Gradient Descent

Review: Gradient Descent

- In step 3, we have to solve the following optimization problem:

$$\theta^* = \arg\min_{\theta} L(\theta)$$

L: loss function θ: parameters

Suppose that θ has two variables $\{\theta_1, \theta_2\}$

Randomly start at $\theta^0 = \begin{bmatrix} \theta_1^0 \\ \theta_2^0 \end{bmatrix}$

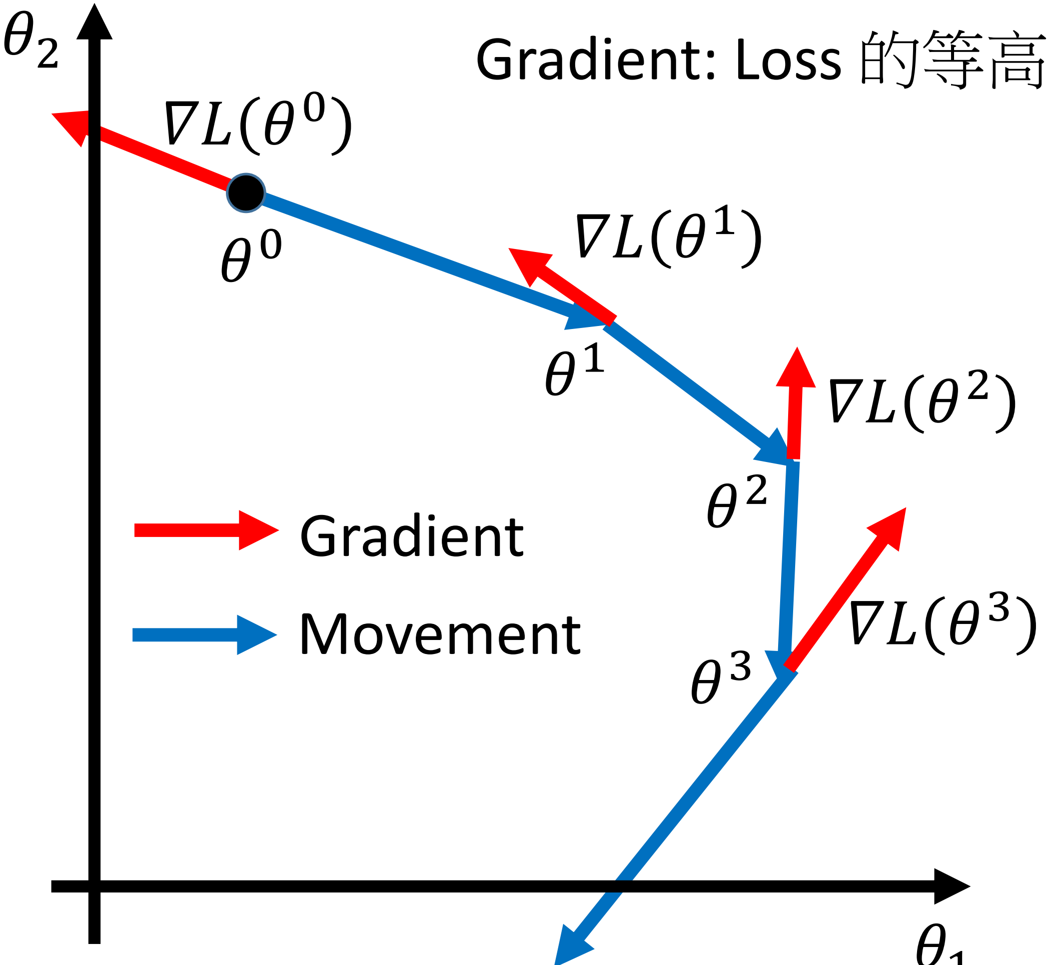
$$\nabla L(\theta) = \begin{bmatrix} \partial L(\theta_1)/\partial \theta_1 \\ \partial L(\theta_2)/\partial \theta_2 \end{bmatrix}$$

$$\begin{bmatrix} \theta_1^1 \\ \theta_2^1 \end{bmatrix} = \begin{bmatrix} \theta_1^0 \\ \theta_2^0 \end{bmatrix} - \eta \begin{bmatrix} \partial L(\theta_1^0)/\partial \theta_1 \\ \partial L(\theta_2^0)/\partial \theta_2 \end{bmatrix} \Rightarrow \theta^1 = \theta^0 - \eta \nabla L(\theta^0)$$

$$\begin{bmatrix} \theta_1^2 \\ \theta_2^2 \end{bmatrix} = \begin{bmatrix} \theta_1^1 \\ \theta_2^1 \end{bmatrix} - \eta \begin{bmatrix} \partial L(\theta_1^1)/\partial \theta_1 \\ \partial L(\theta_2^1)/\partial \theta_2 \end{bmatrix} \Rightarrow \theta^2 = \theta^1 - \eta \nabla L(\theta^1)$$

