Tips for Training Deep Neural Network

Outline

- Activation Function
- Cost Function
- Data Preprocessing
- Optimization
- Generalization

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- Cost Function
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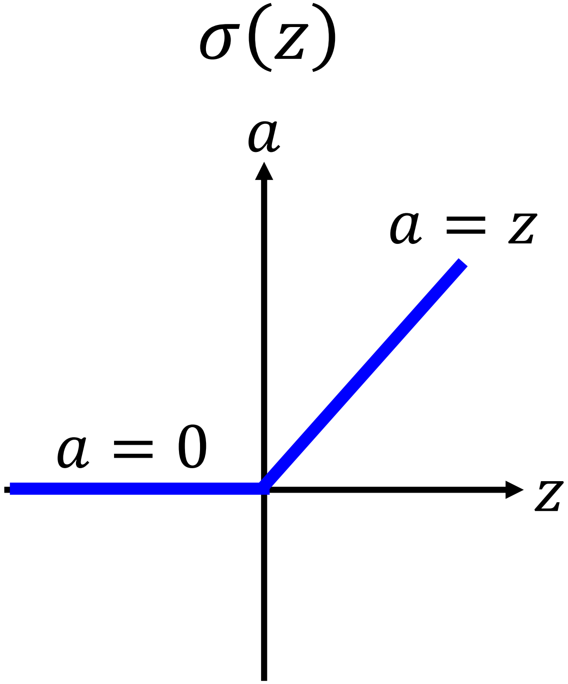
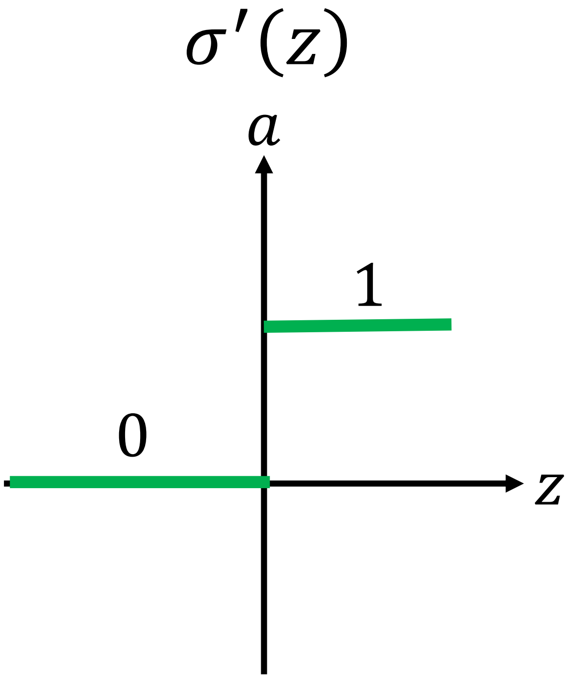
- Generalization

ReLU

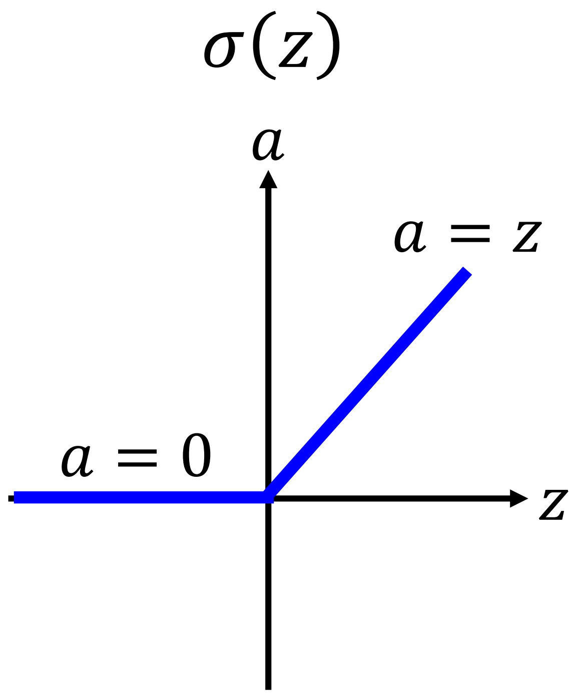
- Rectified Linear Unit (ReLU)





ReLU

- Rectified Linear Unit (ReLU)



Reason:

1. Fast to compute
2. Biological reason
3. Infinite sigmoid with different biases
4. Vanishing gradient problem

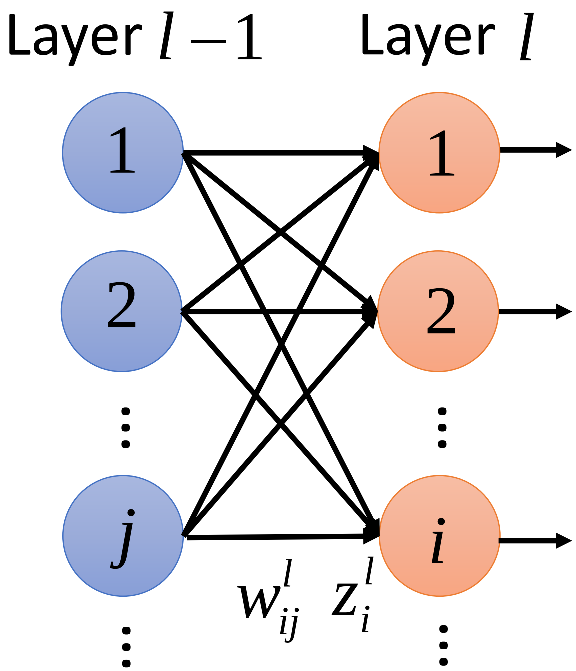
Review: Backpropagation

$$\frac{\partial C_x}{\partial w_{ij}^l} = \boxed{\frac{\partial z_i^l}{\partial w_{ij}^l}} \boxed{\frac{\partial C_x}{\partial z_i^l}}$$

$$\frac{\partial z_i^l}{\partial w_{ij}^l} = \begin{cases} a_j^{l-1} & l > 1 \\ x_j & l = 1 \end{cases}$$

Error signal

$$\frac{\partial C_x}{\partial z_i^l} = \delta_i^l$$



Forward Pass

$$z^1 = W^1 x + b^1$$

$$a^1 = \sigma\left(z^1\right)$$

$$\cdots\cdots$$

$$z^{l-1} = W^{l-1} a^{l-2} + b^{l-1}$$

$$a^{l-1} = \sigma\left(z^{l-1}\right)$$

Backward Pass

$$\delta^L = \sigma'\left(z^L\right) \bullet \nabla C_x(y)$$

$$\delta^{L-1} = \sigma'\left(z^{L-1}\right) \bullet \left(W^L\right)^T \delta^L$$

$$\cdots\cdots$$

$$\delta^l = \sigma'\left(z^l\right) \bullet \left(W^{l+1}\right)^T \delta^{l+1}$$

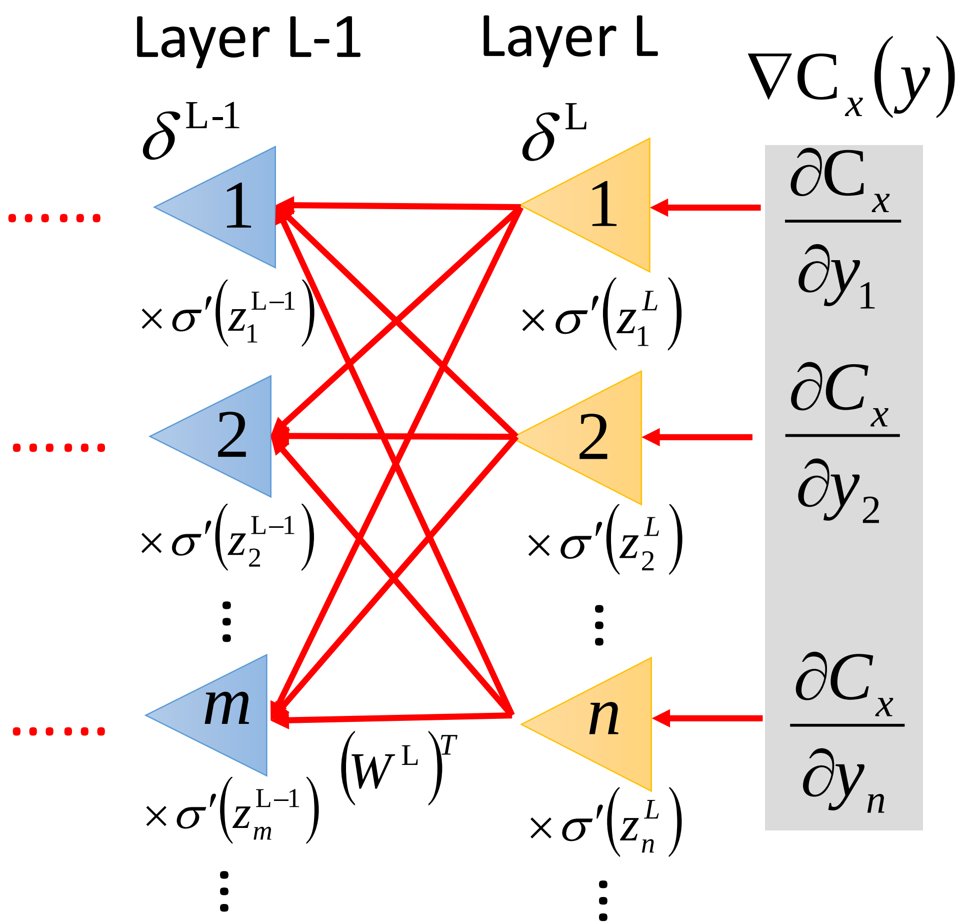
$$\cdots\cdots$$

Review: Backpropagation

$$\frac{\partial C_x}{\partial w_{ij}^l} = \boxed{\frac{\partial z_i^l}{\partial w_{ij}^l}} \boxed{\frac{\partial C_x}{\partial z_i^l}}$$

Error signal

$$\boxed{\delta_i^l}$$



Backward Pass

$$\delta^L = \sigma'(z^L) \bullet \nabla C_x(y)$$

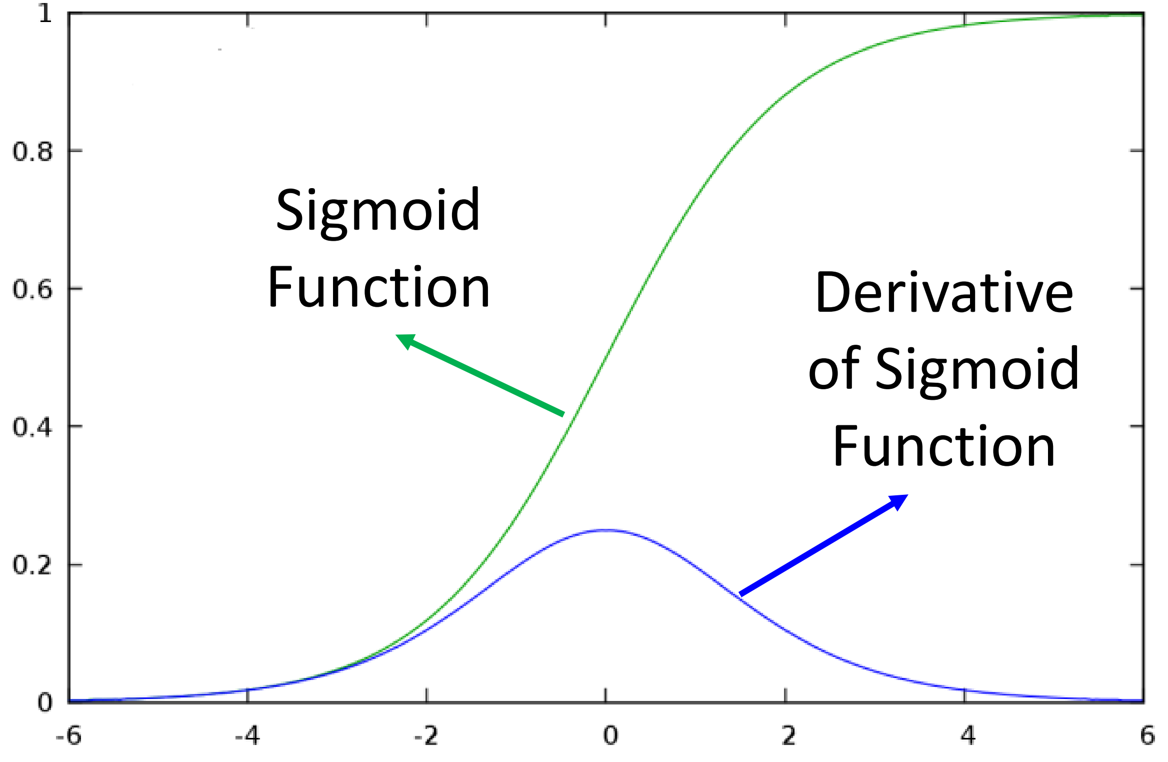
$$\delta^{L-1} = \sigma'(z^{L-1}) \bullet (W^L)^T \delta^L$$

$$\cdots\cdots$$

$$\delta^l = \sigma'(z^l) \bullet (W^{l+1})^T \delta^{l+1}$$

$$\cdots\cdots$$

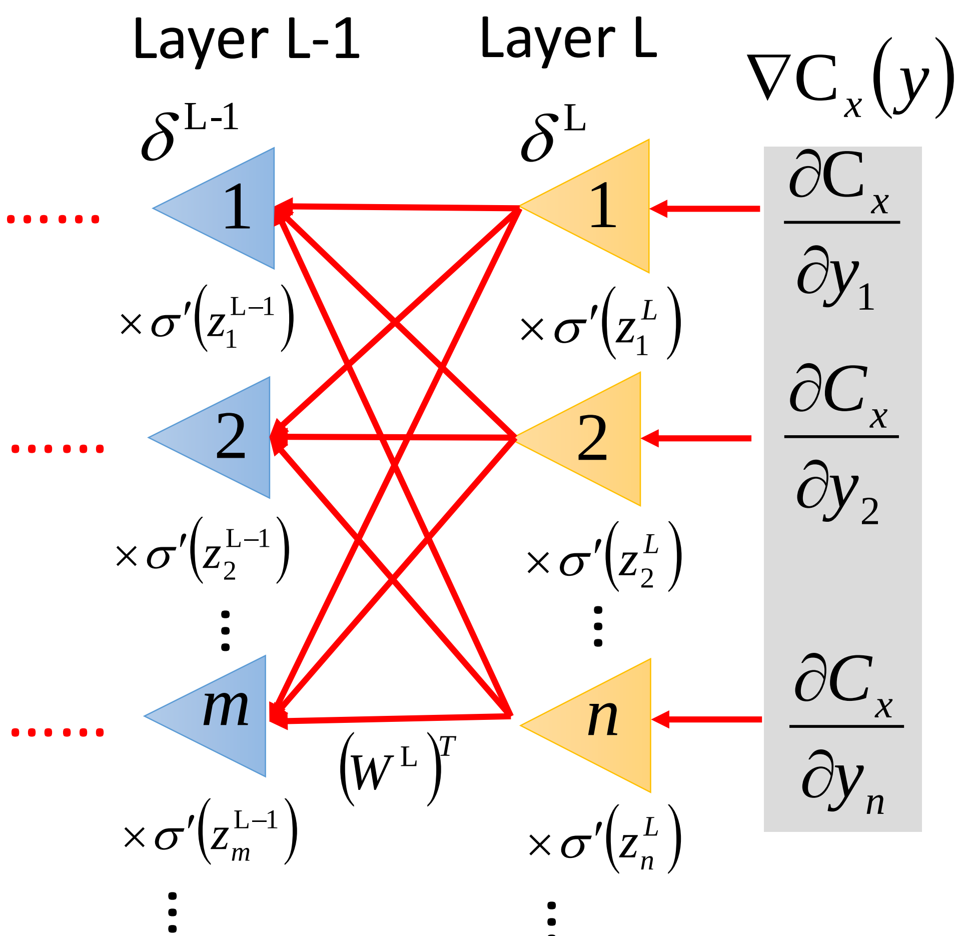
Problem of Sigmoid



Derivative of Sigmoid Function is always smaller than 1

Vanishing Gradient Problem

Backward Pass:

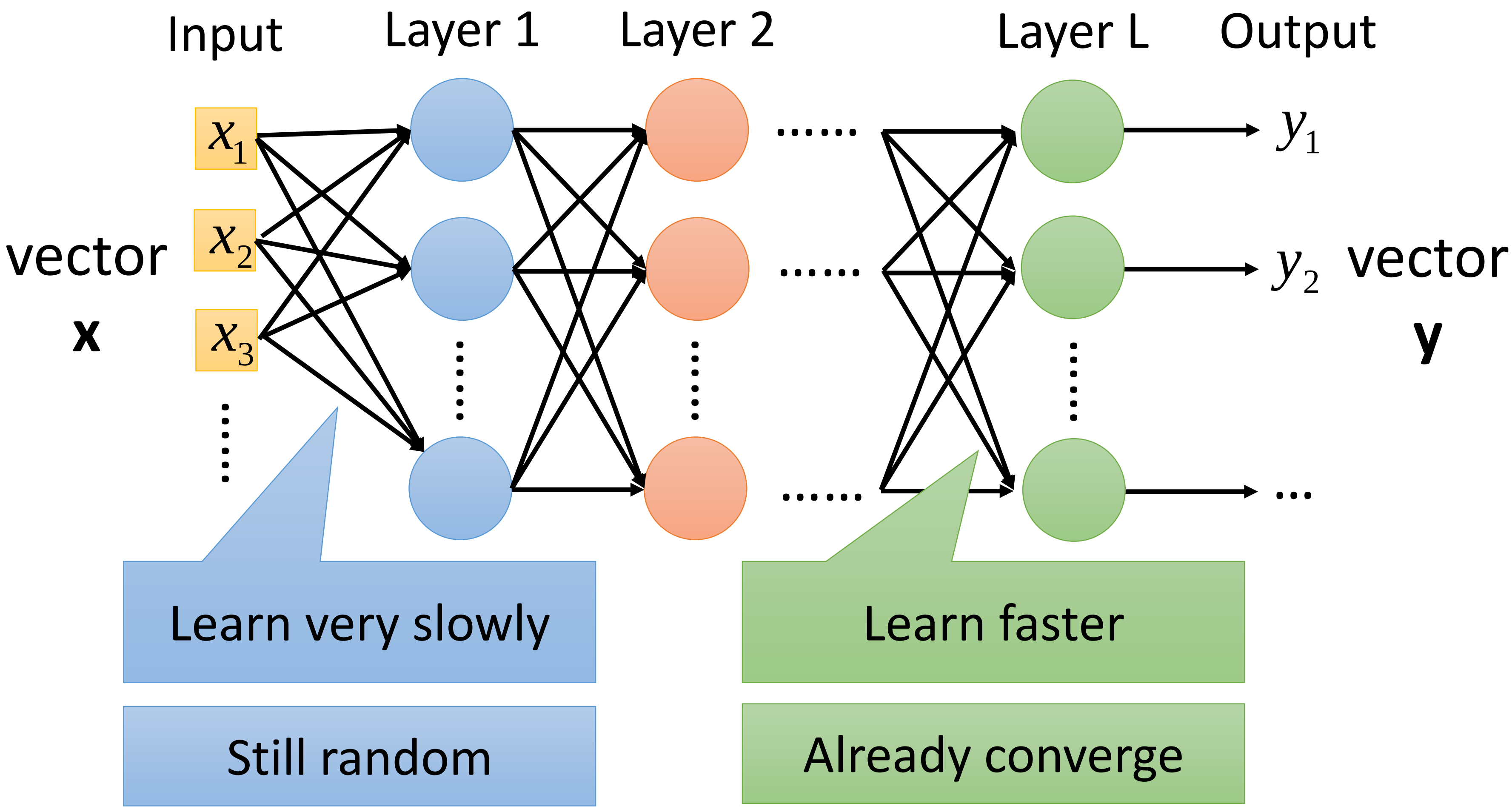


- For sigmoid function, $\sigma'(z)$ always smaller than 1
- Error signal is getting smaller and smaller

Gradient is smaller

$$\frac{\partial C_x}{\partial w_{ij}^l} = \frac{\partial z_i^l}{\partial w_{ij}^l} \boxed{\frac{\partial C_x}{\partial z_i^l}} \rightarrow \boxed{\delta_i^l}$$

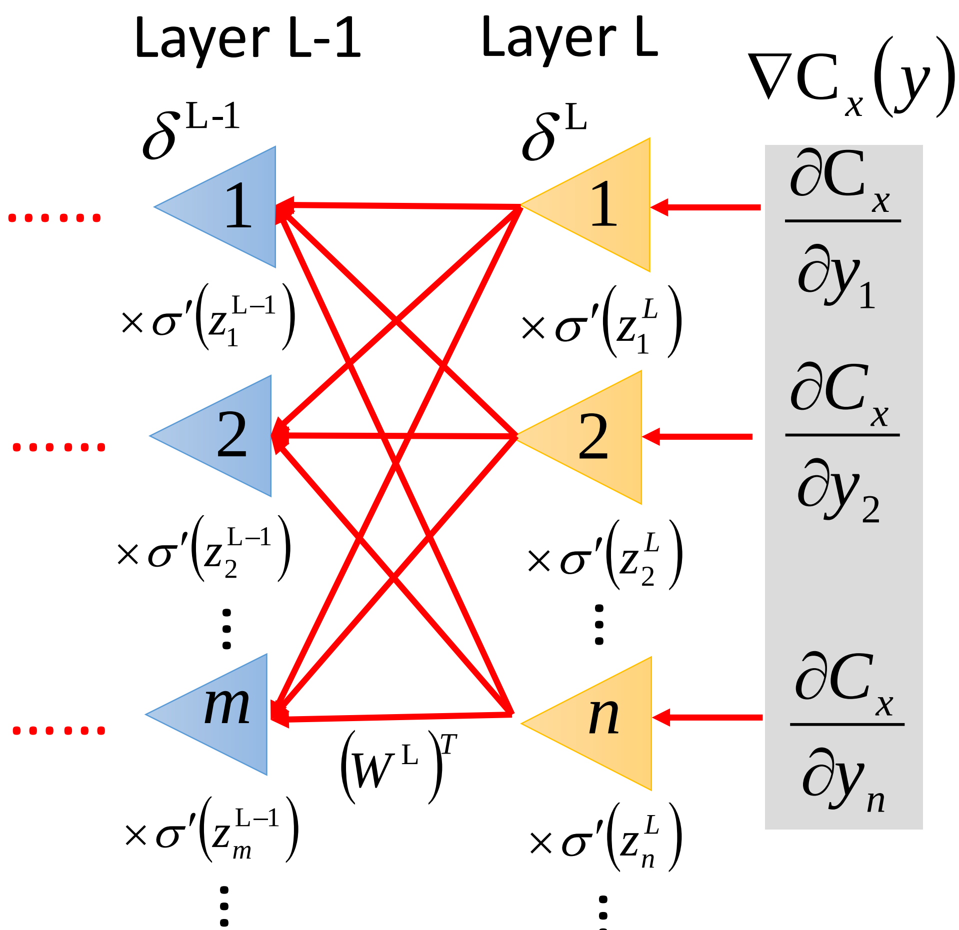
Vanishing Gradient Problem

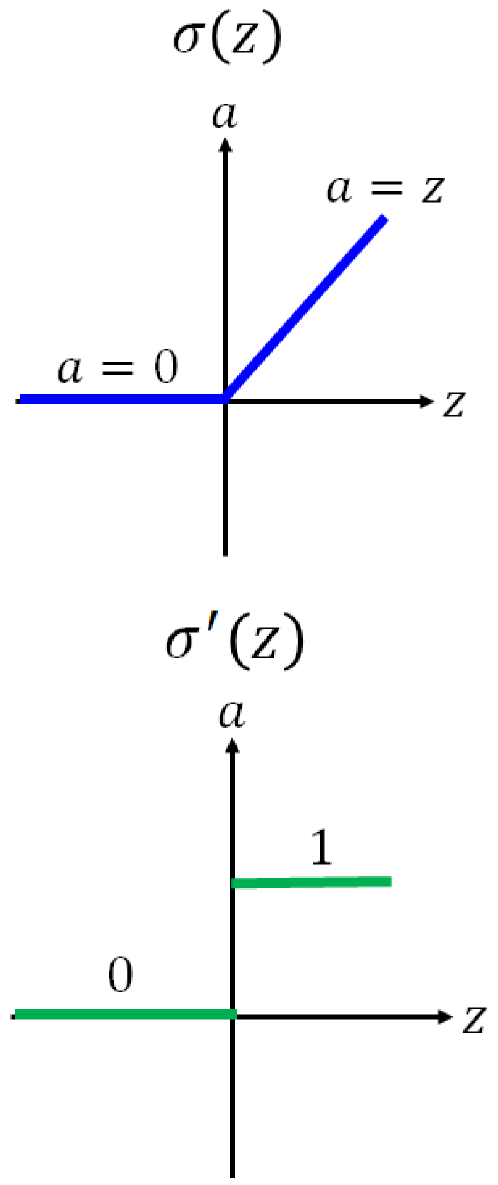


The weights are converged based on random!?

