Gradient descent
導傳遞
Weight Initialization

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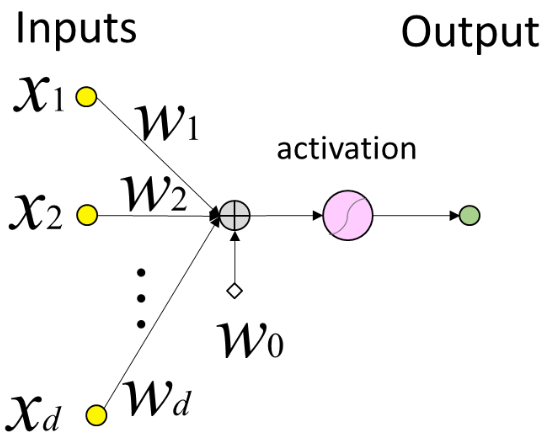
Introduction

神經網路求解方式為利用倒傳遞(back-propagation)方式來更新權重。



權重就是w0, w1,w2,…,wd

怎麼用Gradient descent求解?

此份投影片會利用一些簡單的解釋怎麼利用導數(Derivative)/梯度(Gradient)求最佳解。

微積分求極值

一階微分=0找解，求得的解可能為最大或最小。
二階微分判斷，一階微分找的解為最大或是最小。

$$f(x) = x^2 - 10x + 1$$

$$f'(x) = \frac{\partial f(x)}{\partial x} = 2x - 10 = 0$$

$$\Rightarrow x = 5$$

$$f''(x) = \frac{\partial f'(x)}{\partial x} = 2 > 0$$

此範例有x=5有最小值-24。

微積分求極值

上述範例為close-form可以找到解。

$$f(\boldsymbol{x}) = 0.5x_1 + 2x_2 + 4x_3 + 10$$

$f(\boldsymbol{x})$為三元一次方程式，則此函數的梯度為一個向量方程式:

$$\nabla f = \begin{bmatrix} \frac{\partial f(\boldsymbol{x})}{\partial x_1} \\ \frac{\partial f(\boldsymbol{x})}{\partial x_2} \\ \frac{\partial f(\boldsymbol{x})}{\partial x_3} \end{bmatrix} = \begin{bmatrix} 5 \\ 2 \\ 4 \end{bmatrix}$$

微積分求極值

$f(x)$為一元多次方程式，其對一元的參數作微分稱為求此參數的導數(Derivative)。

$$f'(x)$$

$f(\boldsymbol{x})$為多元多次方程式，其對多元的參數作微分稱為求此參數的梯度(Gradient)。

$$\nabla f = \begin{bmatrix} \frac{\partial f(\boldsymbol{x})}{\partial x_1} \\ \vdots \\ \frac{\partial f(\boldsymbol{x})}{\partial x_d} \end{bmatrix}$$

Hessian Matrix

剛提到梯度順便提一下Hessian Matrix

牛頓法求解用，但相對計算量大，目前還沒被廣泛使用。

$$\mathrm{H}(x) = \nabla^2 f = \nabla \begin{bmatrix} \dfrac{\partial f(\boldsymbol{x})}{\partial x_1} \\ \vdots \\ \dfrac{\partial f(\boldsymbol{x})}{\partial x_d} \end{bmatrix} = \begin{bmatrix} \dfrac{\partial f(\boldsymbol{x})}{\partial x_1 \partial x_1} & \cdots & \dfrac{\partial f(\boldsymbol{x})}{\partial x_1 \partial x_d} \\ \vdots & \ddots & \vdots \\ \dfrac{\partial f(\boldsymbol{x})}{\partial x_d \partial x_1} & \cdots & \dfrac{\partial f(\boldsymbol{x})}{\partial x_d \partial x_d} \end{bmatrix}$$

微積分求極值

上述範例為close-form可以找到解。

現實狀況

$$f(\boldsymbol{x}) = x_1^2 + x_1 - 4x_1x_2 + x_1^3x_2$$

$$\nabla f = \begin{bmatrix} \frac{\partial f(\boldsymbol{x})}{\partial x_1} \\ \frac{\partial f(\boldsymbol{x})}{\partial x_2} \end{bmatrix} = \begin{bmatrix} 2x_1 + 1 - 4x_2 + 3x_1^2x_2 \\ x_1^3 - 4x_1 \end{bmatrix}$$

微積分求極值

上述範例為close-form可以找到解。

現實狀況

$$f(\boldsymbol{x}) = x_1^2 + x_1 - 4x_1x_2 + x_1^3x_2$$

$$\nabla f = \begin{bmatrix} \dfrac{\partial f(\boldsymbol{x})}{\partial x_1} \\ \dfrac{\partial f(\boldsymbol{x})}{\partial x_2} \end{bmatrix} = \begin{bmatrix} 2x_1 + 1 - 4x_2 + 3x_1^2x_2 \\ -4x_1 + x_1^3 \end{bmatrix} = 0$$

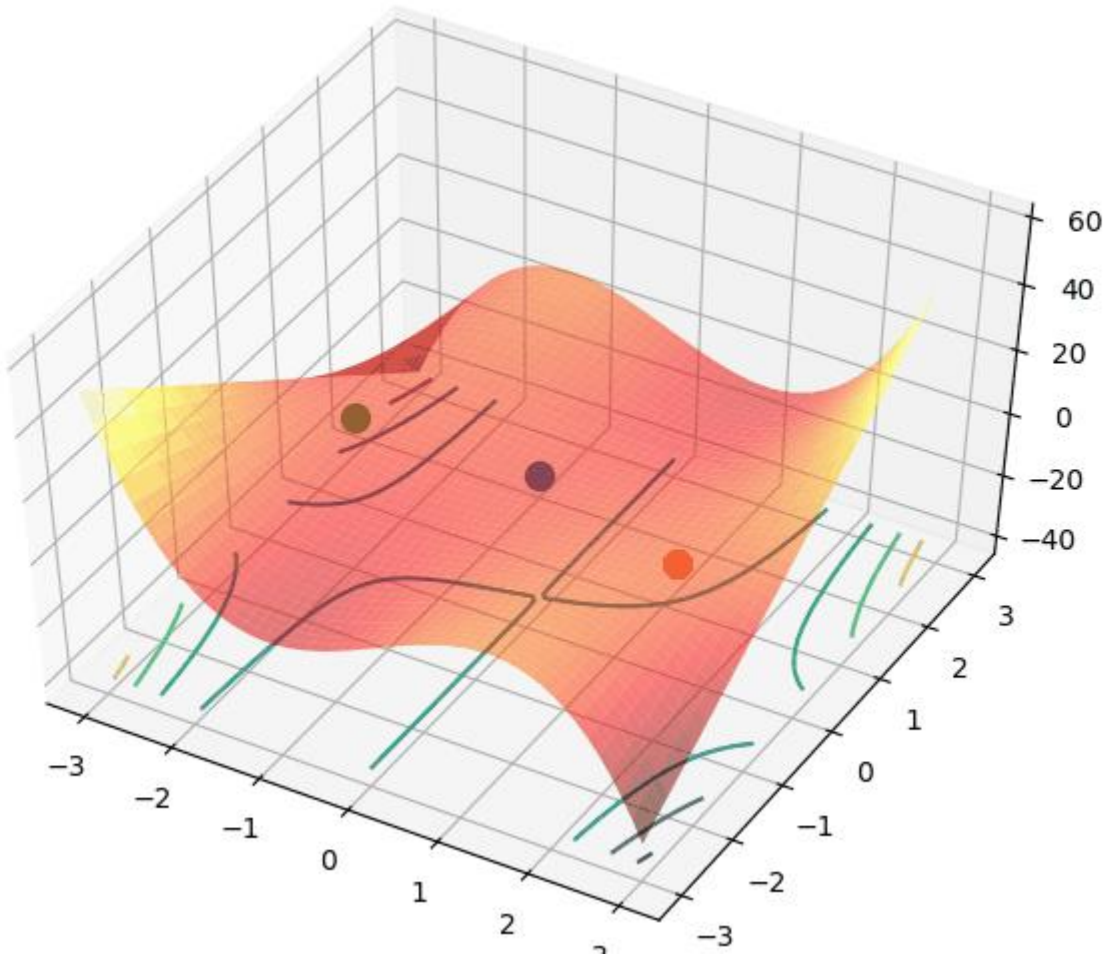
$$x_1 = 0, -2, 2$$

$$(x_1, x_2) = (0, 0.25), (-2, 0.125), (2, -0.625)$$

微積分求極值

$$f(\boldsymbol{x}) = x_1^2 + x_1 - 4x_1x_2 + x_1^3x_2$$
$$f(0, 0.25) = 0$$
$$f(-2, 0.125) = 2$$
$$f(2, -0.625) = 6$$

所以微分得到的解不一定是極值，有可能是鞍點、反曲點。



導數(Derivative)/梯度(Gradient)

- 假設有一個一元的函數為:

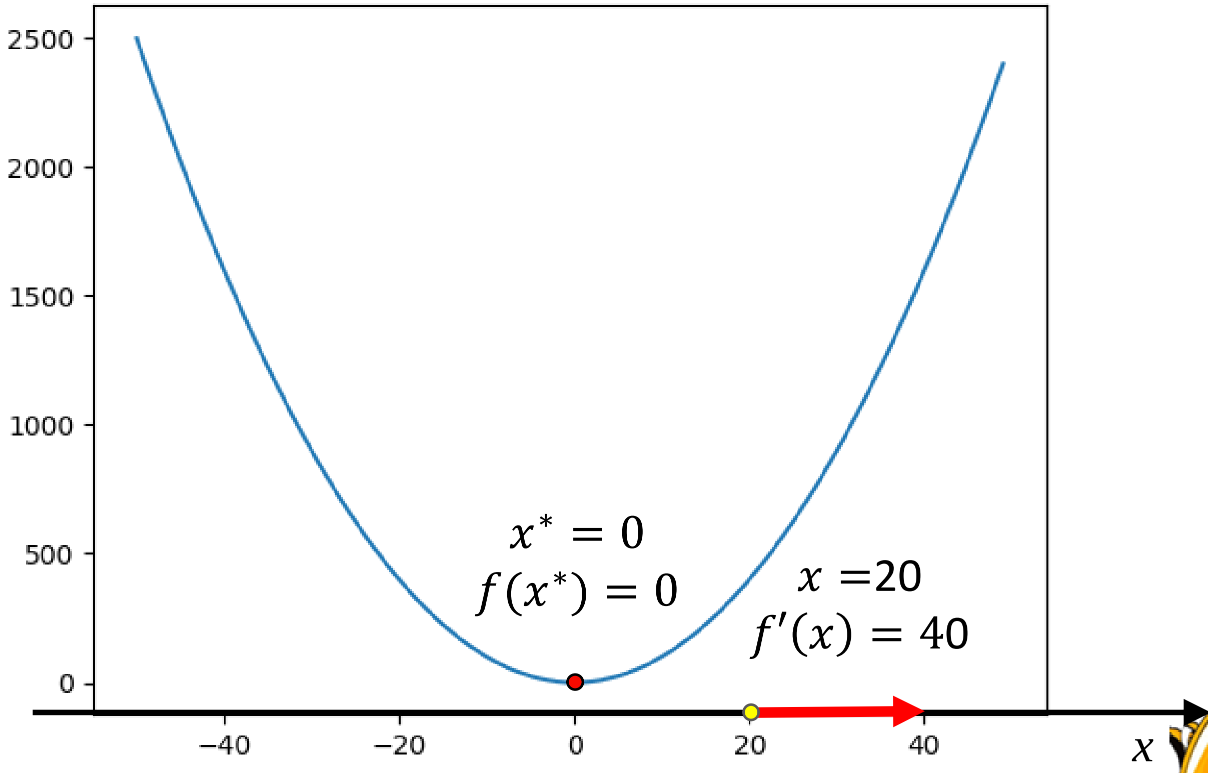
$$f(x) = x^2$$

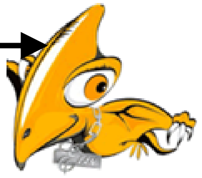
其導數: $f'(x) = 2x$ (導數有方向性)

$x>0 \rightarrow$ 往右(正)的方向

$x<0 \rightarrow$ 往左(負)的方向

導數(Derivative)/梯度(Gradient)往極大值的方向走





導數(Derivative)/梯度(Gradient)

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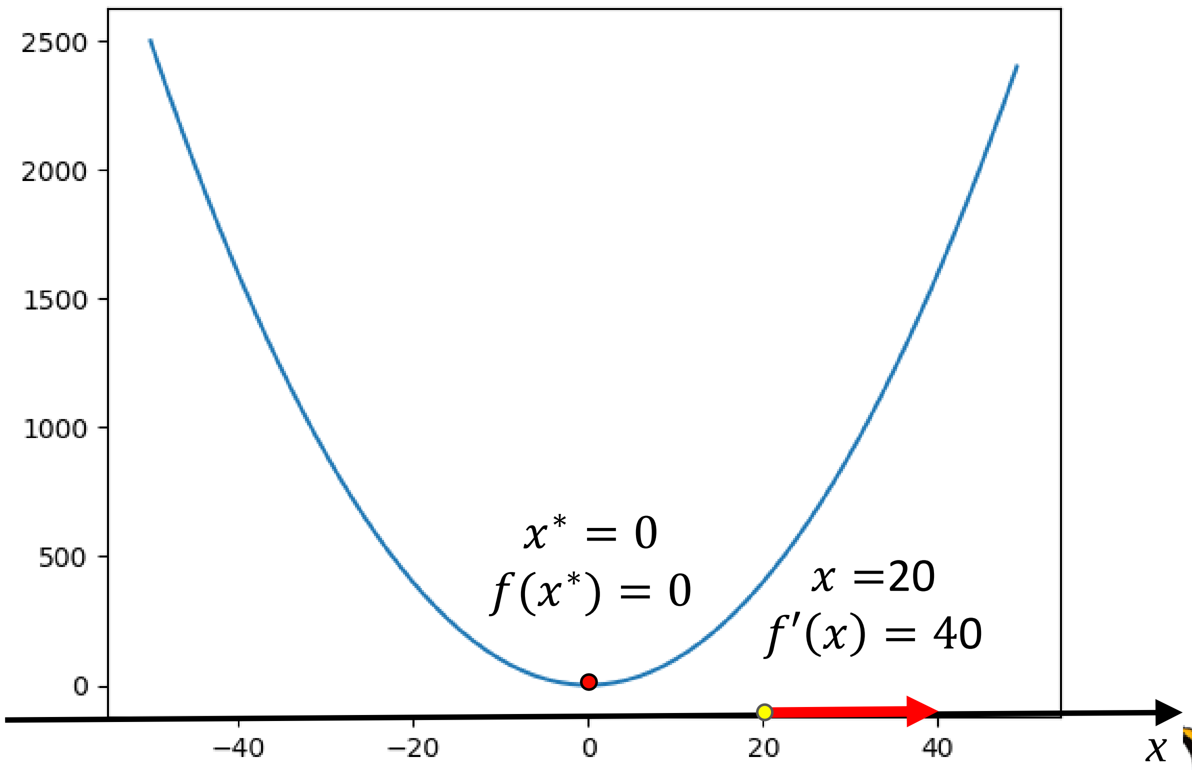
往導數(Derivative)/梯度(Gradient)往極大值的反方向走，則是往極小值

$x^{(t+1)} = x^{(t)} - \alpha f'(x)$

$\alpha = 0.5$

$x^{(0)} = 20, f'(x) = 20, x^{(0)} = 20 - 10 = 10$

梯度下降法(Gradient descent)



梯度(Gradient)

$f(\boldsymbol{x}) = (x_1 - 5)^2 + (x_2)^2$

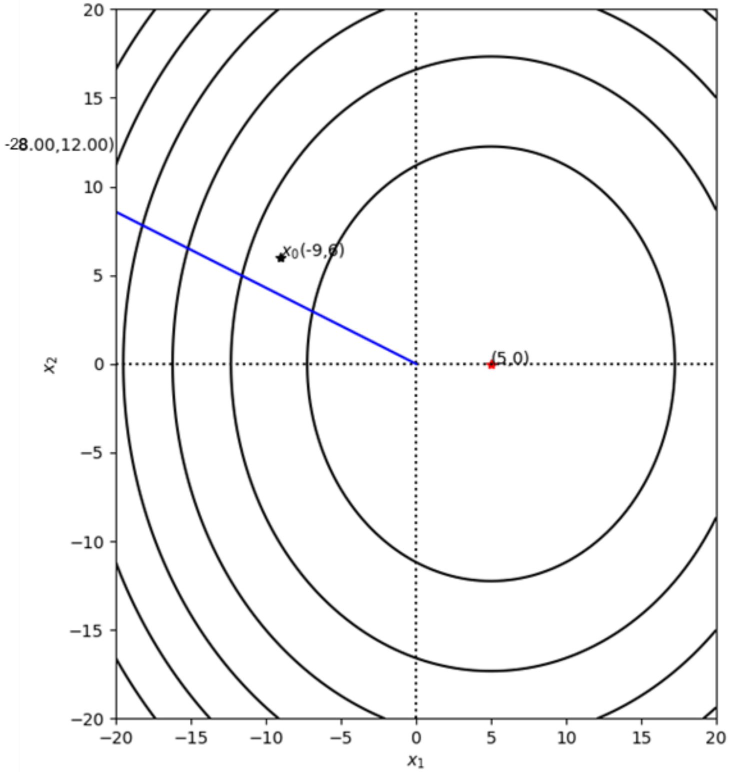
$$\nabla f = \begin{bmatrix} \dfrac{\partial f(\boldsymbol{x})}{\partial x_1} \\ \dfrac{\partial f(\boldsymbol{x})}{\partial x_2} \end{bmatrix} = \begin{bmatrix} 2x_1 - 10 \\ 2x_2 \end{bmatrix}$$

$$\boldsymbol{x}^{(t+1)} = \boldsymbol{x}^{(t)} - \alpha \nabla f\left(\boldsymbol{x}^{(t)}\right), \alpha = 0.1$$

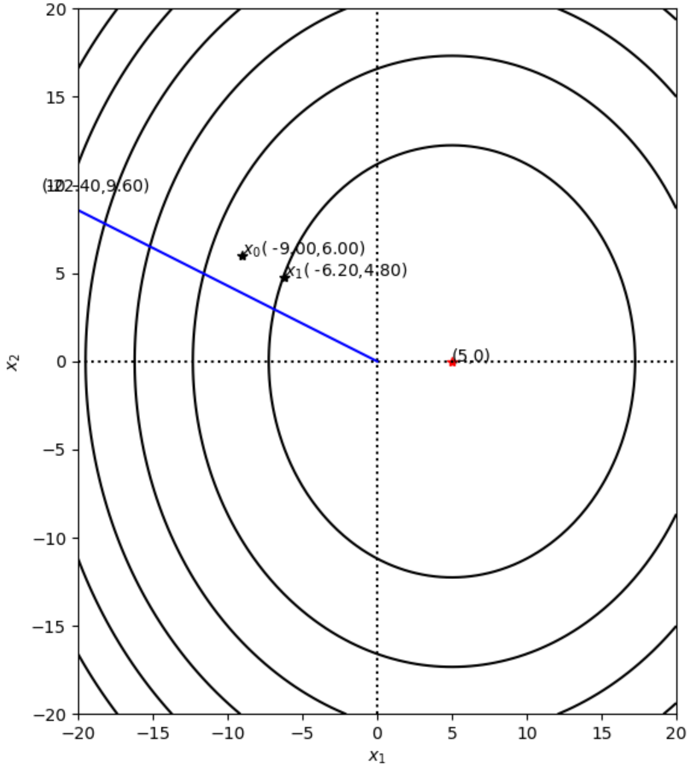
$$\boldsymbol{x}^{(0)} = \begin{bmatrix} -9 \\ 6 \end{bmatrix}, \nabla f\left(\boldsymbol{x}^{(0)}\right) = \begin{bmatrix} -28 \\ 12 \end{bmatrix}$$

$$\boldsymbol{x}^{(1)} = \begin{bmatrix} -6.2 \\ 4.8 \end{bmatrix}, \nabla f\left(\boldsymbol{x}^{(0)}\right) = \begin{bmatrix} -22.4 \\ 9.6 \end{bmatrix}$$

$$\boldsymbol{x}^{(0)} = \begin{bmatrix} -9 \\ 6 \end{bmatrix}$$



$$\boldsymbol{x}^{(1)} = \begin{bmatrix} -6.2 \\ 4.8 \end{bmatrix}$$



藍線為f的Gradient

梯度(Gradient)

$$f(\boldsymbol{x}) = (x_1 - 5)^2 + (x_2)^2$$

$$\nabla f = \begin{bmatrix} \frac{\partial f(\boldsymbol{x})}{\partial x_1} \\ \frac{\partial f(\boldsymbol{x})}{\partial x_2} \end{bmatrix} = \begin{bmatrix} 2x_1 - 10 \\ 2x_2 \end{bmatrix}$$

