1^1)) \cdot a_1^1$$



$$\widehat{w_1^2} = w_1^2 - \eta \cdot \frac{\partial L}{\partial w_1^2}$$

$$\frac{\partial L}{\partial w_1^2} = \frac{\partial L}{\partial \hat{y}} \frac{\partial \hat{y}}{\partial a_1^2} \frac{\partial a_1^2}{\partial z_1^2} \frac{\partial z_1^2}{\partial w_1^2}$$

$$\widehat{w_1^1} = w_1^1 + \eta \cdot (- \quad )$$

$$\widehat{w}_1^1 = w_1^1 - \eta \cdot \frac{\partial L}{\partial w_1^1} \quad \frac{\partial L}{\partial w_1^1} = \frac{\partial L}{\partial \hat{y}} \frac{\partial \hat{y}}{\partial a_1^2} \frac{\partial a_1^2}{\partial z_1^2} \frac{\partial z_1^2}{\partial a_1^1} \frac{\partial a_1^1}{\partial z_1^1} \frac{\partial z_1^1}{\partial w_1^1}$$

$$\frac{\partial L}{\partial w_1^1} = \frac{\partial}{\partial \hat{y}} \overset{L}{\boxed{\frac{1}{2n}(\hat{y} - y)^2}} \frac{\partial}{\partial a_1^2} \overset{\hat{y}}{\boxed{a_1^2}} \frac{\partial}{\partial z_1^2} \overset{a_1^2}{\boxed{\sigma(z_1^2)}} \frac{\partial}{\partial a_1^1} \overset{z_1^2}{\boxed{(w_1^2 a_1^1)}} \frac{\partial}{\partial z_1^1} \overset{a_1^1}{\boxed{\sigma(z_1^1)}} \frac{\partial}{\partial w_1^1} \overset{z_1^1}{\boxed{(w_1^1 \cdot x_1 + w_2^1 \cdot x_2)}}$$

$$= \frac{1}{n} (\hat{y} - y) \cdot \sigma(z_1^2) (1 - \sigma(z_1^2)) w_1^2 \cdot \sigma(z_1^1) (1 - \sigma(z_1^1)) x_1$$



$$\widehat{w}_1^1 = w_1^1 - \eta \cdot (\dots)$$

單純使用連鎖律做計算，的確可以得到梯度的數值，  
然而在越深層的網路中這樣的計算負荷就會急遽增加

$$\widehat{w}_1^2 = w_1^2 - \eta \cdot \frac{\partial L}{\partial w_1^2}$$

$$\frac{\partial L}{\partial w_1^2} = \boxed{\frac{\partial L}{\partial \hat{y}} \frac{\partial \hat{y}}{\partial a_1^2} \frac{\partial a_1^2}{\partial z_1^2}} \frac{\partial z_1^2}{\partial w_1^2}$$