ReLU

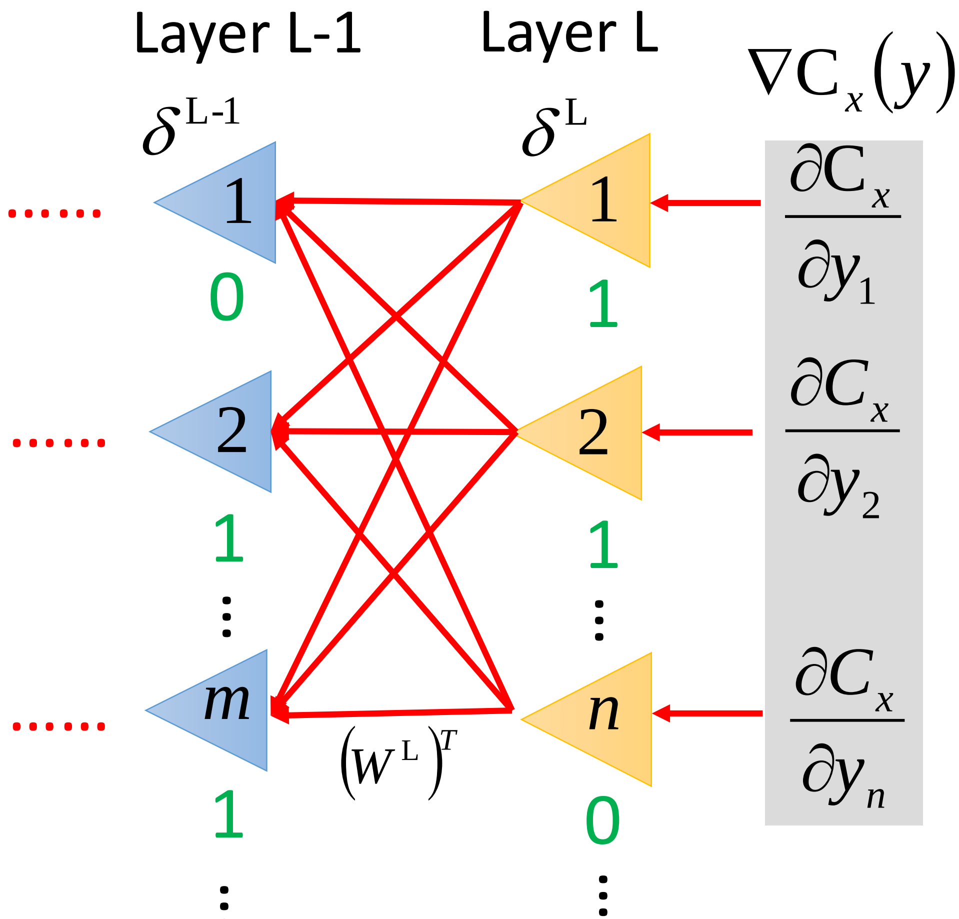
Backward Pass:

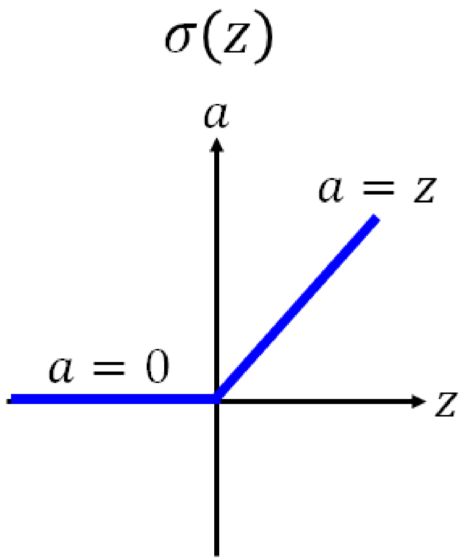


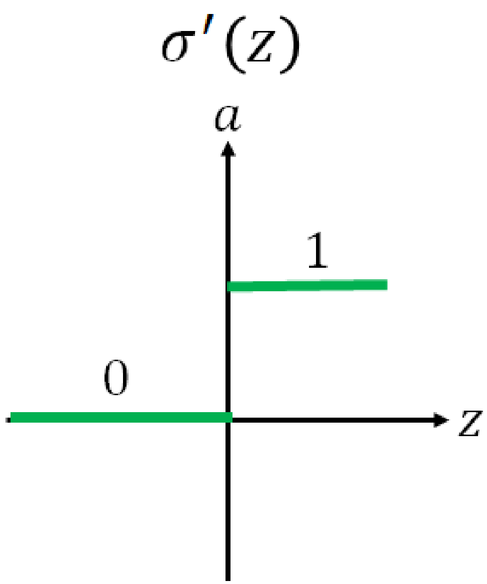


ReLU

Backward Pass:

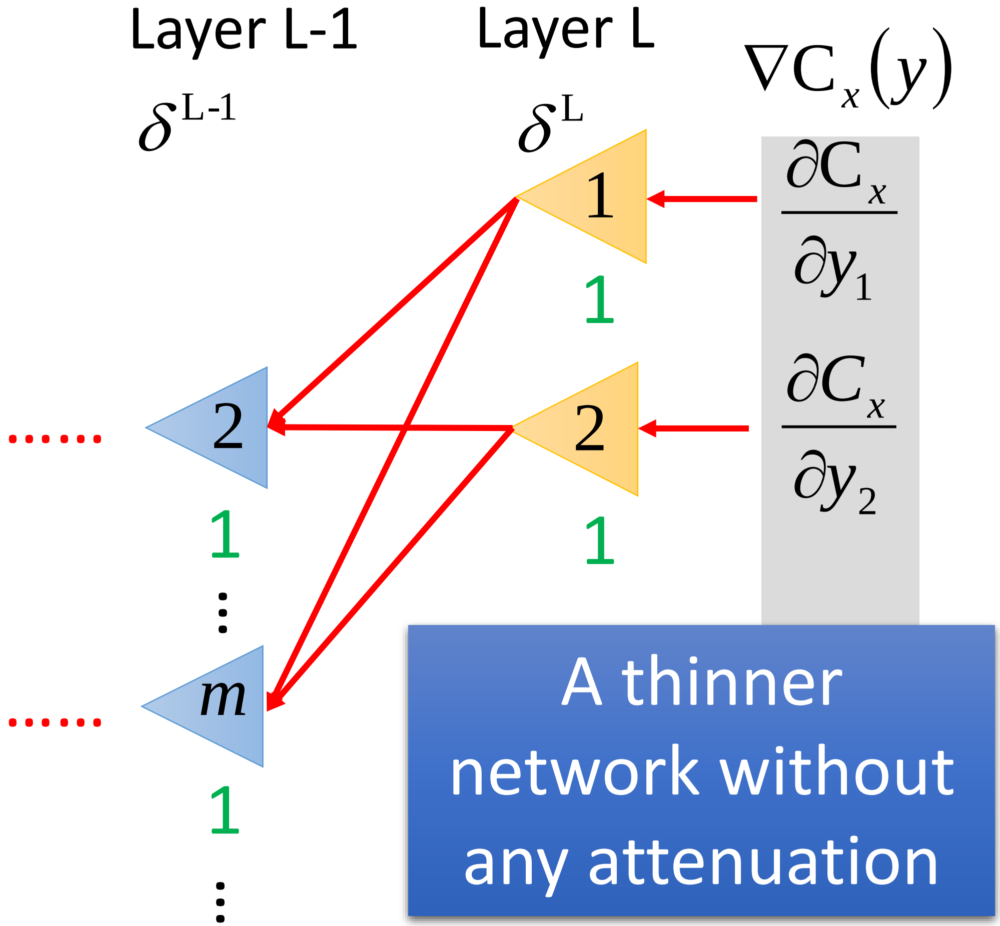




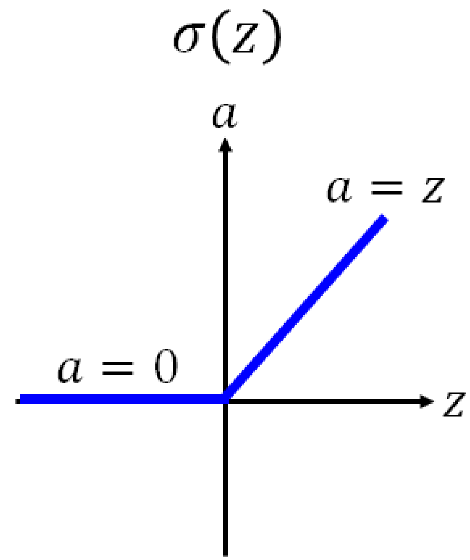


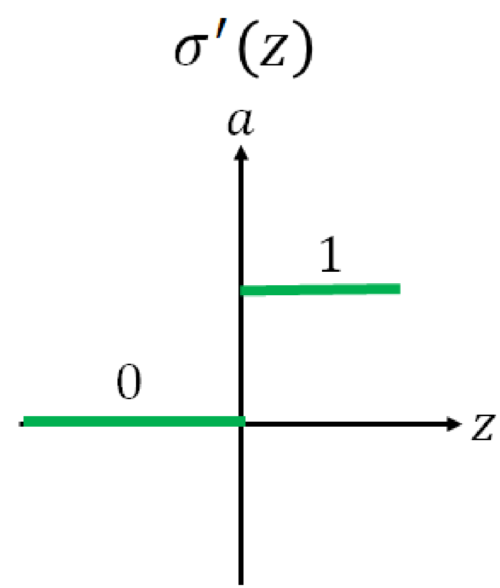
ReLU

Backward Pass:

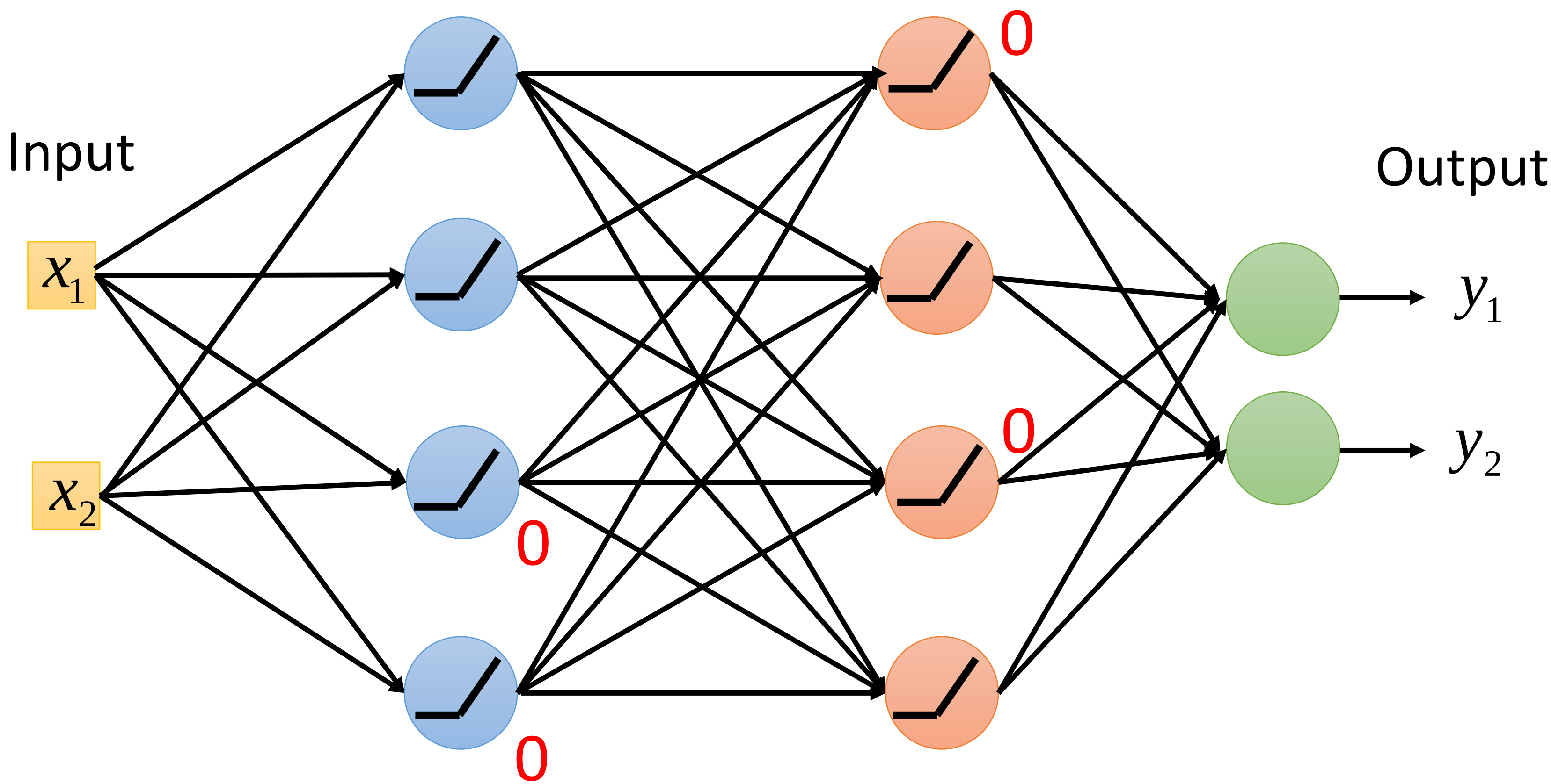


A thinner network without any attenuation

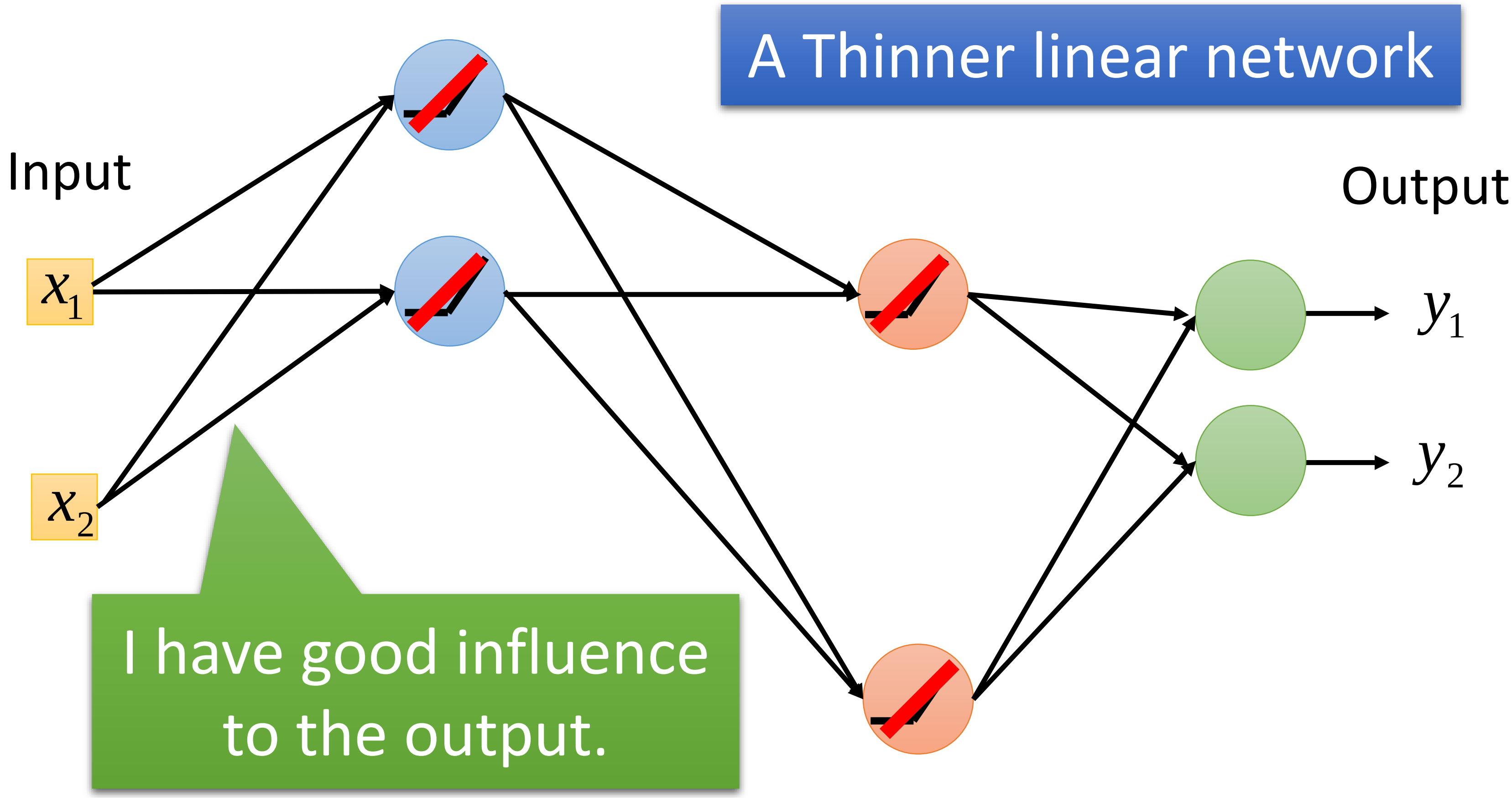




ReLU



ReLU



A Thinner linear network
Input
x_1
x_2
Output
y_1
y_2
I have good influence to the output.

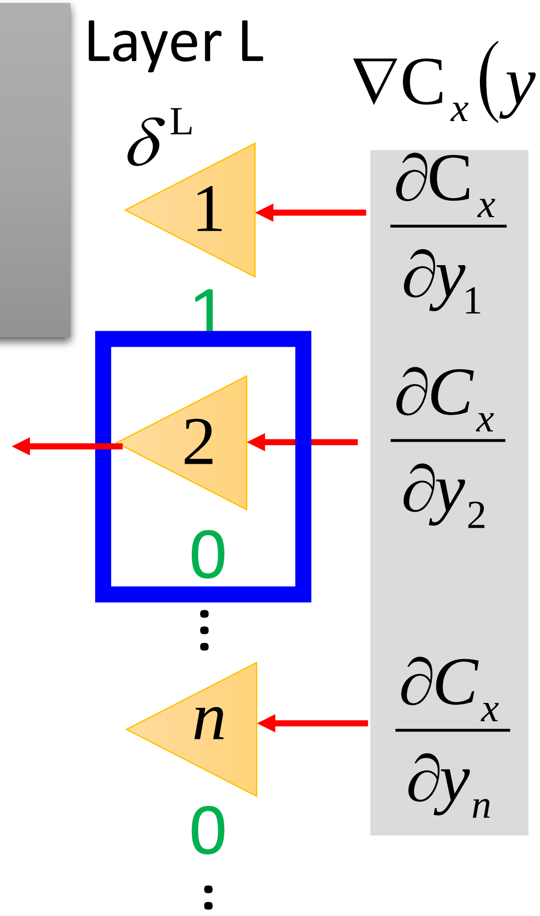
ReLU

$$\frac{\partial C_x}{\partial w_{nj}^L} = \frac{\partial z_n^L}{\partial w_{nj}^L} \frac{\partial C_x}{\partial z_n^L}$$

Backward Pass:

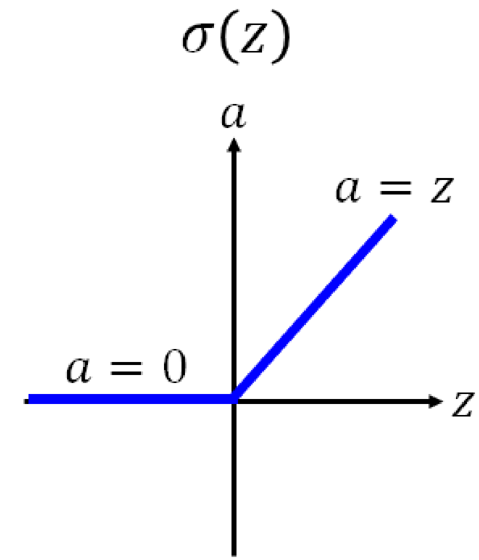
All the weights connected to this neuron will not update.