Review: Gradient Descent

Gradient: Loss 的等高線的法線方向



Start at position θ^0

Compute gradient at θ^0

Move to $\theta^1 = \theta^0 - \eta\nabla L(\theta^0)$

Compute gradient at θ^1

Move to $\theta^2 = \theta^1 - \eta\nabla L(\theta^1)$

⋮

Gradient Descent

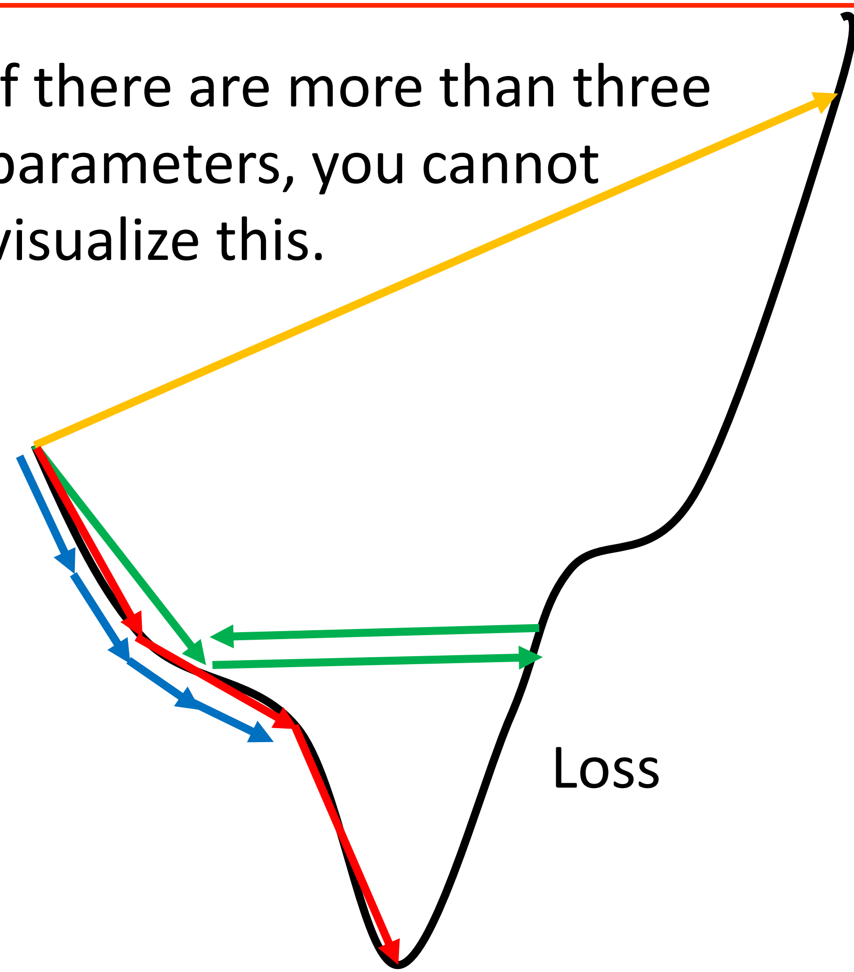
Tip 1: Tuning your learning rates

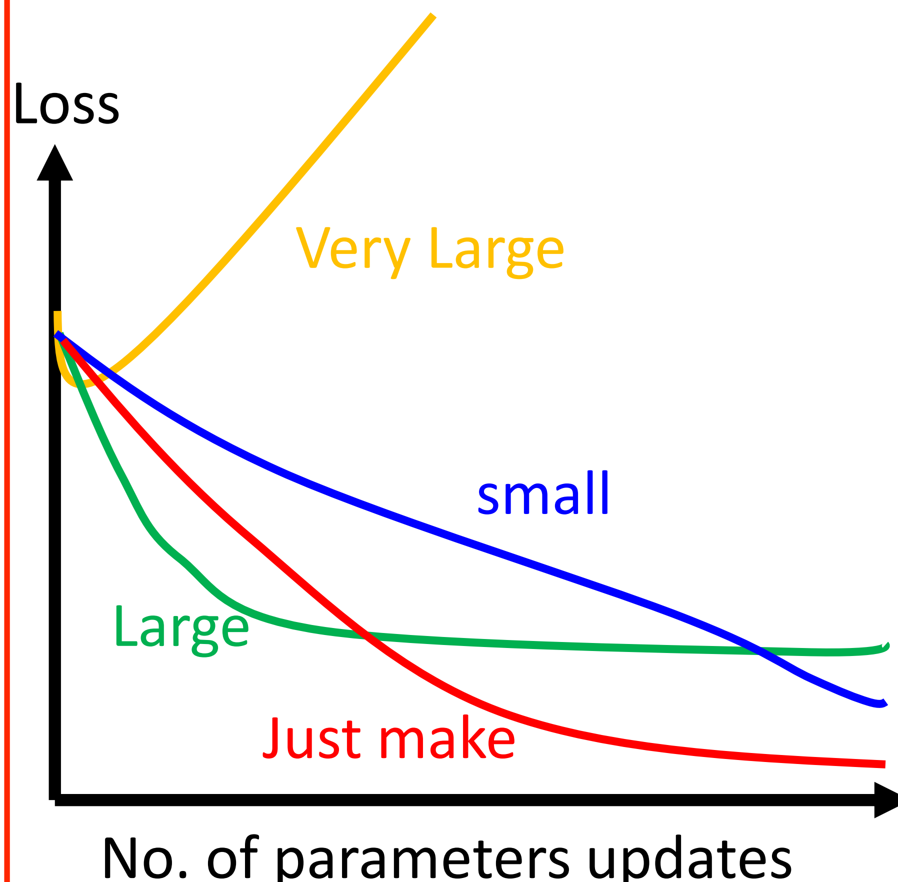
Learning Rate

$$\theta^i = \theta^{i-1} - \eta \nabla L\left(\theta^{i-1}\right)$$

Set the learning rate η carefully

If there are more than three parameters, you cannot visualize this.





But you can always visualize this.

Learning Rate 要依據不同情境「改變」

Adaptive Learning Rates

最簡單的方法

- Popular & Simple Idea: Reduce the learning rate by some factor every few epochs.
  - At the beginning, we are far from the destination, so we use larger learning rate
  - After several epochs, we are close to the destination, so we reduce the learning rate
  - E.g. 1/t decay: $\eta^t = \eta / \sqrt{t+1}$
- Learning rate cannot be one-size-fits-all

進階

  - Giving different parameters different learning rates

Adagrad

$$\boxed{\eta^t = \frac{\eta}{\sqrt{t+1}}}$$

$$\boxed{g^t = \frac{\partial L(\theta^t)}{\partial w}}$$

- Divide the learning rate of each parameter by the ***root mean square of its previous derivatives***

一般的 gradient Descent

Vanilla Gradient descent

$$w^{t+1} \leftarrow w^t - \eta^t g^t$$

w is one parameters

Adagrad

$$w^{t+1} \leftarrow w^t - \frac{\eta^t}{\sigma^t} g^t$$

σ^t: ***root mean square*** of the previous derivatives of parameter w

Parameter dependent

Adagrad

σ^t: ***root mean square*** of the previous derivatives of parameter w

$$w^1 \leftarrow w^0 - \frac{\eta^0}{\sigma^0} g^0 \qquad \sigma^0 = \sqrt{(g^0)^2}$$

$$w^2 \leftarrow w^1 - \frac{\eta^1}{\sigma^1} g^1 \qquad \sigma^1 = \sqrt{\frac{1}{2}\left[(g^0)^2 + (g^1)^2\right]}$$

$$w^3 \leftarrow w^2 - \frac{\eta^2}{\sigma^2} g^2 \qquad \sigma^2 = \sqrt{\frac{1}{3}\left[(g^0)^2 + (g^1)^2 + (g^2)^2\right]}$$

$$\vdots$$

$$w^{t+1} \leftarrow w^t - \frac{\eta^t}{\sigma^t} g^t \qquad \sigma^t = \sqrt{\frac{1}{t+1}\sum_{i=0}^{t}(g^i)^2}$$

Adagrad

- Divide the learning rate of each parameter by the ***root mean square of its previous derivatives***

$$\eta^t = \frac{\eta}{\sqrt{\cancel{t+1}}}$$

1/t decay

$$w^{t+1} \leftarrow w^t - \frac{\eta^t}{\sigma^t} g^t$$

$$\sigma^t = \sqrt{\frac{1}{\cancel{t+1}} \sum_{i=0}^{t} (g^i)^2}$$

Adagrad 最終樣子

$$\boxed{w^{t+1} \leftarrow w^t - \frac{\eta}{\sqrt{\sum_{i=0}^{t} (g^i)^2}} g^t}$$

針對 Adagrad 參數更新式的「分母」討論！

Contradiction?

$$\eta^t = \frac{\eta}{\sqrt{t+1}} \qquad g^t = \frac{\partial L(\theta^t)}{\partial w}$$

Vanilla Gradient descent

$$w^{t+1} \leftarrow w^t - \eta^t \underline{g^t}$$

Larger gradient, larger step

Adagrad

$$w^{t+1} \leftarrow w^t - \frac{\eta}{\sqrt{\underline{\sum_{i=0}^{t}(g^i)^2}}} \underline{g^t}$$

Larger gradient, larger step

Larger gradient, smaller step

Intuitive Reason

$$\eta^t = \frac{\eta}{\sqrt{t+1}} \quad g^t = \frac{\partial C(\theta^t)}{\partial w}$$