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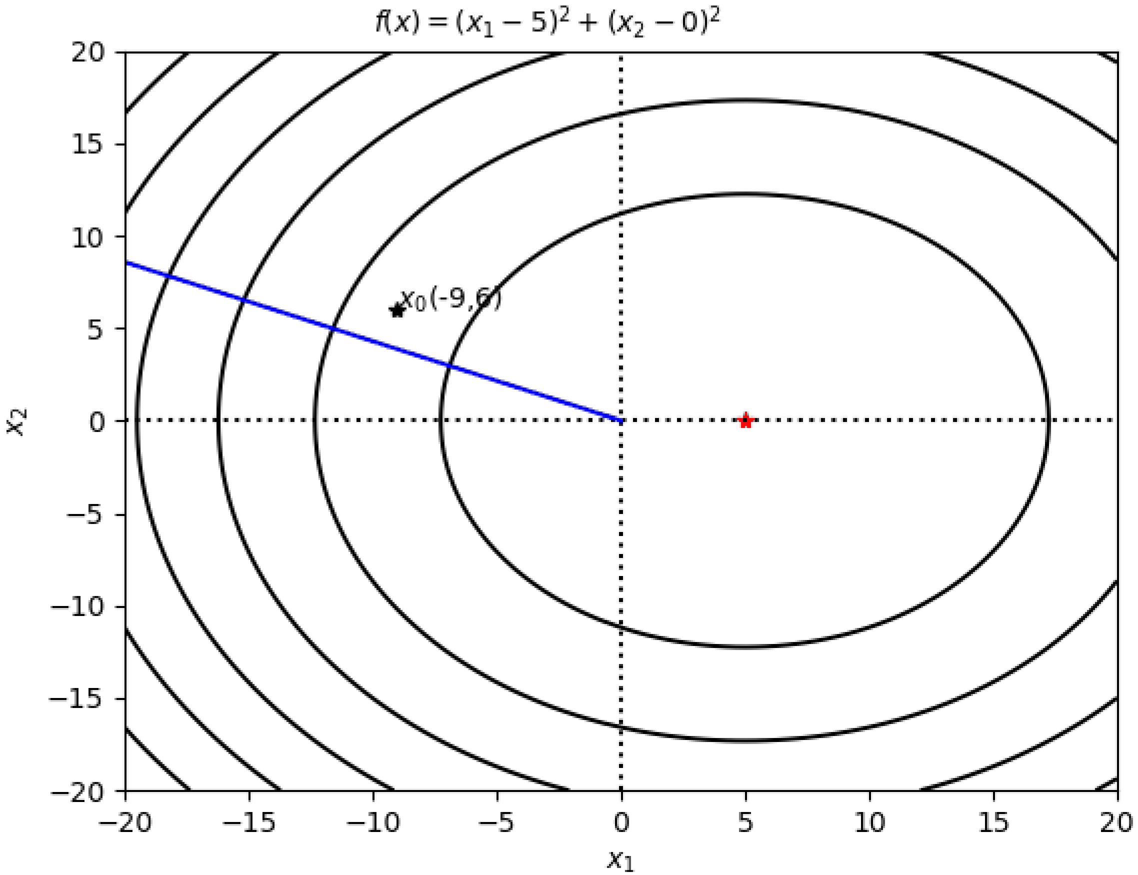


藍線為f的Gradient

梯度下降法(Gradient descent)

梯度下降法(Gradient descent)公式:

$$\boldsymbol{x}^{(t+1)} = \boldsymbol{x}^{(t)} - \gamma \nabla f\left(\boldsymbol{x}^{(t)}\right)$$

t: 第*t*次迭代

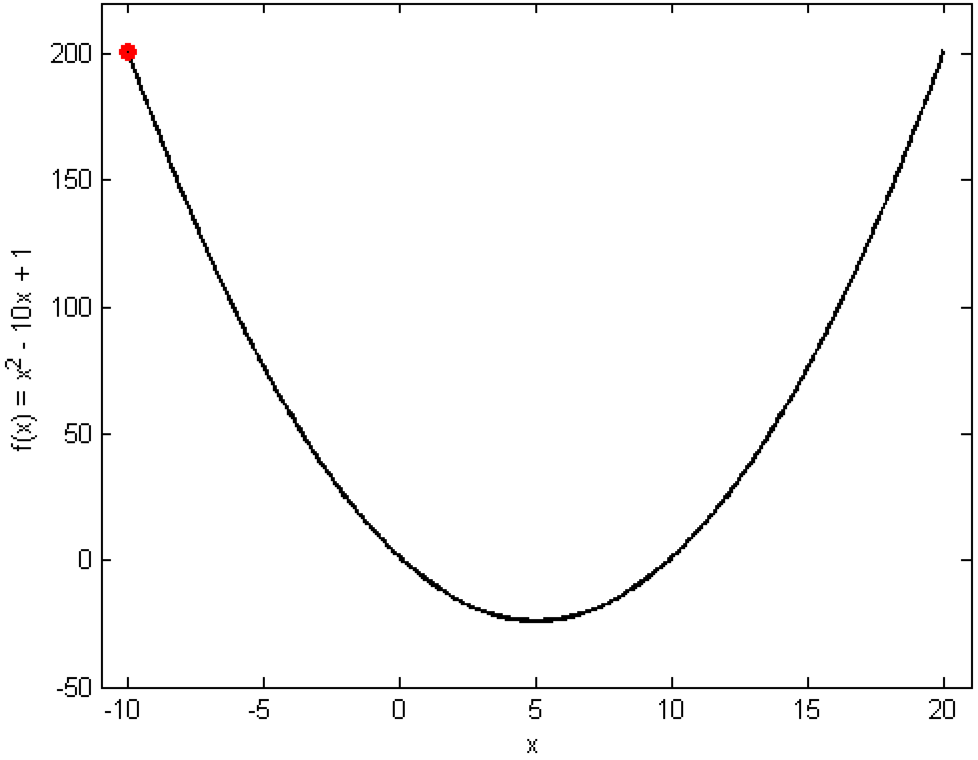
∇f:函數f的Gradient

γ: learning rate

梯度下降法-範例

$$f(x) = x^2 - 10x + 1$$
$$f'(x) = 2x - 10$$

$$x^{(t+1)} = x^{(t)} - \gamma f'\left(x^{(t)}\right)$$
$$\Rightarrow x^{(t+1)} = x^{(t)} - \gamma\left(2x^{(t)} - 10\right) = (1-2\gamma)x^{(t)} + 10\gamma$$
$$\Rightarrow x^{(t+1)} = (1-2\gamma)x^{(t)} + 10\gamma$$

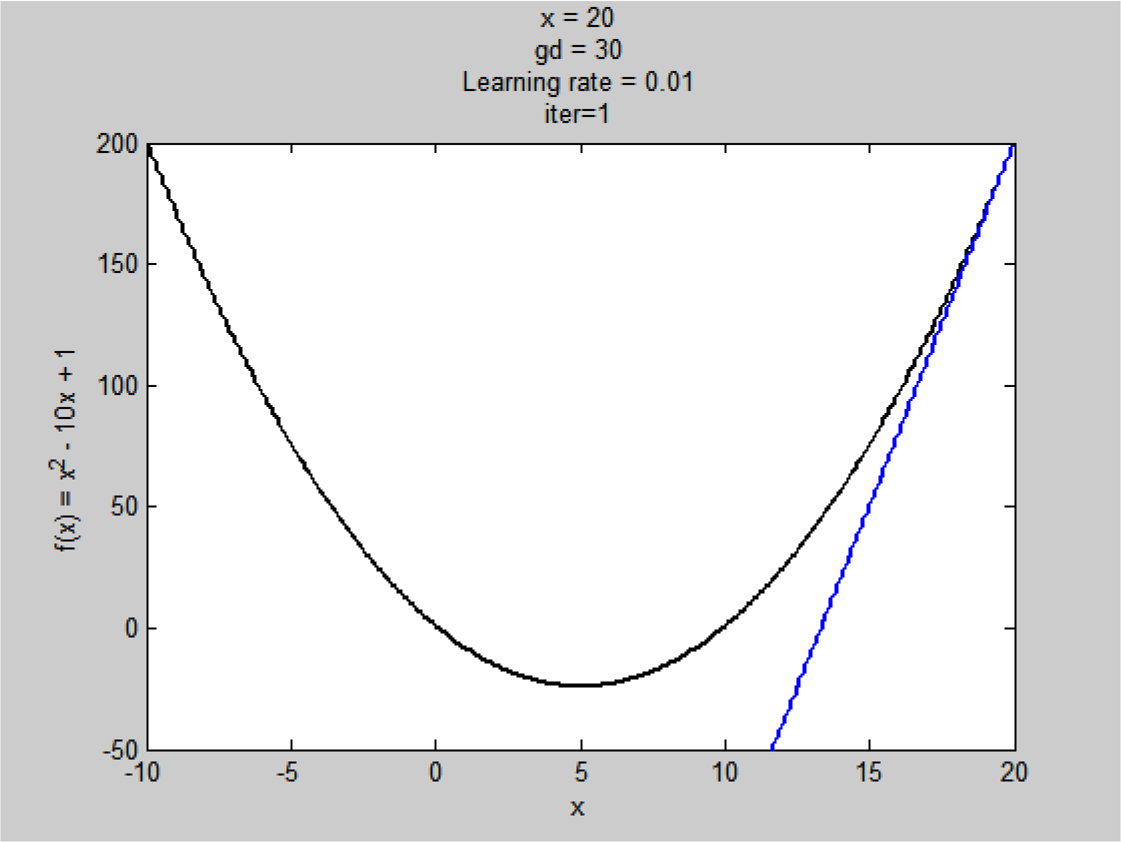


梯度下降法-範例

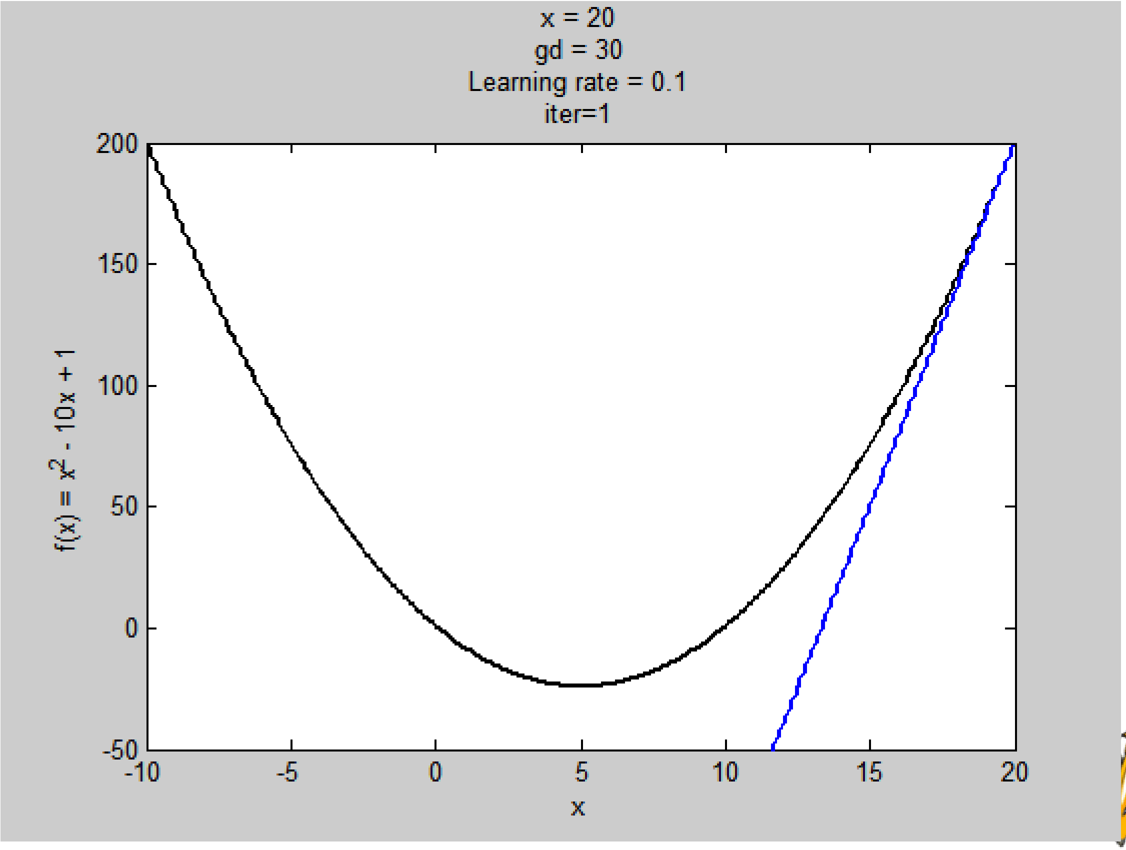
Learning rate 越大越快找到解

$$f(x) = x^2 - 10x + 1$$

Learning rate =0.01

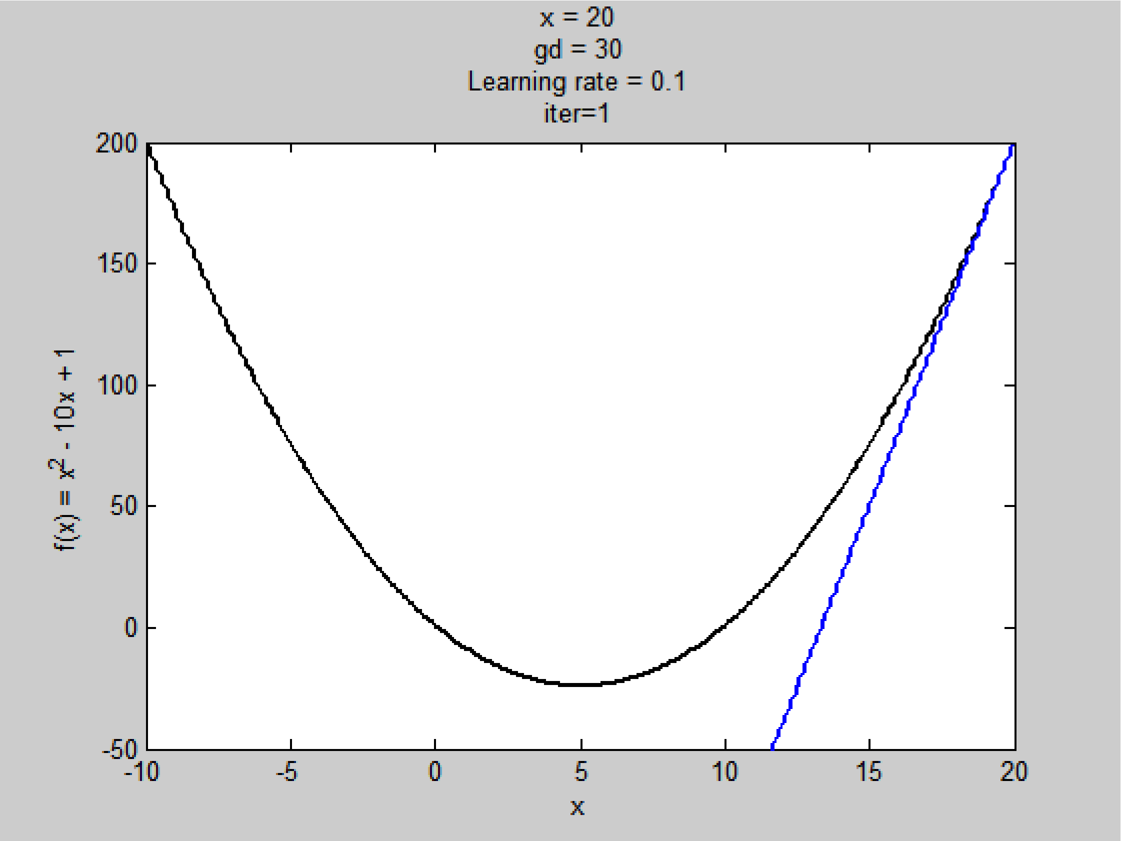


Learning rate =0.1

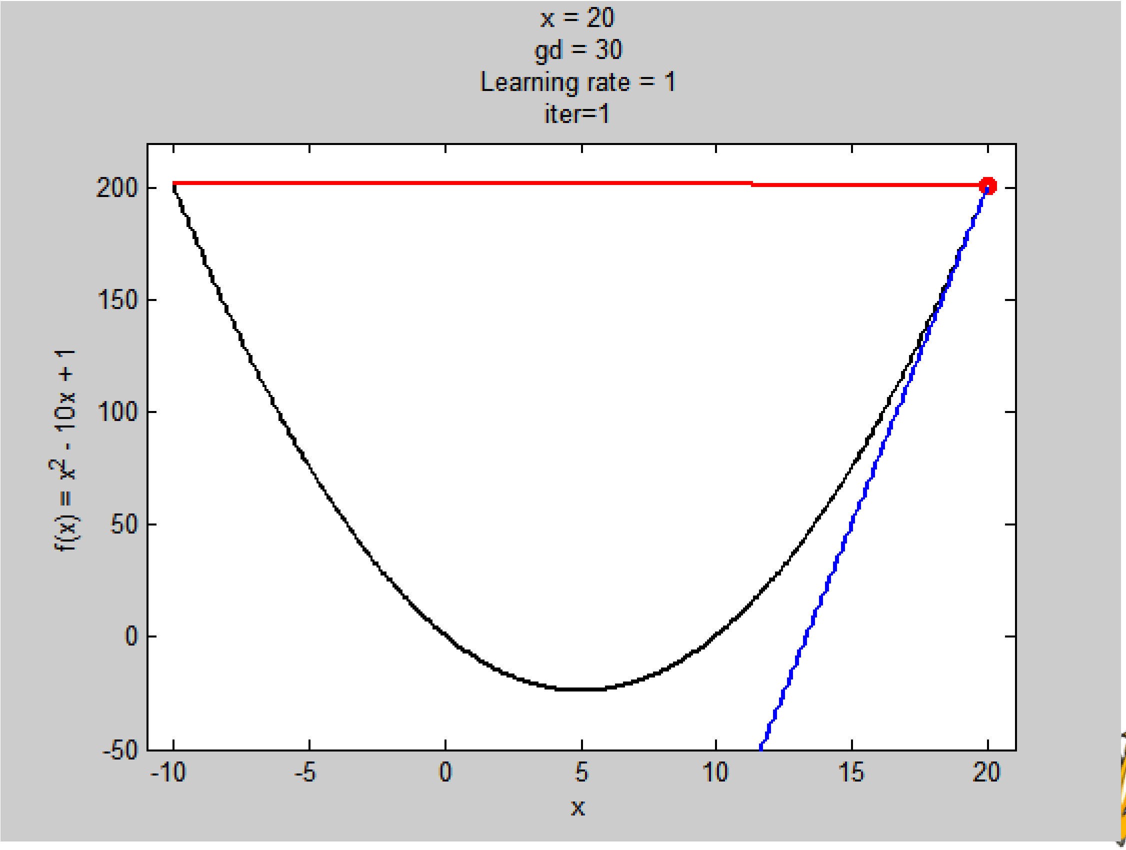


梯度下降法 (學習率過大)