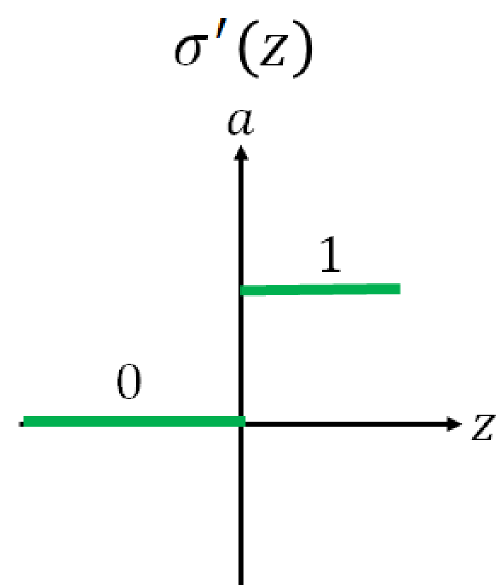
$$\delta_n^L = \frac{\partial C_x}{\partial z_n^L} = 0$$



Possible solution:

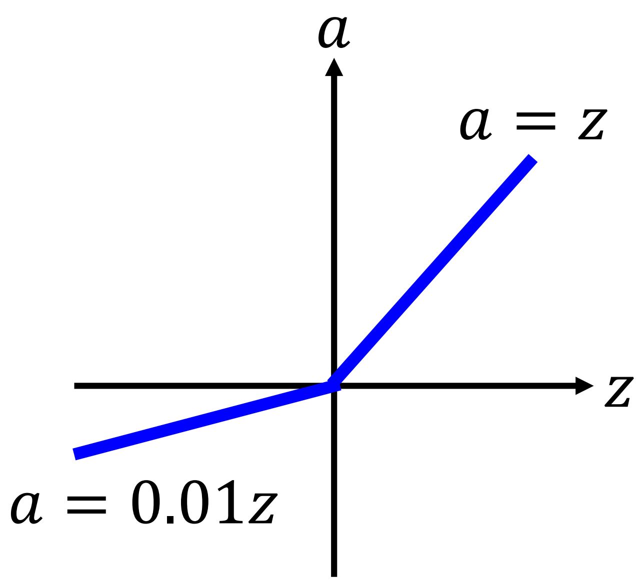
1. softplus
2. Initialize with large bias



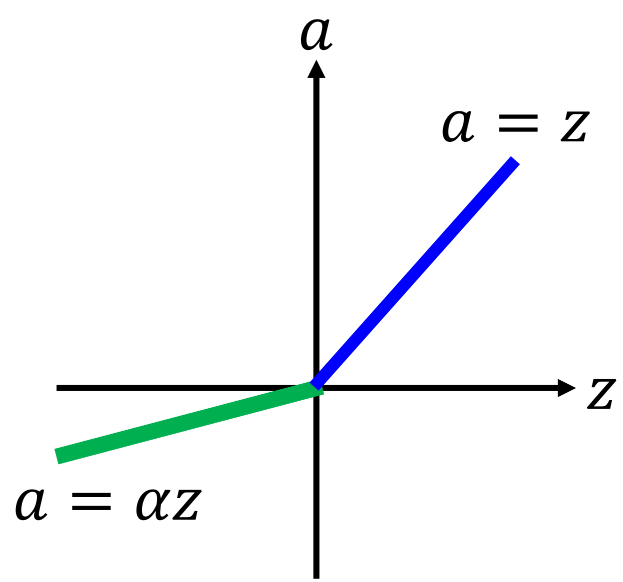


ReLU - variant

$Leaky\ ReLU$



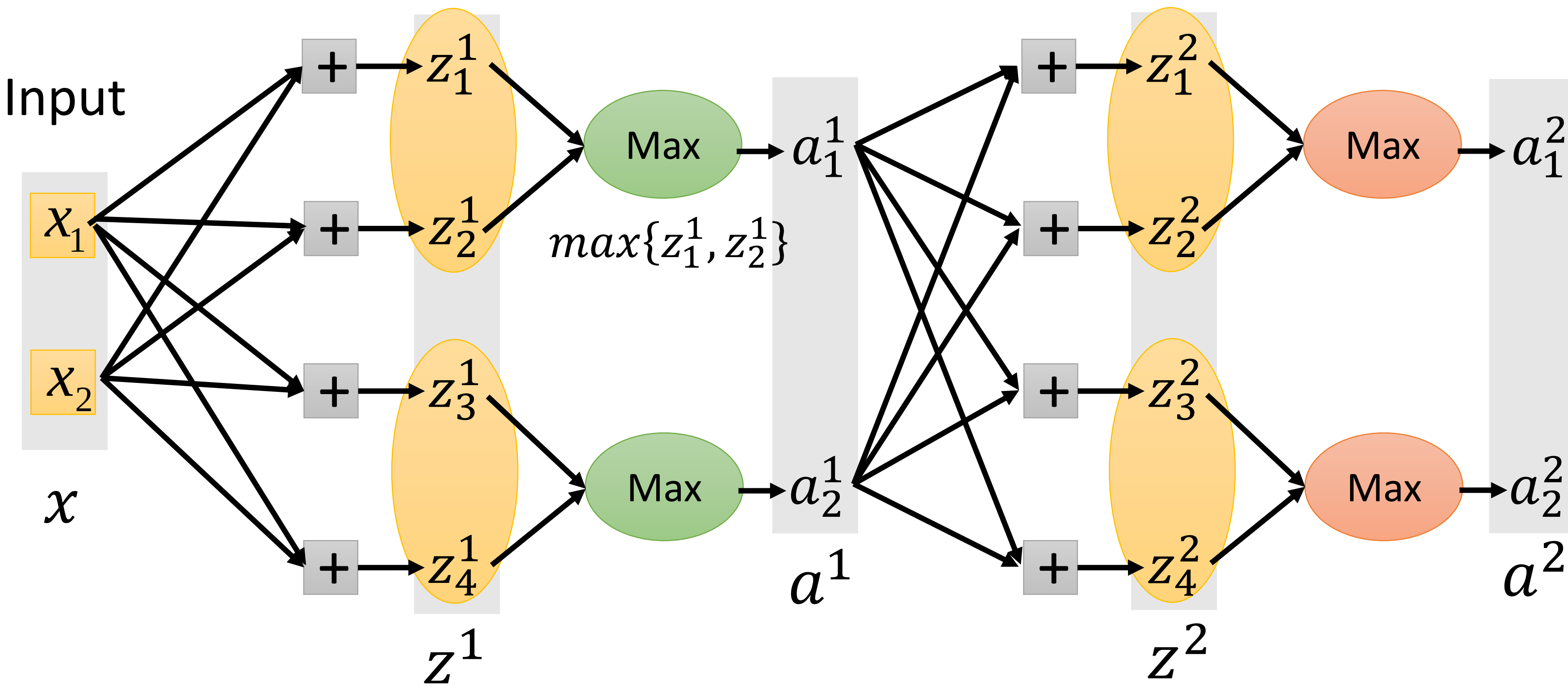
$Parametric\ ReLU$



α also learned by gradient descent

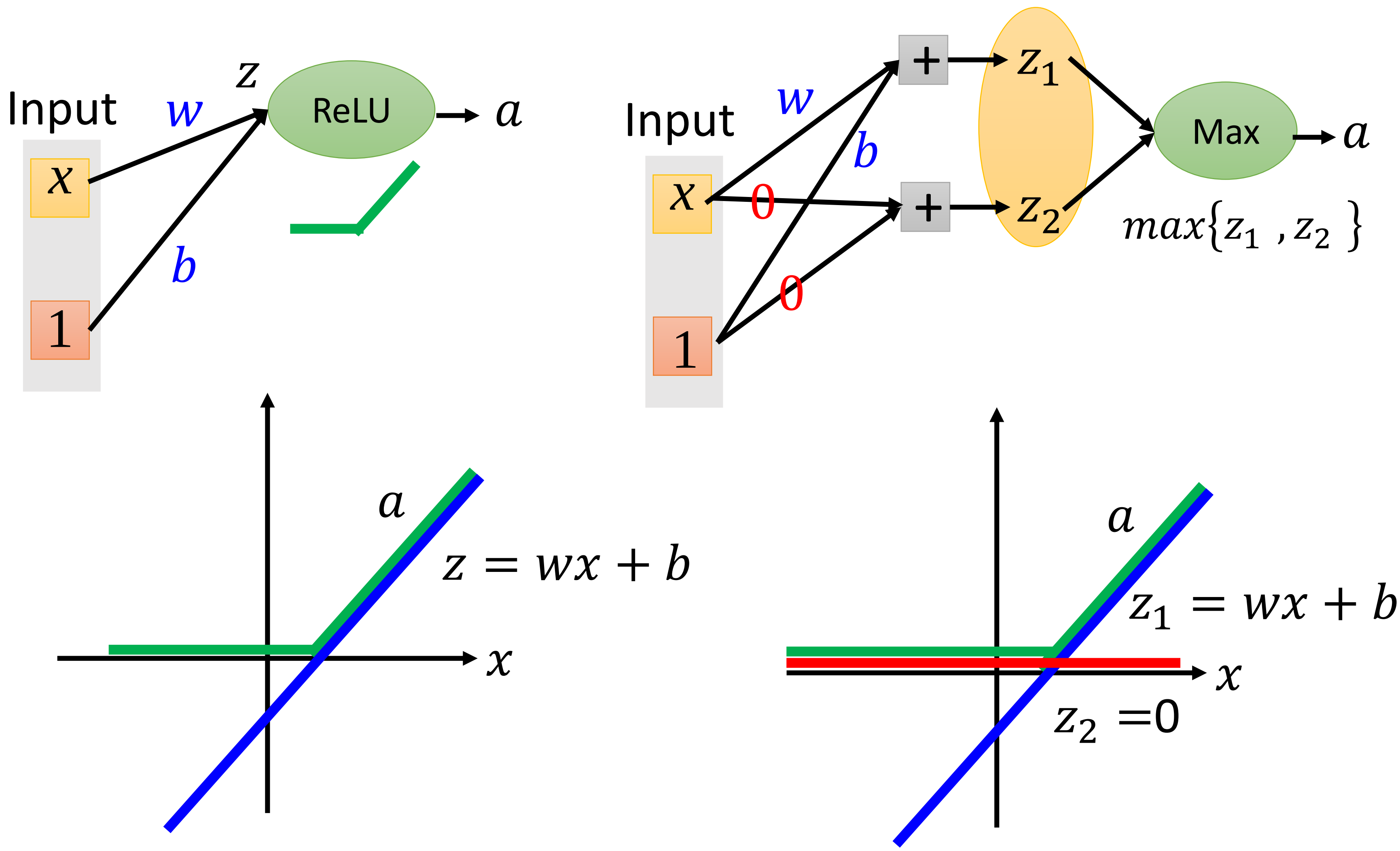
Maxout

- All ReLU variants are just special cases of Maxout

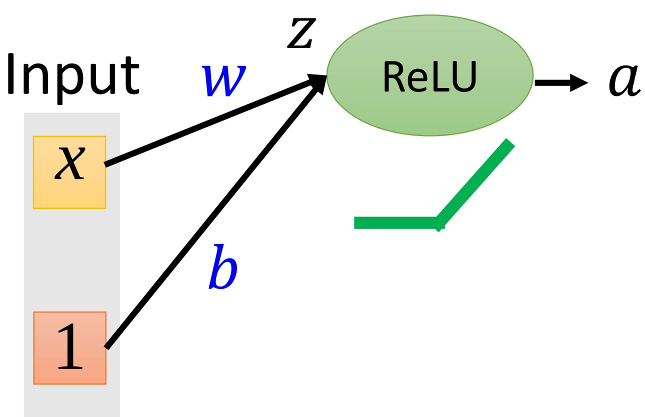


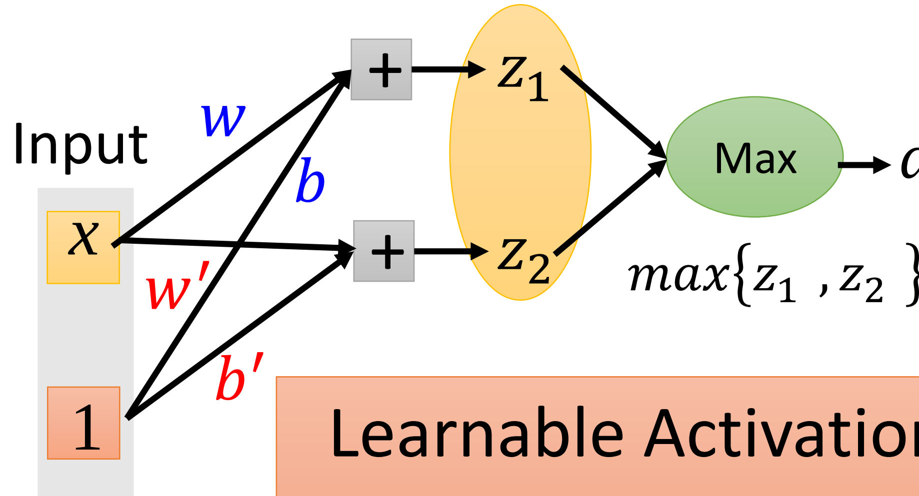
$z^1 = W^1 x$ $z^2 = W^2 a^1$

Maxout – ReLU is special case

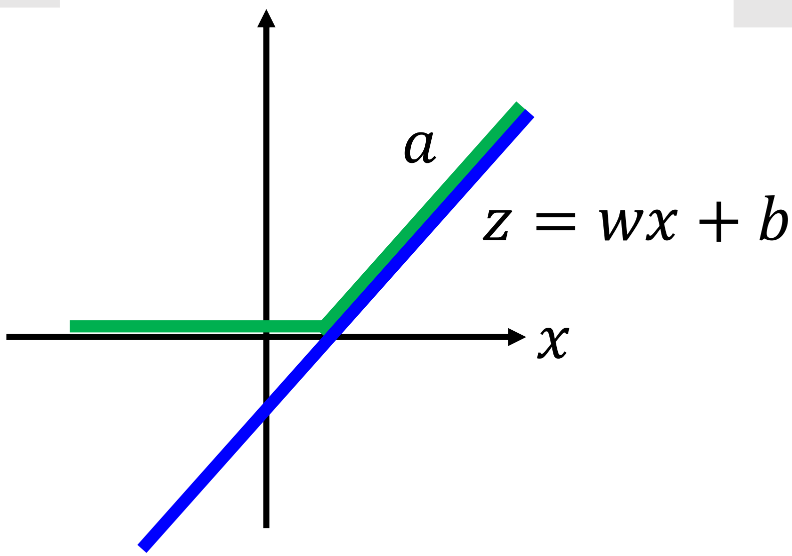


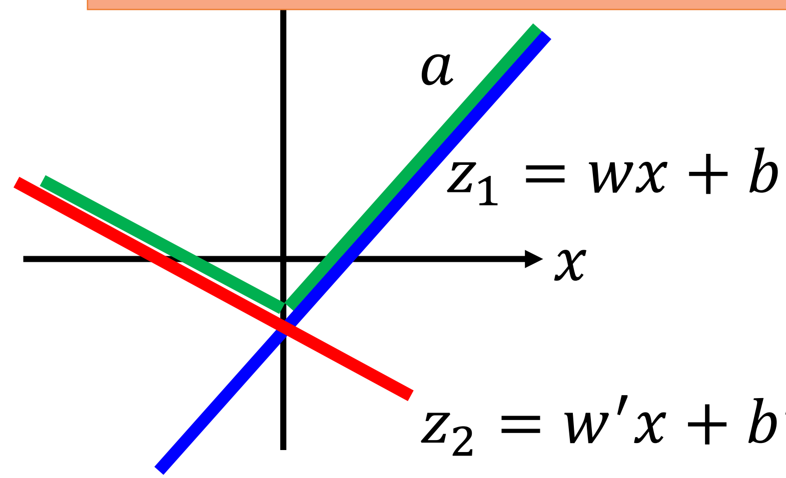
Maxout – ReLU is special case





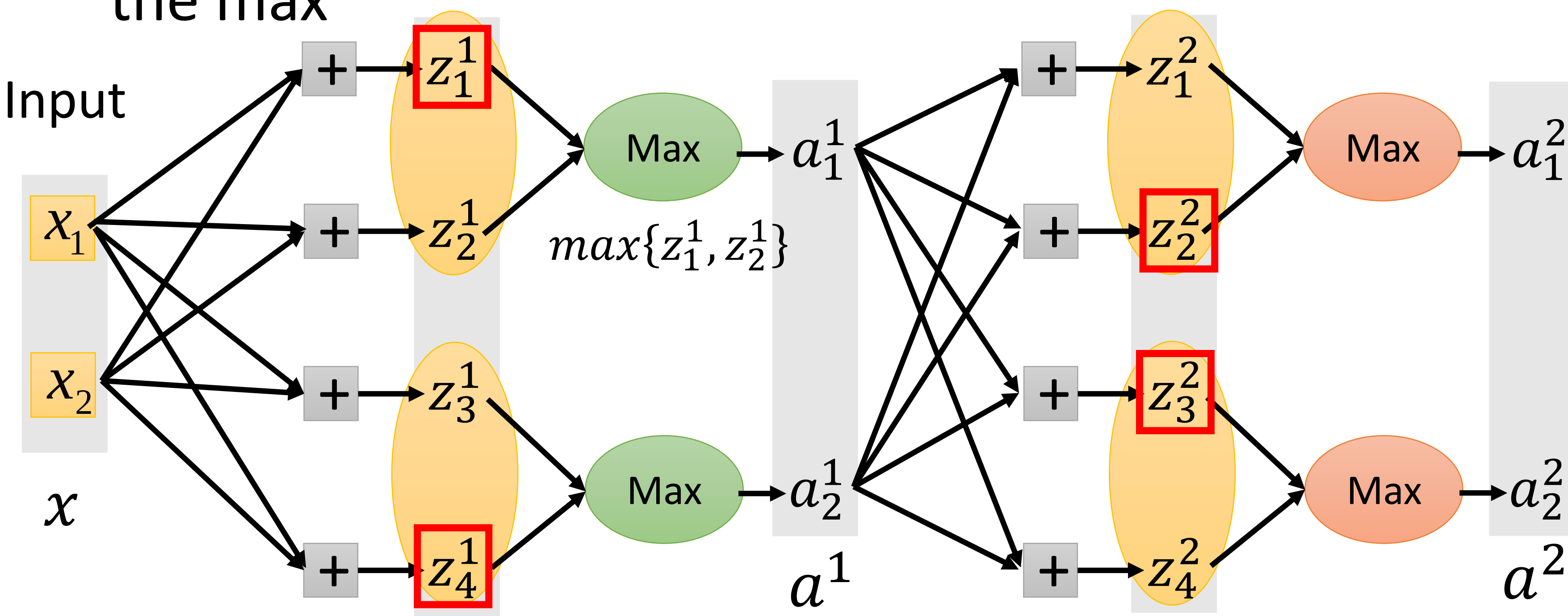
Learnable Activation Function





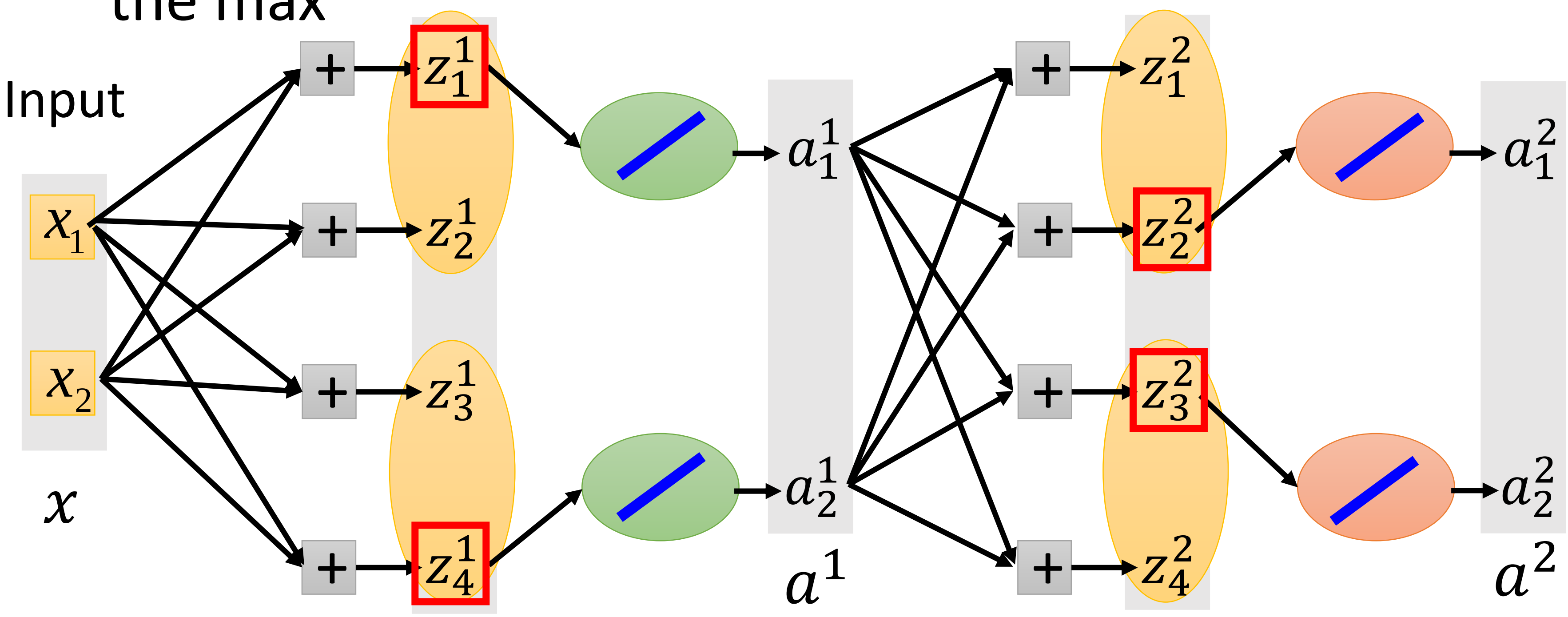
Maxout - Training

- Given a training data x, we know which z would be the max



Maxout - Training

- Given a training data x, we know which z would be the max



- Train this thin and linear netowrk

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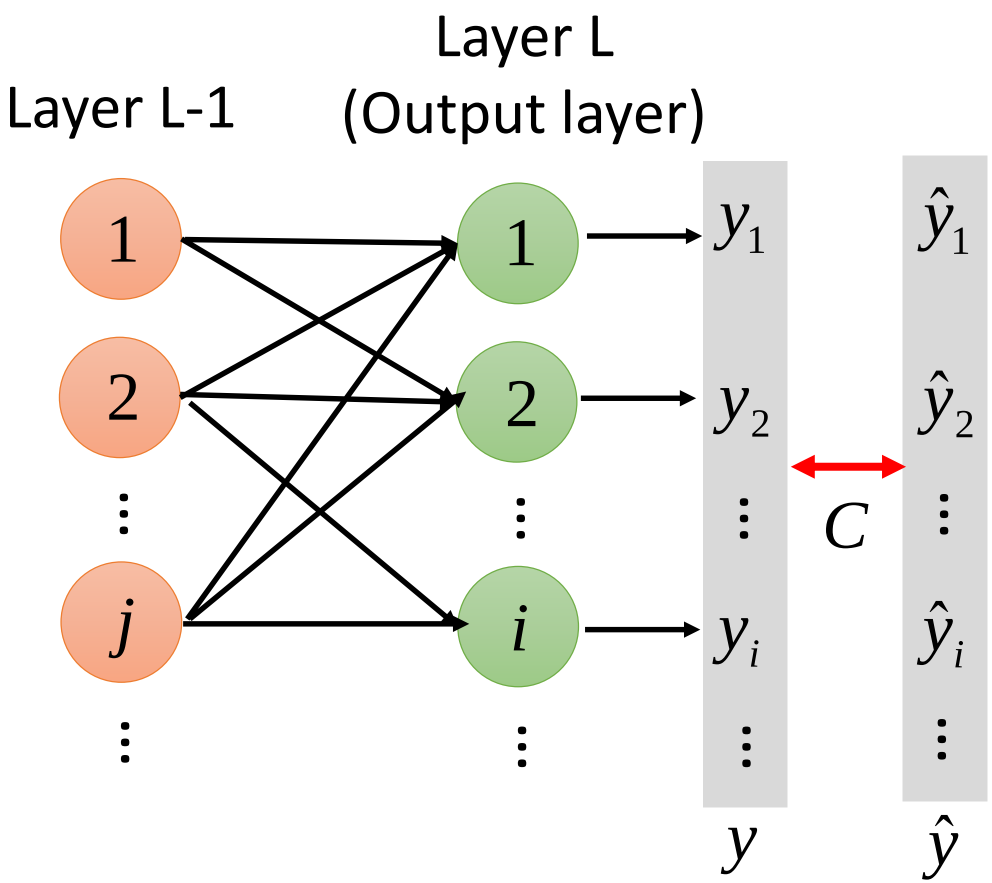
Cost Function