- How surprise it is 反差

特別大

g^0	g^1	g^2	g^3	g^4	……
0.001	0.001	0.003	0.002	0.1	……

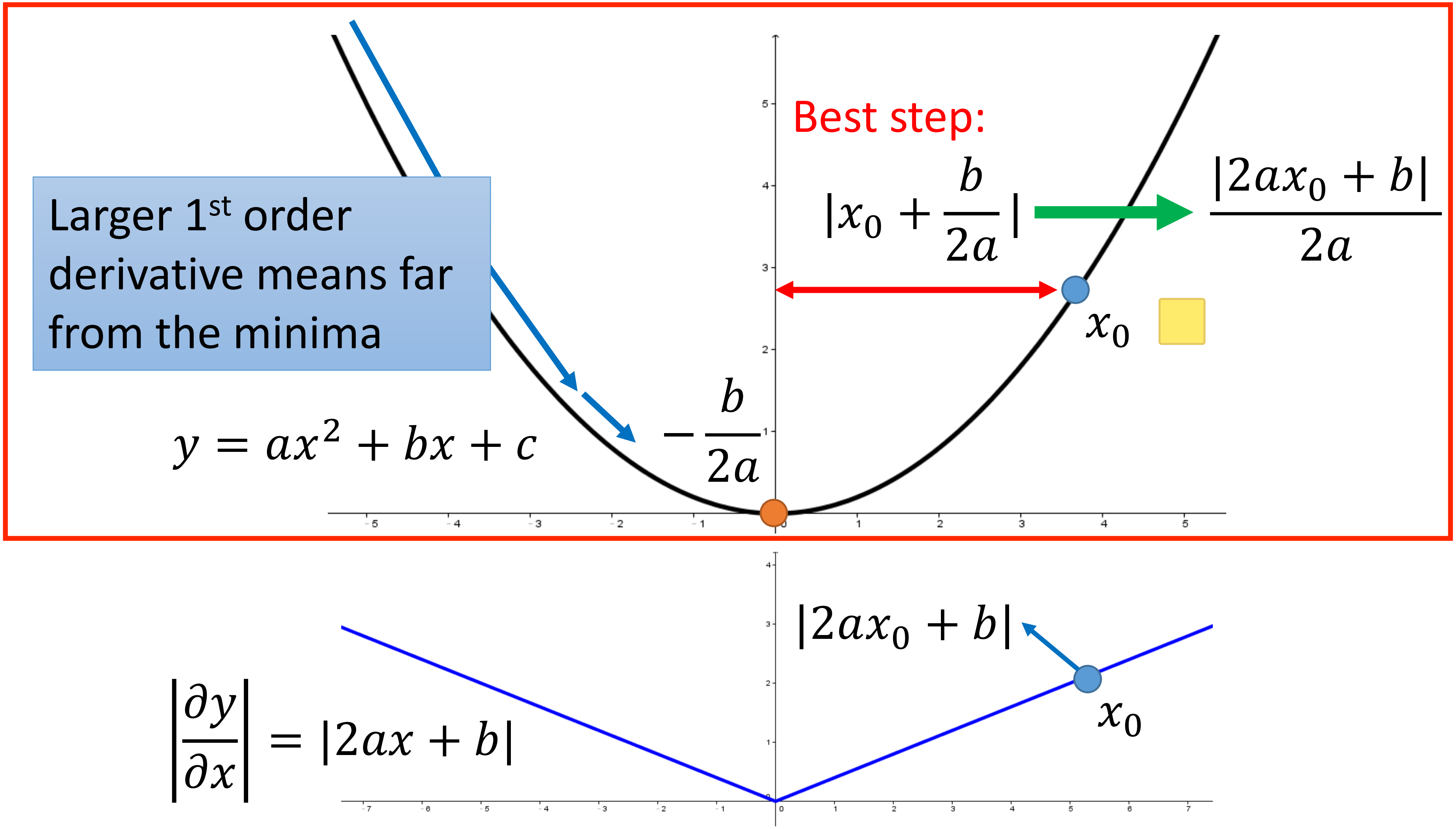
g^0	g^1	g^2	g^3	g^4	……
10.8	20.9	31.7	12.1	0.1	……

特別小

$$w^{t+1} \leftarrow w^t - \frac{\eta}{\sqrt{\underline{\sum_{i=0}^{t}(g^i)^2}}} g^t$$

$\rightarrow$ 造成反差的效果

Larger gradient, larger steps?



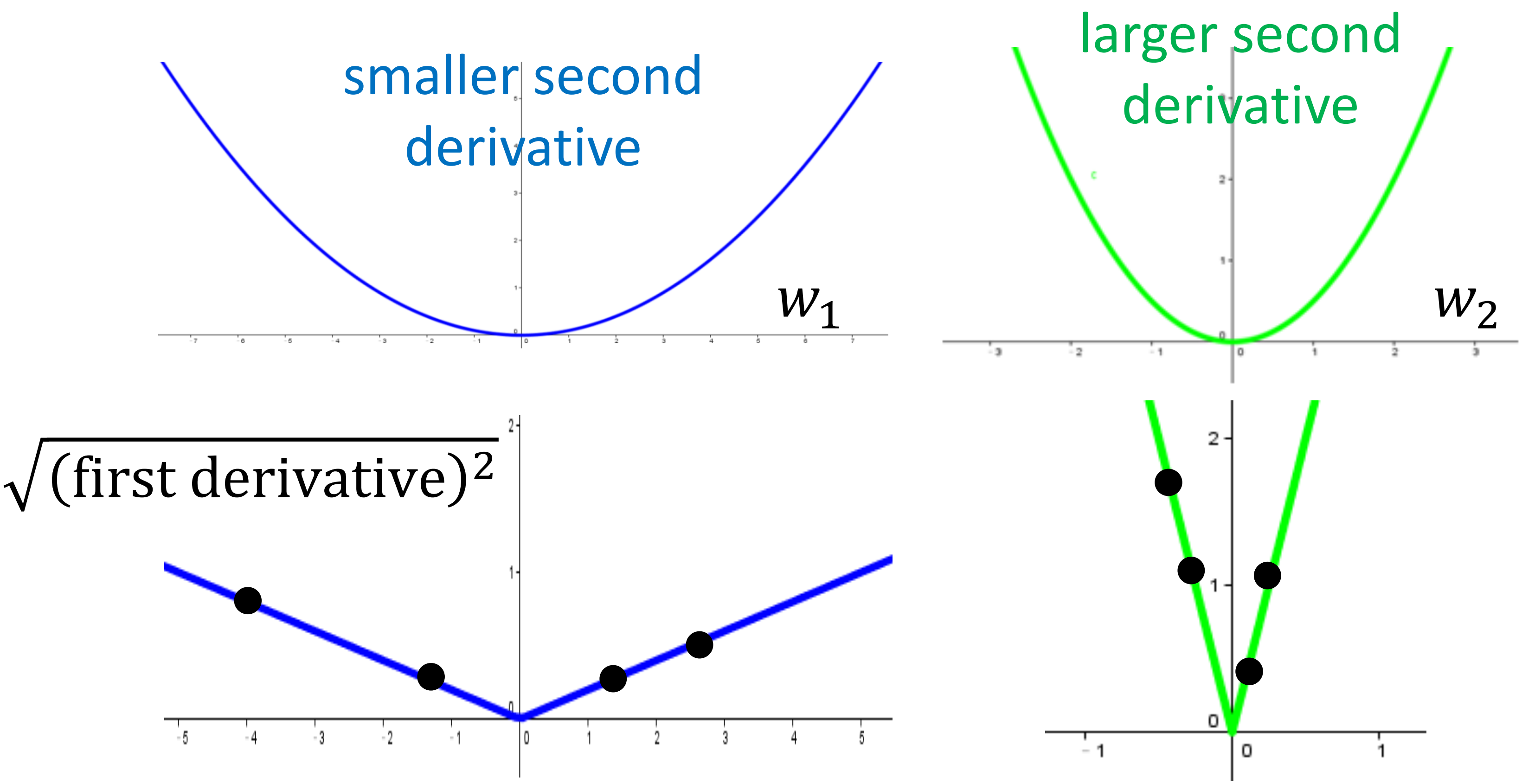
$$w^{t+1} \leftarrow w^t - \frac{\eta}{\sqrt{\sum_{i=0}^{t}(g^i)^2}} g^t$$