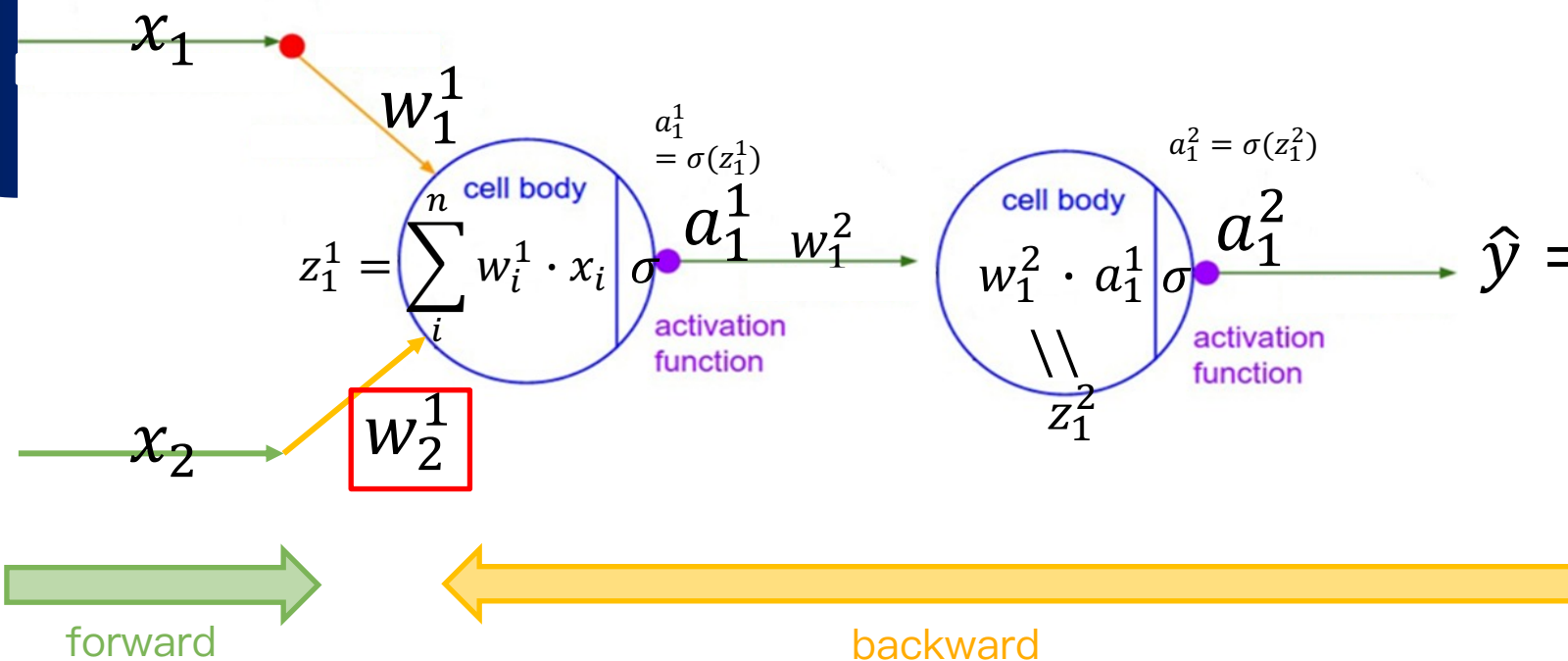
$$\widehat{w}_1^1 = w_1^1 - \eta \cdot \frac{\partial L}{\partial w_1^1}$$

$$\frac{\partial L}{\partial w_1^1} = \boxed{\frac{\partial L}{\partial \hat{y}} \frac{\partial \hat{y}}{\partial a_1^2} \frac{\partial a_1^2}{\partial z_1^2}} \frac{\partial z_1^2}{\partial a_1^1} \frac{\partial a_1^1}{\partial z_1^1} \frac{\partial z_1^1}{\partial w_1^1}$$

已被計算過的部分

$$\begin{aligned} \frac{\partial L}{\partial w_1^1} &= \boxed{\frac{\partial}{\partial \hat{y}} \frac{1}{2n} (\hat{y} - y)^2 \frac{\partial}{\partial a_1^2} a_1^2 \frac{\partial}{\partial z_1^2} \sigma(z_1^2)} \frac{\partial}{\partial a_1^1} (w_1^2 a_1^1) \frac{\partial}{\partial z_1^1} \sigma(z_1^1) \frac{\partial}{\partial w_1^1} (w_1^1 \cdot x_1 + w_2^1 \cdot x_2) \\ &= \boxed{\frac{1}{n} (\hat{y} - y) \cdot \sigma(z_1^2) (1 - \sigma(z_1^2))} w_1^2 \cdot \sigma(z_1^1) (1 - \sigma(z_1^1)) x_1 \end{aligned}$$