$$C = \frac{1}{2}\left\|y - \hat{y}\right\|^2$$

$$= \frac{1}{2}\sum_n \left(y_n - \hat{y}_n\right)^2$$

Output Layer

$$\hat{y} = \begin{bmatrix} 0 \\ 0 \\ \vdots \\ 1 \\ \vdots \end{bmatrix}$$

More similar?

ReLU

$$y = \begin{bmatrix} 0 \\ 0 \\ \vdots \\ 1.2 \\ \vdots \end{bmatrix}$$

ReLU

$$y = \begin{bmatrix} 0 \\ 0 \\ \vdots \\ 2 \\ \vdots \end{bmatrix}$$

- Larger output means larger confidence

Better?

<u>Classification Task:</u>

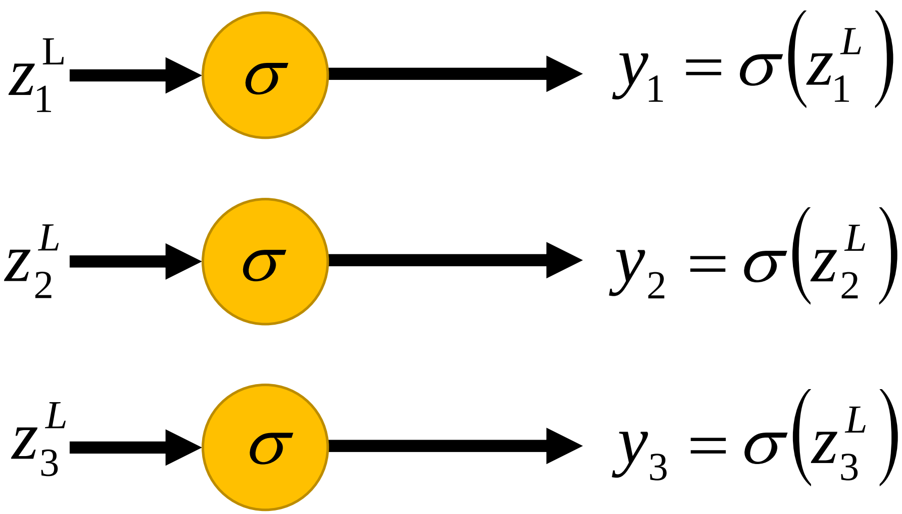
Only one dimension is 1, and others are all 0

It is better to let the output bounded.

Softmax

- Softmax layer as the output layer

<u>Ordinary Output layer</u>



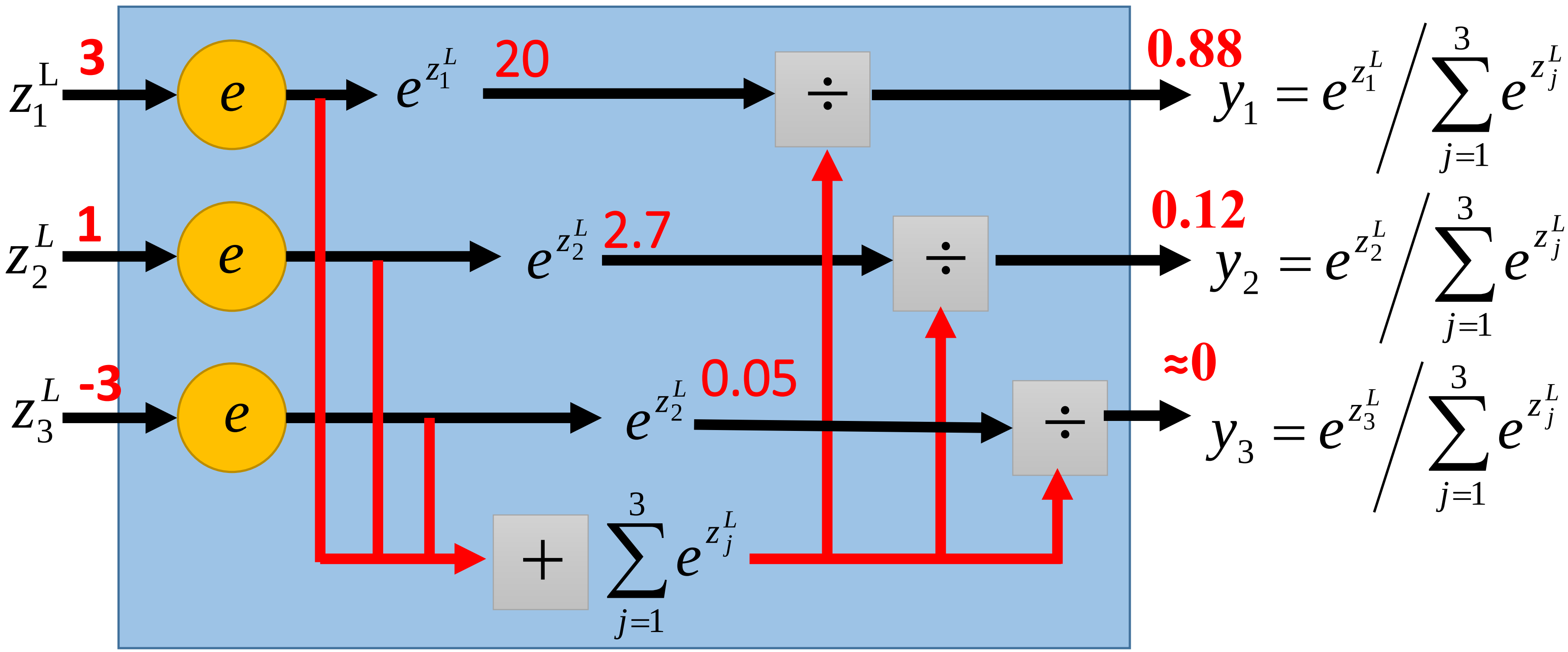
Softmax

- Softmax layer as the output layer

Probability:

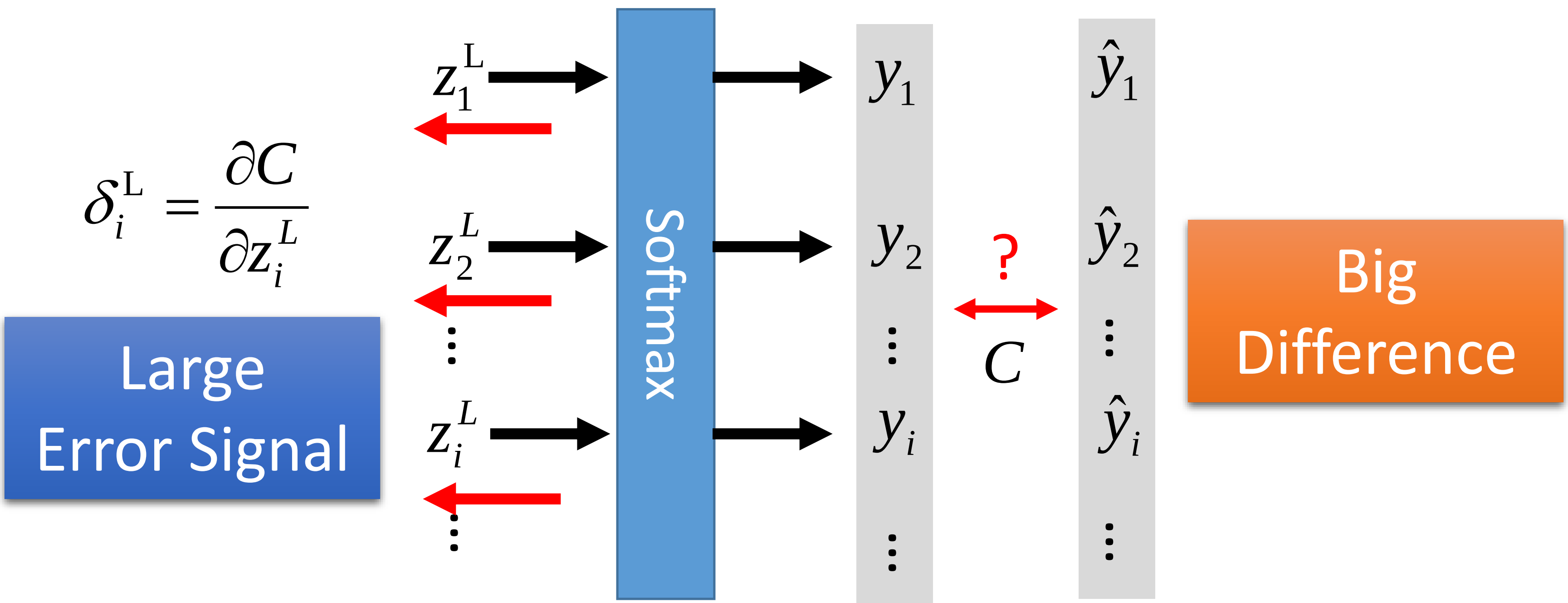
- $1 > y_i > 0$
- $\sum_i y_i = 1$

Softmax Layer



Softmax

- What kind of cost function should we used for softmax layer output?



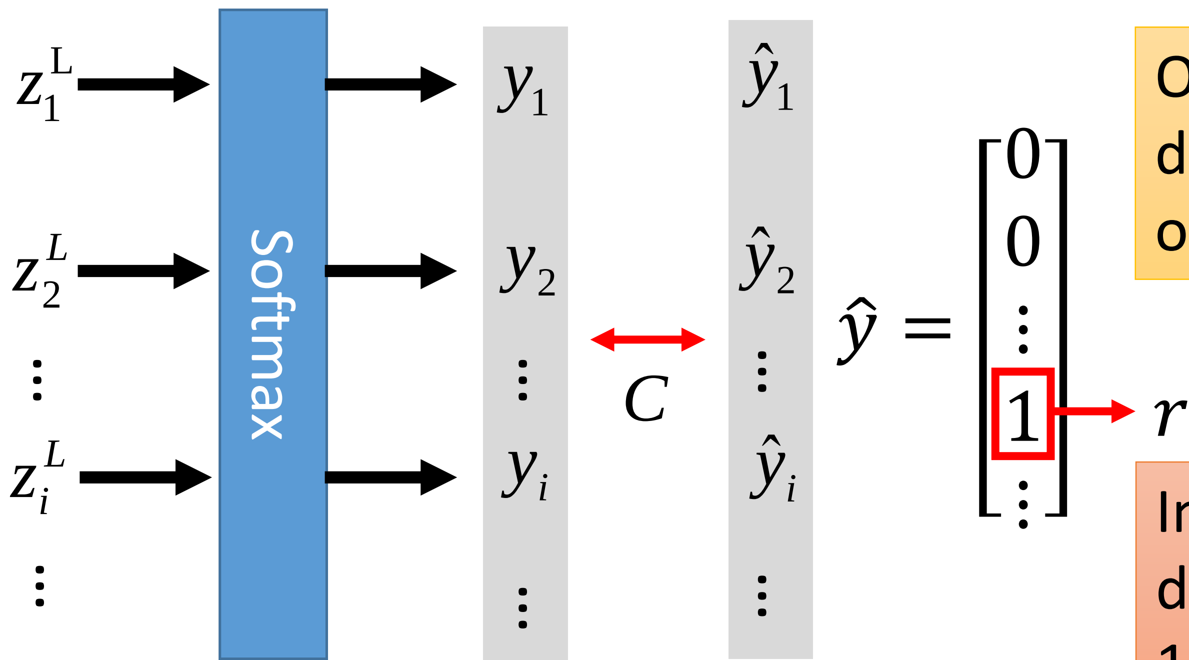
Softmax

Define cost: $C = -log y_r$

Cross Entropy

$$y_i = \frac{e^{z_i^L}}{\sum_j e^{z_j^L}}$$

Do we have to consider other dimensions?



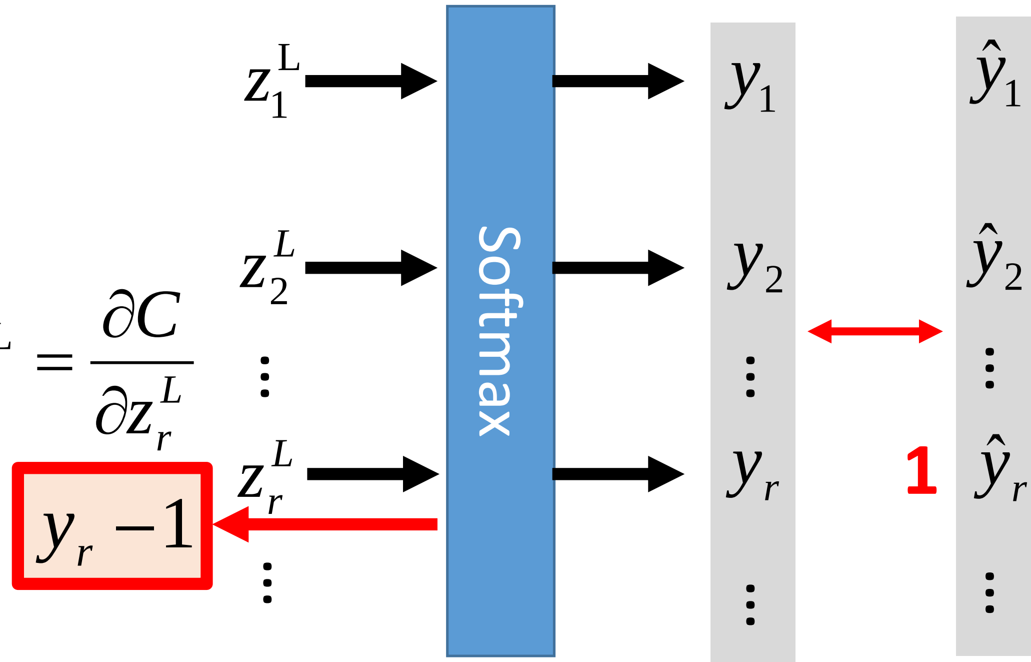
Only one dimension is 1, and others are all 0

Index of the dimension which is 1

$$y_i = \frac{e^{z_i^L}}{\sum_j e^{z_j^L}}$$

$$C = -\log y_r$$

$$\delta_r^L = \frac{\partial C}{\partial z_r^L}$$



$$\frac{\partial C}{\partial y_r} \frac{\partial y_r}{\partial z_r^L}$$

$$\delta_r^L = \frac{\partial C}{\partial z_r^L} = -\frac{1}{y_r} \frac{\partial y_r}{\partial z_r^L} = -\frac{1}{y_r}\left(y_r - y_r^2\right) = \underline{y_r - 1}$$

The absolute value of δ_r^L is larger when y_r is far from 1

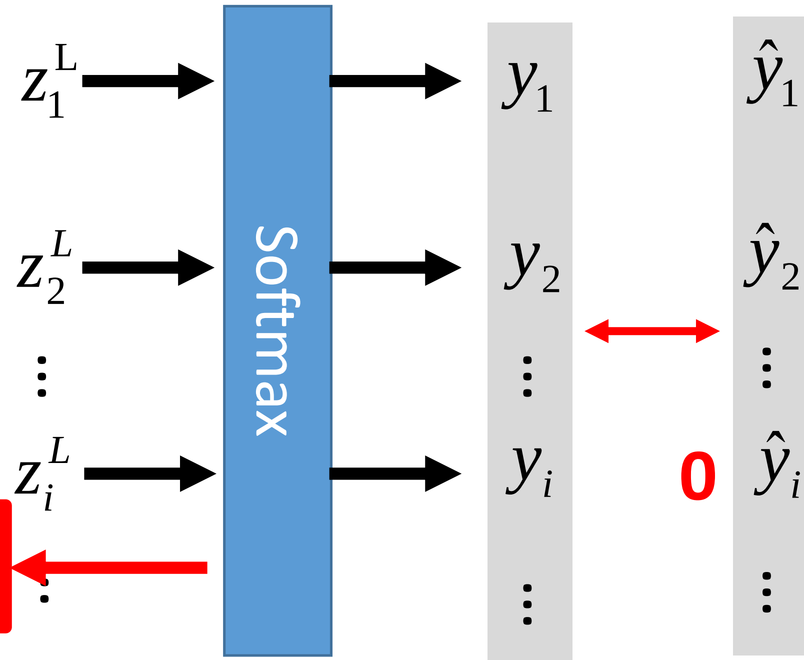
$$y_r = \frac{e^{z_r^L}}{\sum_j e^{z_j^L}}$$

z_r^L appears in both numerator and denominator

$$y_i = \frac{e^{z_i^L}}{\sum_j e^{z_j^L}}$$

$$C = -log y_r$$

$$\delta_i^{\mathrm{L}} = \frac{\partial C}{\partial z_i^L}$$



$$\boxed{y_i - 0}$$

$$\frac{\partial C}{\partial y_r}\frac{\partial y_r}{\partial z_i^L}$$

$$i \neq r$$

$$\delta_i^{\mathrm{L}} = \frac{\partial C}{\partial z_i^L} = -\frac{1}{y_r}\frac{\partial y_r}{\partial z_i^L} = -\frac{1}{y_r}\left(-y_r y_i\right) = \underline{y_i}$$

$$y_r = \frac{e^{z_r^L}}{\sum_j e^{z_j^L}}$$

z_i^L appears only in denominator

The absolute value of δ_i^L is larger when y_i is larger

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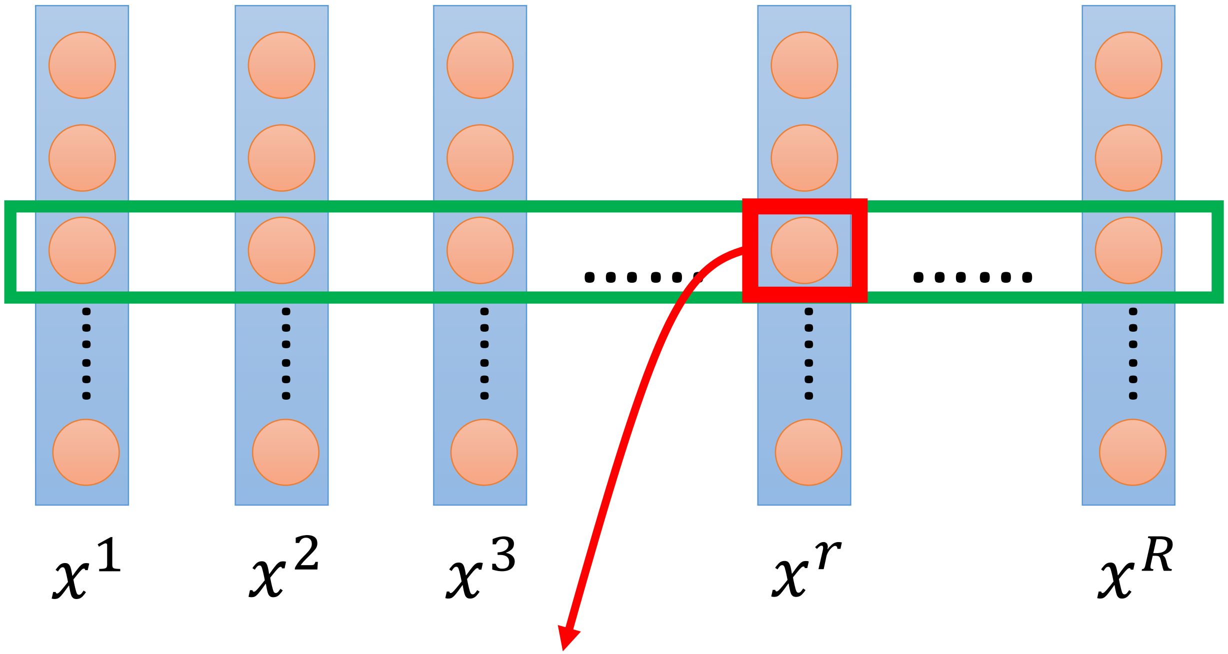
Normalizing Input



For each dimension i:

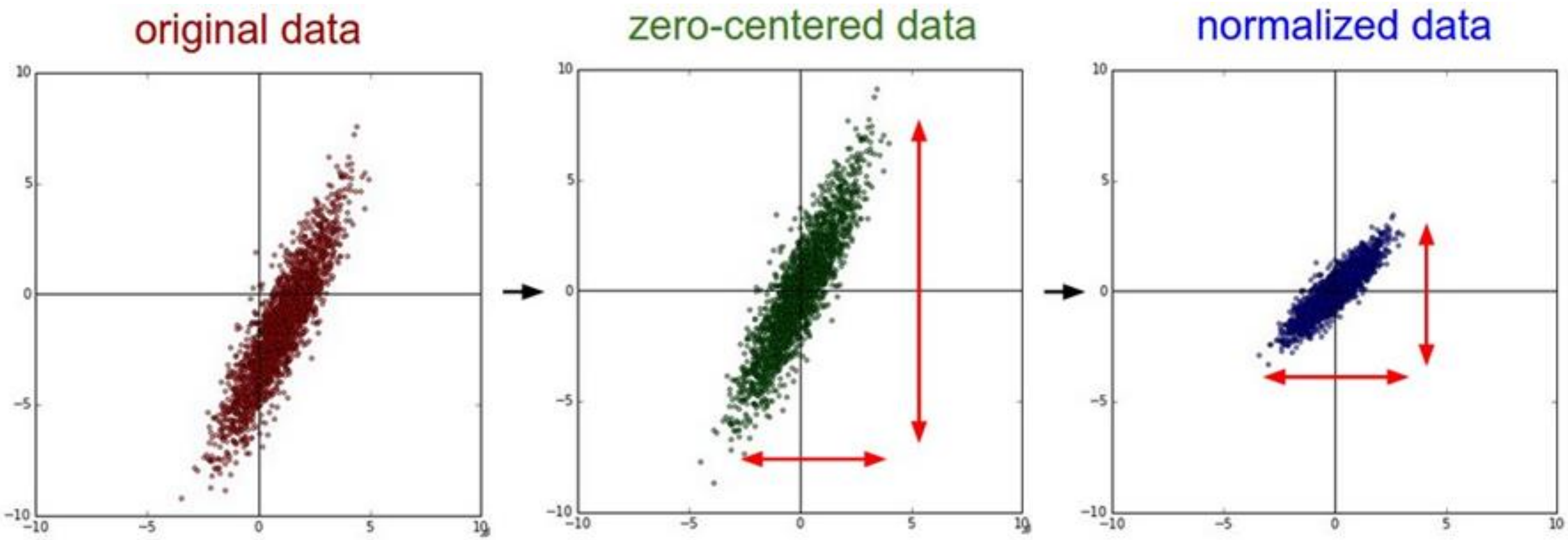
mean: m_i

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

Normalizing Input



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

Normalizing your training and testing data in the same way.