The best step is

$$\frac{|\text{First derivative}|}{\text{Second derivative}}$$

?

Use *first derivative* to estimate *second derivative*



Gradient Descent

Tip 2: Stochastic Gradient Descent

Make the training faster

Stochastic Gradient Descent

$$L = \sum_n \left(\hat{y}^n - \left(b + \sum w_i x_i^n \right) \right)^2$$

Loss is the summation over all training examples

◆ ***Gradient Descent*** $\theta^i = \theta^{i-1} - \eta \nabla L\left(\theta^{i-1}\right)$

◆ ***Stochastic Gradient Descent***

Faster!

Pick an example x^n

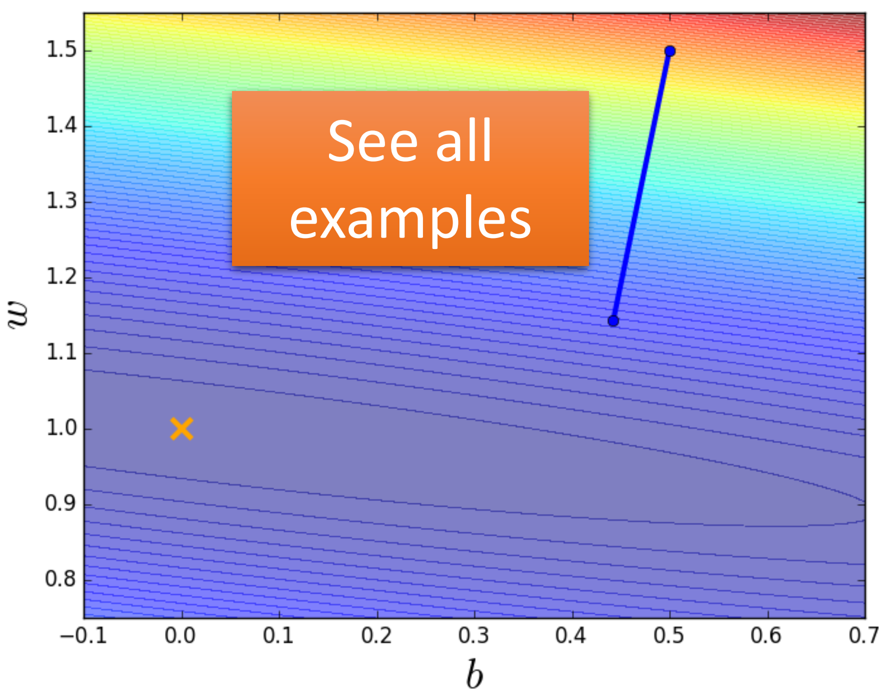
$$L^n = \left(\hat{y}^n - \left(b + \sum w_i x_i^n \right) \right)^2 \qquad \theta^i = \theta^{i-1} - \eta \nabla L^n\left(\theta^{i-1}\right)$$

Loss for only one example

Stochastic Gradient Descent

Gradient Descent

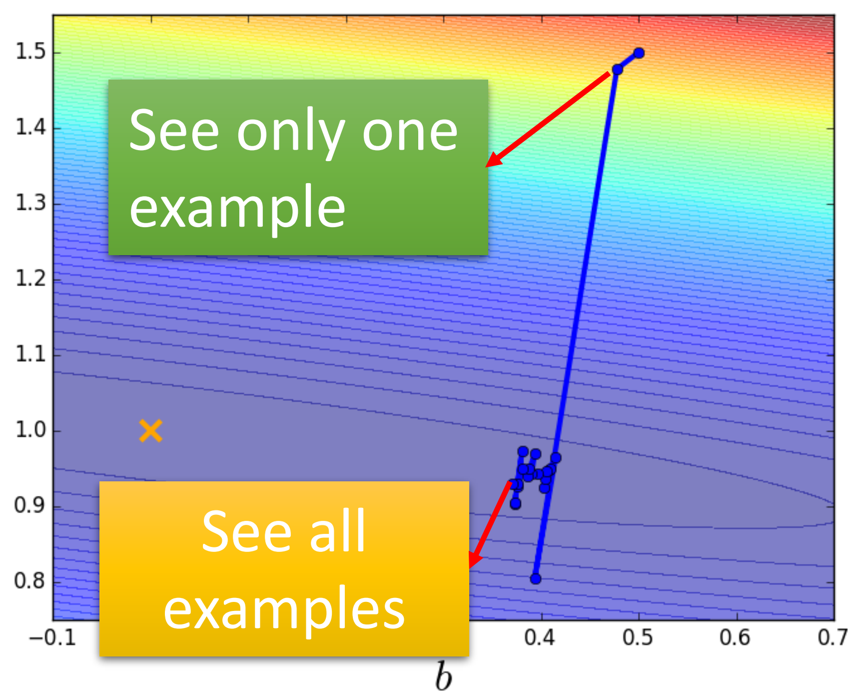
Update after seeing all examples



Stochastic Gradient Descent

Update for each example

If there are 20 examples, 20 times faster.