Learning rate =0.1



Learning rate = 1



梯度下降法-範例2

$$f(x) = x^4 - 50x^3 - x + 1$$
$$f'(x) = 4x^3 - 150x^2 - 1$$

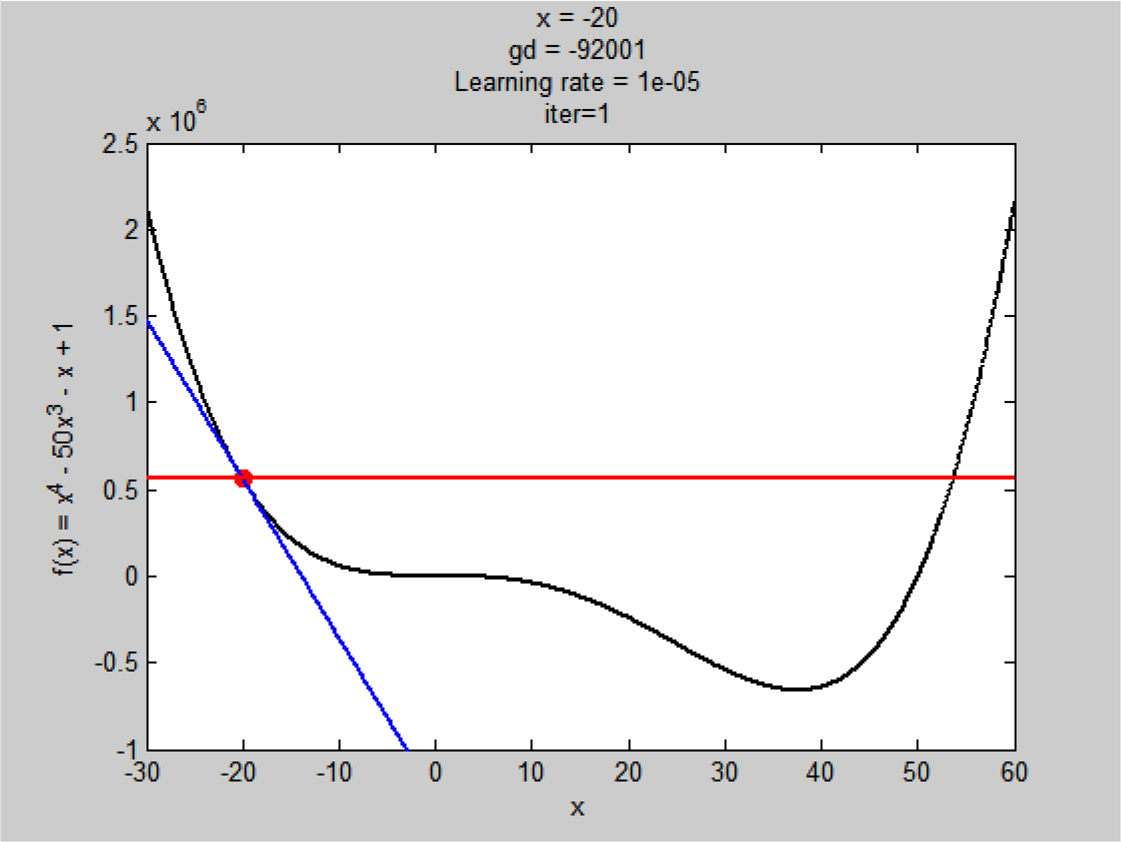
$$x^{(t+1)} = x^{(t)} - \gamma f'\left(x^{(t)}\right)$$
$$\Rightarrow x^{(t+1)} = x^{(t)} - \gamma\left(4{x^{(t)}}^3 - 150{x^{(t)}}^2 - 1\right)$$
$$\Rightarrow x^{(t+1)} = -4\gamma {x^{(t)}}^3 + 150\gamma {x^{(t)}}^2 + x^{(t)} + \gamma$$

梯度下降法-範例2

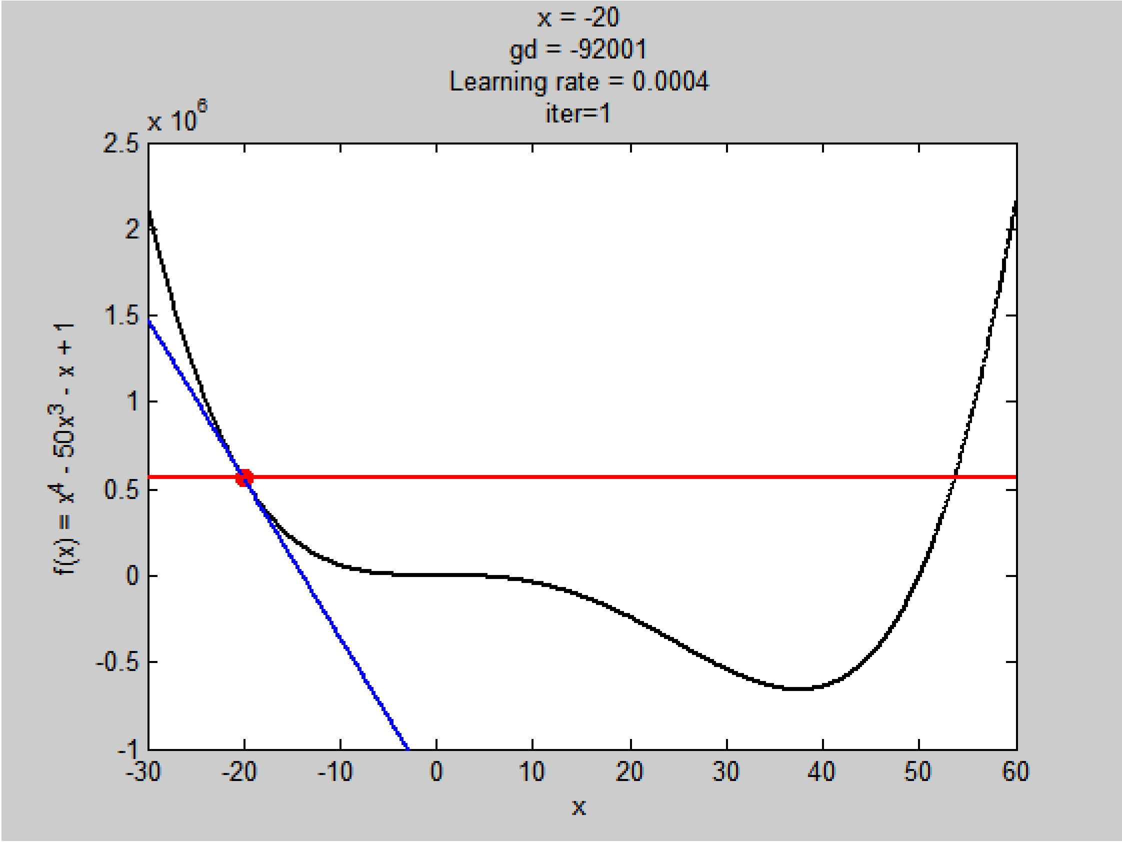
Learning rate 過小容易掉到local minima

$$f(x) = x^4 - 50x^3 - x + 1$$

Learning rate =0.00001

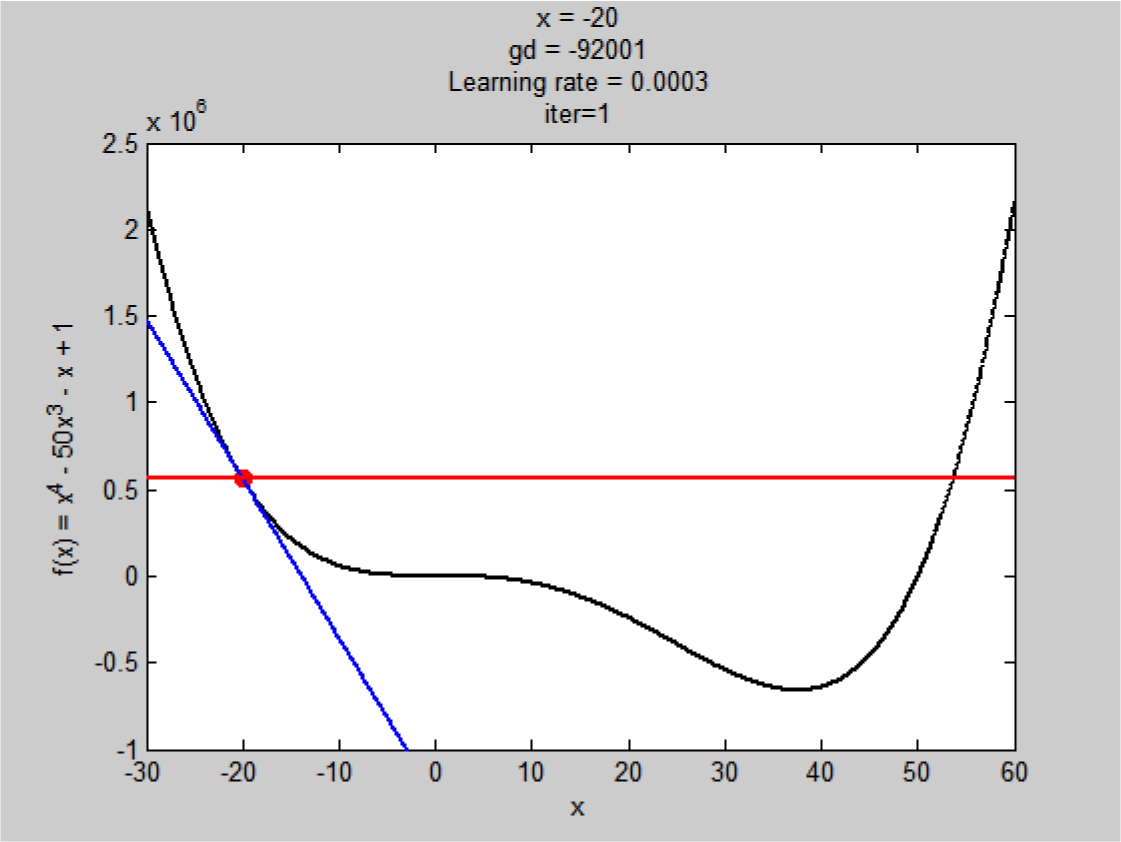


Learning rate =0.0004



梯度下降法-範例2

Learning rate =0.0003



Learning rate =0.00001
過小掉到local minima

Learning rate =0.0004
過大雖然跳出local minima，但走不進global minima

Learning rate =0.0003
最合適

梯度下降法

梯度下降法: 學習率是非常重要的一個參數因子。

因此梯度下降研究就可以展開了

梯度下降法

大家比較常看到的function為Stochastic gradient descent (SGD)、Momentum、Adagrad、RMSProp、Adam。

SGD跟前面提到GD的差異。

一般在神經網路/深度學習，訓練數量可能達到幾百萬筆

一筆資料就update模型一次(很沒有效率): 一筆資料訓練假設要1秒，一萬筆都跑過模型就要1萬秒(2.7個小時)

Mini-batch update模型一次: 假設100筆一個mini-batch，訓練要兩秒，一萬筆只需要3.3分鐘。

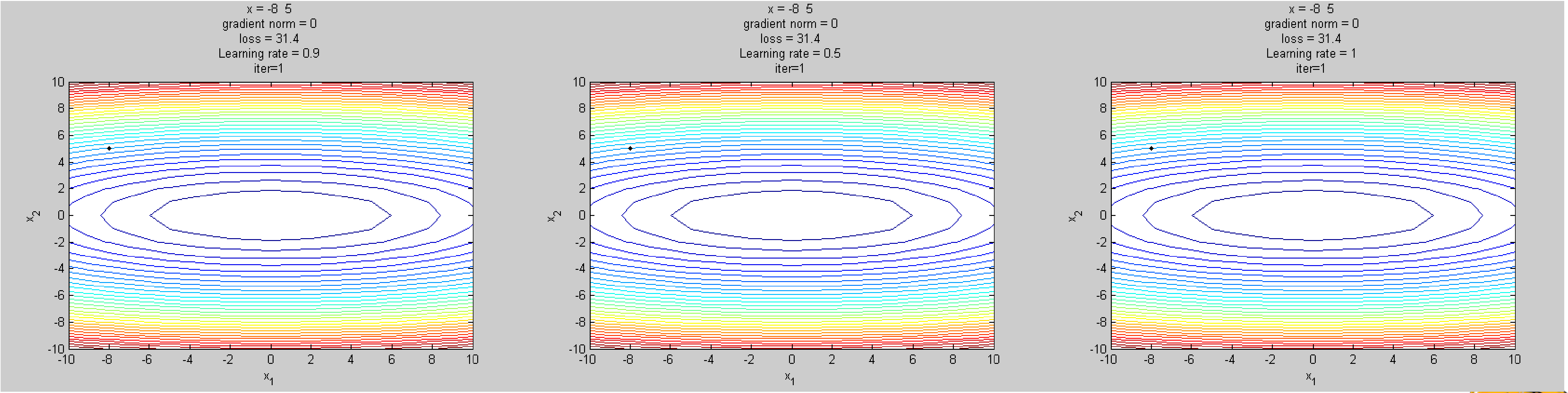
SGD: 就是一次跑一個小批次(Mini-batch)後的平均梯度模型即更新一次，這個mini-batch為隨機抽取出，所以用Stochastic。

SGD

$$f(x_1, x_2) = 0.1x_1^2 + x_2^2$$

Initial point=[-8,5]

Learning rate = 0.9 | Learning rate = 0.5 | Learning rate = 1



Momentum

Momentum是架構在SGD上的算法

$$\boldsymbol{v}^{(t)} = \begin{cases} \gamma \boldsymbol{g}_t & t = 0 \\ m\boldsymbol{v}^{(t-1)} + \gamma \boldsymbol{g}_t & t \geq 1 \end{cases}$$

$$\boldsymbol{x}^{(t+1)} = \boldsymbol{x}^{(t)} - \boldsymbol{v}^{(t)}$$

$$\boldsymbol{g}_t = \nabla f\left(\boldsymbol{x}^{(t)}\right)$$

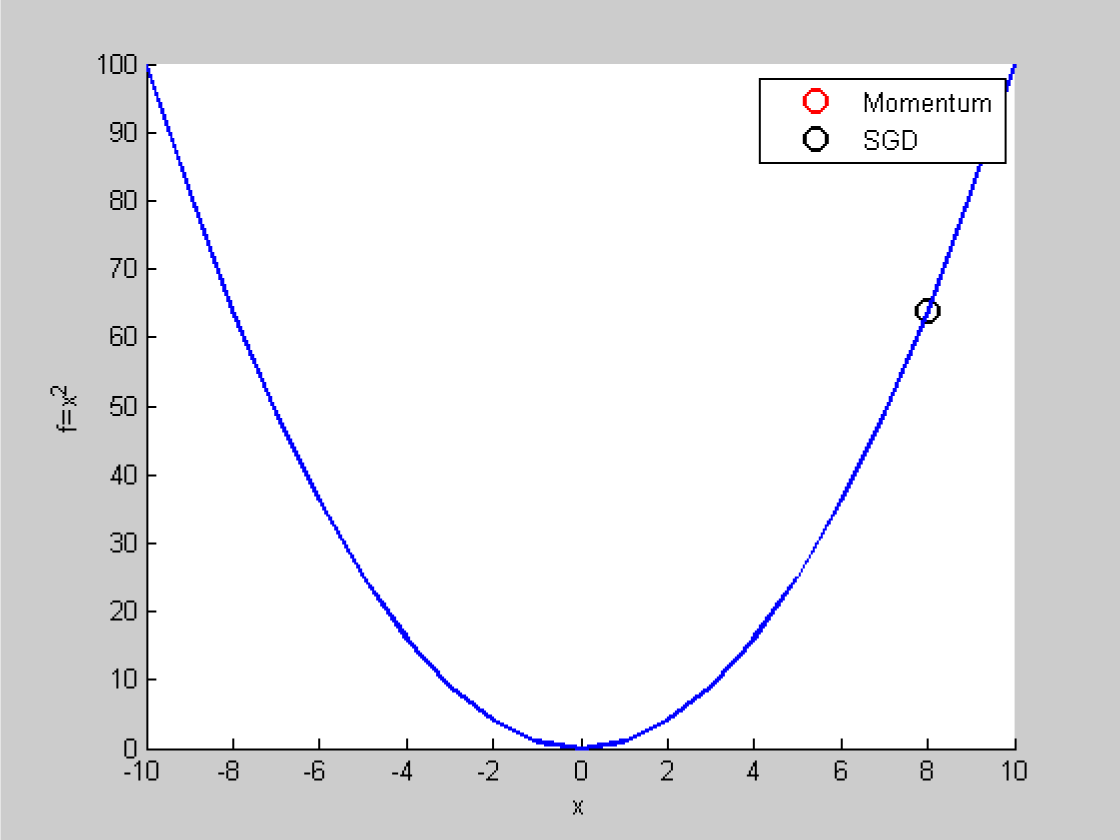
$\boldsymbol{g}_t$:第t次迭代的gradient。

$\boldsymbol{v}^{(t)}$:第t次參數要更新的幅度(歷史的梯度和)。

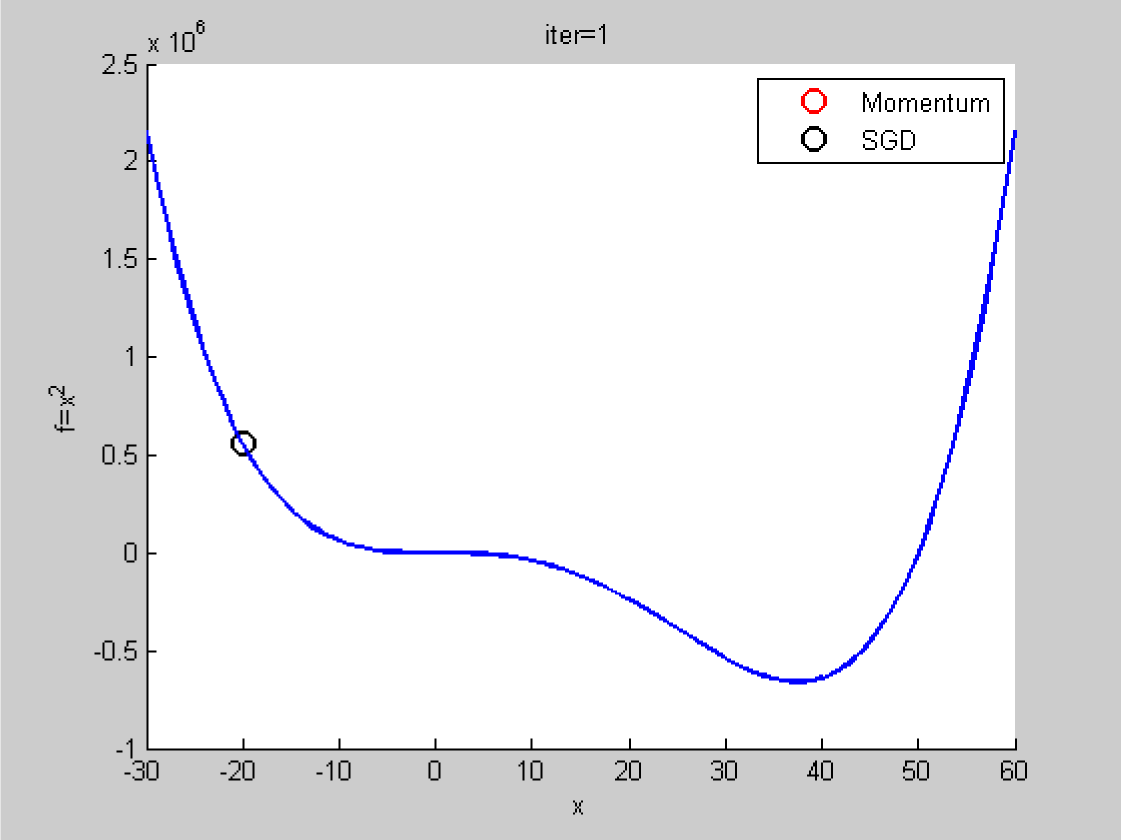
如果過去的梯度方向和當下的梯度方向一致，代表這個更新方向是對的，會增強這個方向的梯度。

如果過去的和當下方向不一致，則梯度會有消融作用(衰退)，只會微幅調整參數。

Momentum



Learning rate = 0.00001



基本上API用的SGD都有Momentum可以設定。

Adagrad

- SGD和momentum在更新參數時，都是用同一個學習率(γ)
- Adagrad算法則是在學習過程中對學習率不斷的調整，這種技巧叫做「學習率衰減(Learning rate decay)」。
- Ada這個字跟是Adaptive縮寫。