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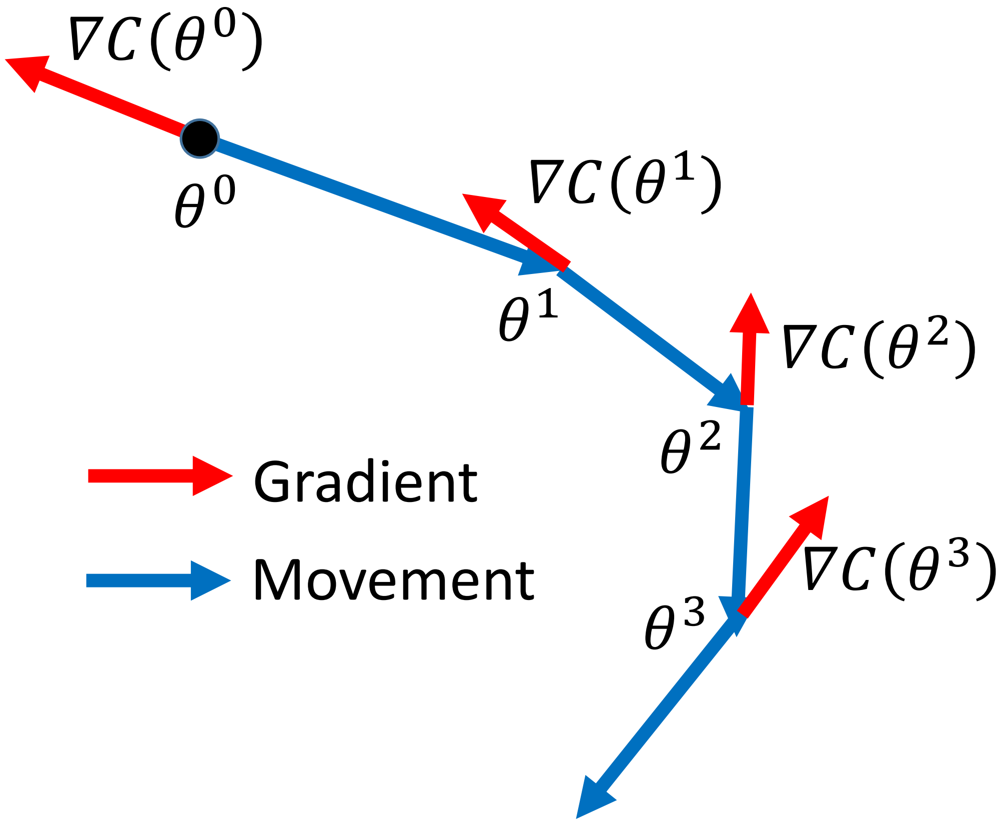
Vanilla Gradient Descent



Start at position θ^0

Compute gradient at θ^0

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

Compute gradient at θ^1

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

⋮

Stop until $\nabla C(\theta^t) \approx 0$

1. How to determine the learning rates
2. Stuck at local minima or saddle points

Outline

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- Optimization
  - Learning Rate
  - Momentum
- Generalization

Outline

Activation Function

Cost Function

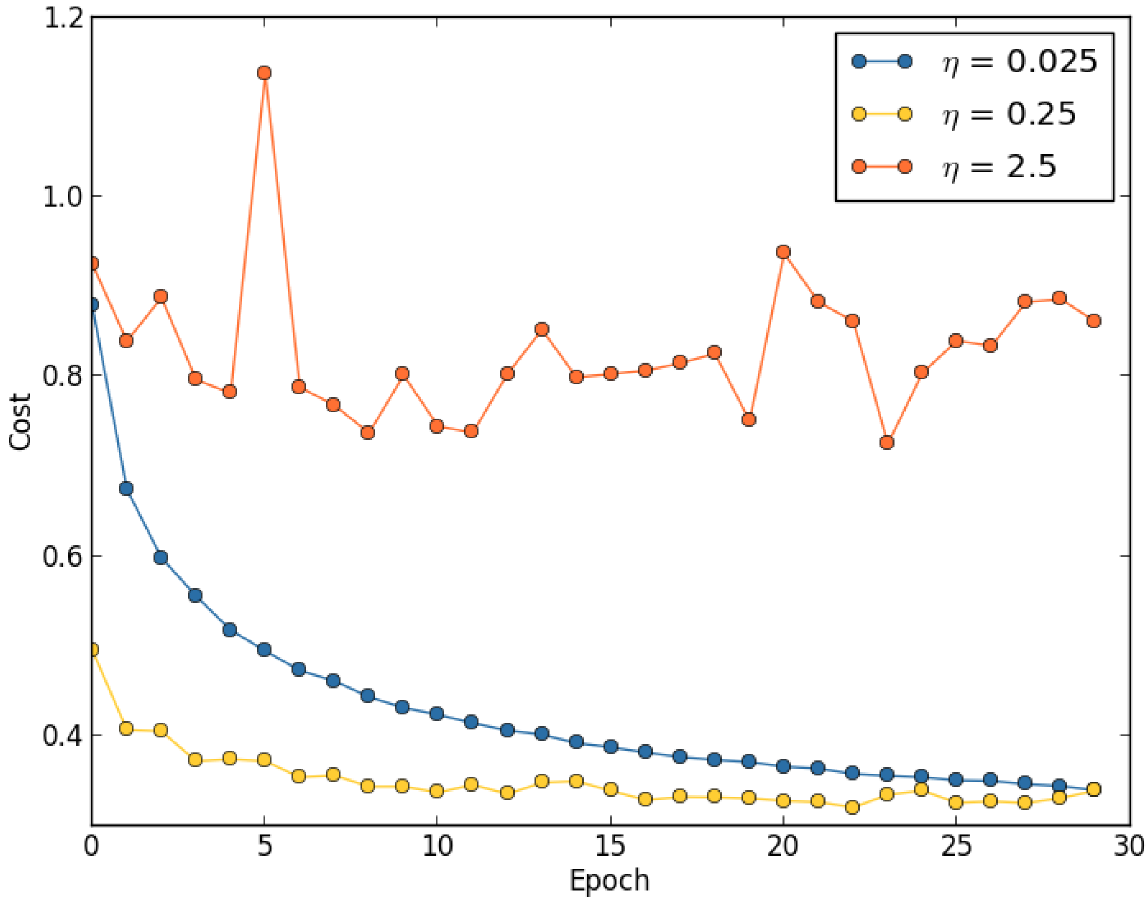
Data Preprocessing

Optimization

Learning Rate | Momentum

Generalization

Learning Rates



Source:
http://neuralnetworksanddeeplearning.com/chap3.html

Learning Rates

- 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
  - Give different parameters different learning rates

Adagrad

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

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

<u>Vanilla Gradient descent</u>

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

w is one parameters

<u>Adagrad</u>

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

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

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

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

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

$$\vdots$$

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

Adagrad

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

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

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

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

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

Contradiction?

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

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

- *反差*

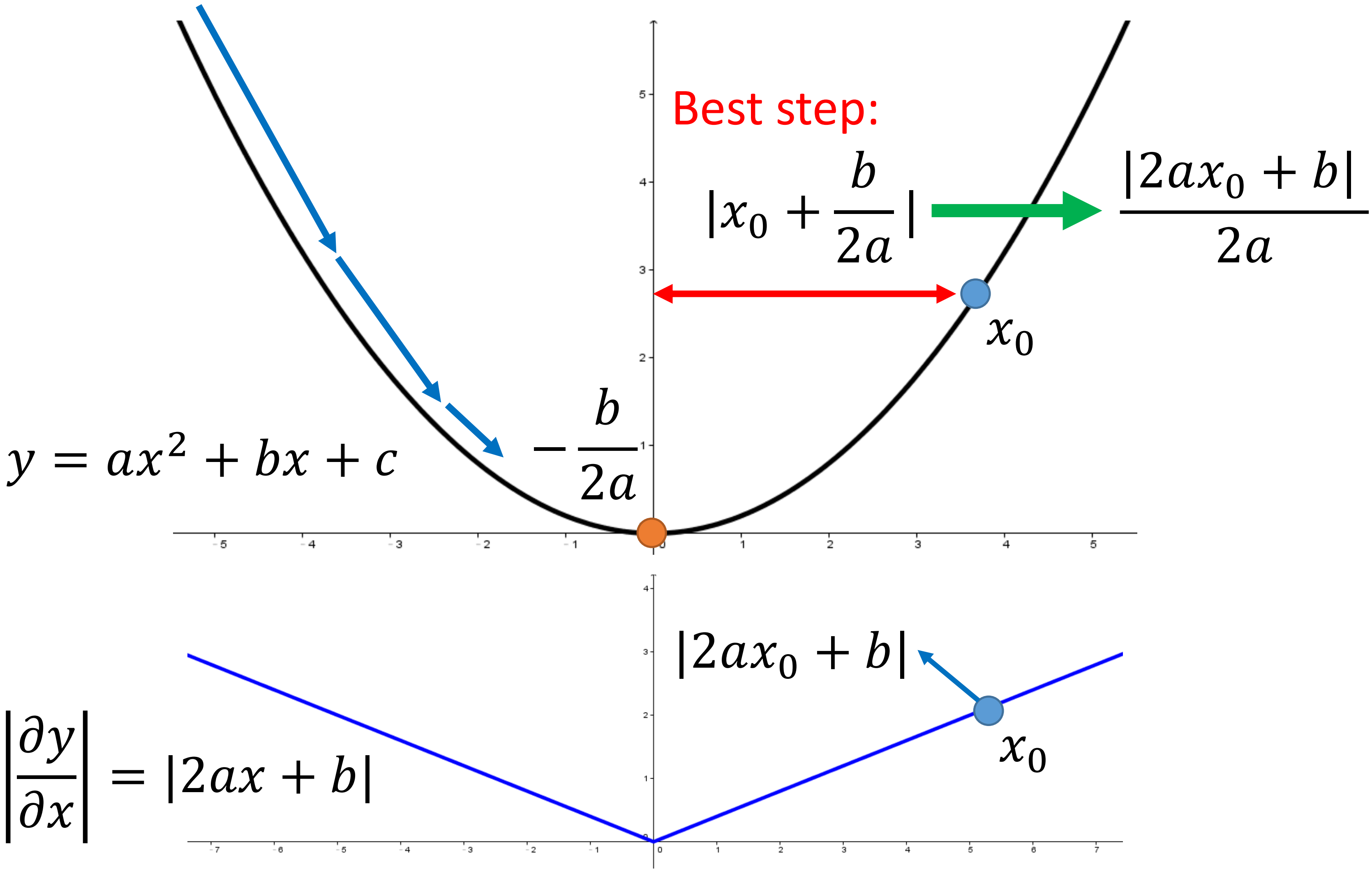
g^0	g^1	g^2	g^3	g^4	……
0.001	0.001	0.003	0.002	0.1	……

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

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

造成反差的效果

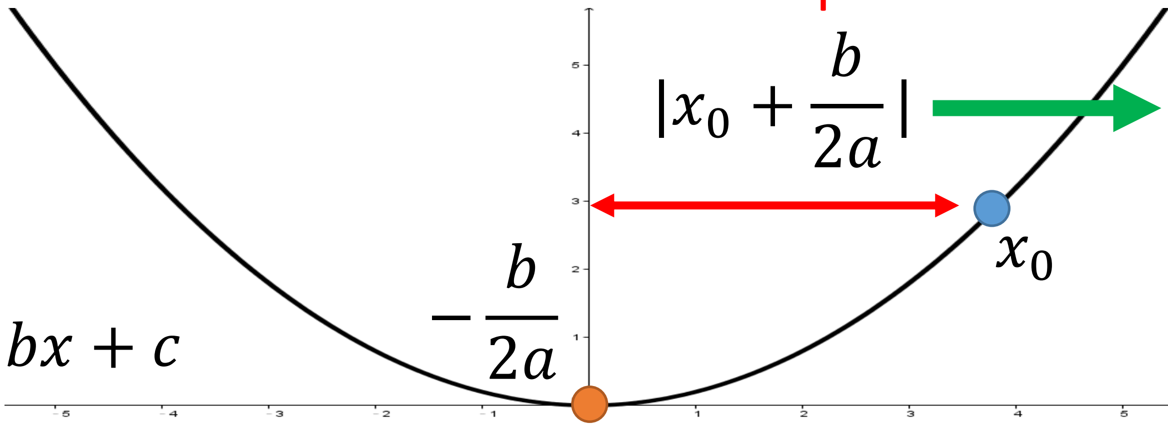
Larger gradient, larger steps?



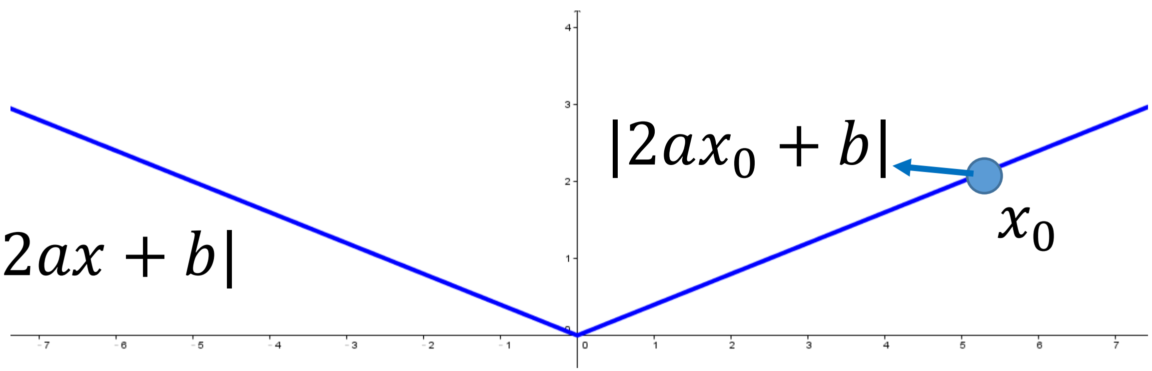
Second Derivative

Best step:

$$\left|x_0 + \frac{b}{2a}\right| \longrightarrow \frac{|2ax_0 + b|}{\boxed{2a}}$$



$$y = ax^2 + bx + c$$



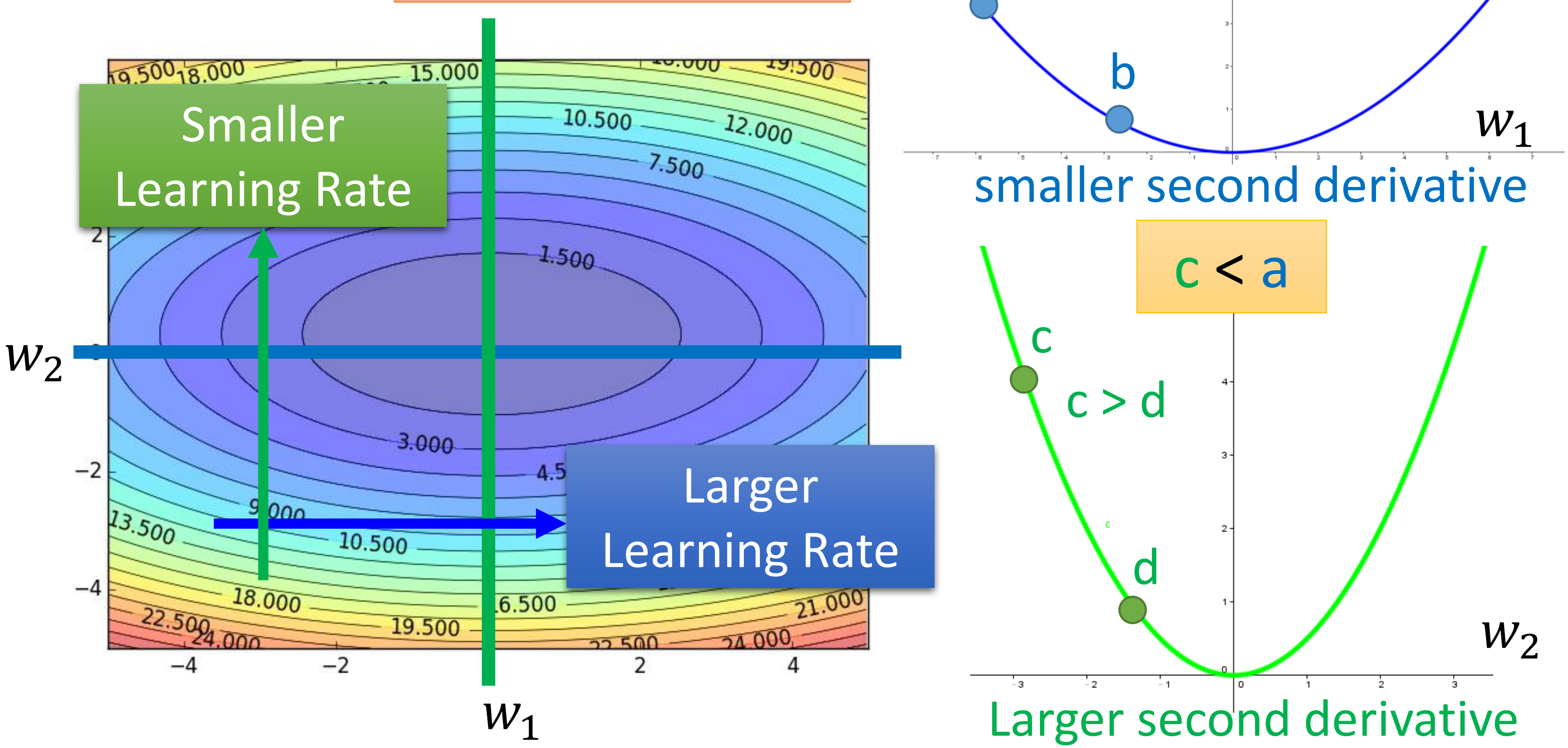
$$\left|\frac{\partial y}{\partial x}\right| = |2ax + b|$$

$$\frac{\partial^2 y}{\partial x^2} = 2a$$

The best step is $\dfrac{|\text{First derivative}|}{\text{Second derivative}}$

More than one parameters

The best step is $\dfrac{|\text{First derivative}|}{\text{Second derivative}}$

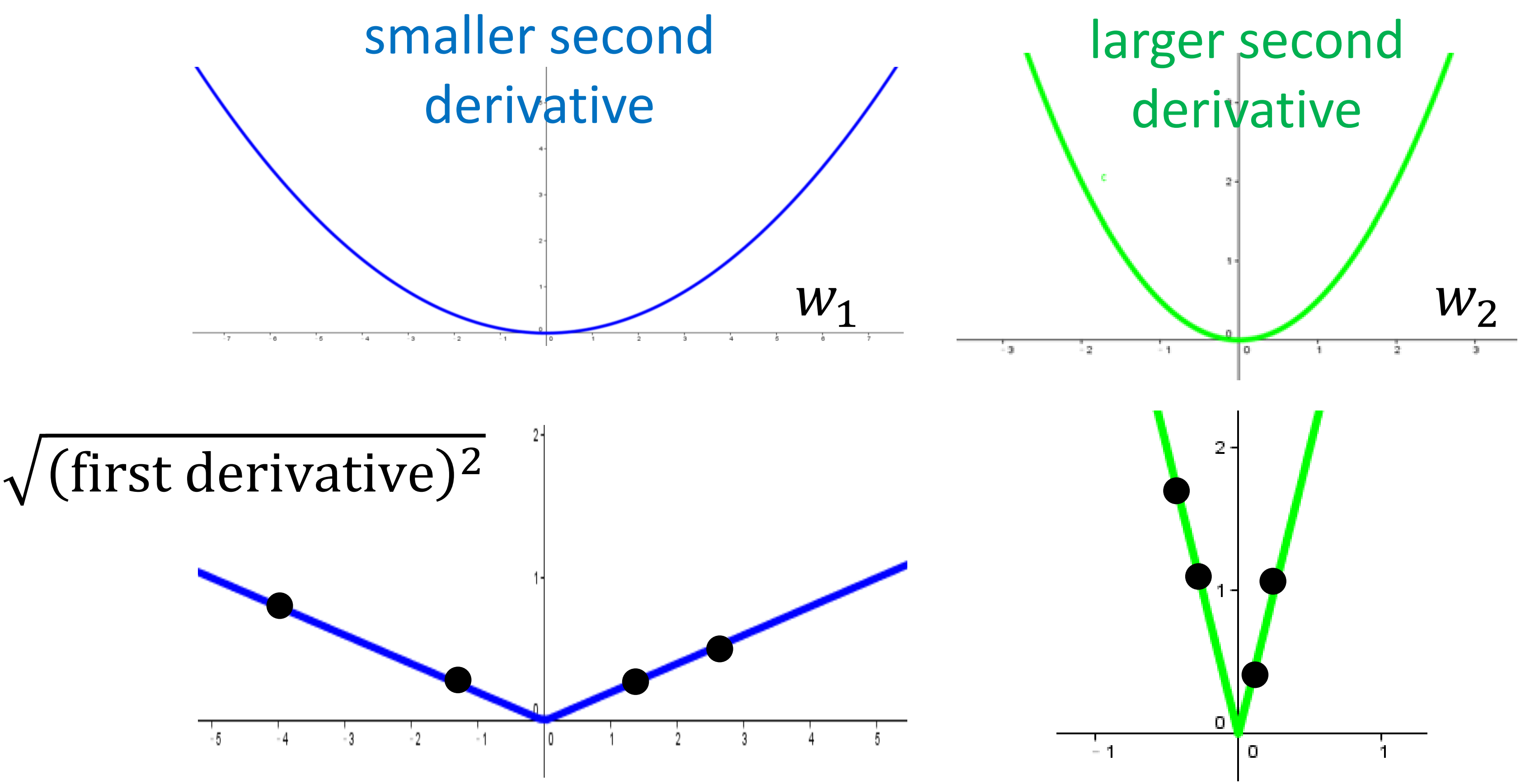


What to do with Adagrad?