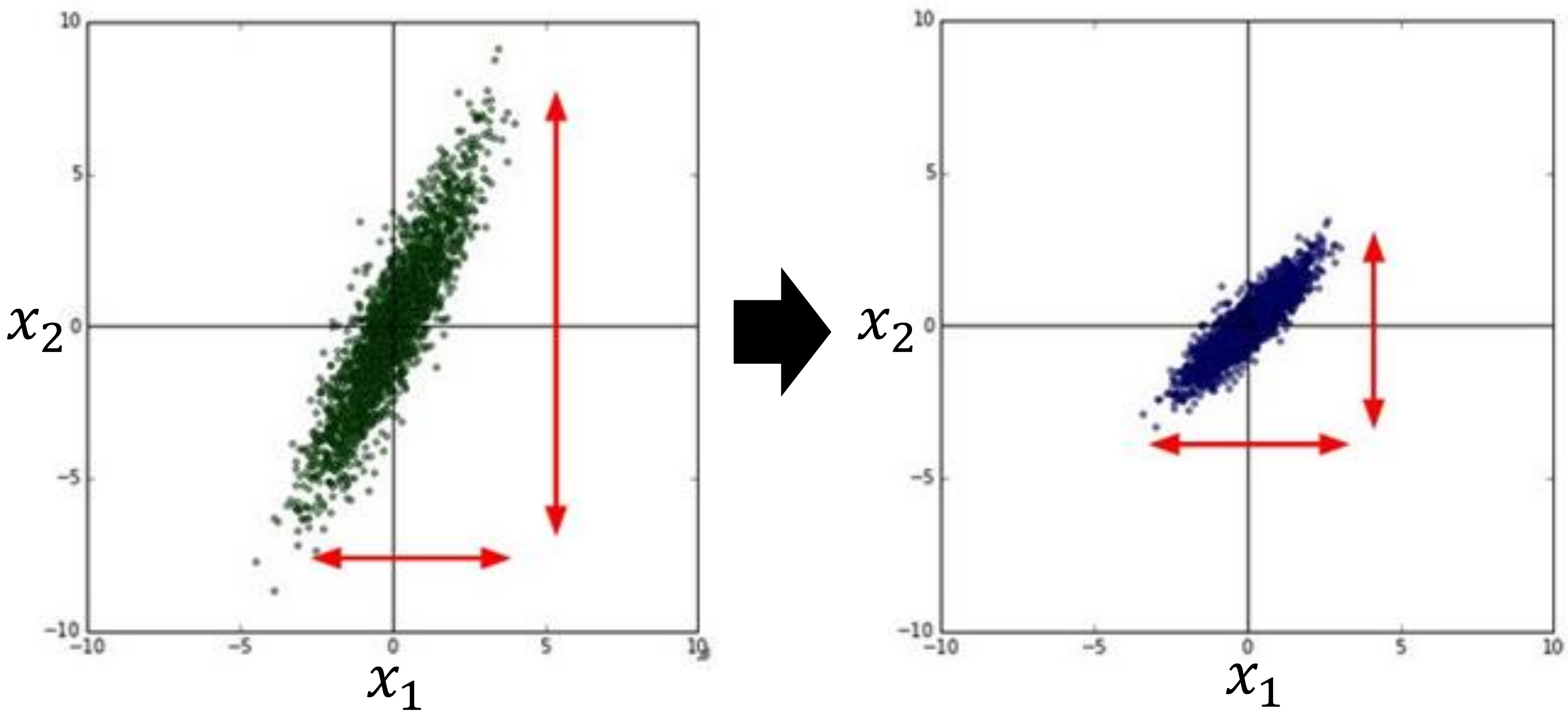
Gradient Descent

Tip 3: Feature Scaling

Feature Scaling

Source of figure: http://cs231n.github.io/neural-networks-2/

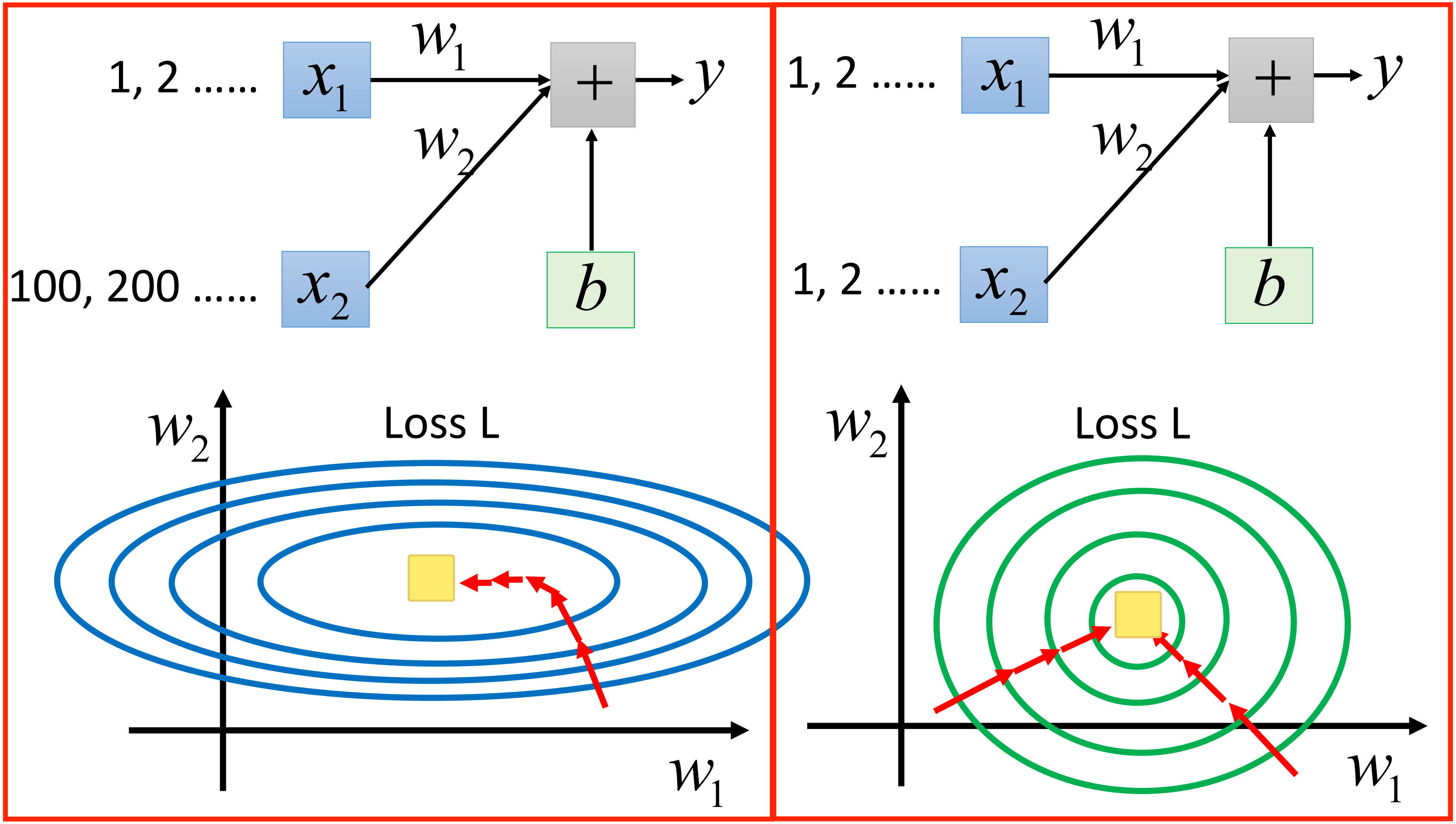
$$y = b + w_1 x_1 + w_2 x_2$$



Make different features have the same scaling

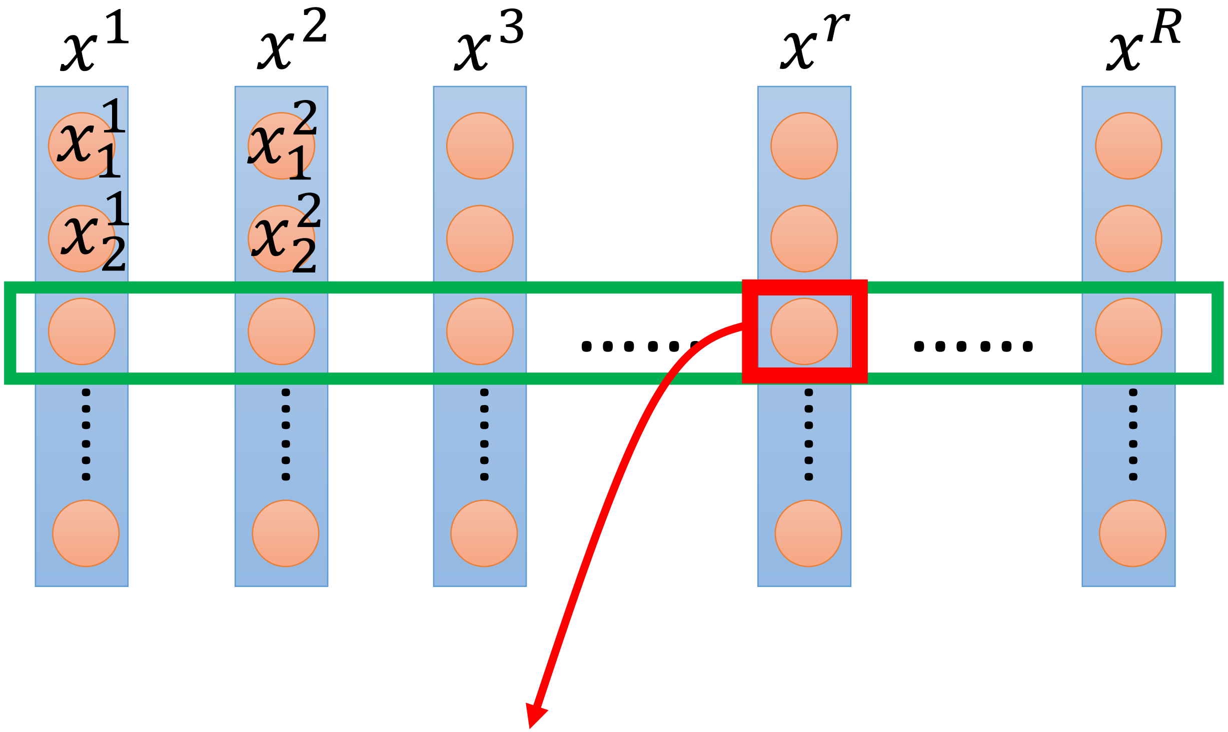
Feature Scaling

$$y = b + w_1 x_1 + w_2 x_2$$



Feature Scaling 的一種方法：Normalization => 對所有 Example 的同一種 Feature 進行標準化

Feature Scaling



For each dimension i:

mean: m_i

standard deviation: σ_i

$$x_i^r \leftarrow \frac{x_i^r - m_i}{\sigma_i}$$

The means of all dimensions are 0, and the variances are all 1