Gradient: $$g_{t,i} = \nabla_{x_i} f\left(x_i^{(t)}\right)$$

SGD: $$x_i^{(t+1)} = x_i^{(t)} - \gamma g_{t,i}$$

Adagrad : $$x_i^{(t+1)} = x_i^{(t)} - \frac{\gamma}{\boxed{\sqrt{G_{t,ii} + \varepsilon}}} g_{t,i}$$

Adagrad

$$x_i^{(t+1)} = x_i^{(t)} - \frac{\gamma}{\sqrt{G_{t,ii} + \varepsilon}} g_{t,i} \qquad \boldsymbol{x} = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_d \end{bmatrix} \in \mathbb{R}^{d\times 1}$$

$$G_t = \begin{bmatrix} \sum_{t'=1}^{t} (g_{t',1} \times g_{t',1}) & 0 & 0 \\ 0 & \ddots & 0 \\ 0 & 0 & \sum_{t'=1}^{t} (g_{t',d} \times g_{t',d}) \end{bmatrix} \in \mathbb{R}^{d\times d}$$

$$G_{t,ii} = \sum_{t'=1}^{t} (g_{t',i} \times g_{t',i})$$

Adagrad

$$x_i^{(t+1)} = x_i^{(t)} - \frac{\gamma}{\sqrt{G_{t,ii} + \varepsilon}} g_{t,i} \qquad \boldsymbol{x} = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_d \end{bmatrix} \in \mathbb{R}^{d\times 1}$$

$$G_{t,ii} = \sum_{t'=1}^{t} \left(g_{t',i} \times g_{t',i}\right)$$

- 隨著迭代次數越多，分母(Gradient平方和開根號)越大，學習率會越低，達到前期學習率高，後期學習率低的目的。
- 缺點: 學習中後期，分母有可能因為累積過大導致最後更新的參數趨近於0，所以無法有效學習。

RMSProp

- RMSprop是Geoff Hinton 提出未發表的方法，和Adagrad一樣是自適應的方法，但**Adagrad的分母是從第1次梯度到第t次梯度的和**，所以和可能過大，**RMSprop則是算對應的平均值**，因此可以緩解Adagrad學習率下降過快的問題。

Adagrad

$$x_i^{(t+1)} = x_i^{(t)} - \frac{\gamma}{\sqrt{G_{t,ii} + \varepsilon}} g_{t,i}$$

$$G_{t,ii} = \sum_{t'=1}^{t} \left(g_{t',i} \times g_{t',i}\right)$$

RMSprop

$$x_i^{(t+1)} = x_i^{(t)} - \frac{\gamma}{\sqrt{E\left[g_i^2\right]_t + \varepsilon}} g_{t,i}$$

$$E\left[g_i^2\right]_t = \rho E\left[g_i^2\right]_{t-1} + (1-\rho) g_{t,i}^2$$

Adam

- **Momentum**: 考慮過去梯度的方向和當前梯度的方向做合成 (沒直接修改learning rate)
- **Adagrad、 RMSprop**: 考慮過去梯度的大小用來修改learning rate (Learning rate decay)
- **Adam(Adaptive Moment Estimation)**則是兩者合併加強版本(Momentum+RMSprop+各自做偏差的修正)

Adam

Momentum

$$\boldsymbol{v}^{(t)} = \begin{cases} \gamma \boldsymbol{g}_t & t = 0 \\ \boxed{m v^{(t-1)} + \gamma \boldsymbol{g}_t} & t \geq 1 \end{cases}$$

$$\boldsymbol{x}^{(t+1)} = \boldsymbol{x}^{(t)} - \boldsymbol{v}^{(t)}$$

$$\boldsymbol{g}_t = \nabla f\left(\boldsymbol{x}^{(t)}\right)$$

RMSProp

$$x_i^{(t+1)} = x_i^{(t)} - \frac{\gamma}{\sqrt{E[g_i^2]_t + \varepsilon}} g_{t,i}$$

$$E[g_i^2]_t = \boxed{\rho E[g_i^2]_{t-1} + (1-\rho) g_{t,i}^2}$$

$$\boldsymbol{m}_t = \boxed{\beta_1 \boldsymbol{m}_{t-1} + (1-\beta_1)\boldsymbol{g}_t}$$

$$\boldsymbol{v}_t = \boxed{\beta_2 \boldsymbol{v}_{t-1} + (1-\beta_2)\boldsymbol{g}_t^2}$$

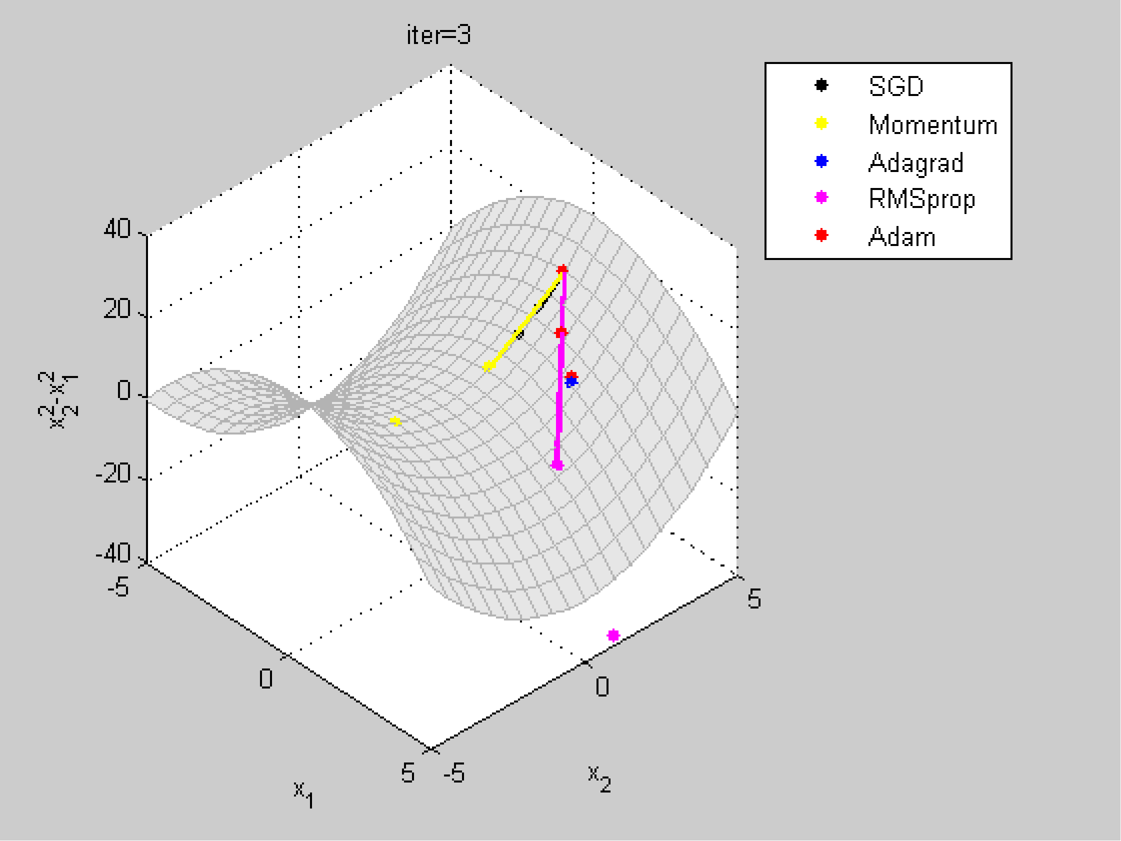
$$\widehat{\boldsymbol{m}}_t = \frac{\boldsymbol{m}_t}{1-\beta_1^t}$$

$$\widehat{\boldsymbol{v}}_t = \frac{\boldsymbol{v}_t}{1-\beta_2^t}$$

$$\boldsymbol{x}^{(t+1)} = \boldsymbol{x}^{(t)} - \frac{\gamma}{\sqrt{\widehat{\boldsymbol{v}}_t} + \varepsilon} \widehat{\boldsymbol{m}}_t$$

Example

$$f(x_1, x_2) = x_2^2 - x_1^2$$



導傳遞

- 神經網路如何利用導傳遞找解
- 神經網路太深層的問題:

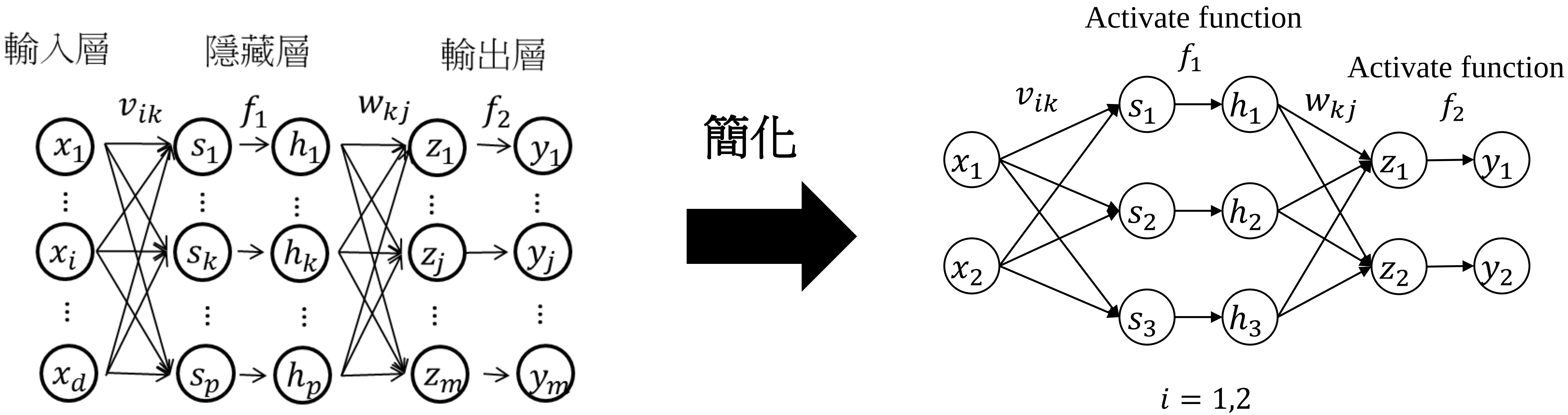
梯度消失問題(Vanishing gradient)/梯度爆炸問題（exploding gradient problem）。

Activation Function為什麼要採用ReLU，而不是用Sigmoid。

Residual block克服神經網路不能太深層的問題。

神經網路如何利用導傳遞找解

- 下圖為一個三層的MLP



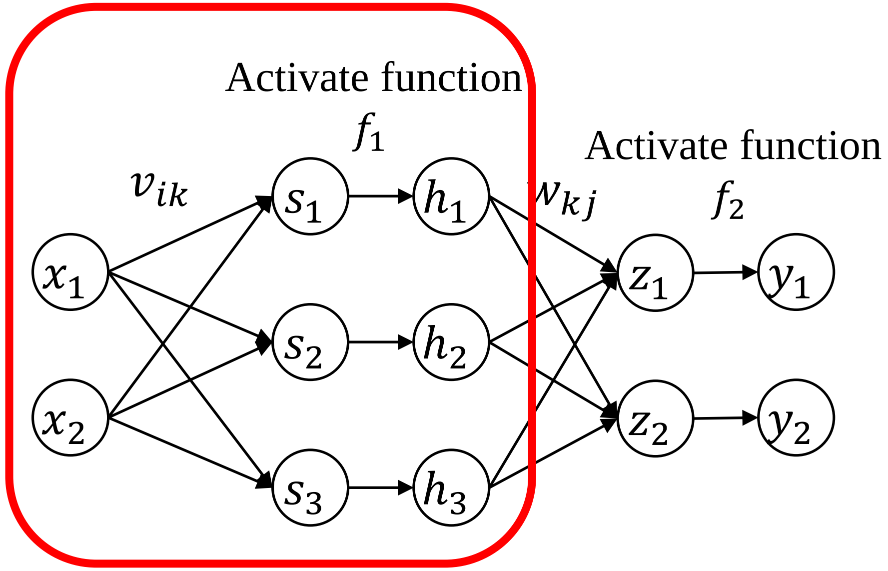
$i = 1,2$

$k = 1,2,3$

$\mathrm{j} = 1,2$

Forward propagation

輸入層→隱藏層



$i = 1,2$
$k = 1,2,3$
$\mathrm{j} = 1,2$

$$s_1 = v_{11}x_1 + v_{21}x_2 = \boldsymbol{v}_1^T\boldsymbol{x}$$
$$s_2 = v_{12}x_1 + v_{22}x_2 = \boldsymbol{v}_2^T\boldsymbol{x}$$
$$s_3 = v_{13}x_1 + v_{23}x_2 = \boldsymbol{v}_3^T\boldsymbol{x}$$

$$\boldsymbol{x} = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}, \boldsymbol{v}_k = \begin{bmatrix} v_{1k} \\ v_{2k} \end{bmatrix}, k = 1,2,3$$

$$s_k = \sum_{i=1}^{2} v_{ik}x_i$$

$$\boldsymbol{s} = \boldsymbol{v}^T\boldsymbol{x}$$

$$\boldsymbol{s} = \begin{bmatrix} s_1 \\ s_2 \\ s_3 \end{bmatrix}$$

$$\boldsymbol{v} = [\boldsymbol{v}_1 \quad \boldsymbol{v}_2 \quad \boldsymbol{v}_2] = \begin{bmatrix} v_{11} & v_{12} & v_{13} \\ v_{21} & v_{22} & v_{23} \end{bmatrix}$$

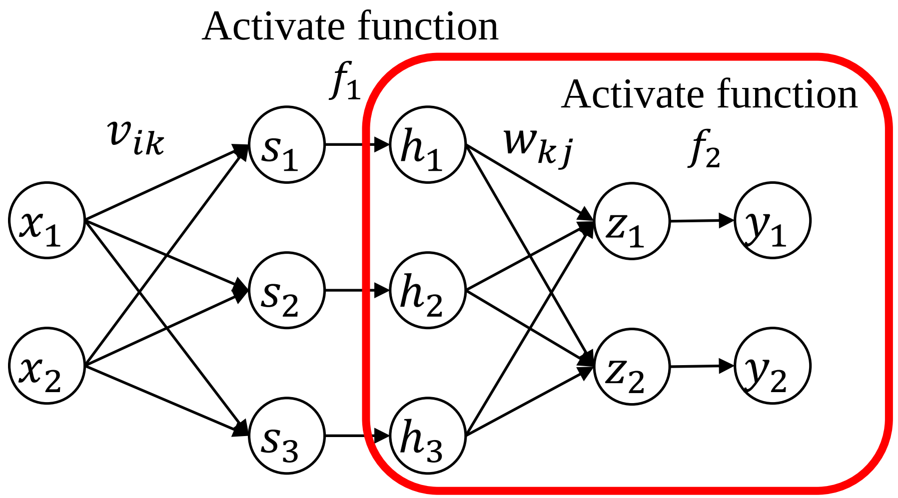
Activate function

$$\boldsymbol{h} = f_1(\boldsymbol{s})$$

$$\boldsymbol{h} = \begin{bmatrix} h_1 \\ h_2 \\ h_3 \end{bmatrix}$$

Forward propagation

隱藏層→輸出層



$i = 1,2$
$k = 1,2,3$
$\mathrm{j} = 1,2$

$$z_1 = w_{11}h_1 + w_{21}h_2 + w_{31}h_3 = \boldsymbol{w}_1^T\boldsymbol{h}$$
$$z_2 = w_{12}h_1 + w_{22}h_2 + w_{32}h_3 = \boldsymbol{w}_2^T\boldsymbol{h}$$

$$\boldsymbol{w}_j = \begin{bmatrix} w_{1j} \\ w_{2j} \\ w_{3j} \end{bmatrix}, j = 1,2$$

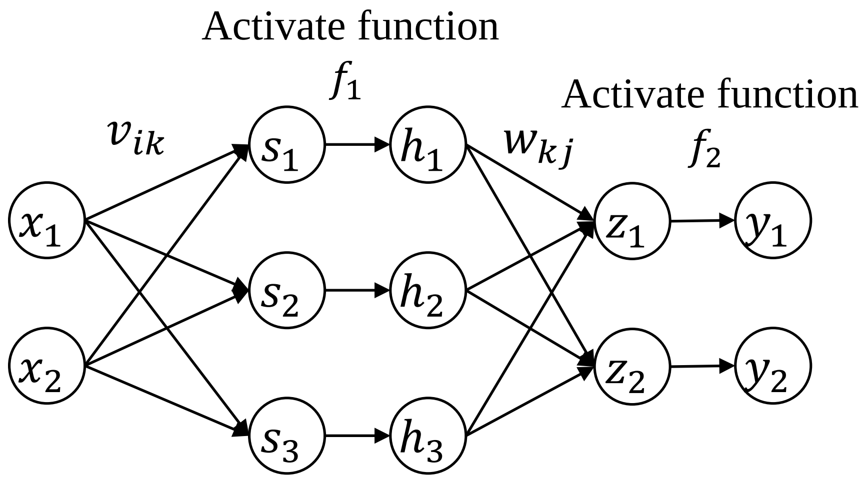
$$\boldsymbol{z} = \boldsymbol{w}^T\boldsymbol{h}$$
$$\boldsymbol{z} = \begin{bmatrix} z_1 \\ z_2 \end{bmatrix}$$

$$\boldsymbol{w} = [\boldsymbol{w}_1 \quad \boldsymbol{w}_2] = \begin{bmatrix} w_{11} & w_{12} \\ w_{21} & w_{22} \\ w_{31} & w_{32} \end{bmatrix}$$

Activate function

$$\boldsymbol{y} = f_2(\boldsymbol{z})$$
$$\boldsymbol{y} = \begin{bmatrix} y_1 \\ y_2 \end{bmatrix}$$

Forward propagation



$$i = 1,2$$
$$k = 1,2,3$$
$$\mathrm{j} = 1,2$$

輸入層→隱藏層

$$\boldsymbol{s} = \boldsymbol{v}^{\boldsymbol{T}}\boldsymbol{x}$$
$$\boldsymbol{h} = f_1(\boldsymbol{s})$$

隱藏層→輸出層

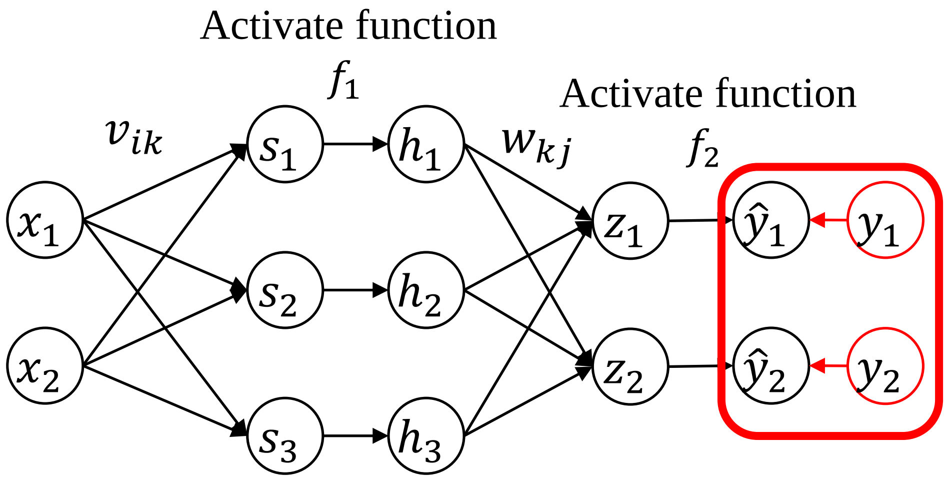
$$\boldsymbol{z} = \boldsymbol{w}^{\boldsymbol{T}}\boldsymbol{h}$$
$$\boldsymbol{y} = f_2(\boldsymbol{z})$$

=

$$\boldsymbol{y} = f_2\left(\boldsymbol{w}^{\boldsymbol{T}} f_1(\boldsymbol{v}^{\boldsymbol{T}}\boldsymbol{x}\,)\right)$$

參數為$\boldsymbol{v}$和$\boldsymbol{w}$。

Back-propagation



$$\hat{\boldsymbol{y}} = f_2\left(\boldsymbol{w}^{\boldsymbol{T}} f_1(\boldsymbol{v}^{\boldsymbol{T}}\boldsymbol{x})\right) \qquad \boldsymbol{y} = \begin{bmatrix} y_1 \\ y_2 \end{bmatrix}$$