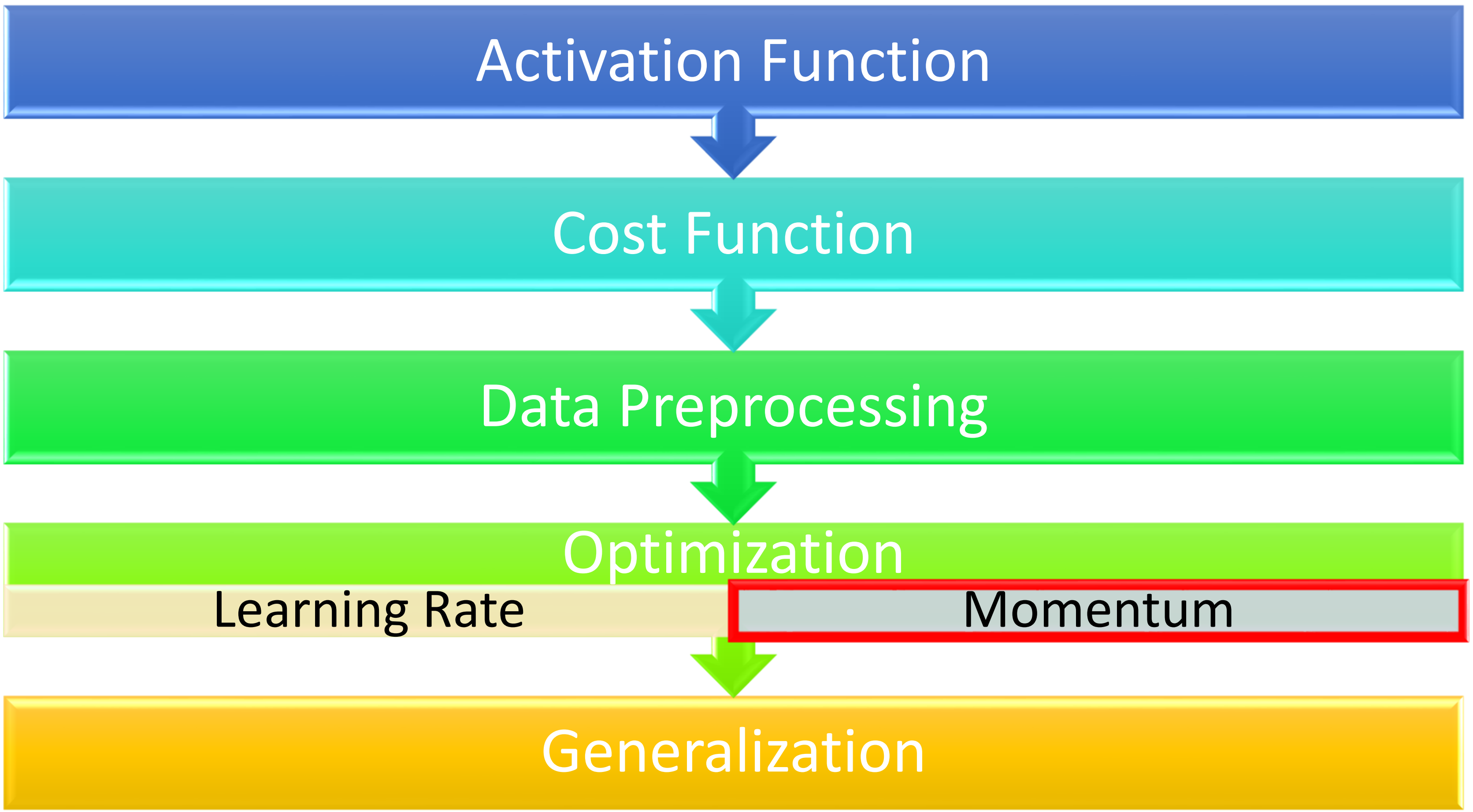
The best step is

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

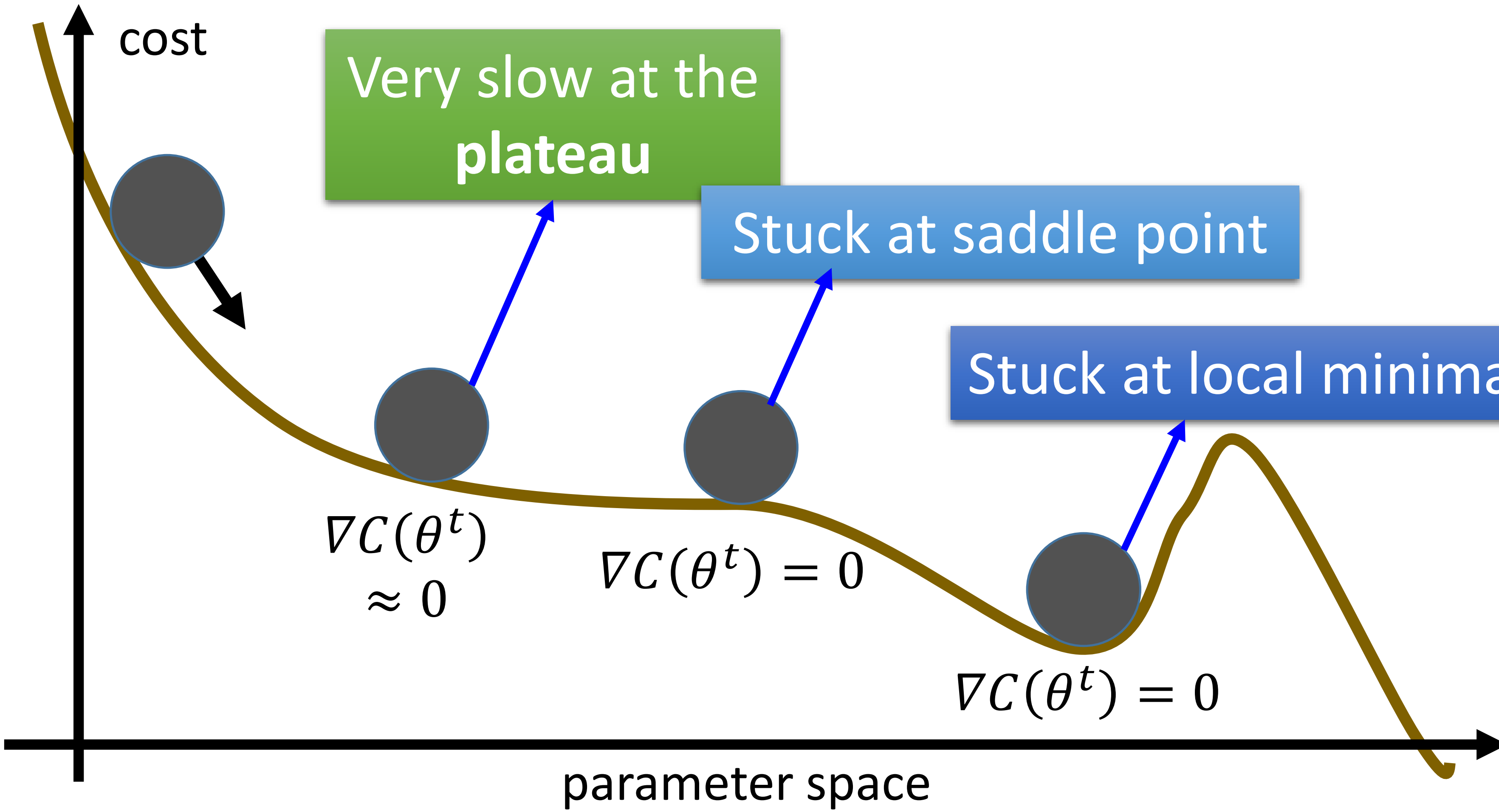
Use *first derivative* to estimate *second derivative*



Outline

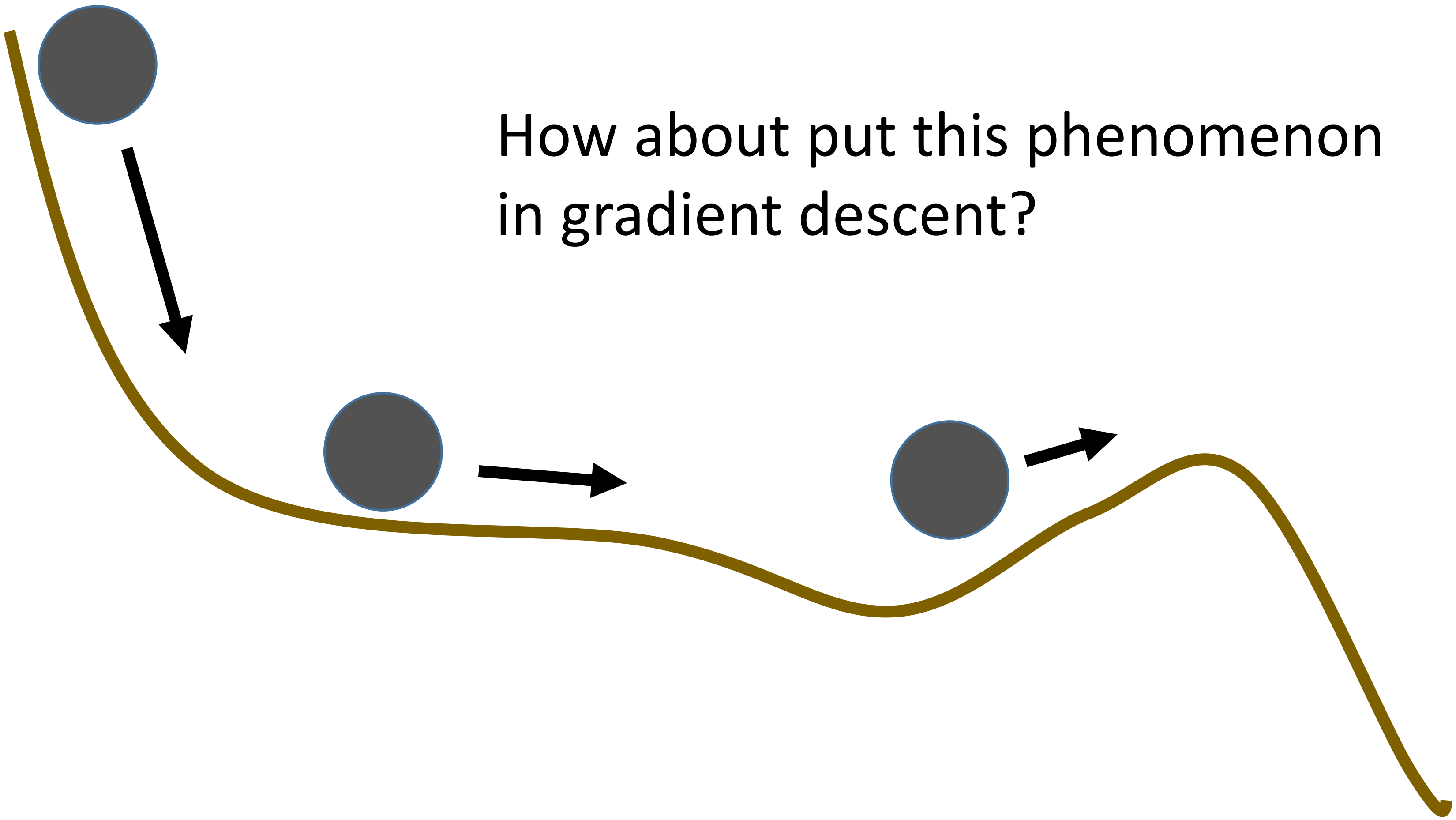

Activation Function
Cost Function
Data Preprocessing
Optimization
Learning Rate
Momentum
Generalization

Easy to stuck



In physical world ……

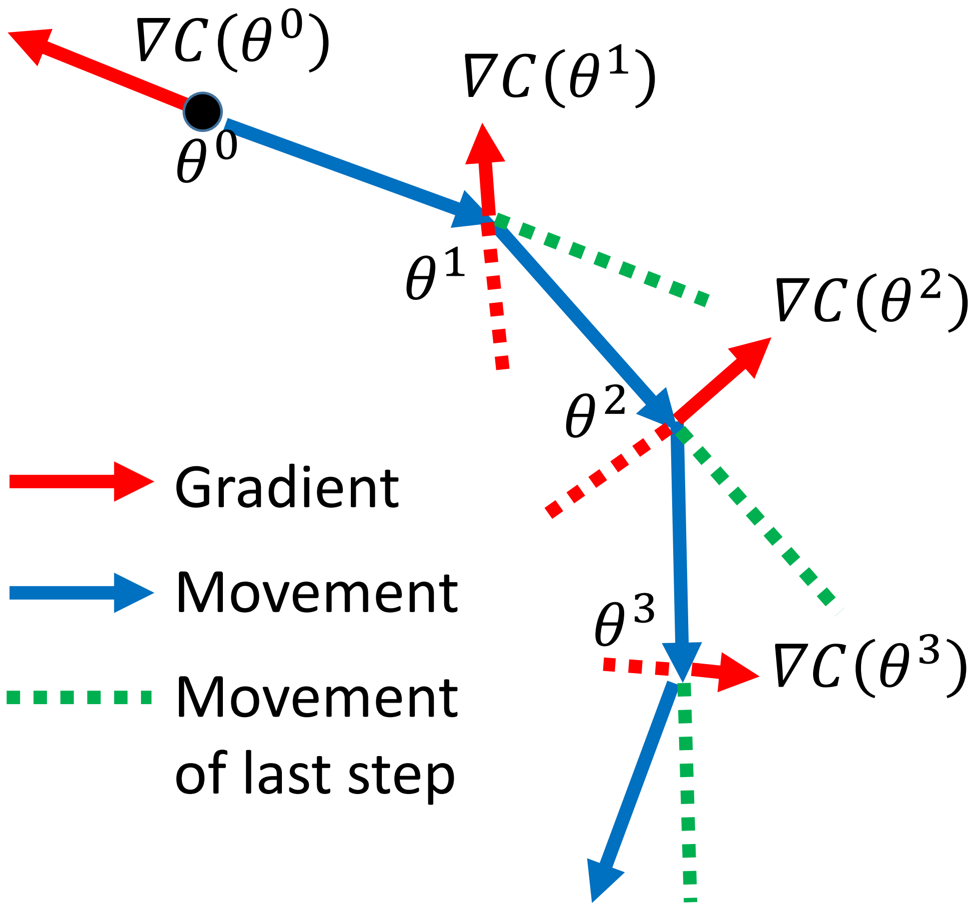
- Momentum



How about put this phenomenon in gradient descent?

Momentum

Movement: movement of last step minus gradient at present



Start at point θ^0

Movement $v^0=0$

Compute gradient at θ^0

Movement $v^1 = \lambda v^0 - \eta \nabla C(\theta^0)$

Move to $\theta^1 = \theta^0 + v^1$

Compute gradient at θ^1

Movement $v^2 = \lambda v^1 - \eta \nabla C(\theta^1)$

Move to $\theta^2 = \theta^1 + v^2$

Movement not just based on gradient, but previous movement.

Momentum

Movement: movement of last step minus gradient at present

v^i is actually the weighted sum of all the previous gradient: $\nabla C(\theta^0)$,$\nabla C(\theta^1)$, … $\nabla C(\theta^{i-1})$