Gradient Descent

Theory

Question

- When solving:

$$\theta^* = \arg\min_{\theta} L(\theta) \quad \text{by gradient descent}$$

- $\boxed{\begin{array}{l}\text{Each time we update the parameters, we obtain } \theta \\ \text{that makes } L(\theta) \text{ smaller.} \\[1em] L(\theta^0) > L(\theta^1) > L(\theta^2) > \cdots\end{array}}$

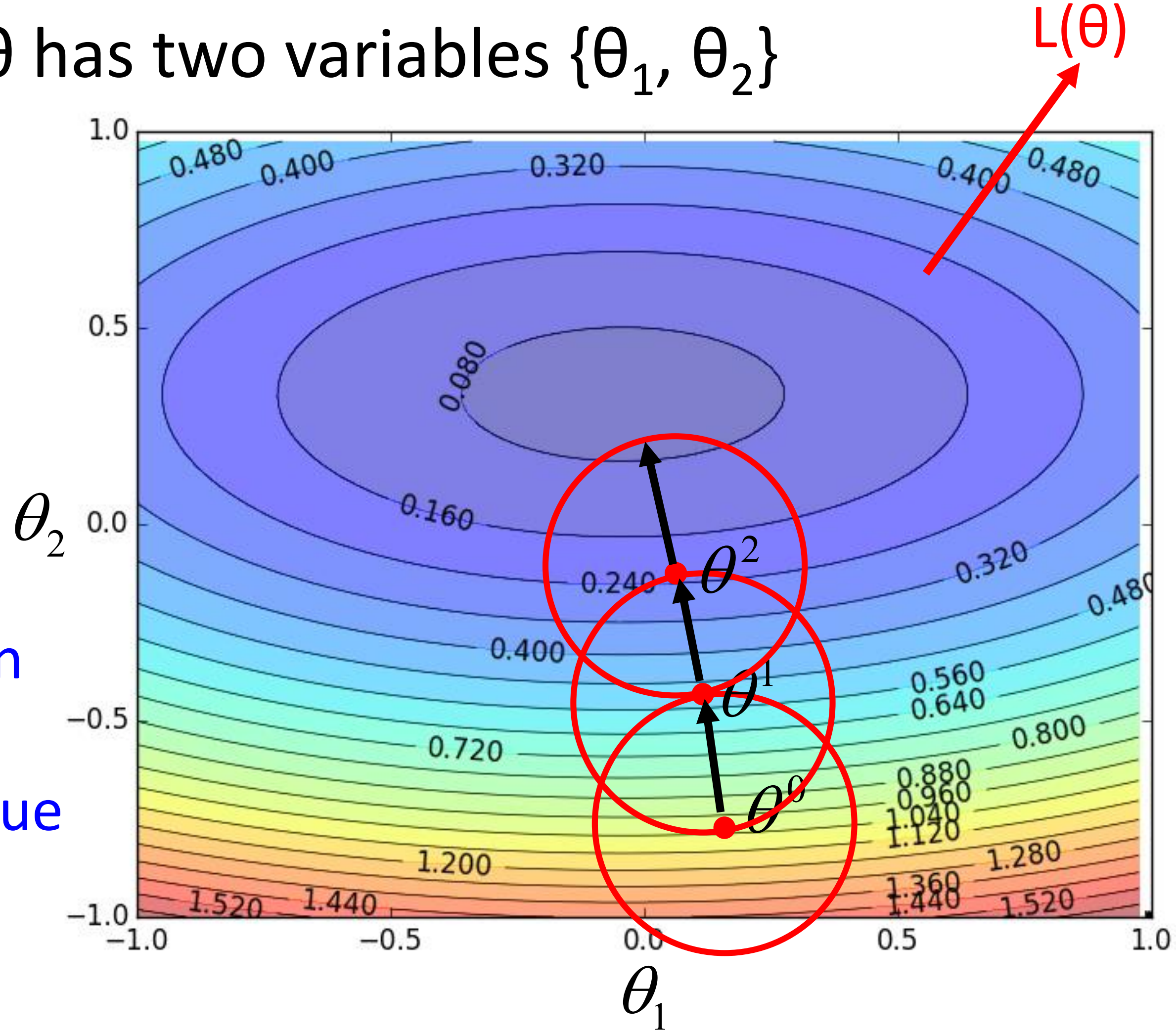
Is this statement correct?

錯！並不是每次更新參數都會讓 Loss Function 的 Value 更小！

Warning of Math

Formal Derivation

- Suppose that θ has two variables $\{\theta_1, \theta_2\}$



Given a point, we can easily find the point with the smallest value nearby. How?