在更新 $w_1^2$ 時就已經計算到部分的梯度，因此不需重複計算，可直接使用已計算完的數值



另外，同一個神經元的不同權重只有在forward部分不同，因此同樣可以不需重複計算

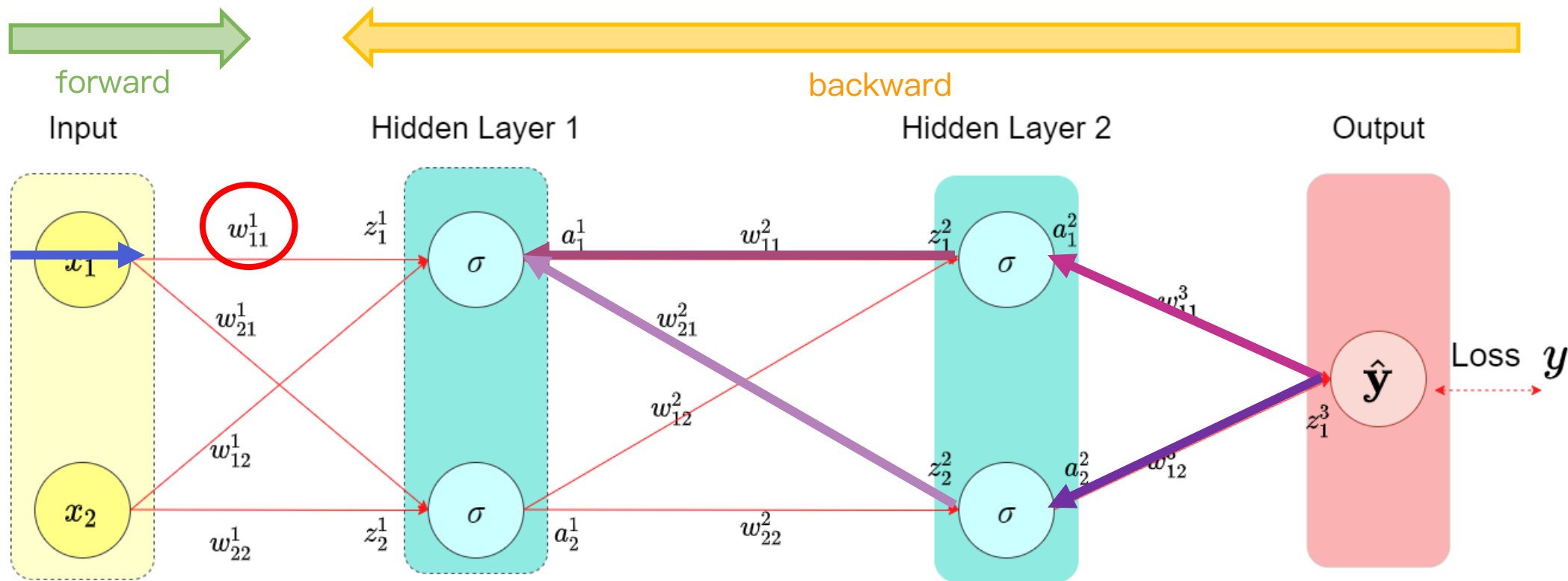
$$\widehat{w}_1^1 = w_1^1 - \eta \cdot \frac{\partial L}{\partial w_1^1}$$

$$\widehat{w}_2^1 = w_2^1 - \eta \cdot \frac{\partial L}{\partial w_2^1}$$

$$\frac{\partial L}{\partial w_1^1} = \boxed{\frac{\partial L}{\partial \hat{y}} \frac{\partial \hat{y}}{\partial a_1^2} \frac{\partial a_1^2}{\partial z_1^2} \frac{\partial z_1^2}{\partial a_1^1} \frac{\partial a_1^1}{\partial z_1^1}} \frac{\partial z_1^1}{\partial w_1^1}$$

$$\frac{\partial L}{\partial w_2^1} = \boxed{\frac{\partial L}{\partial \hat{y}} \frac{\partial \hat{y}}{\partial a_1^2} \frac{\partial a_1^2}{\partial z_1^2} \frac{\partial z_1^2}{\partial a_1^1} \frac{\partial a_1^1}{\partial z_1^1}} \frac{\partial z_1^1}{\partial w_2^1}$$