我們用SSE來當作loss function

$$loss(\boldsymbol{y}, \hat{\boldsymbol{y}}) = \frac{1}{2}(\boldsymbol{y} - \hat{\boldsymbol{y}})^{\boldsymbol{T}}(\boldsymbol{y} - \hat{\boldsymbol{y}})$$

利用gradient descent找最佳參數解(參數只有$\boldsymbol{w}$和$\boldsymbol{v}$)

$$\boldsymbol{w}^{(t+1)} = \boldsymbol{w}^{(t)} - \alpha \nabla \boldsymbol{w}^{(t)}$$
$$\boldsymbol{v}^{(t+1)} = \boldsymbol{v}^{(t)} - \alpha \nabla \boldsymbol{v}^{(t)}$$

輸入層→隱藏層

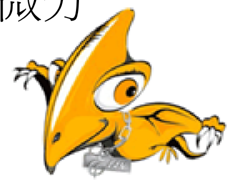
$$\boldsymbol{s} = \boldsymbol{v}^{\boldsymbol{T}}\boldsymbol{x}$$
$$\boldsymbol{h} = f_1(\boldsymbol{s})$$

隱藏層→輸出層

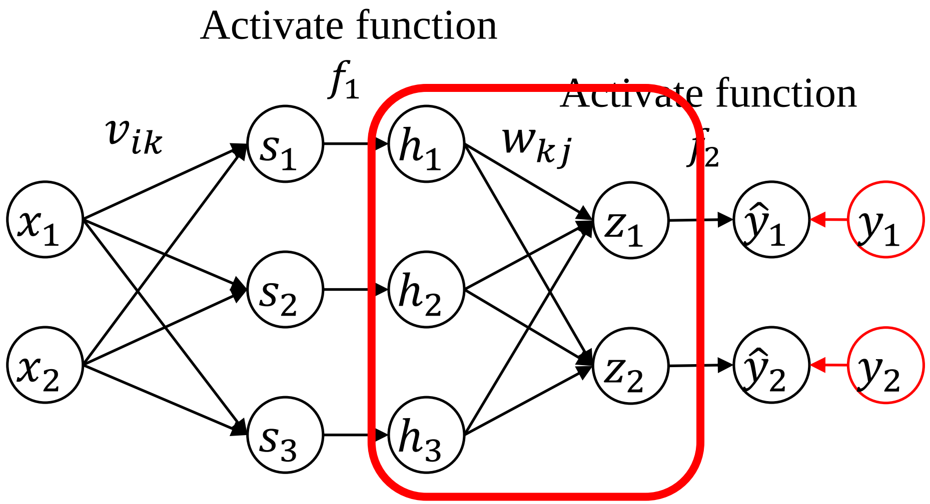
$$\boldsymbol{z} = \boldsymbol{w}^{\boldsymbol{T}}\boldsymbol{h}$$
$$\boldsymbol{y} = f_2(\boldsymbol{z})$$

$\nabla \boldsymbol{w} = \dfrac{\partial loss(\boldsymbol{y}, \hat{\boldsymbol{y}})}{\partial \boldsymbol{w}}$ 輸出層→隱藏層參數為$\boldsymbol{w}$，對loss進行$\boldsymbol{w}$的偏微分

$\nabla \boldsymbol{v} = \dfrac{\partial loss(\boldsymbol{y}, \hat{\boldsymbol{y}})}{\partial \boldsymbol{v}}$ 隱藏層→輸入層參數為$\boldsymbol{v}$，對loss進行$\boldsymbol{v}$的偏微分



Back-propagation
輸出層→隱藏層



$$loss(\boldsymbol{y},\hat{\boldsymbol{y}}) = \frac{1}{2}(\boldsymbol{y}-\hat{\boldsymbol{y}})^{\boldsymbol{T}}(\boldsymbol{y}-\hat{\boldsymbol{y}})$$
$$= \frac{1}{2}\left(\boldsymbol{y}-f_2(\boldsymbol{z})\right)^{\boldsymbol{T}}\left(\boldsymbol{y}-f_2(\boldsymbol{z})\right)$$
$$= \frac{1}{2}\left(\boldsymbol{y}-f_2(\boldsymbol{w}^{\boldsymbol{T}}\boldsymbol{h})\right)^{\boldsymbol{T}}\left(\boldsymbol{y}-f_2(\boldsymbol{w}^{\boldsymbol{T}}\boldsymbol{h})\right)$$

Chain rule

$$\Delta\boldsymbol{w} = \frac{\partial loss(\boldsymbol{y},\hat{\boldsymbol{y}})}{\partial \boldsymbol{w}} = \boxed{\frac{\partial loss(\boldsymbol{y},\hat{\boldsymbol{y}})}{\partial \boldsymbol{z}}}\boxed{\frac{\partial \boldsymbol{z}}{\partial \boldsymbol{w}}}$$

隱藏層→輸出層

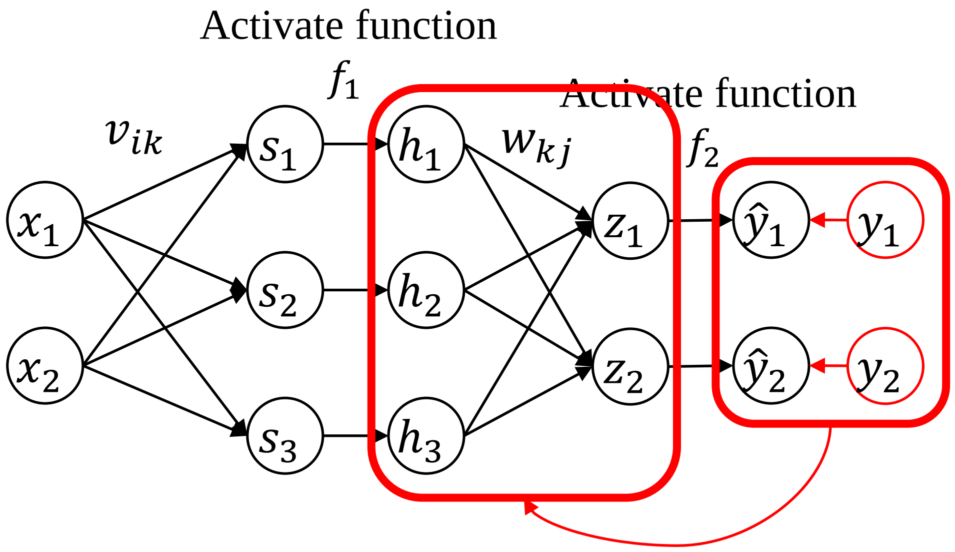
$$\boldsymbol{z} = \boldsymbol{w}^{\boldsymbol{T}}\boldsymbol{h}$$
$$\boldsymbol{y} = f_2(\boldsymbol{z})$$

參數為$\boldsymbol{w}$，因此我們對loss進行$\boldsymbol{w}$的偏微分

$$\boxed{\begin{aligned}\frac{\partial loss(\boldsymbol{y},\hat{\boldsymbol{y}})}{\partial \boldsymbol{z}} &= \frac{\frac{1}{2}\left(\boldsymbol{y}-f_2(\boldsymbol{z})\right)^{\boldsymbol{T}}\left(\boldsymbol{y}-f_2(\boldsymbol{z})\right)}{\partial \boldsymbol{z}}\\ &= \left(\boldsymbol{y}-f_2(\boldsymbol{z})\right)\frac{\partial f_2(\boldsymbol{z})}{\partial \boldsymbol{z}} = (\boldsymbol{y}-\hat{\boldsymbol{y}})f_2{}'(\boldsymbol{z})\end{aligned}}$$

$$\boxed{\frac{\partial \boldsymbol{z}}{\partial \boldsymbol{w}} = \frac{\partial \boldsymbol{w}^{\boldsymbol{T}}\boldsymbol{h}}{\partial \boldsymbol{w}} = \boldsymbol{h}}$$

Back-propagation
輸出層→隱藏層



隱藏層→輸出層

$$\boldsymbol{z} = \boldsymbol{w}^T \boldsymbol{h}$$

$$\boldsymbol{y} = f_2(\boldsymbol{z})$$

參數為$\boldsymbol{w}$，因此我們對loss進行$\boldsymbol{w}$的偏微分

$$loss(\boldsymbol{y}, \hat{\boldsymbol{y}}) = \frac{1}{2}(\boldsymbol{y} - \hat{\boldsymbol{y}})^T(\boldsymbol{y} - \hat{\boldsymbol{y}})$$

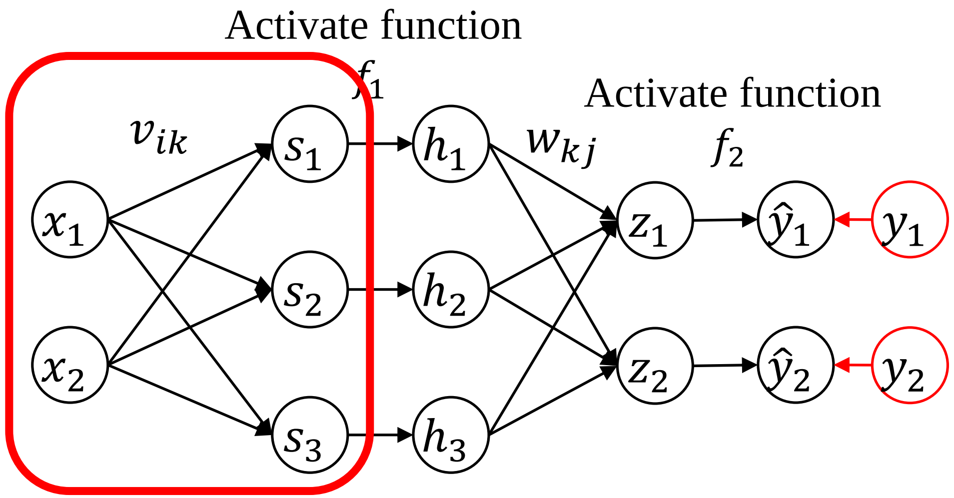
$$= \frac{1}{2}\left(\boldsymbol{y} - f_2(\boldsymbol{z})\right)^{\boldsymbol{T}}\left(\boldsymbol{y} - f_2(\boldsymbol{z})\right)$$

$$= \frac{1}{2}\left(\boldsymbol{y} - f_2(\boldsymbol{w}^T\boldsymbol{h})\right)^{\boldsymbol{T}}\left(\boldsymbol{y} - f_2(\boldsymbol{w}^T\boldsymbol{h})\right)$$

$$\Delta \boldsymbol{w} = \frac{\partial loss(\boldsymbol{y}, \hat{\boldsymbol{y}})}{\partial \boldsymbol{w}} = \frac{\partial loss(\boldsymbol{y}, \hat{\boldsymbol{y}})}{\partial \boldsymbol{z}} \frac{\partial \boldsymbol{z}}{\partial \boldsymbol{w}}$$

$$= (\boldsymbol{y} - \hat{\boldsymbol{y}}) f_2{}'(\boldsymbol{z}) \boldsymbol{h}$$

Back-propagation
隱藏層→輸入層



$$loss(\boldsymbol{y},\widehat{\boldsymbol{y}}) = \left(\boldsymbol{y} - f_2(\boldsymbol{z})\right)^{\boldsymbol{T}}\left(\boldsymbol{y} - f_2(\boldsymbol{z})\right)$$

$$= \frac{1}{2}\left(\boldsymbol{y} - f_2\left(\boldsymbol{w}^{\boldsymbol{T}} f_1(\boldsymbol{s})\right)\right)^{\boldsymbol{T}}\left(\boldsymbol{y} - f_2\left(\boldsymbol{w}^{\boldsymbol{T}} f_1(\boldsymbol{s})\right)\right)$$

$$= \frac{1}{2}\left(\boldsymbol{y} - f_2\left(\boldsymbol{w}^{\boldsymbol{T}} f_1(\boldsymbol{v}^{\boldsymbol{T}}\boldsymbol{x})\right)\right)^{\boldsymbol{T}}\left(\boldsymbol{y} - f_2\left(\boldsymbol{w}^{\boldsymbol{T}} f_1(\boldsymbol{v}^{\boldsymbol{T}}\boldsymbol{x})\right)\right)$$

Chain rule

$$\Delta\boldsymbol{v} = \frac{\partial loss(\boldsymbol{y},\widehat{\boldsymbol{y}})}{\partial\boldsymbol{v}} = \frac{\partial loss(\boldsymbol{y},\widehat{\boldsymbol{y}})}{\partial\boldsymbol{s}}\frac{\partial\boldsymbol{s}}{\partial\boldsymbol{v}} = \boxed{\frac{\partial loss(\boldsymbol{y},\widehat{\boldsymbol{y}})}{\partial\boldsymbol{z}}}\frac{\partial\boldsymbol{z}}{\partial\boldsymbol{s}}\frac{\partial\boldsymbol{s}}{\partial\boldsymbol{v}}$$

前面解過了

$$\frac{\partial loss(\boldsymbol{y},\widehat{\boldsymbol{y}})}{\partial\boldsymbol{z}} = (\boldsymbol{y} - \widehat{\boldsymbol{y}}) f_2{}'(\boldsymbol{z})$$

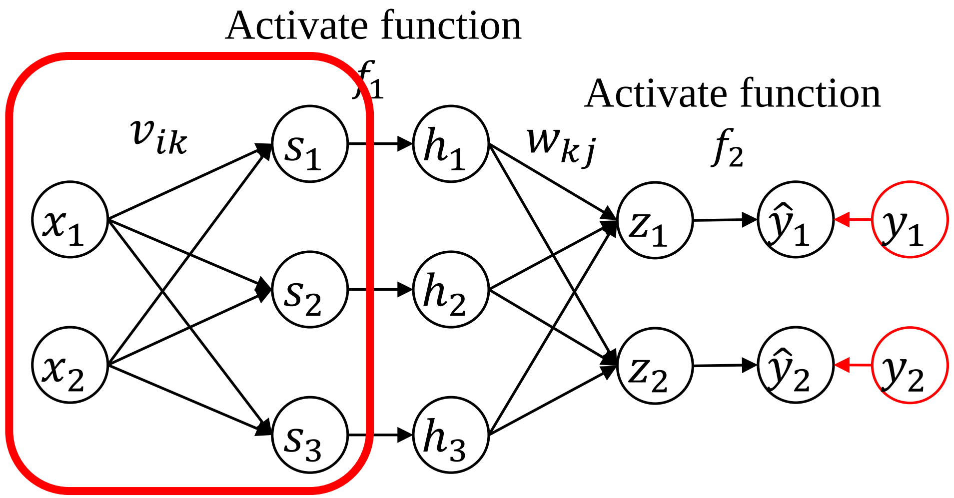
隱藏層→輸入層

$$\boldsymbol{s} = \boldsymbol{v}^{\boldsymbol{T}}\boldsymbol{x}$$

$$\boldsymbol{h} = f_1(\boldsymbol{s})$$

參數為$\boldsymbol{v}$，因此我們對loss進行$\boldsymbol{v}$的偏微分

Back-propagation
隱藏層→輸入層



$$loss(\boldsymbol{y}, \hat{\boldsymbol{y}}) = (\boldsymbol{y} - f_2(\boldsymbol{z}))^{\boldsymbol{T}} (\boldsymbol{y} - f_2(\boldsymbol{z}))$$
$$= \frac{1}{2}\left(\boldsymbol{y} - f_2\left(\boldsymbol{w}^{\boldsymbol{T}} f_1(\boldsymbol{s})\right)\right)^{\boldsymbol{T}} \left(\boldsymbol{y} - f_2\left(\boldsymbol{w}^{\boldsymbol{T}} f_1(\boldsymbol{s})\right)\right)$$
$$= \frac{1}{2}\left(\boldsymbol{y} - f_2\left(\boldsymbol{w}^{\boldsymbol{T}} f_1(\boldsymbol{v}^{\boldsymbol{T}}\boldsymbol{x})\right)\right)^{\boldsymbol{T}} \left(\boldsymbol{y} - f_2\left(\boldsymbol{w}^{\boldsymbol{T}} f_1(\boldsymbol{v}^{\boldsymbol{T}}\boldsymbol{x})\right)\right)$$

Chain rule

$$\Delta \boldsymbol{v} = \frac{\partial loss(\boldsymbol{y}, \hat{\boldsymbol{y}})}{\partial \boldsymbol{v}} = \frac{\partial loss(\boldsymbol{y}, \hat{\boldsymbol{y}})}{\partial \boldsymbol{s}} \frac{\partial \boldsymbol{s}}{\partial \boldsymbol{v}} = \frac{\partial loss(\boldsymbol{y}, \hat{\boldsymbol{y}})}{\partial \boldsymbol{z}} \boxed{\frac{\partial \boldsymbol{z}}{\partial \boldsymbol{s}}} \boxed{\frac{\partial \boldsymbol{s}}{\partial \boldsymbol{v}}}$$

隱藏層→輸入層

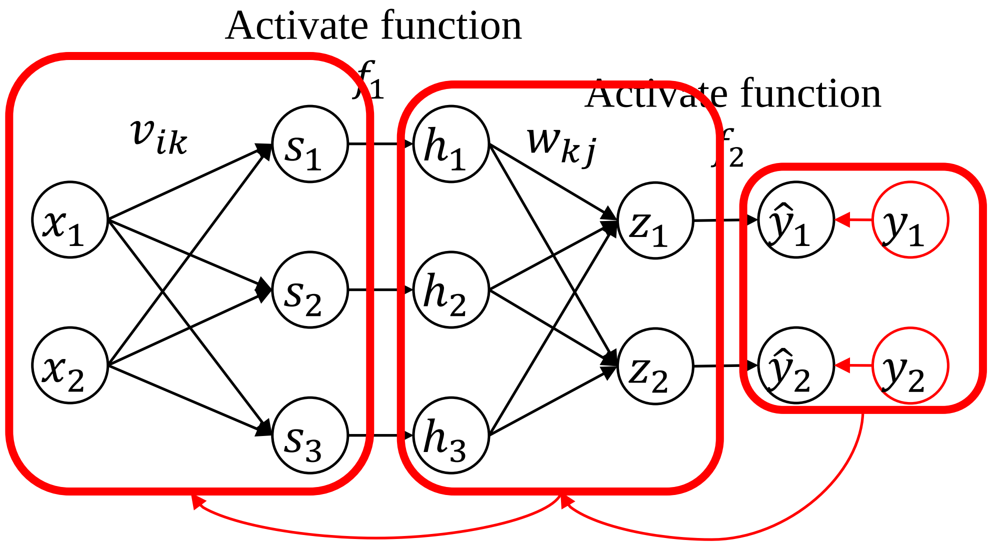
$$\boldsymbol{s} = \boldsymbol{v}^{\boldsymbol{T}} \boldsymbol{x}$$
$$\boldsymbol{h} = f_1(\boldsymbol{s})$$

參數為$\boldsymbol{v}$，因此我們對loss進行$\boldsymbol{v}$的偏微分

$$\boxed{\frac{\partial \boldsymbol{z}}{\partial \boldsymbol{s}} = \frac{\partial \boldsymbol{w}^{\boldsymbol{T}} f_1(\boldsymbol{s})}{\partial \boldsymbol{s}} = \boldsymbol{w}^{\boldsymbol{T}} f_1{}'(\boldsymbol{s})}$$

$$\boxed{\frac{\partial \boldsymbol{s}}{\partial \boldsymbol{v}} = \frac{\partial \boldsymbol{v}^{\boldsymbol{T}} \boldsymbol{x}}{\partial \boldsymbol{v}} = \boldsymbol{x}}$$