Taylor Series

- **Taylor series**: Let h(x) be any function infinitely differentiable around $x = x_0$.

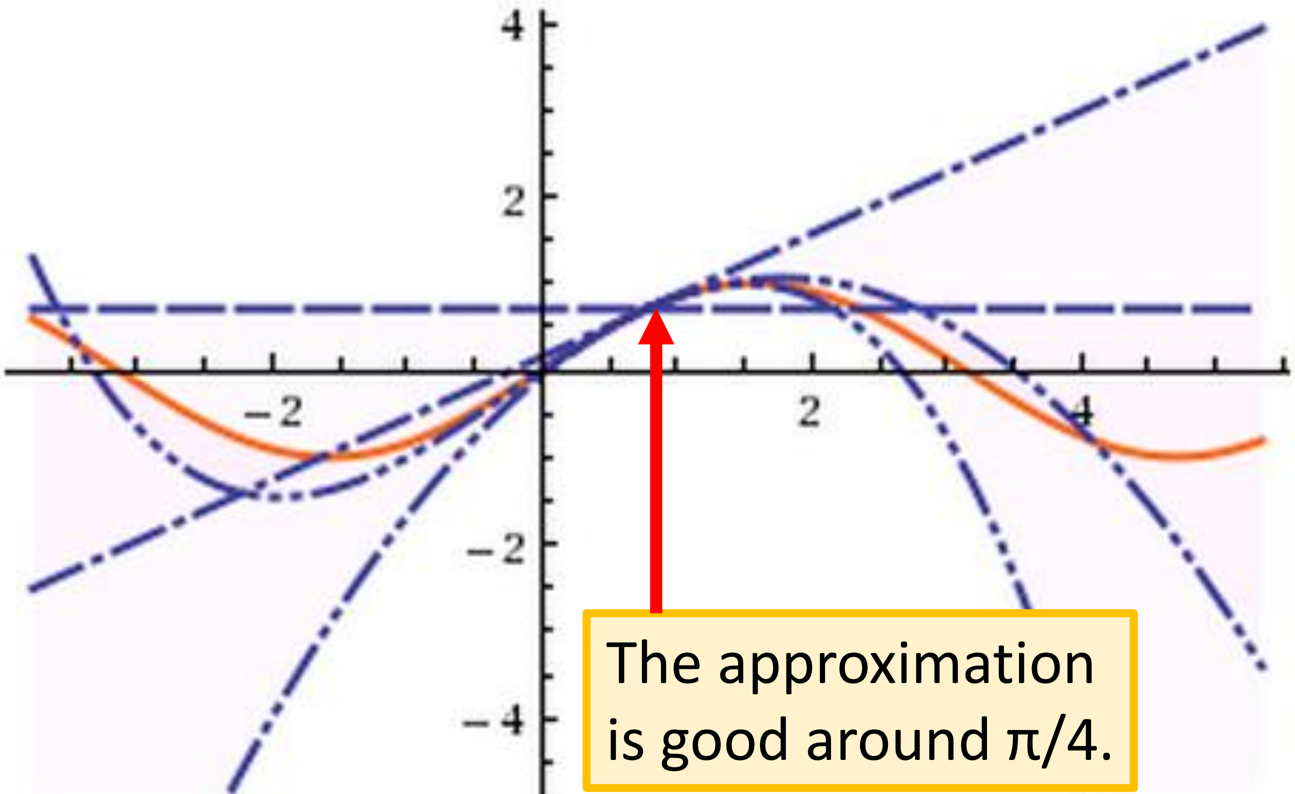
$$\mathrm{h}(\mathrm{x}) = \sum_{k=0}^{\infty} \frac{\mathrm{h}^{(k)}(x_0)}{k!}(x - x_0)^k$$

$$= h(x_0) + h'(x_0)(x - x_0) + \frac{h''(x_0)}{2!}(x - x_0)^2 + \ldots$$

When x is close to x_0 ➡ $h(x) \approx h(x_0) + h'(x_0)(x - x_0)$

E.g. Taylor series for h(x)=sin(x) around $x_0=\pi/4$

$$\sin(x)=\frac{1}{\sqrt{2}}+\frac{x-\frac{\pi}{4}}{\sqrt{2}}-\frac{\left(x-\frac{\pi}{4}\right)^2}{2\sqrt{2}}-\frac{\left(x-\frac{\pi}{4}\right)^3}{6\sqrt{2}}+\frac{\left(x-\frac{\pi}{4}\right)^4}{24\sqrt{2}}+\frac{\left(x-\frac{\pi}{4}\right)^5}{120\sqrt{2}}-\frac{\left(x-\frac{\pi}{4}\right)^6}{720\sqrt{2}}-\frac{\left(x-\frac{\pi}{4}\right)^7}{5040\sqrt{2}}+\frac{\left(x-\frac{\pi}{4}\right)^8}{40\,320\sqrt{2}}+\frac{\left(x-\frac{\pi}{4}\right)^9}{362\,880\sqrt{2}}-\frac{\left(x-\frac{\pi}{4}\right)^{10}}{3\,628\,800\sqrt{2}}+\ldots\ldots$$



Multivariable Taylor Series

$$h(x, y) = h(x_0, y_0) + \frac{\partial h(x_0, y_0)}{\partial x}(x - x_0) + \frac{\partial h(x_0, y_0)}{\partial y}(y - y_0)$$

+ something related to $(x-x_0)^2$ and $(y-y_0)^2$ + ……

When x and y is close to x_0 and y_0

$$h(x, y) \approx h(x_0, y_0) + \frac{\partial h(x_0, y_0)}{\partial x}(x - x_0) + \frac{\partial h(x_0, y_0)}{\partial y}(y - y_0)$$

Back to Formal Derivation

Based on Taylor Series:

If the red circle is ***small enough***, in the red circle

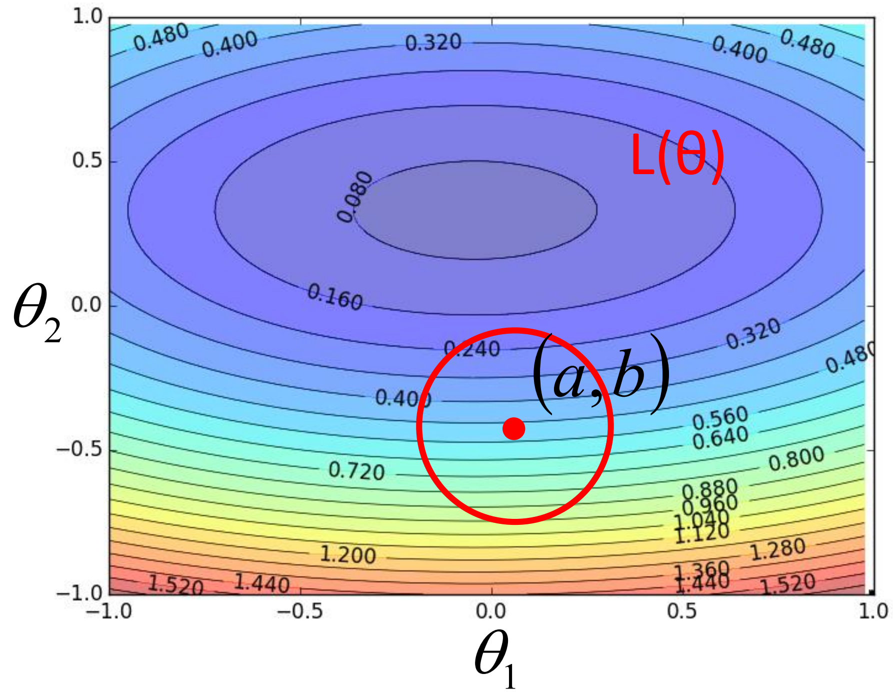
$$L(\theta) \approx L(a,b) + \frac{\partial L(a,b)}{\partial \theta_1}(\theta_1 - a) + \frac{\partial L(a,b)}{\partial \theta_2}(\theta_2 - b)$$