# 反向傳播 Back propagation



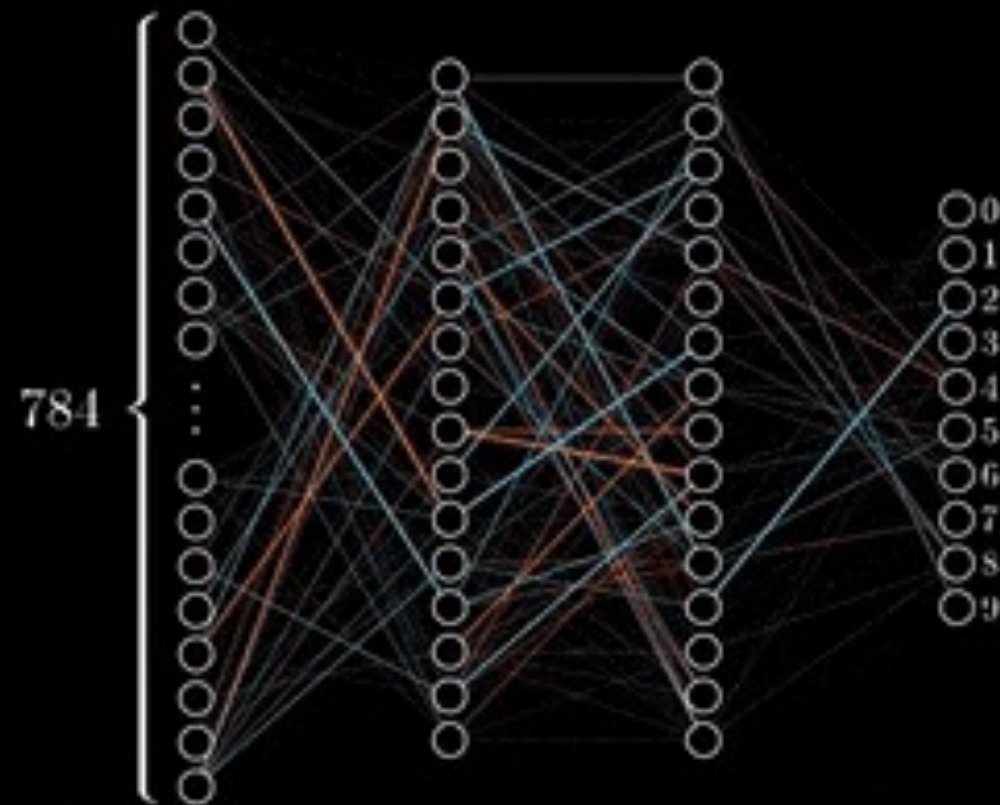
$$\hat{w}_{11}^1 = w_{11}^1 - \eta \cdot \frac{\partial L}{\partial w_{11}^1} \quad \frac{\partial L}{\partial w_{11}^1} = \frac{\partial L}{\partial \hat{y}} \frac{\partial \hat{y}}{\partial z_1^3} \left( \frac{\partial z_1^3}{\partial a_1^2} \frac{\partial a_1^2}{\partial z_1^2} \frac{\partial z_1^2}{\partial a_1^1} \right) \frac{\partial a_1^1}{\partial w_{11}^1}$$