$v^0 = 0$

$v^1 = -\eta\nabla C(\theta^0)$

$v^2 = -\lambda\,\eta\nabla C(\theta^0) - \eta\nabla C(\theta^1)$

⋮

Start at point θ^0

Movement v^0=0

Compute gradient at θ^0

Movement $v^1 = \lambda v^0 - \eta\nabla C(\theta^0)$

Move to $\theta^1 = \theta^0 + v^1$

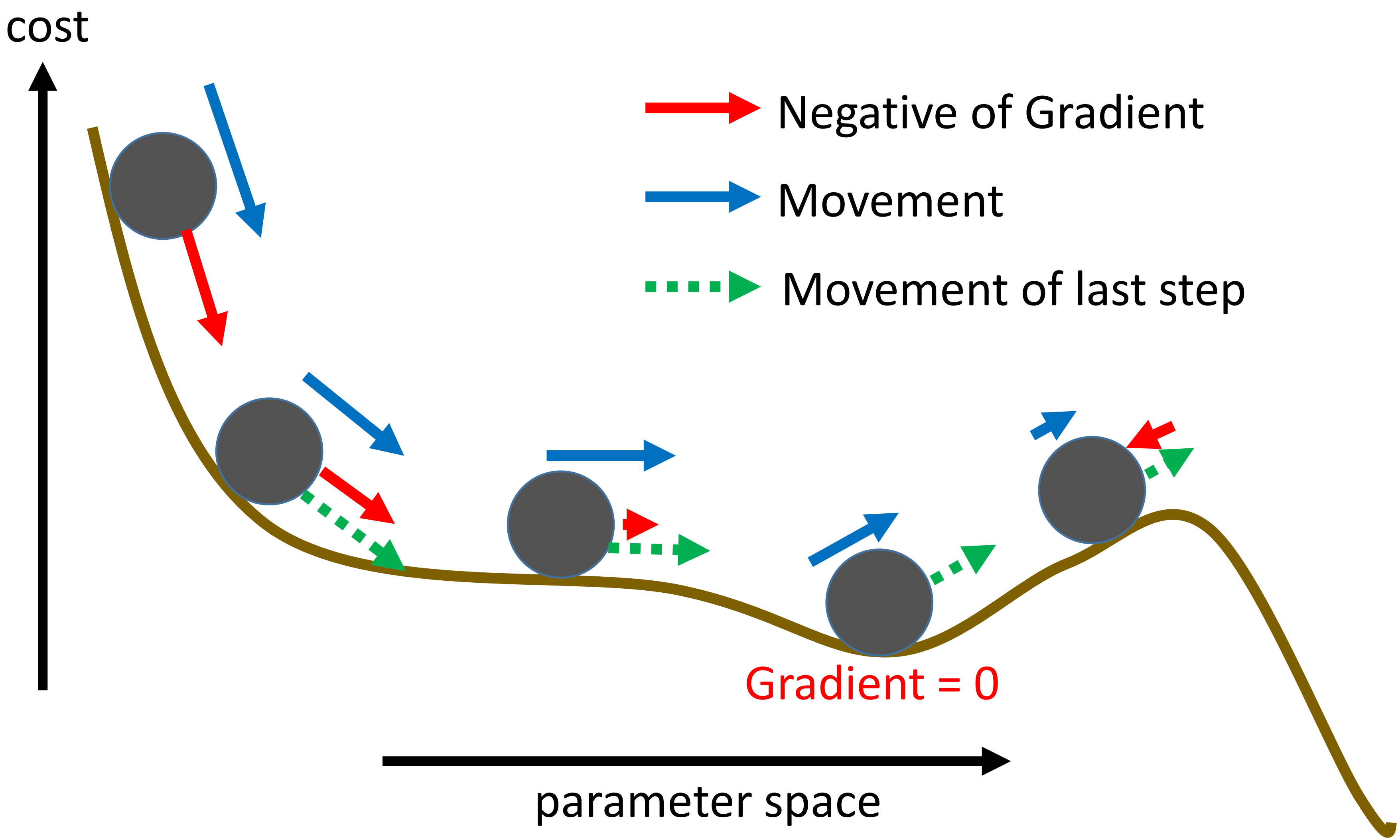
Compute gradient at θ^1

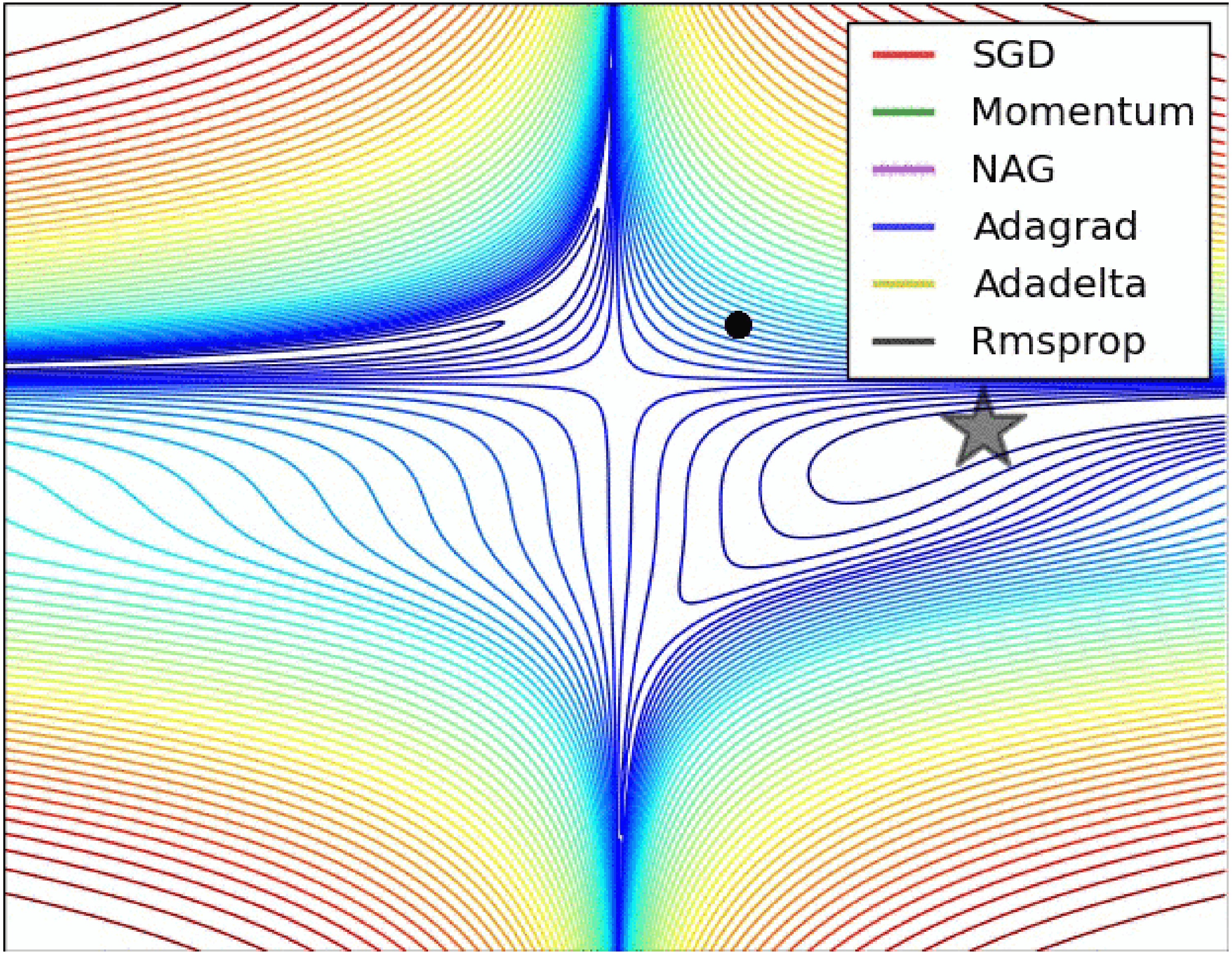
Movement $v^2 = \lambda v^1 - \eta\nabla C(\theta^1)$

Move to $\theta^2 = \theta^1 + v^2$

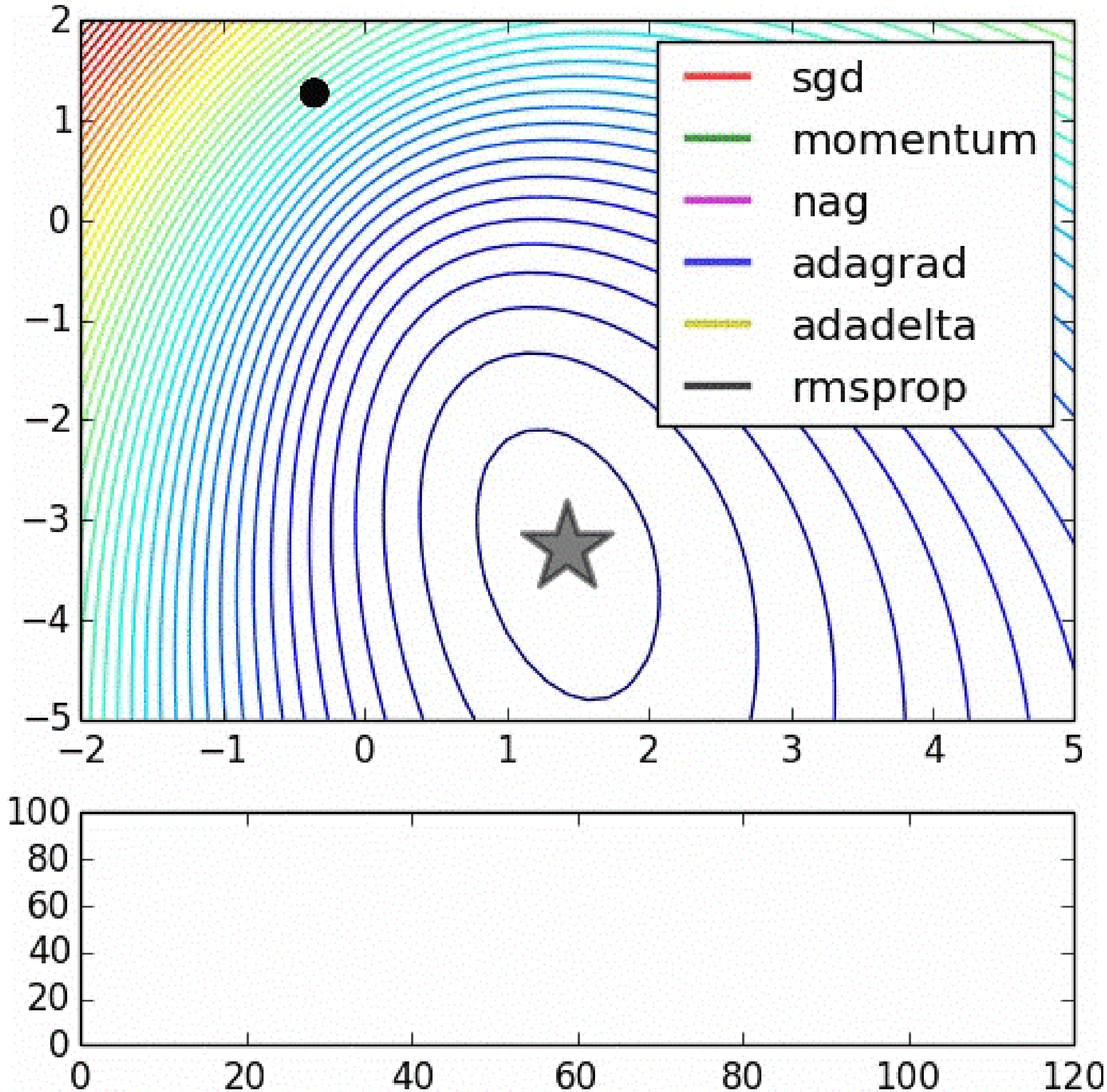
Movement not just based on gradient, but previous movement

Momentum


cost
Negative of Gradient
Movement
Movement of last step
Gradient = 0
parameter space



http://www.reddit.com/r/MachineLearning/comments/2gopfa/visualizing_gradient_optimization_techniques/cklhott (**By Alec Radford**)



http://www.reddit.com/r/MachineLearning/comments/2gopfa/visualizing_gradient_optimization_techniques/cklhott **(By Alec Radford)**

Outline

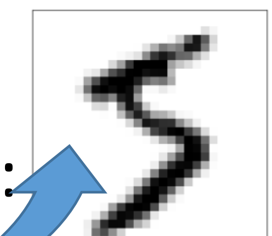
- Activation Function
- Cost Function
- Data Preprocessing
- Optimization
- Generalization

Panacea

- Have more training data
- ***Create*** more training data (?)

Handwriting recognition:

Original Training Data: 

Created Training Data: 

Shift 15 °

Outline

- Activation Function
- Cost Function
- Data Preprocessing
- Optimization
- Generalization
  - Early Stopping
  - Weight Decay
  - Dropout

Outline

Activation Function

Cost Function

Data Preprocessing

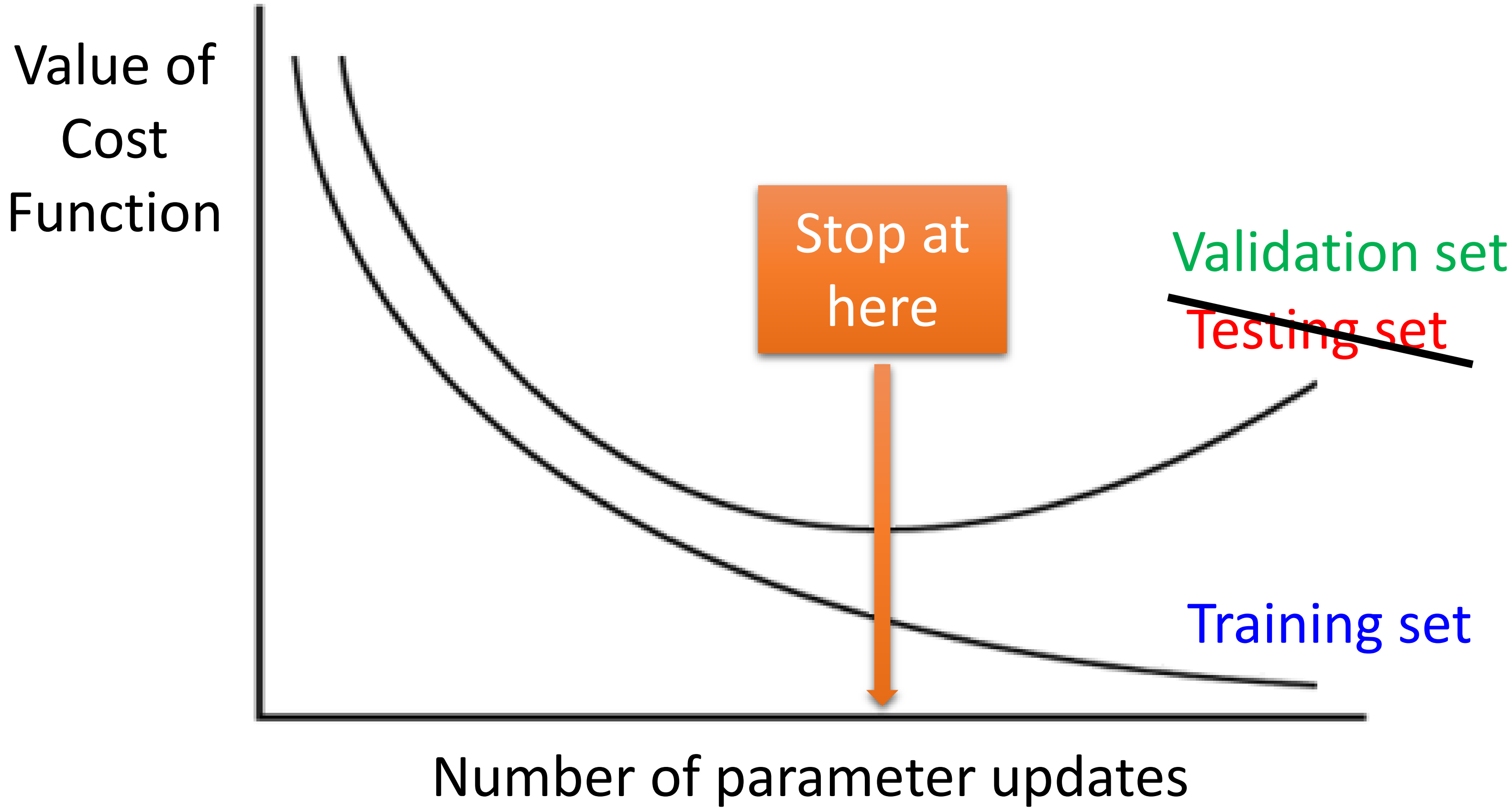
Optimization

Generalization

Early Stopping | Weight Decay | Dropout

Early Stopping

How many parameter updates do we need?



Outline

Activation Function

Cost Function

Data Preprocessing

Optimization

Generalization

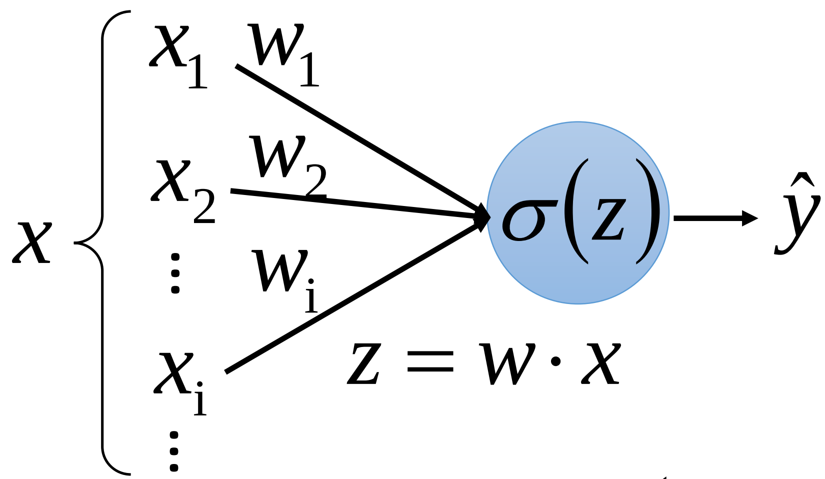
Early Stopping	Weight Decay	Dropout

Weight Decay

- The parameters closer to zero is preferred.

Training data:

$$\{(x, \hat{y}), \ldots\}$$



Testing data:

$$\{(x', \hat{y}), \ldots\} \qquad x' = x + \varepsilon$$

$$\begin{aligned} z' &= w \cdot (x + \varepsilon) \\ &= w \cdot x + w \cdot \varepsilon \\ &= z + w \cdot \varepsilon \end{aligned}$$

To minimize the effect of noise, we want w close to zero.

Weight Decay

- New cost function to be minimized
  - Find a set of weight not only minimizing original cost but also close to zero

$$\mathrm{C}'(\theta) = \underbrace{C(\theta)}_{\text{Original cost}} + \lambda \frac{1}{2} \underline{\|\theta\|^2}$$

→ Regularization term:

$$\theta = \{\mathrm{W}^1, \mathrm{W}^2, \ldots\}$$

$$\|\theta\|^2 = \left(w_{11}^1\right)^2 + \left(w_{12}^1\right)^2 + \ldots$$

$$+ \left(w_{11}^2\right)^2 + \left(w_{12}^2\right)^2 + \ldots$$

(not consider biases. why?)

Original cost
(e.g. minimize square error, cross entropy …)

Weight Decay

$$\|\theta\|^2 = \left(w_{11}^1\right)^2 + \left(w_{12}^1\right)^2 + \ldots$$
$$+ \left(w_{11}^2\right)^2 + \left(w_{12}^2\right)^2 + \ldots$$

- New cost function to be minimized

$$\mathrm{C}'(\theta) = C(\theta) + \lambda \frac{1}{2}\|\theta\|^2$$

Gradient: $$\frac{\partial \mathrm{C}'}{\partial w} = \frac{\partial \mathrm{C}}{\partial w} + \lambda w$$

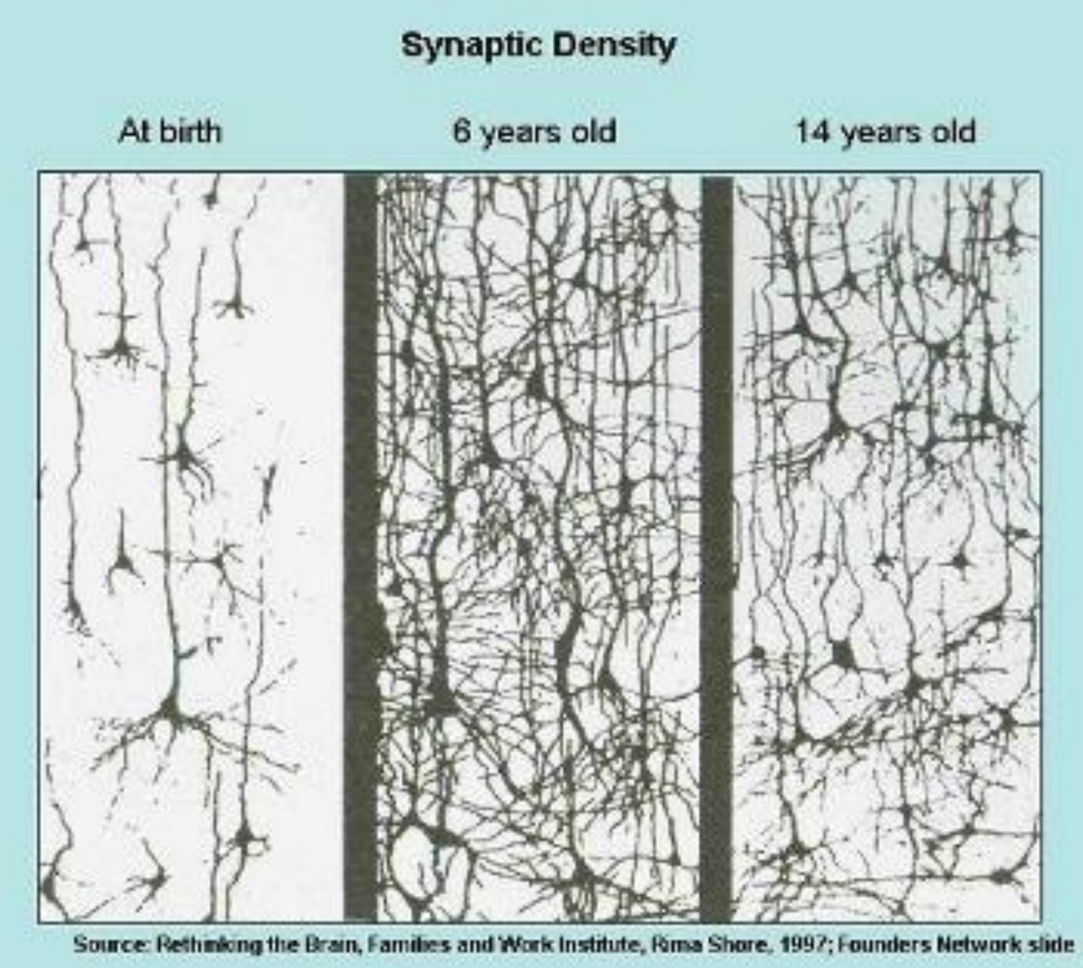
Update: $$w^{t+1} \rightarrow w^t - \eta \frac{\partial \mathrm{C}'}{\partial w} = w^t - \eta\left(\frac{\partial \mathrm{C}}{\partial w} + \lambda w^t\right)$$

$$= (1 - \eta\lambda) w^t - \eta \frac{\partial \mathrm{C}}{\partial w}$$

Smaller and smaller

Weight Decay

- Our Brain



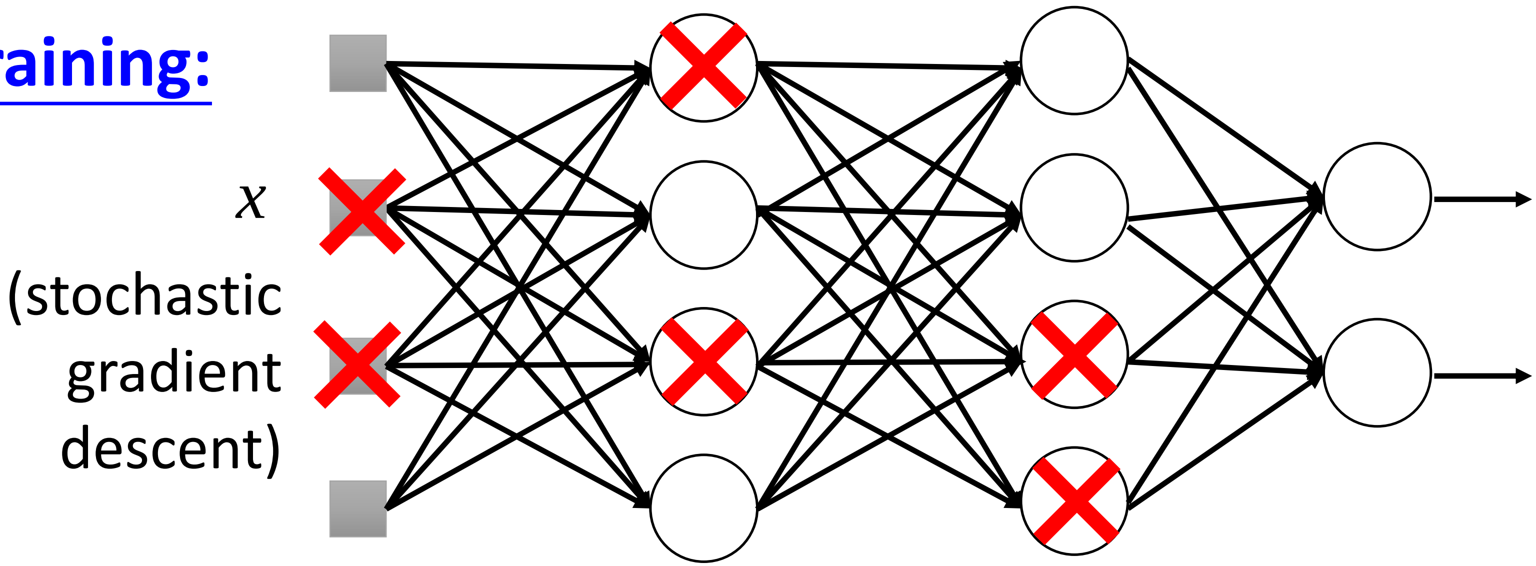
Outline

- Activation Function
- Cost Function
- Data Preprocessing
- Optimization
- Generalization
  - Early Stopping
  - Weight Decay
  - Dropout