$$s = L(a,b)$$

$$u = \frac{\partial L(a,b)}{\partial \theta_1}, v = \frac{\partial L(a,b)}{\partial \theta_2}$$

$$L(\theta)$$

$$\approx s + u(\theta_1 - a) + v(\theta_2 - b)$$



Back to Formal Derivation

Based on Taylor Series:

If the red circle is ***small enough***, in the red circle

constant

$$s = L(a,b)$$

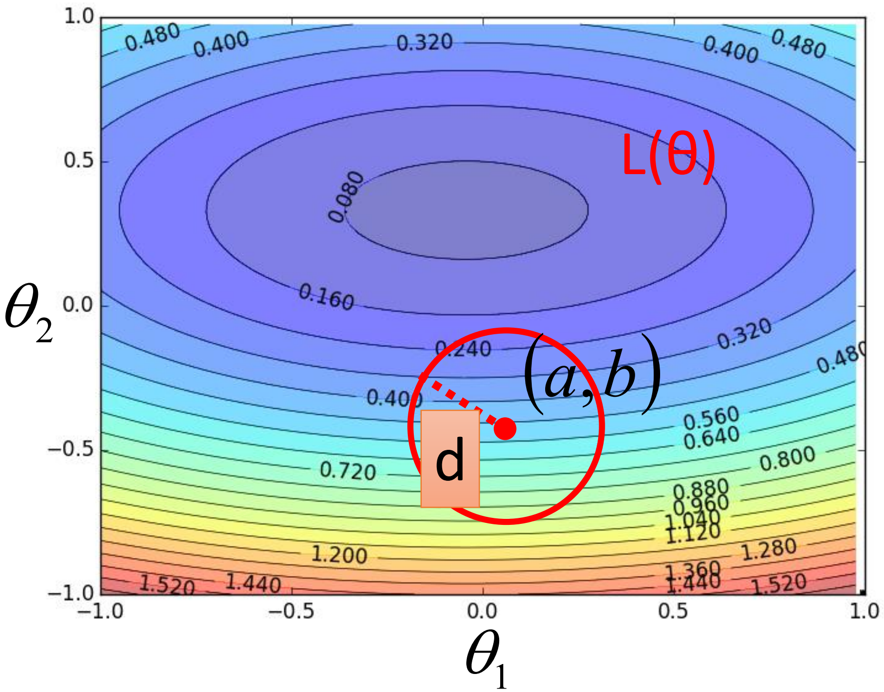
$$u = \frac{\partial L(a,b)}{\partial \theta_1}, v = \frac{\partial L(a,b)}{\partial \theta_2}$$

$$L(\theta) \approx s + u(\theta_1 - a) + v(\theta_2 - b)$$

Find θ_1 and θ_2 in the red circle ***minimizing*** L(θ)

$$(\theta_1 - a)^2 + (\theta_2 - b)^2 \leq d^2$$

Simple, right?



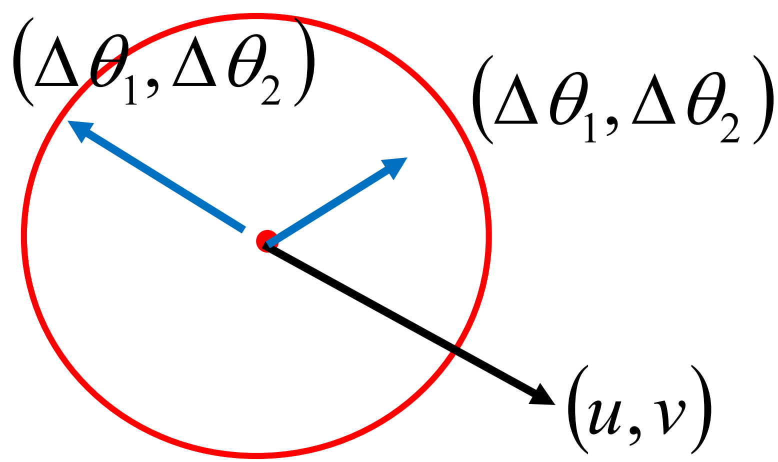
Gradient descent – two variables

Red Circle: (If the radius is small)

$$\mathrm{L}(\theta) \approx \cancel{s} + u\underbrace{(\theta_1 - a)}_{\Delta\theta_1} + v\underbrace{(\theta_2 - b)}_{\Delta\theta_2}$$

Find θ_1 and θ_2 in the red circle ***minimizing*** $\mathrm{L}(\theta)$

$$\underbrace{(\theta_1 - a)}_{\Delta\theta_1}^2 + \underbrace{(\theta_2 - b)}_{\Delta\theta_2}^2 \le d^2$$



To minimize $\mathrm{L}(\theta)$

$$\begin{bmatrix} \Delta\theta_1 \\ \Delta\theta_2 \end{bmatrix} = -\eta \begin{bmatrix} u \\ v \end{bmatrix} \Rightarrow \begin{bmatrix} \theta_1 \\ \theta_2 \end{bmatrix} = \begin{bmatrix} a \\ b \end{bmatrix} - \eta \begin{bmatrix} u \\ v \end{bmatrix}$$

Back to Formal Derivation

Based on Taylor Series:

If the red circle is ***small enough***, in the red circle

constant

$$s = \mathrm{L}(a,b)$$

$$\mathrm{L}(\theta) \approx s + u(\theta_1 - a) + v(\theta_2 - b)$$

$$u = \frac{\partial \mathrm{L}(a,b)}{\partial \theta_1}, v = \frac{\partial \mathrm{L}(a,b)}{\partial \theta_2}$$

Find θ_1 and θ_2 yielding the smallest value of $L(\theta)$ in the circle

$$\begin{bmatrix} \theta_1 \\ \theta_2 \end{bmatrix} = \begin{bmatrix} a \\ b \end{bmatrix} - \eta \begin{bmatrix} u \\ v \end{bmatrix} = \begin{bmatrix} a \\ b \end{bmatrix} - \eta \begin{bmatrix} \frac{\partial \mathrm{L}(a,b)}{\partial \theta_1} \\ \frac{\partial \mathrm{L}(a,b)}{\partial \theta_2} \end{bmatrix}$$

This is gradient descent.

Not satisfied if the red circle (learning rate) is not small enough

You can consider the second order term, e.g. Newton's method.

End of Warning

More Limitation of Gradient Descent