Back-propagation
隱藏層→輸入層



隱藏層→輸入層

$$\boldsymbol{s} = \boldsymbol{v}^T\boldsymbol{x}$$

$$\boldsymbol{h} = f_1(\boldsymbol{s})$$

參數為$\boldsymbol{v}$，因此我們對loss進行$\boldsymbol{v}$的偏微分

$$loss(\boldsymbol{y},\hat{\boldsymbol{y}}) = \left(\boldsymbol{y} - f_2(\boldsymbol{z})\right)^{\boldsymbol{T}}\left(\boldsymbol{y} - f_2(\boldsymbol{z})\right)$$

$$= \frac{1}{2}\left(\boldsymbol{y} - f_2\left(\boldsymbol{w}^{\boldsymbol{T}} f_1(\boldsymbol{s})\right)\right)^{\boldsymbol{T}}\left(\boldsymbol{y} - f_2\left(\boldsymbol{w}^{\boldsymbol{T}} f_1(\boldsymbol{s})\right)\right)$$

$$= \frac{1}{2}\left(\boldsymbol{y} - f_2\left(\boldsymbol{w}^{\boldsymbol{T}} f_1(\boldsymbol{v}^{\boldsymbol{T}}\boldsymbol{x})\right)\right)^{\boldsymbol{T}}\left(\boldsymbol{y} - f_2\left(\boldsymbol{w}^{\boldsymbol{T}} f_1(\boldsymbol{v}^{\boldsymbol{T}}\boldsymbol{x})\right)\right)$$

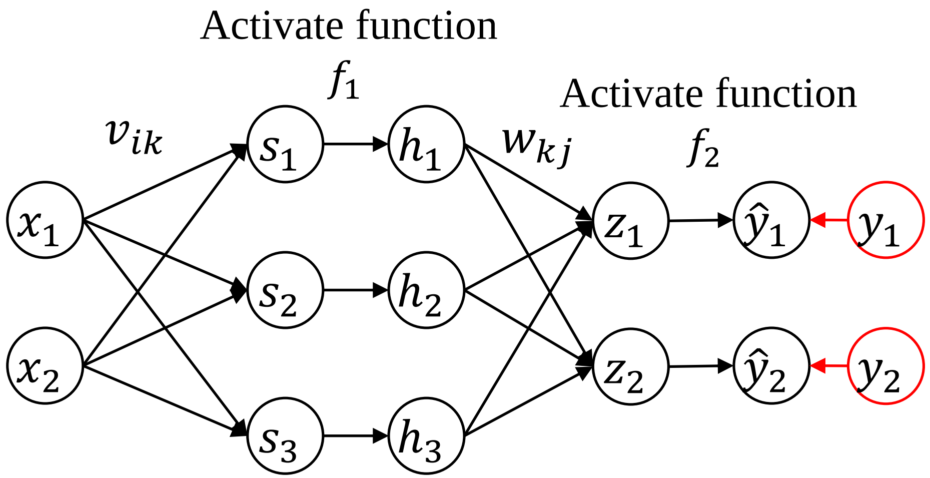
$$\Delta\boldsymbol{v} = \frac{\partial loss(\boldsymbol{y},\hat{\boldsymbol{y}})}{\partial\boldsymbol{v}} = \frac{\partial loss(\boldsymbol{y},\hat{\boldsymbol{y}})}{\partial\boldsymbol{s}}\frac{\partial\boldsymbol{s}}{\partial\boldsymbol{v}} = \frac{\partial loss(\boldsymbol{y},\hat{\boldsymbol{y}})}{\partial\boldsymbol{z}}\frac{\partial\boldsymbol{z}}{\partial\boldsymbol{s}}\frac{\partial\boldsymbol{s}}{\partial\boldsymbol{v}}$$

$$= [(\boldsymbol{y} - \hat{\boldsymbol{y}})f_2{}'(\boldsymbol{z})][\boldsymbol{w}^{\boldsymbol{T}} f_1{}'(\boldsymbol{s})]\boldsymbol{x}$$

Back-propagation

$$\boldsymbol{w}^{(t+1)} = \boldsymbol{w}^{(t)} - \alpha\Delta\boldsymbol{w}^{(t)}$$

$$\boldsymbol{v}^{(t+1)} = \boldsymbol{v}^{(t)} - \alpha\Delta\boldsymbol{v}^{(t)}$$



輸出層→隱藏層參數為$\boldsymbol{w}$

$$\Delta\boldsymbol{w} = \boxed{(\boldsymbol{y} - \hat{\boldsymbol{y}})f_2{}'(\boldsymbol{z})}\boldsymbol{h}$$

隱藏層→輸入層參數為$\boldsymbol{v}$

$$\Delta\boldsymbol{v} = \boxed{[(\boldsymbol{y} - \hat{\boldsymbol{y}})f_2{}'(\boldsymbol{z})]}\boxed{[\boldsymbol{w}^{\boldsymbol{T}} f_1{}'(\boldsymbol{s})]}\boldsymbol{x}$$

輸入層→隱藏層

$$\boldsymbol{s} = \boldsymbol{v}^{\boldsymbol{T}}\boldsymbol{x}$$
$$\boldsymbol{h} = f_1(\boldsymbol{s})$$

隱藏層→輸出層

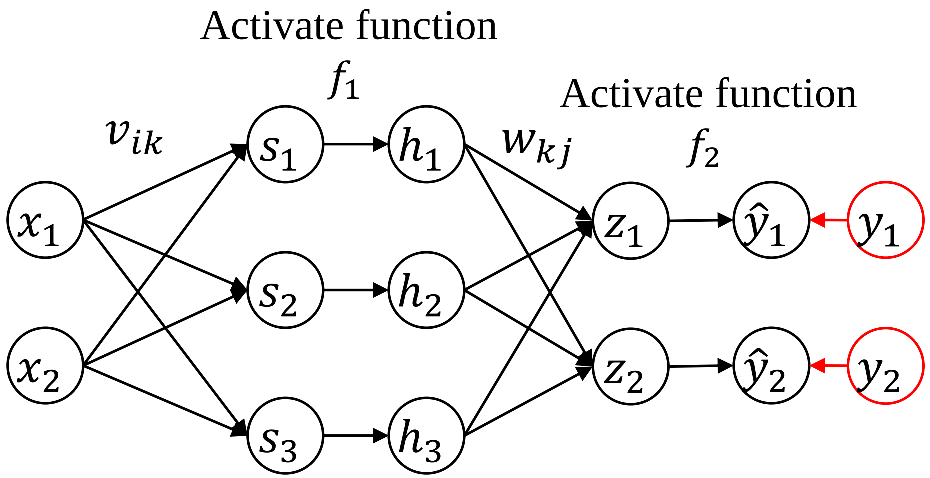
$$\boldsymbol{z} = \boldsymbol{w}^{\boldsymbol{T}}\boldsymbol{h}$$
$$\boldsymbol{y} = f_2(\boldsymbol{z})$$

前面層的gradient
會是由後面所有層的gradient和現在這層的疊乘。

神經網路太深層的問題

神經網路太深層的問題

Sigmoid在神經網路太深層的問題



輸出層→隱藏層參數為$\boldsymbol{w}$

$$\Delta \boldsymbol{w} = \boxed{(\boldsymbol{y}-\hat{\boldsymbol{y}}) f_2'(\boldsymbol{z})}\boldsymbol{h}$$

隱藏層→輸入層參數為$\boldsymbol{v}$

$$\Delta \boldsymbol{v} = \boxed{[(\boldsymbol{y}-\hat{\boldsymbol{y}}) f_2'(\boldsymbol{z})]}\boxed{[\boldsymbol{w}^{\boldsymbol{T}} f_1'(\boldsymbol{s})]}\boldsymbol{x}$$

Sigmoid : $f(x) = \frac{1}{1+e^{-x}}$

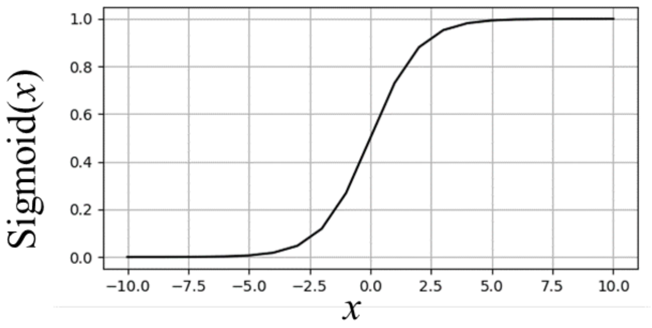
$$f' = f(x)(1-f(x))$$

輸入層→隱藏層

$$\boldsymbol{s} = \boldsymbol{v}^{\boldsymbol{T}}\boldsymbol{x}$$
$$\boldsymbol{h} = f_1(\boldsymbol{s})$$

隱藏層→輸出層

$$\boldsymbol{z} = \boldsymbol{w}^{\boldsymbol{T}}\boldsymbol{h}$$
$$\boldsymbol{y} = f_2(\boldsymbol{z})$$

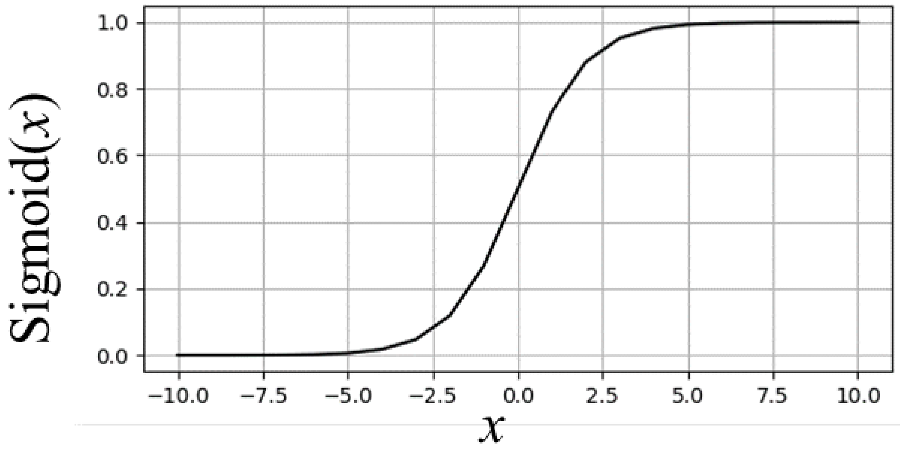


Sigmoid在神經網路太深層的問題

Sigmoid : $f(x) = \frac{1}{1+e^{-x}}$

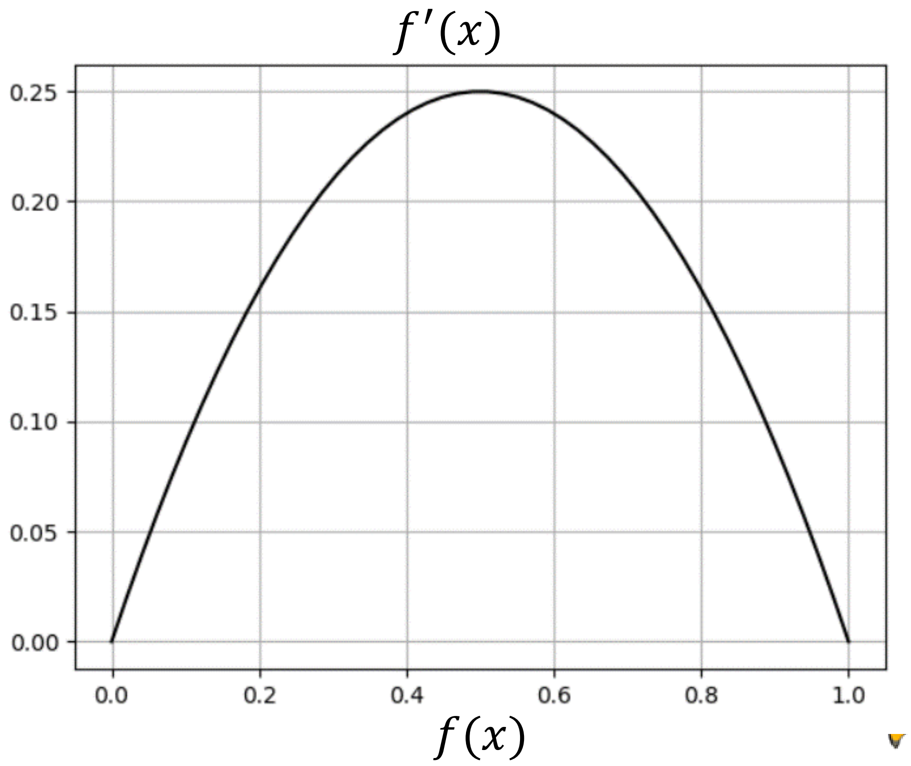
$f'(x) = f(x)\big(1 - f(x)\big)$

$f(x)$輸出介於0~1



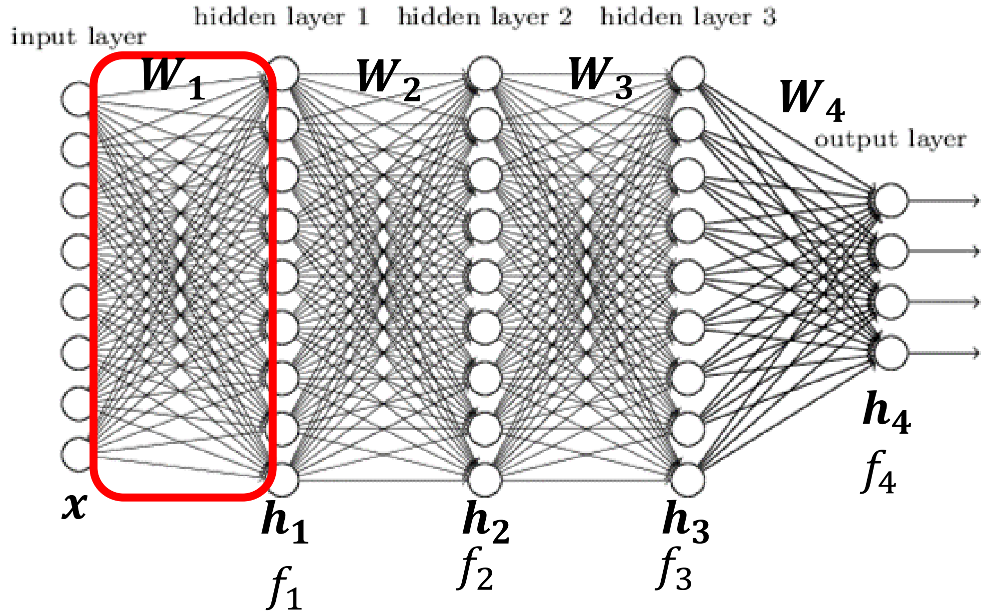
$f'(x)$會更小，最大值為0.25

$f(x) = 0.5$，$f'(x) = 0.5 \times 0.5 = 0.25$



Sigmoid在神經網路太深層的問題

MLP



$$\Delta W_1 = [(y-\hat{y})f_4'(h_4)][W_3^T f_3'(h_3)][W_2^T f_2'(h_2)][W_1^T f_1'(h_1)]x$$

所以當層數到100層時候，對於第一層的gradient會有100個activate function的導數相乘。

剛剛sigmoid已經說了，其導數最大為0.25。

所以$0.25^{100} \approx 0$

這就是梯度消失問題(Vanishing gradient)

如果導數值單調大於1時，就會發生**梯度爆炸問題（exploding gradient problem）**。

如何舒緩Gradient造成的問題

- 1. 重新設計網路架構: 更少的層。
- 2. Rectified Linear Activation (ReLU)
- 3. Gradient Clipping (Keras預設 clipnorm = 1.0和clipvalue = 0.5。)
- 4. Weight Regularization (L1 or L2 Regularizers)

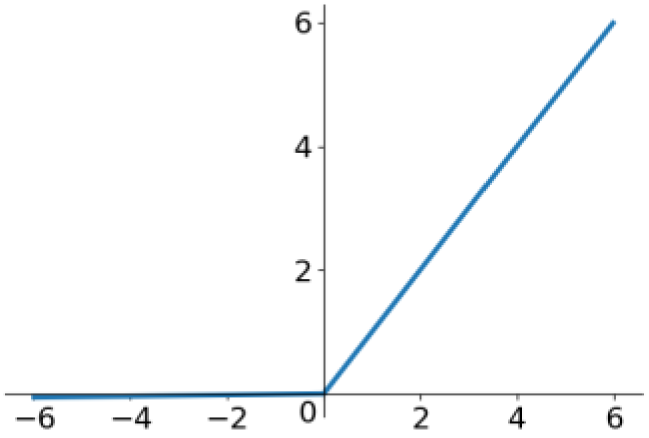
實際解決神經網路太深層的方法: Residual block。

本次介紹不考慮RNN系列的設計。

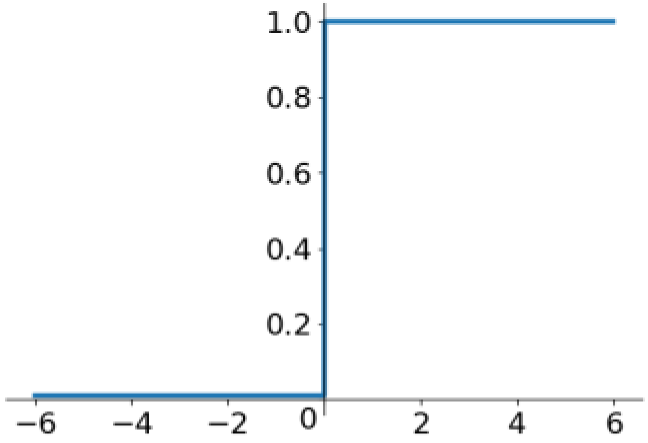
ReLu在神經網路如何舒緩Gradient的問題

- $\mathrm{ReLU}(x) = \max(0, x) = \begin{cases} x & if\ x > 0 \\ 0 & O.W. \end{cases}$
- $\mathrm{ReLU}(x)$的導數 $= \begin{cases} 1 & if\ x > 0 \\ 0 & O.W. \end{cases}$

ReLU函數並不是全區間皆可微分，但是不可微分的部分可以使用Sub-gradient進行取代



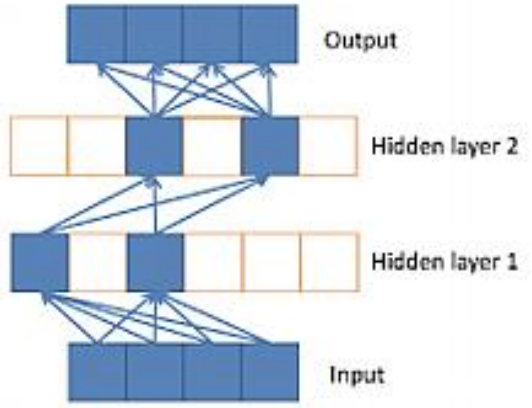
ReLU(x)



ReLU(x)導數

ReLu在神經網路如何舒緩Gradient的問題

- ReLU激勵函數會使負數部分的神經元輸出為0，可以讓網路變得更加多樣性，如同Dropout的概念，可以緩解過擬合(Over fitting)之問題。



- **衍生Dead ReLU的問題**，當某個神經元輸出為0後，就難以再度輸出值，當遇到以下兩種情形時容易導致dead ReLU發生。
- 初始化權重設定為不能被激活的數值。
- 學習率設置過大，在剛開始進行誤差反向傳遞時，容易修正權重值過大，導致權重梯度為0，神經元即再也無法被激活。

ResNet

此Residual block有兩層，第一層權重為w_1，第二層權重為w_1
第一層輸出:

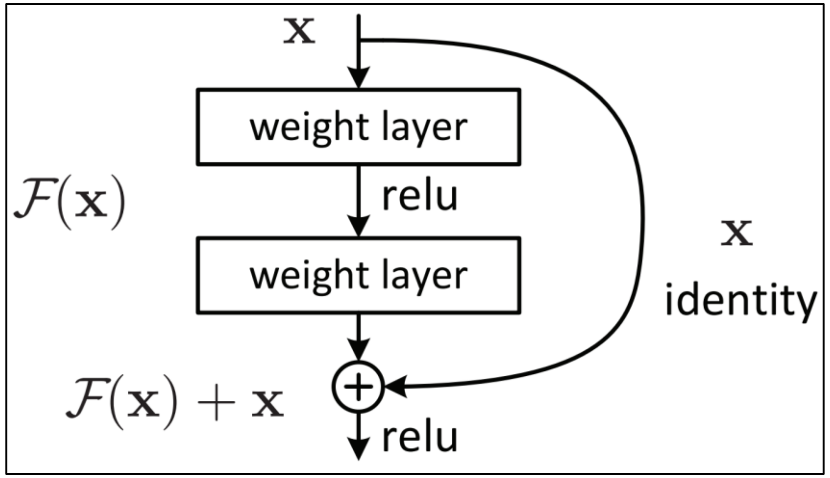
$$\text{relu}(w_1 x)$$

第二層輸出:

$$F(x) = w_2 \text{relu}(w_1 x)$$

最後element-add後結果:

$$H(x) = F(x) + x$$



假設神經網路太深對應用沒有幫助

1. 沒有shortcut connection (residual) ，兩層的輸出結果叫做$H(x)$

最理想狀況就是 $H(x)$ = **$F(x) = x$** (identity mapping)