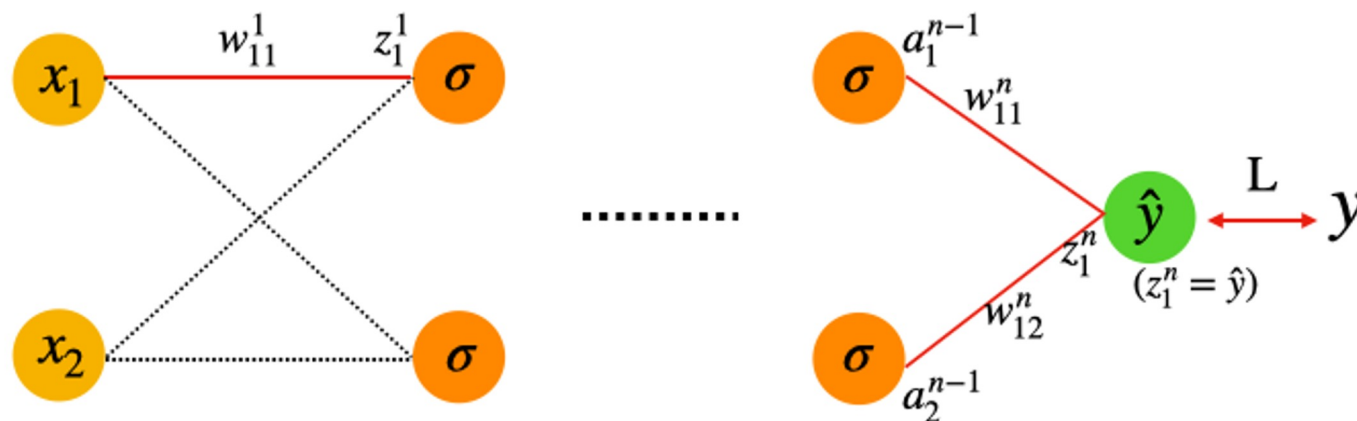
# 為什麼需要反向傳播？

利用反向傳播（Back Propagation），  
我們可以用**有效率**的方式找到損失函數對於權重的梯度，  
進而利用梯度下降法來最佳化每一個權重。

# Training in progress...



# 梯度消失



$$\hat{w}_{11}^1 = w_{11}^1 - \eta \cdot \frac{\partial L}{\partial w_{11}^1} \rightarrow 0$$

## • 3 layers

$$\frac{\partial L}{\partial w_{11}^1} = \frac{1}{n}(\hat{y} - y) \left[ \sum_i w_{1i}^3 \sigma'(z_i^2) w_{i1}^2 \right] \sigma'(z_1^1) x_1$$

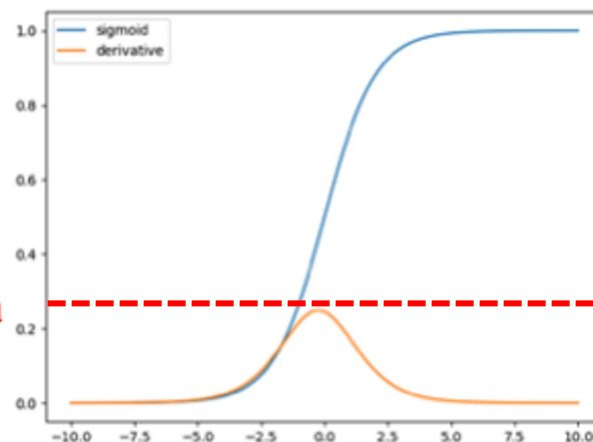
## • n layers

$$\frac{\partial L}{\partial w_{11}^1} = \frac{1}{n}(\hat{y} - y) \underbrace{w \sigma'(z)} \underbrace{w \sigma'(z)} \underbrace{w \sigma'(z)} \cdots x_1$$

Too many **activation function**

藍線：sigmoid

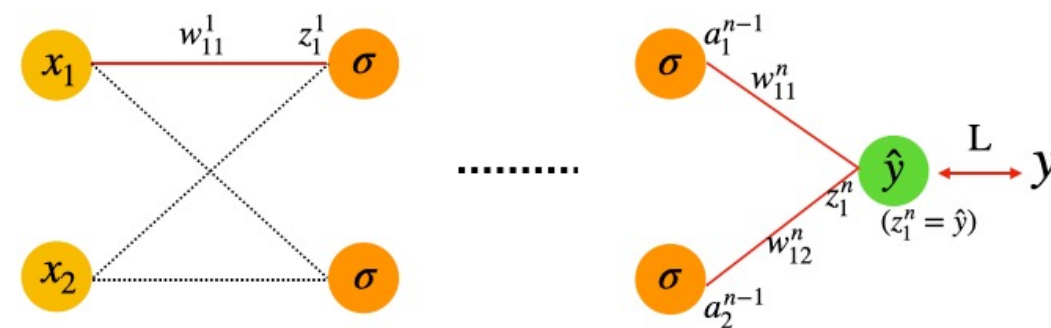
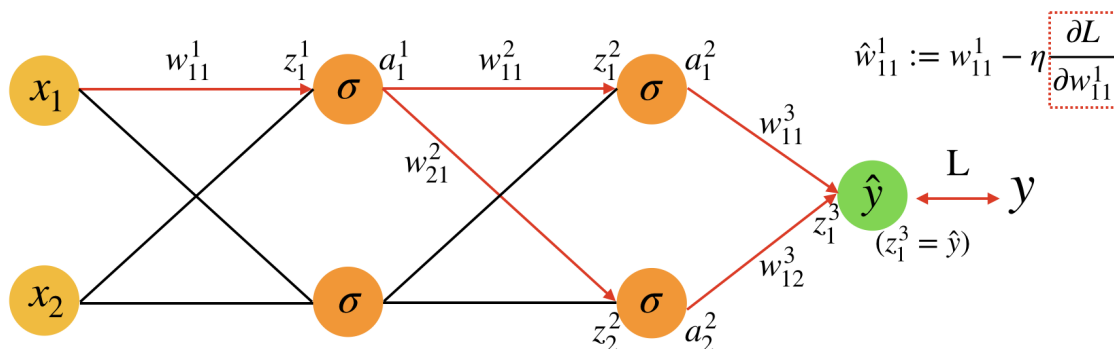
橘線：sigmoid函數的微分



0.25

# 梯度消失

影響  $w_{11}^1$  Gradient 的因素:



3 Layers:

$$\frac{\partial L}{\partial w_{11}^1} = \frac{1}{n} (\hat{y} - y) [\sum_{i=1}^2 w_{1i}^3 \sigma'(z_i^2) w_{i1}^2] \sigma'(z_1^1) x_1$$

$$0.25 \times 0.25 = 0.0625$$

$n$  Layers:

$$\frac{\partial L}{\partial w_{11}^1} = \frac{1}{n} (\hat{y} - y) w \sigma'(z) w \sigma'(z) w \sigma'(z) \dots x_1$$

Gradient vanishing  
梯度消失

# 總結：如何避免梯度消失和梯度爆炸

- 如何避免梯度消失？
  - 使用別種激勵函數，例如ReLU、Mish、Swish
  - 降低層數
  - 使用其他輔助的神經網路層，例如 BatchNormalization
  - 嘗試使用機器學習模型，例如XGBoost，有時機器學習模型表現比 DNN 還要好
- 如何避免梯度爆炸？
  - 使用 Gradient clip 限制梯度的值域大小
  - 使用 Weight clip 限制每次更新後的權重大小

# 總結：如何設計合適的網路架構

- 網路該多深？

- 一般來說，特徵數量以及資料量越多，層數會跟著加深，而訓練時間、記憶體用量也隨之增加。

- 每一層的神經元數量該怎麼設定？

- 以全連結層（DNN）為例：  
大原則是隨著層數堆疊，每一層的神經元數量會先變多再變少，  
例如：64 → 128 → 256 → 64 → 2。  
輸出層的神經元數量由任務類型決定，例如分類任務中的類別數量。

不同的資料集，其適合的網路架構都有所不同，在建模時除了參考類似任務的架構外，可以多嘗試以找到最合適者。