2. 有shortcut connection，$H(x) = F(x) + x \rightarrow \boxed{F(x) = H(x) - x}$

最理想狀況就是 **$F(x) = 0$**

2的優化找weight解會比1容易。

ResNet

假設我們的residual block只有一層權重為w

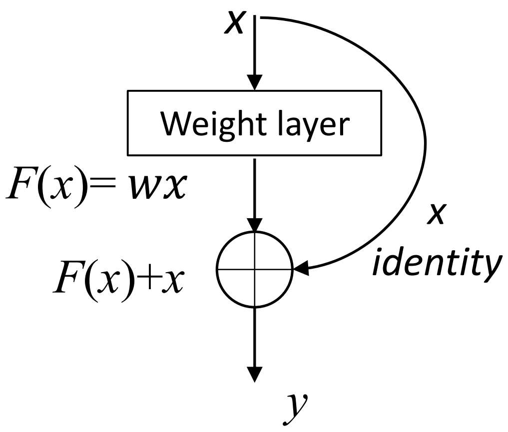
1. 沒有shortcut connection(residual) ，兩層的輸出結果叫做$H(x)$

$$F(x) = wx = x$$

2. 有**shortcut connection**，$H(x) = F(x) + x \rightarrow F(x) = H(x) - x$

$$F(x) = wx = 0$$

residual block



Gradient:

1. $\frac{\partial E}{\partial w} = \frac{(\hat{y}-y)^2}{\partial w} = \frac{(wx-y)^2}{\partial w} = 2(wx-y)x$

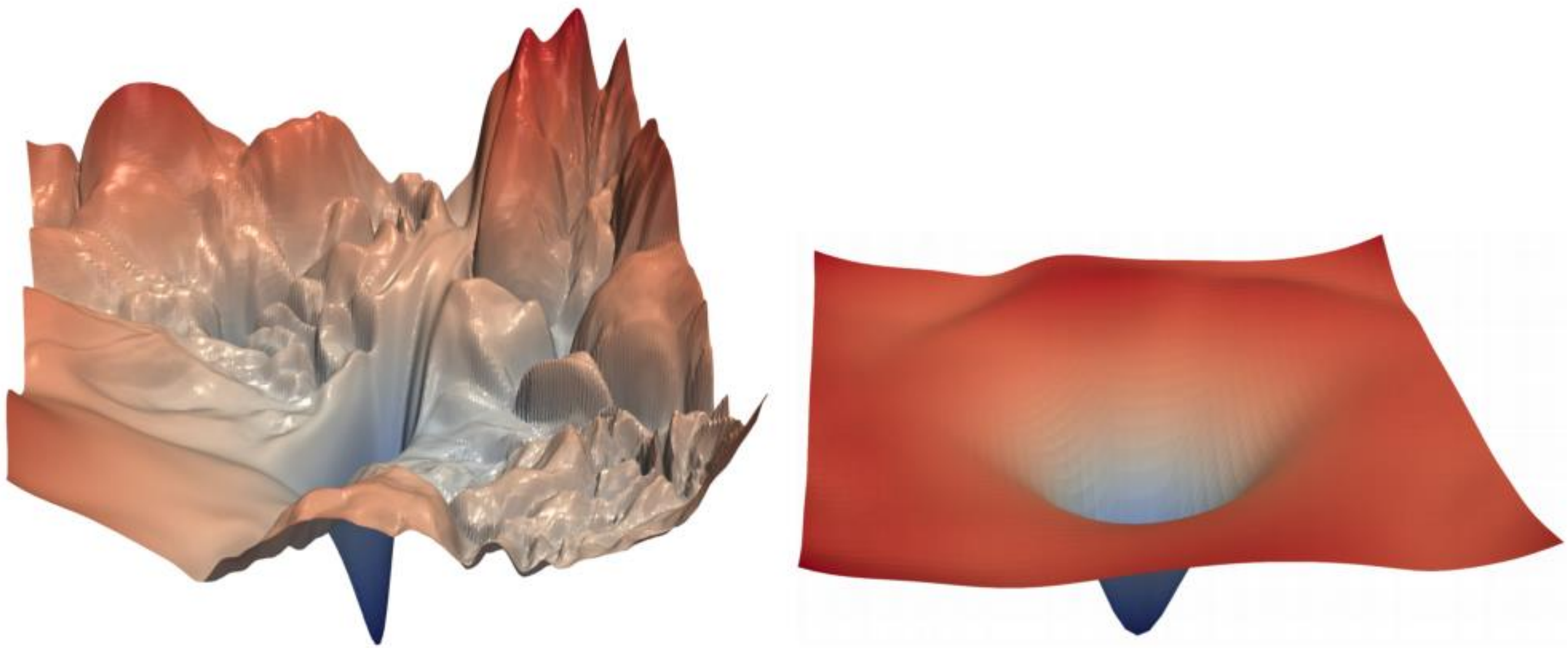
2. $\frac{\partial E}{\partial w} = \frac{(\hat{y}-y)^2}{\partial w} = \frac{(wx+x-y)^2}{\partial w} = 2(wx-y)x + \mathbf{2x^{2}}$

接近0

假設越後面層的Gradient很小，甚至Gradient vanish)。

$$\Delta \boldsymbol{W_1} = [(\boldsymbol{y}-\hat{\boldsymbol{y}})f_4'(\boldsymbol{h_4})][\boldsymbol{W_3^T}f_3'(\boldsymbol{h_3})][\boldsymbol{W_2^T}f_2'(\boldsymbol{h_2})][\boldsymbol{W_1^T}f_1'(\boldsymbol{h_1})]\boldsymbol{x}$$

題外話: 有Residual block的loss space



(a) without skip connections (b) with skip connections

Figure 1: The loss surfaces of ResNet-56 with/without skip connections. The proposed filter normalization scheme is used to enable comparisons of sharpness/flatness between the two figures.

Visualizing the Loss Landscape of Neural Nets

導傳遞

- 神經網路如何利用導傳遞找解
- 神經網路太深層的問題:

梯度消失問題(Vanishing gradient)/梯度爆炸問題（exploding gradient problem）。

Activation Function為什麼要採用ReLU，而不是用Sigmoid。

Residual block克服神經網路不能太深層的問題。

Weight initialization

- 神經網路結構設定完成後，最重要的是

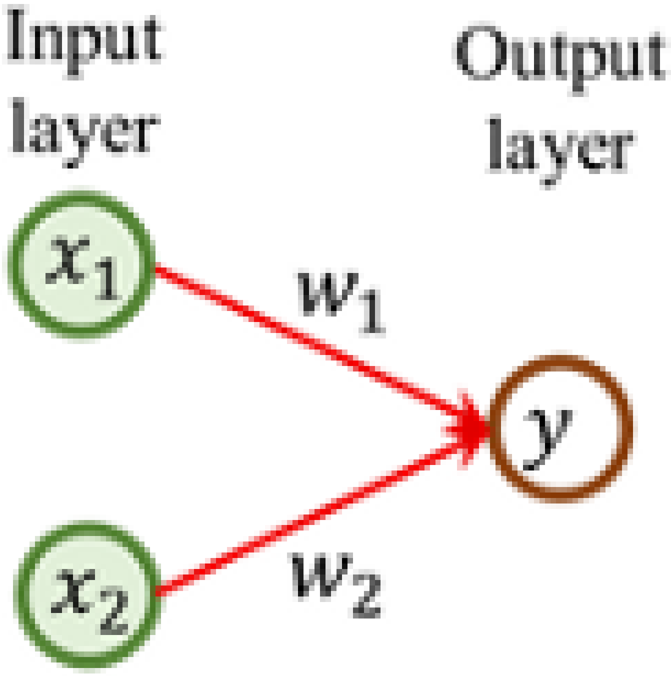
1. 如何更新權重 (梯度下降法)
2. 權重如何初始設定

- Weight initialization和□Batch Normalization

Outline

- 1. weight初始值是0
- 2. Random initialization
- 3. Xavier initialization
- 4. He initialization
- 5. Batch Normalization

weight初始值是0



$$y = w_1x_1 + w_2x_2$$

Backward update:

$$w_i = w_i - \eta\Delta w_i$$

Forward:

$$\hat{y} = w_1x_1 + w_2x_2 = 0$$

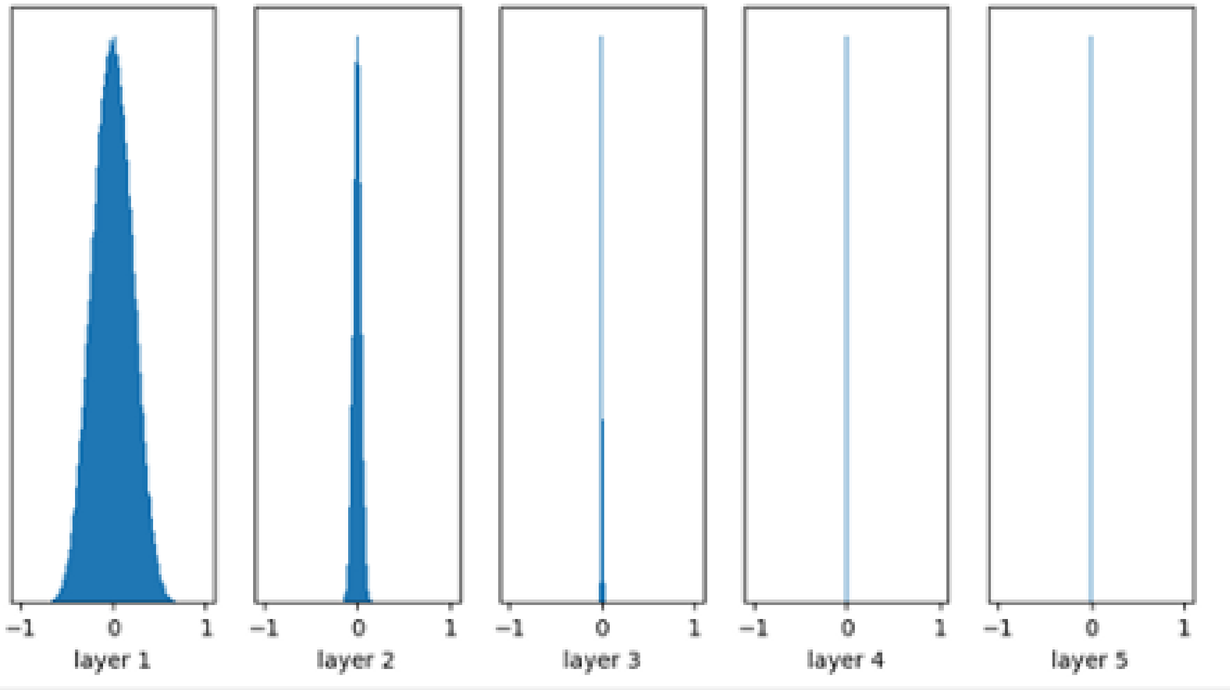
weight的gradient

$$\Delta w_i = \frac{\partial E}{\partial w_i} = \frac{\frac{1}{2}y^2}{\partial w_i} = 0$$

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

Random initialization

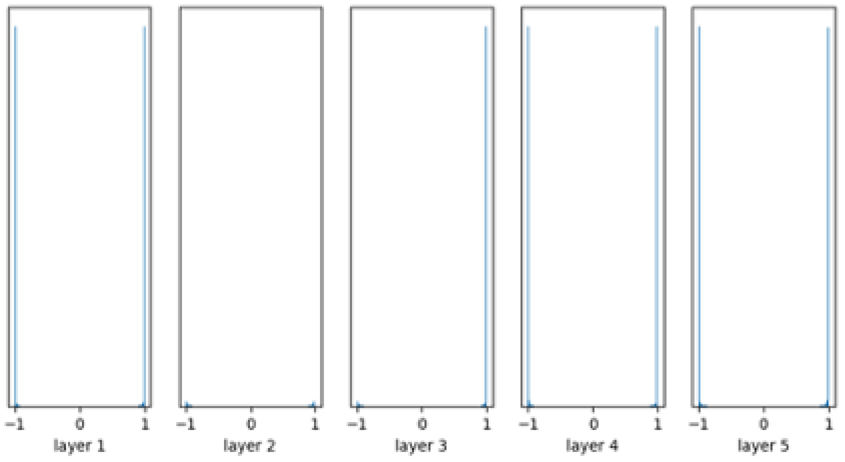
所以第二個最簡單的想法，初始權重用隨機方式建立。
我們建立一個6層的MLP，每一層輸出的activation用tanh。
Weight從**常態分佈(平均數為0，標準差為0.01)**生成



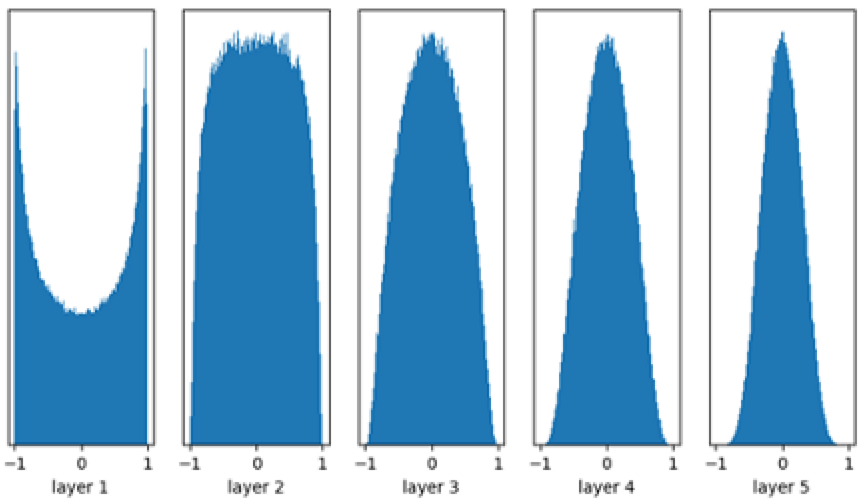
input mean 0.00065 and std 0.99949
layer 1 mean 0.00025 and std 0.21350
layer 2 mean -0.00002 and std 0.04516
layer 3 mean -0.00001 and std 0.00899
layer 4 mean -0.00000 and std 0.00168
layer 5 mean -0.00000 and std 0.00029

Random initialization

實驗2. 常態分佈(平均數為0，標準差為1)

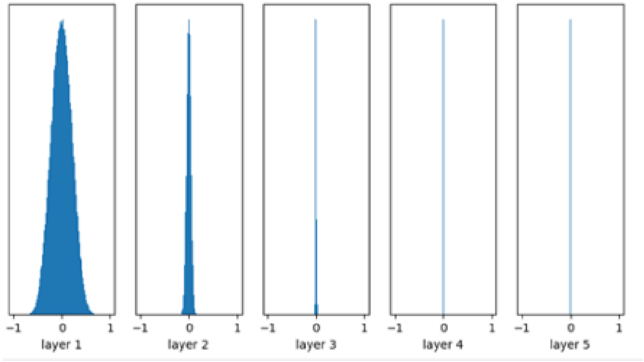


實驗3. 常態分佈(平均數為0，標準差為0.05)

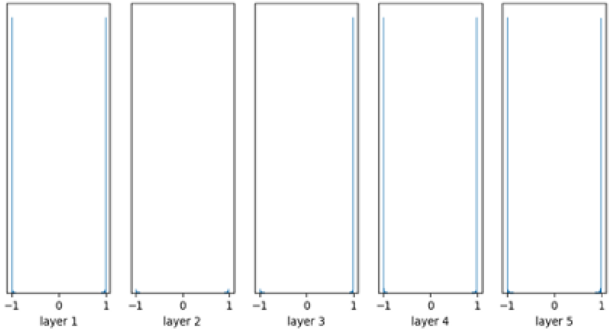


Random initialization

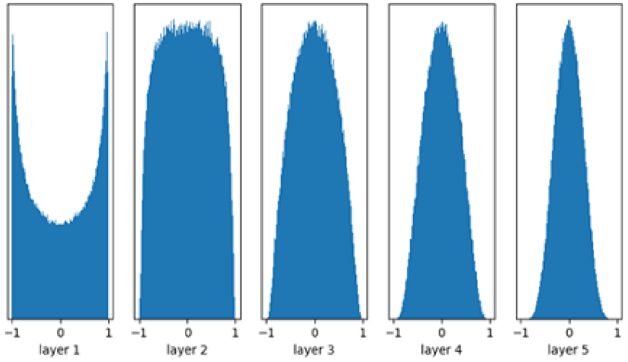
常態分佈
(平均數為0，標準差為0.02)



常態分佈
(平均數為0，標準差為1)



常態分佈
(平均數為0，標準差為0.05)



weight初始值從常態分布(也可以用均勻分布)的標準差變化會影響結果。

Xavier initialization

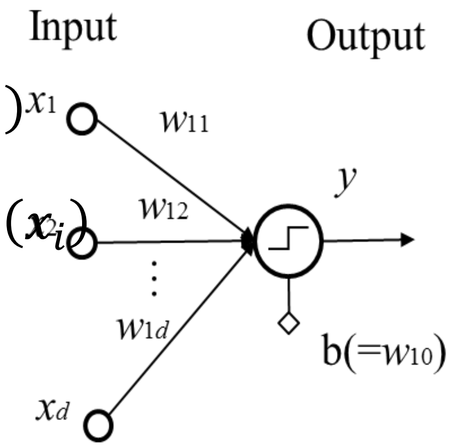
- 由Random initialization得知weight權重的生成會影響神經元的輸出太集中或是過於飽和。
- Xavier的論文(Understanding the difficulty of training deep feedforward neural networks)的想法是希望神經元輸入(*xi*, *i=1,2,…,d*)和輸出(*y*)的變異數(variance，標準差的平方)保持一致。

Suppose $x_i, w_i \overset{iid}{\sim} Distribution(mean = 0)$

$$y = w_1x_1 + w_2x_2 + \cdots + w_dx_d \text{ (bias先不考慮)}$$

$$Var(y) = Var(w_1x_1 + w_2x_2 + \cdots + w_dx_d) = \sum_i^d Var(w_ix_i)$$

$$Var(w_ix_i) = \mathrm{E}(x_i)^2Var(w_i) + \mathrm{E}(w_i)^2Var(x_i) + Var(w_i)Var(x_i)$$



Xavier initialization

$$Var(y) = Var(w_1x_1 + w_2x_2 + \cdots + w_dx_d) = \sum_{i}^{d} Var(w_ix_i)$$

$$Var(w_ix_i) = Var(w_i)Var(x_i)$$

$$Var(y) = \sum_{i}^{d} Var(w_ix_i) = \sum_{i}^{d} Var(w_i)Var(x_i) = d \times Var(w_i)Var(x_i)$$

- Xavier initialization的想法是希望$Var(y)$=1

$$Var(y) = d \times Var(w_i)Var(x_i) = 1 \Rightarrow Var(w_i) = \frac{1}{d \times Var(x_i)}$$

因為前一層的輸出我們也希望其variance=1 (所以資料前處理很常做z-score處理)

$$Var(w_i) = \frac{1}{d} = \frac{1}{n_{inputnode}}$$

Xavier initialization

同樣得程序在back-propagation也推一遍就可以得到

$$Var(w_i) = \frac{1}{n_{outputnode}}$$

為了希望forward和backward的variance可以一致，除非$n_{inputnode} = n_{outputnode}$，文章就直接取

$$Var(w_i) = \frac{2}{n_{inputnode} + n_{outputnode}}$$

$$Var(y) = d \times Var(w_i) = = \frac{2n_{inputnode}}{n_{inputnode} + n_{outputnode}}$$

Xavier initialization

如果採用相加除以2:

$$\frac{\left(\frac{1}{n_{inputnode}}+\frac{1}{n_{outputnode}}\right)}{2}=\left(\frac{n_{inputnode}+n_{outputnode}}{2n_{outputnode}n_{inputnode}}\right)$$

Suppose

Layer 1 node=32, Layer 2 node=64, Layer 3 node=128

$$Var(w_i)=\frac{2}{n_{inputnode}+n_{outputnode}}$$

Layer 1 = 2/(32+64)=2/96=0.021, Layer 2= 2/(64+128)=2/192=0.01

Layer 1 = (32+64)/(2*32*64)=0.023, Layer 2= (32+64)/(2*64*128)=0.00586

Note how both constraints are satisfied when all layers have the same width.

constraints: $Var(w_i)=\frac{1}{n_{inputnode}}$, $Var(w_i)=\frac{1}{n_{outputnode}}$

Xavier initialization

- 文章提到假設每一層的node數一樣

$$Var(w_i) = \frac{2}{n_{inputnode} + n_{outputnode}}$$

$$\forall i, Var\left[\frac{\partial Cost}{\partial s^i}\right] = \boxed{\left[nVar[W]\right]^{d-i}} Var[x] \qquad (13)$$

$$\forall i, Var\left[\frac{\partial Cost}{\partial w^i}\right] = \boxed{\left[nVar[W]\right]^{d}} Var[x] Var\left[\frac{\partial Cost}{\partial s^d}\right] \qquad (14)$$

所以這個方法只能盡量緩和gradient vanish/explode，不能避免。

Xavier initialization

$$w_i \overset{iid}{\sim} U(a, b)$$

$$var(w_i) = \frac{(b-a)^2}{12}$$

一般用均匀分布

$$w_i \overset{iid}{\sim} U(-\frac{1}{\sqrt{n}}, \frac{1}{\sqrt{n}})$$

$$var(w_i) = \frac{\left(\frac{2}{\sqrt{n}}\right)^2}{12} = \frac{1}{3n} = n\ var(w_i) = \frac{1}{3}$$

論文建議用他們提出來的normalized initialization

$$w \sim U\left(-\sqrt{\frac{6}{n_{inputnode} + n_{outputnode}}}, \sqrt{\frac{6}{n_{inputnode} + n_{outputnode}}}\right)$$

Xavier initialization

$$w_i \overset{iid}{\sim} U(-b, b)$$

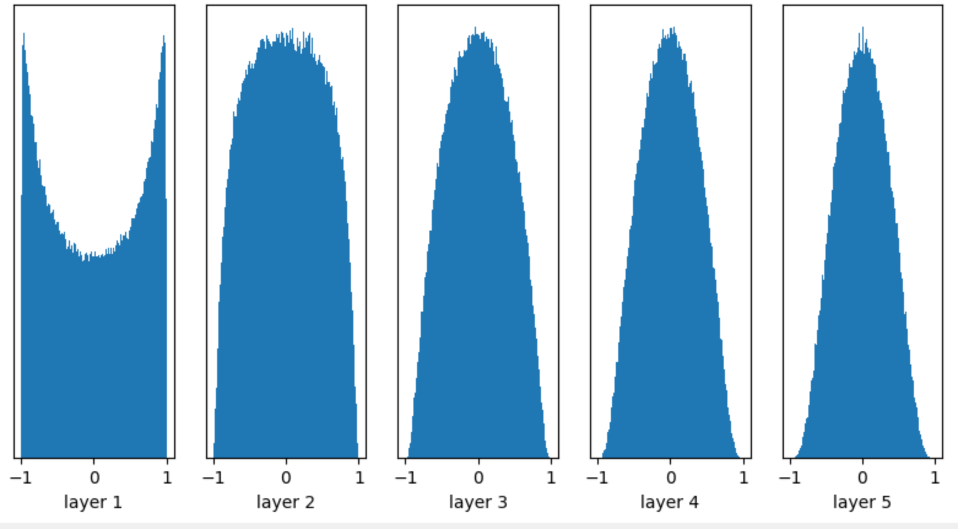
$$var(w_i) = \frac{(b-a)^2}{12} = \frac{b^2}{3} = \frac{2}{n_{inputnode} + n_{outputnode}}$$

$$\Rightarrow b^2 = \frac{6}{n_{inputnode} + n_{outputnode}}$$

$$\Rightarrow b = \sqrt{\frac{6}{n_{inputnode} + n_{outputnode}}}$$

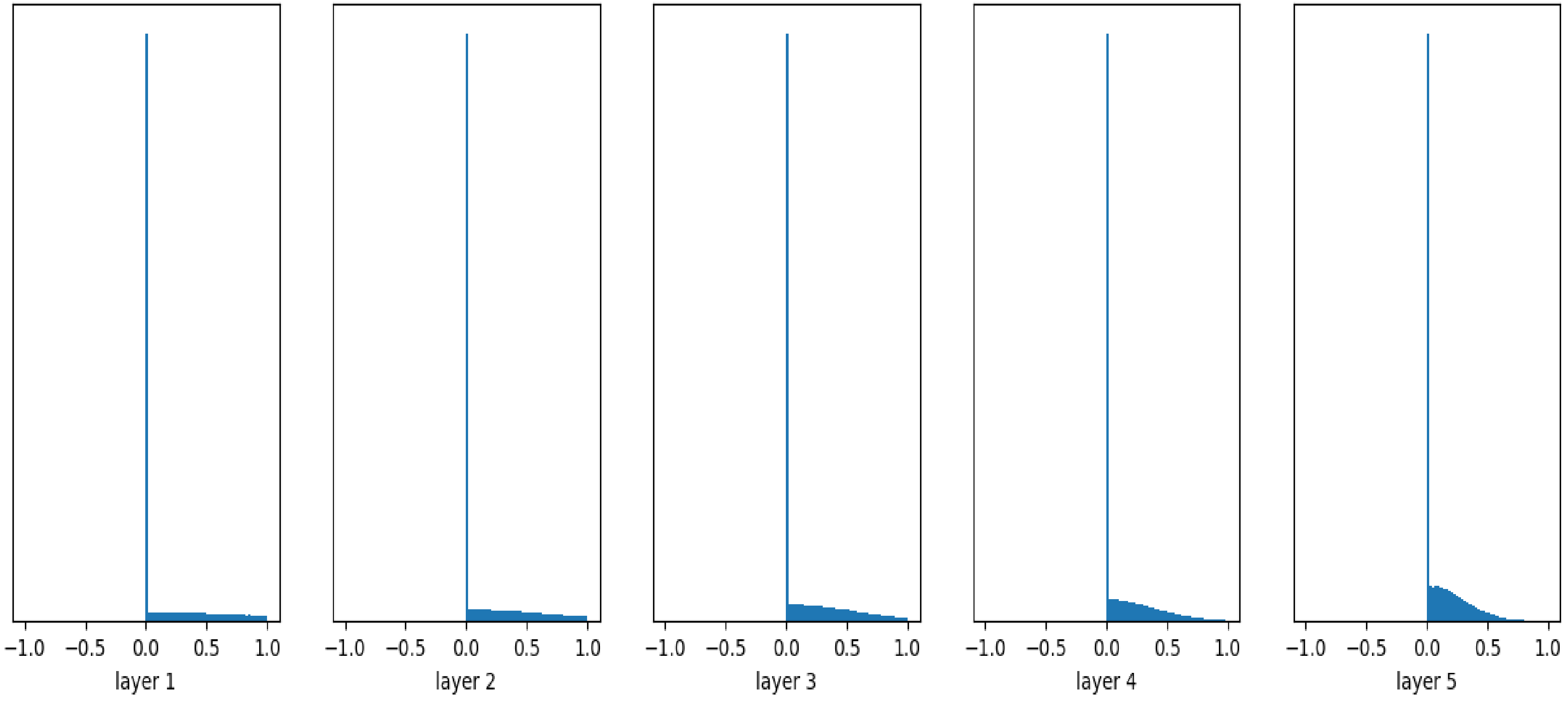
Xavier initialization

實驗一: 用Xavier initialization，神經網路activation function採用tanh輸出。



Xavier initialization

實驗二: 用Xavier initialization，神經網路activation function採用ReLU輸出。後深層值會越接近0。



He initialization

He initialization為何鎧明的文章[Delving deep into rectifiers: Surpassing human-level performance on ImageNet classification]

$$Var(y) = d \times Var(w_i)Var(x_i)$$

因為He initialization的推導稍微複雜一點，需要引入前層和當層的關係，所以我將公式修改成

$$Var(y_l) = n_l \times Var(w_l)Var(x_l)$$

- y_l:第*l*層的輸出
- n_l: 第*l*層輸入神經元數量
- w_l: 第*l*層的權重
- x_l: 第*l*層的輸入，且$x_l = f(y_{l-1}), f$: ReLU

He initialization

w_{l-1}是對稱於0的分佈，所以y_{l-1}的結果也是對稱於0的分佈(平均數等於0)

$$Var(x_l) = Var\left(f(y_{l-1})\right) = \frac{1}{2}Var(y_{l-1})$$

$$Var(y_l) = \frac{n_l}{2} \times Var(w_l)Var(y_{l-1})$$

$$Var(y_L) = \frac{n_L}{2} \times Var(w_L)Var(y_{L-1})$$

$$= \frac{n_L}{2} \times Var(w_L) \times \frac{n_{L-1}}{2}Var(w_{L-1})Var(y_{L-2}) = \cdots$$

$$= Var(y_1)\left(\prod_{l=2}^{L}\frac{n_l}{2}Var(w_l)\right)$$

只要這個variance大於1或是小於1都會因為層數增加造成vanish或是explosion

He initialization

$$\frac{n_l}{2} Var(w_l) = 1 \Rightarrow Var(w_l) = \frac{2}{n_l}, \forall l$$

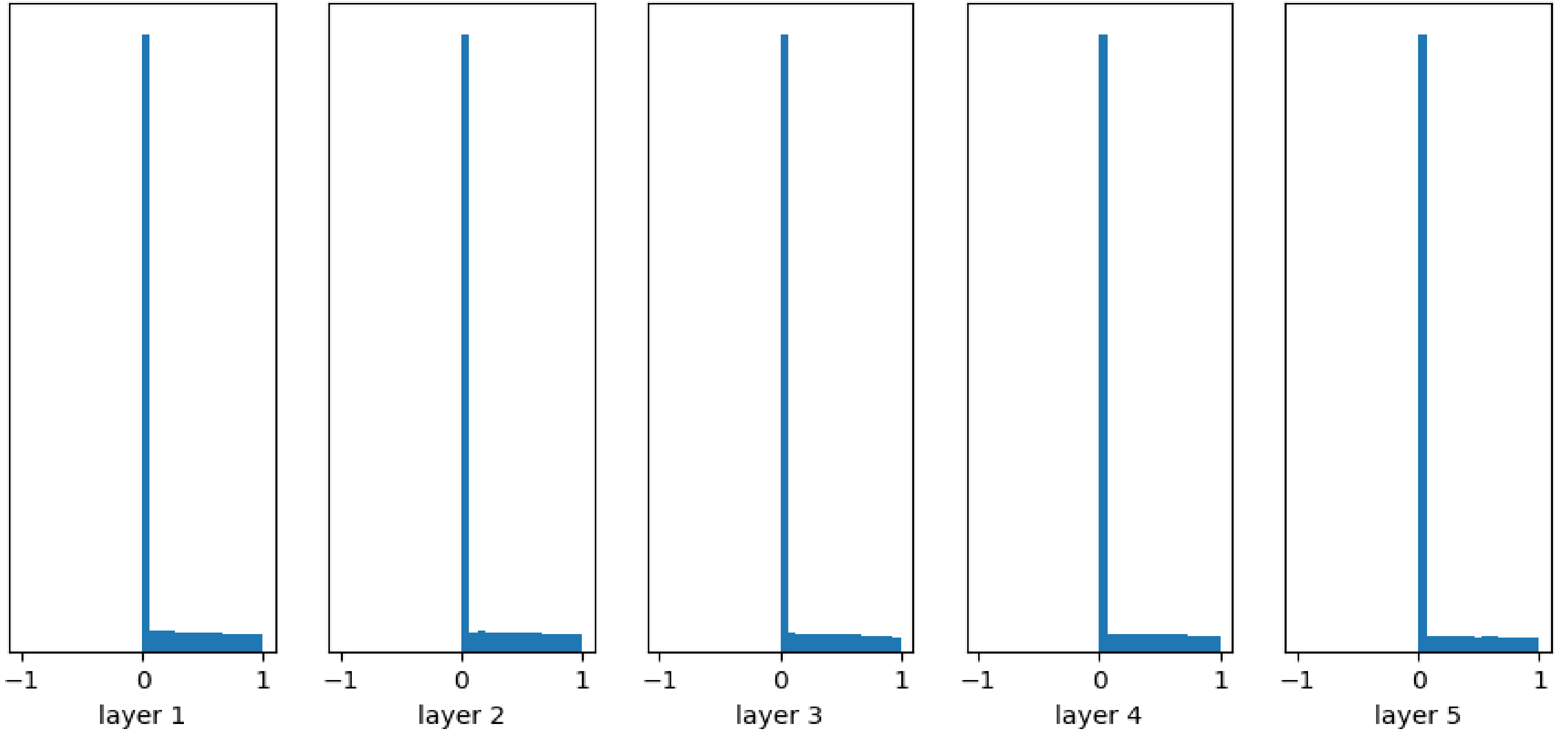
$$w_i \overset{iid}{\sim} U(-b, b)$$

$$var(w_i) = \frac{(b-(-b))^2}{12} = \frac{2}{n_l} \Rightarrow b^2 = \frac{6}{n_l} \Rightarrow b = \sqrt{\frac{6}{n_l}}$$

$$w \sim U\left(-\sqrt{\frac{6}{n_l}}, \sqrt{\frac{6}{n_l}}\right)$$

He initialization

實驗: 剛剛 Xavier initialization發生問題的例子，改用He initialization，神經網路activation function採用ReLU輸出。



Batch Normalization

- Weight Initialization前面說了這麼多，不外乎是要怎麼有效決定weight生成時分佈的參數。
- 有沒有不管參數生成方法都可以避免發生問題的方法: Batch Normalization(BN)。(Batch Normalization: Accelerating Deep Network Training by Reducing Internal Covariate Shift)
- 我們剛剛前面都希望輸出的變異數等於1 ($Var(y) = 1$)

最簡單的方式統計學的z-score

假設資料是$x \sim N(\mu, \sigma)$

$$\frac{x-\mu}{\sigma} \sim N(0,1)$$

Batch Normalization

Input: Values of x over a mini-batch: $\mathcal{B} = \{x_{1...m}\}$;
Parameters to be learned: γ, β

Output: $\{y_i = \mathrm{BN}_{\gamma,\beta}(x_i)\}$

$$\mu_{\mathcal{B}} \leftarrow \frac{1}{m}\sum_{i=1}^{m} x_i \qquad \text{// mini-batch mean}$$

$$\sigma_{\mathcal{B}}^2 \leftarrow \frac{1}{m}\sum_{i=1}^{m} (x_i - \mu_{\mathcal{B}})^2 \qquad \text{// mini-batch variance}$$

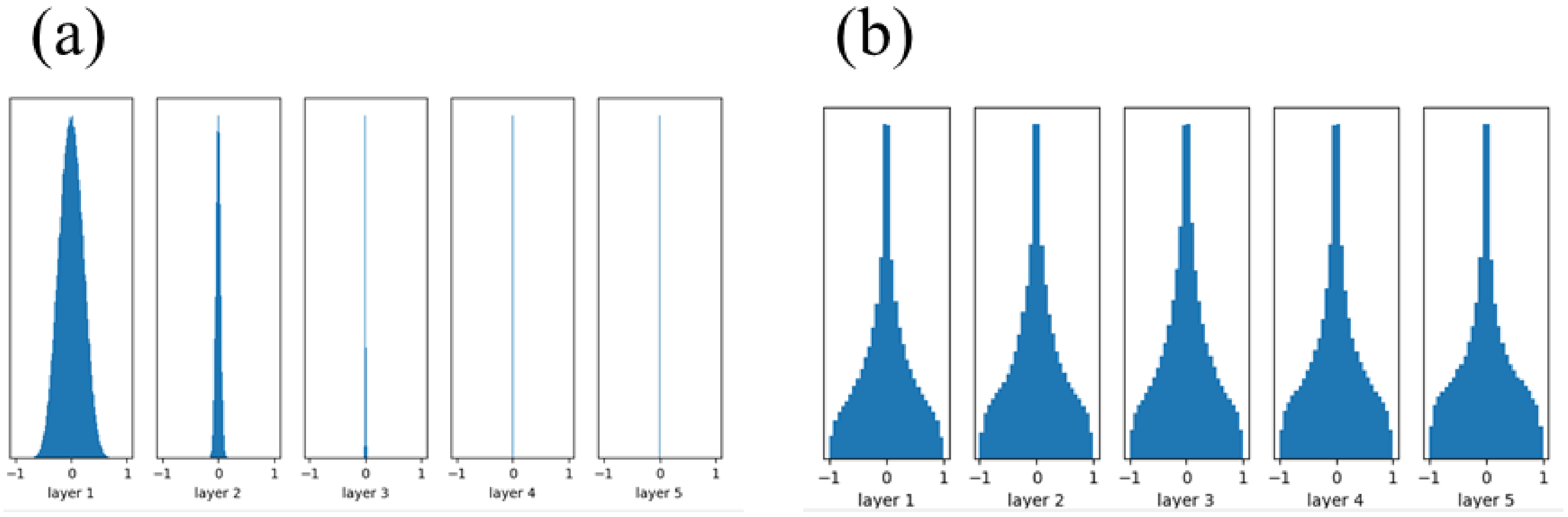
強制把值拉到標準常態:$\frac{x-\mu}{\sigma} \sim N(0,1)$

$$\widehat{x}_i \leftarrow \frac{x_i - \mu_{\mathcal{B}}}{\sqrt{\sigma_{\mathcal{B}}^2 + \epsilon}} \qquad \text{// normalize}$$

$$y_i \leftarrow \gamma \widehat{x}_i + \beta \equiv \mathrm{BN}_{\gamma,\beta}(x_i) \qquad \text{// scale and shift}$$

Batch Normalization

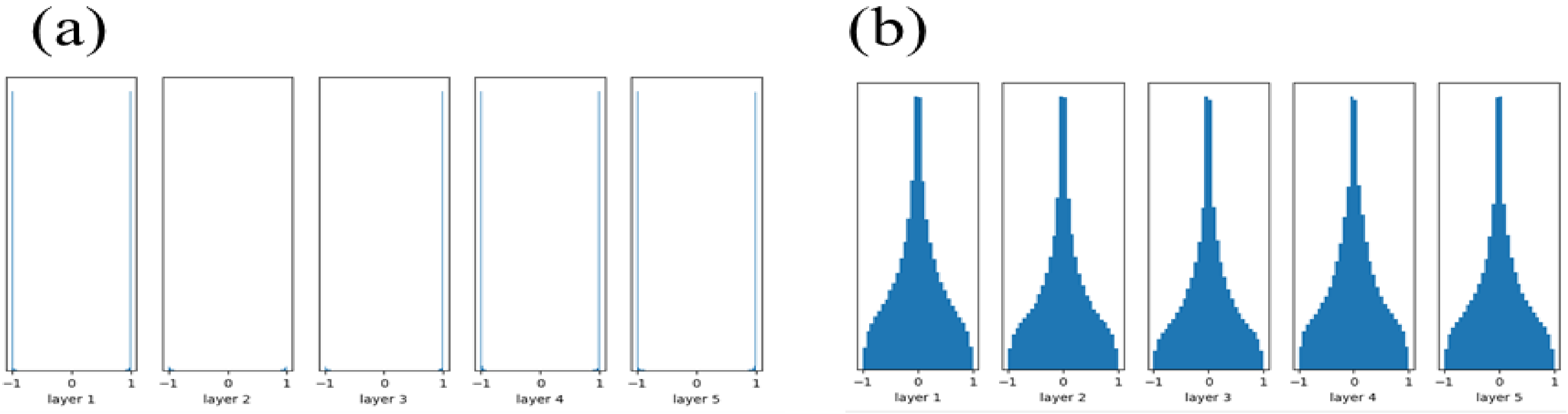
實驗1. Weight是由常態分佈隨機生成(平均數為0，標準差為0.01)。



(a) 神經網路沒有加Batch normalization，(b)神經網路加入Batch normalization。

Batch Normalization

實驗2. Weight是由常態分佈隨機生成(平均數為0，標準差為1)。



(a) 神經網路沒有加Batch normalization，(b)神經網路加入Batch normalization。