Dropout

$$\theta^t \leftarrow \theta^{t-1} - \eta \nabla C_x(\theta^{t-1})$$

Training:

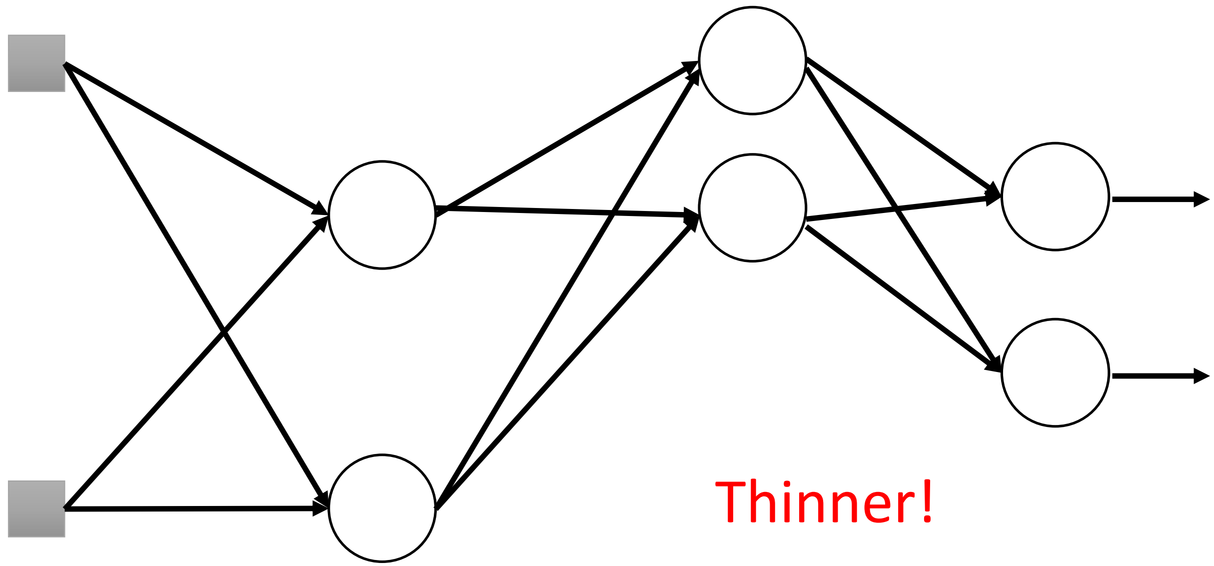


- In each ***iteration***
  - Each neuron has p% to dropout

Dropout

$$\theta^t \leftarrow \theta^{t-1} - \eta \nabla C_x(\theta^{t-1})$$

Training:



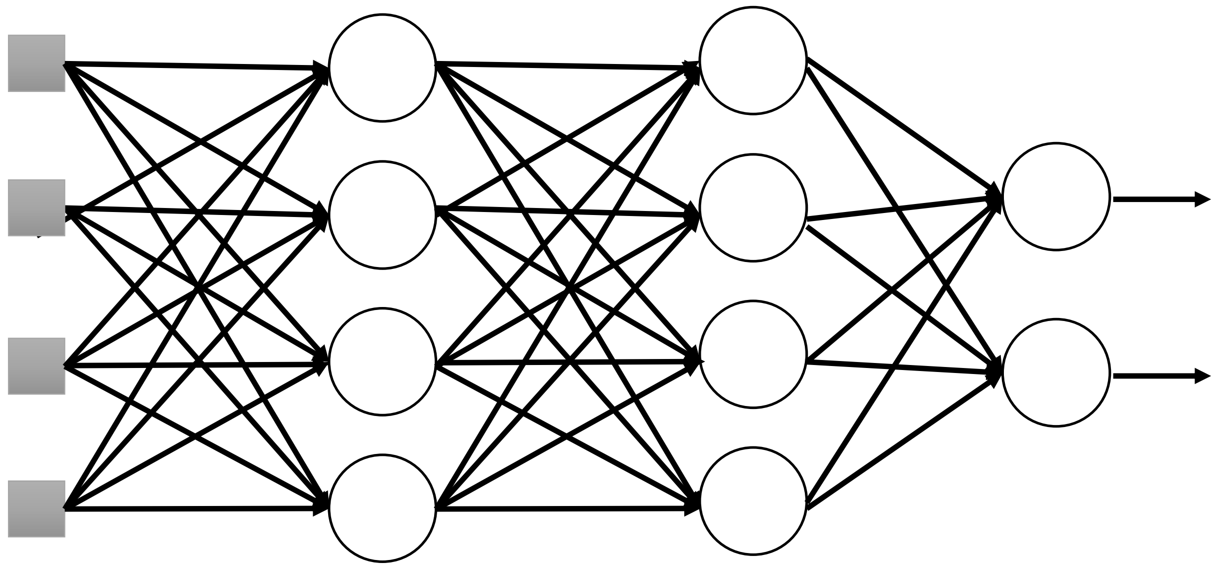
- In each ***iteration***
  - Each neuron has p% to dropout

    The structured of the network is changed.
  - Using the new network for training

For each iteration, we resample the dropout neurons

Dropout

Testing:



- **No dropout**
  - If the dropout rate at training is p%, all the weights times (1-p)%
  - Assume that the dropout rate is 50%. If $w_{ij}^{l} = 1$ from training, set $w_{ij}^{l} = 0.5$ for testing.

Dropout
- Intuitive Reason

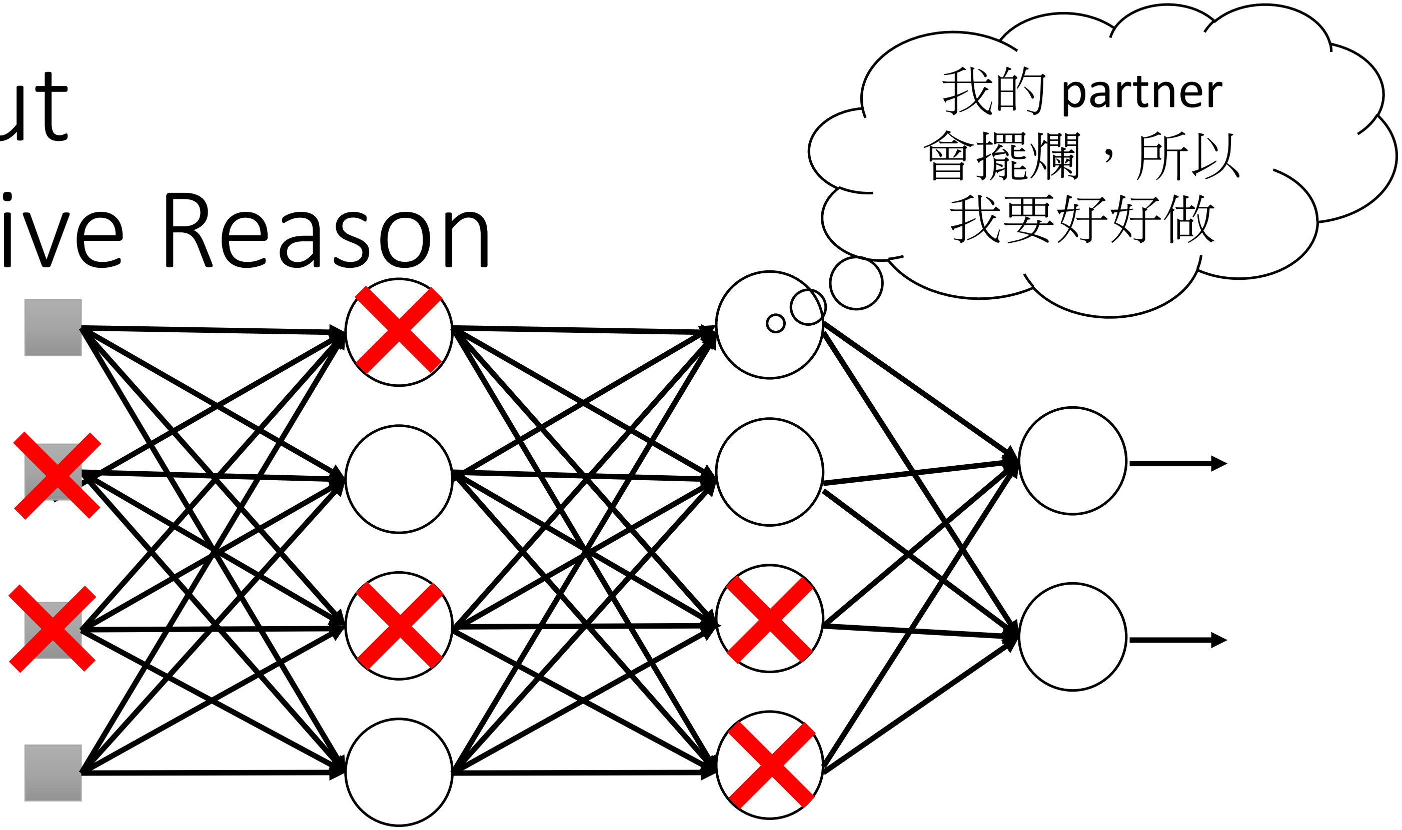
Testing

No dropout
(拿下重物後就變很強)

Training

Dropout (腳上綁重物)

Dropout
- Intuitive Reason



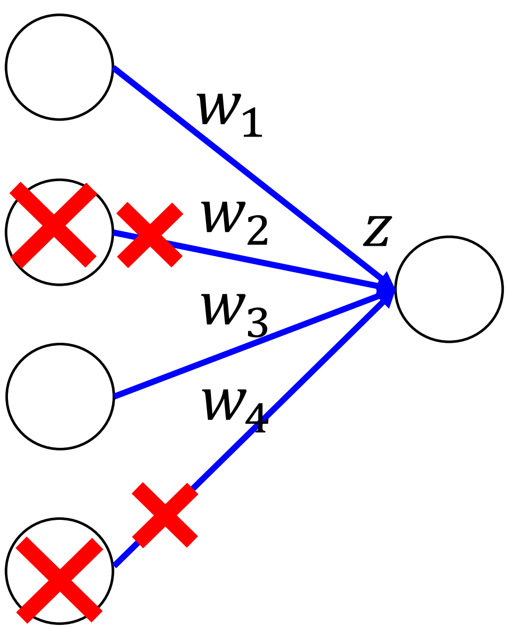
- When teams up, if everyone expect the partner will do the work, nothing will be done finally.
- However, if you know your partner will dropout, you will do better.
- When testing, no one dropout actually, so obtaining good results eventually.

Dropout
- Intuitive Reason

- Why the weights should multiply (1-p)% (dropout rate) when testing?

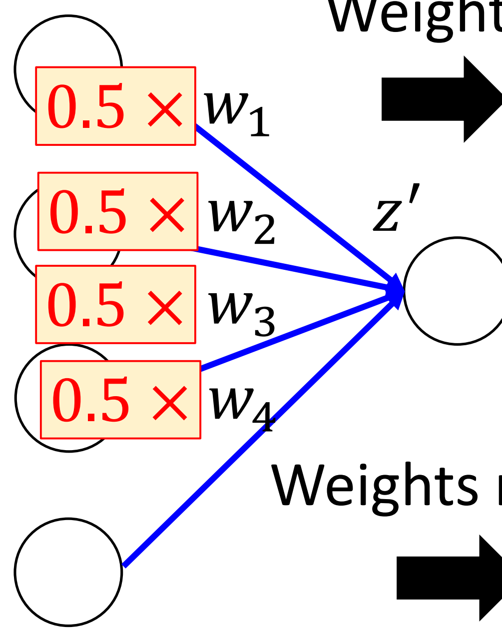
Training of Dropout

Assume dropout rate is 50%



Testing of Dropout

No dropout



Weights from training

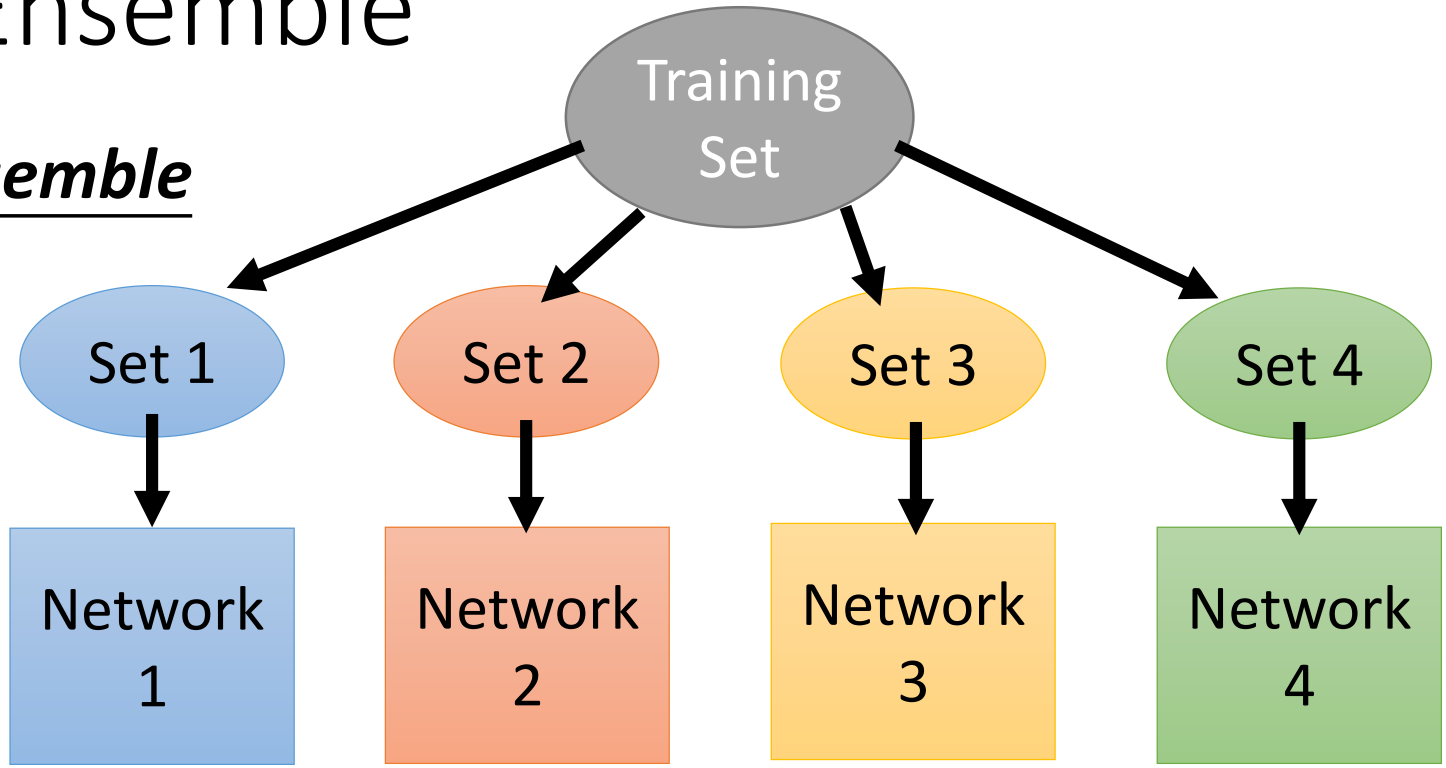
$\Rightarrow z' \approx 2z$

Weights multiply (1-p)%

$\Rightarrow z' \approx z$

Dropout
- Ensemble

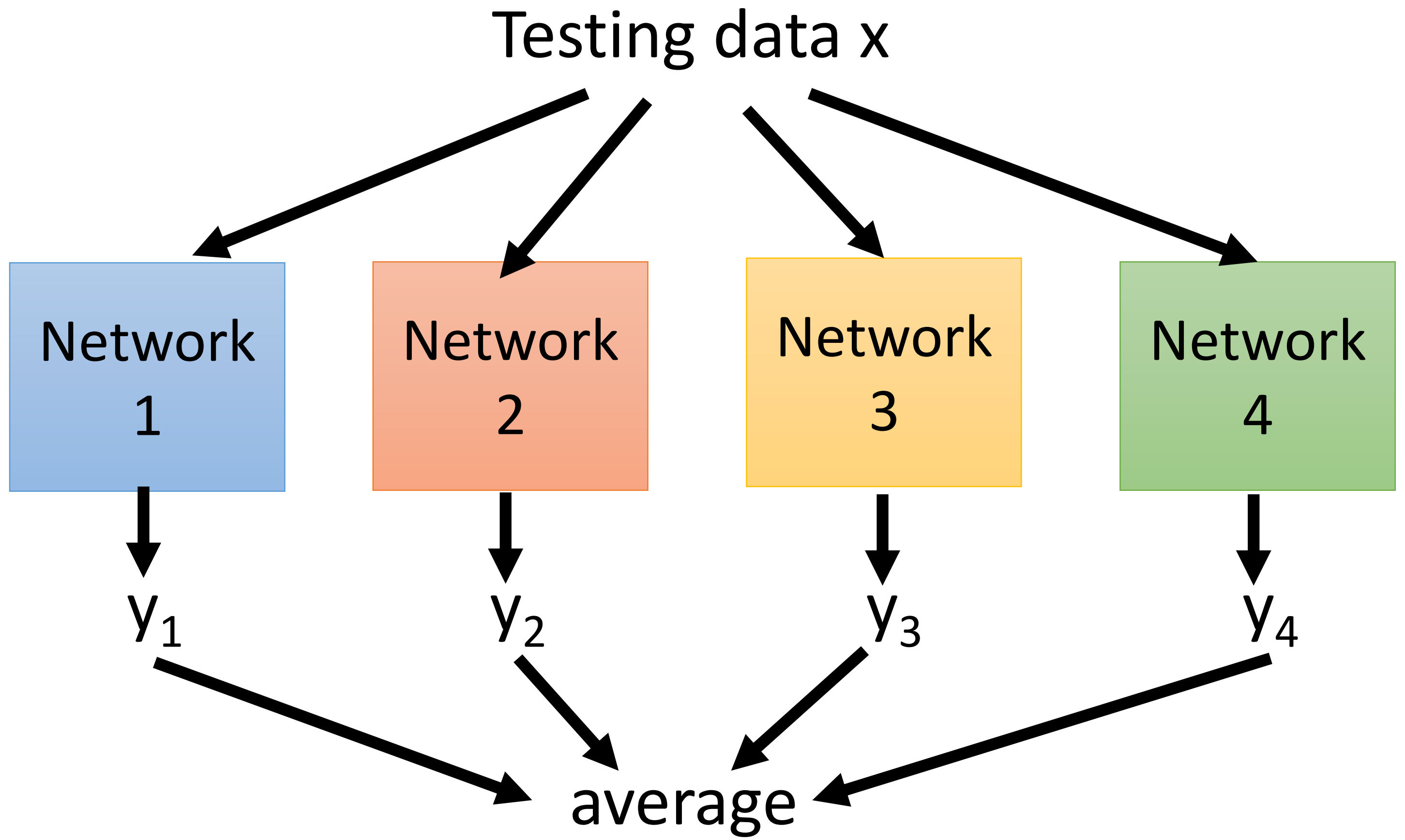
Ensemble



Train a bunch of networks with different structures

Dropout
- Ensemble

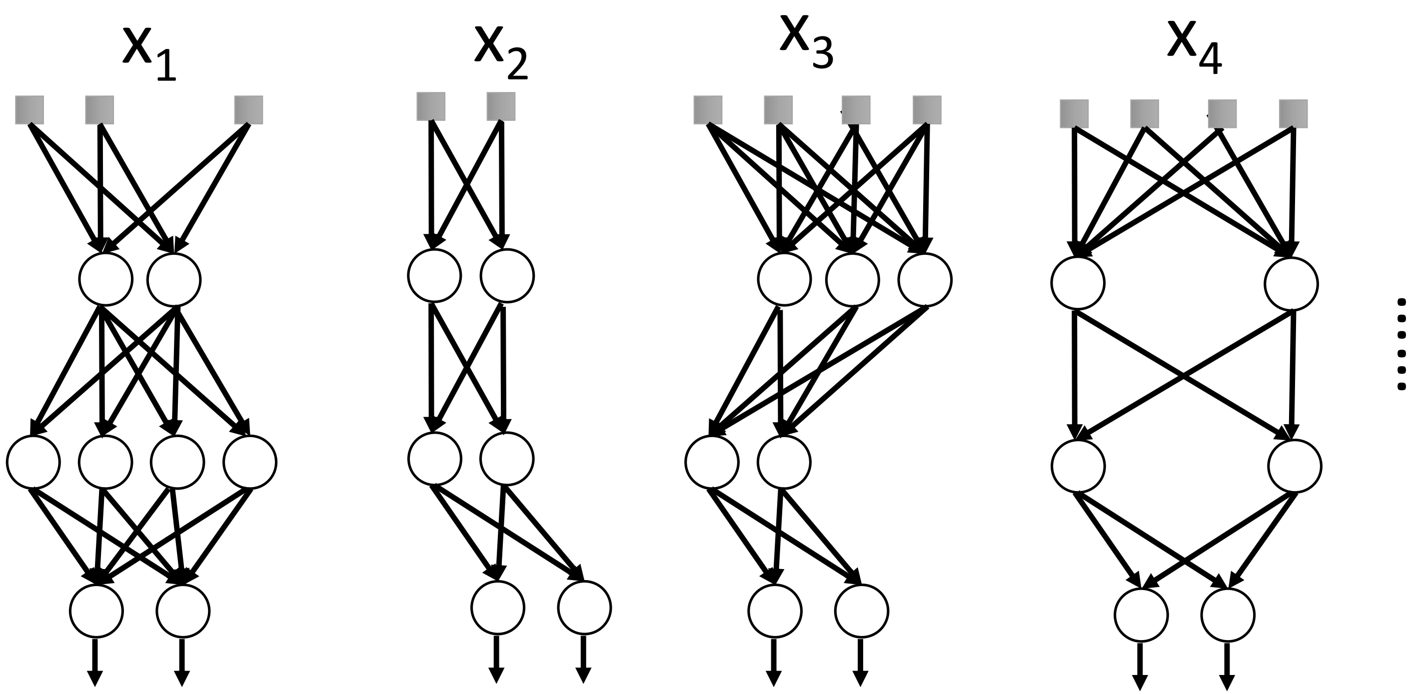
Ensemble



Dropout
- Ensemble

***Dropout* ≈ *Ensemble*.**

Training of Dropout



M neurons

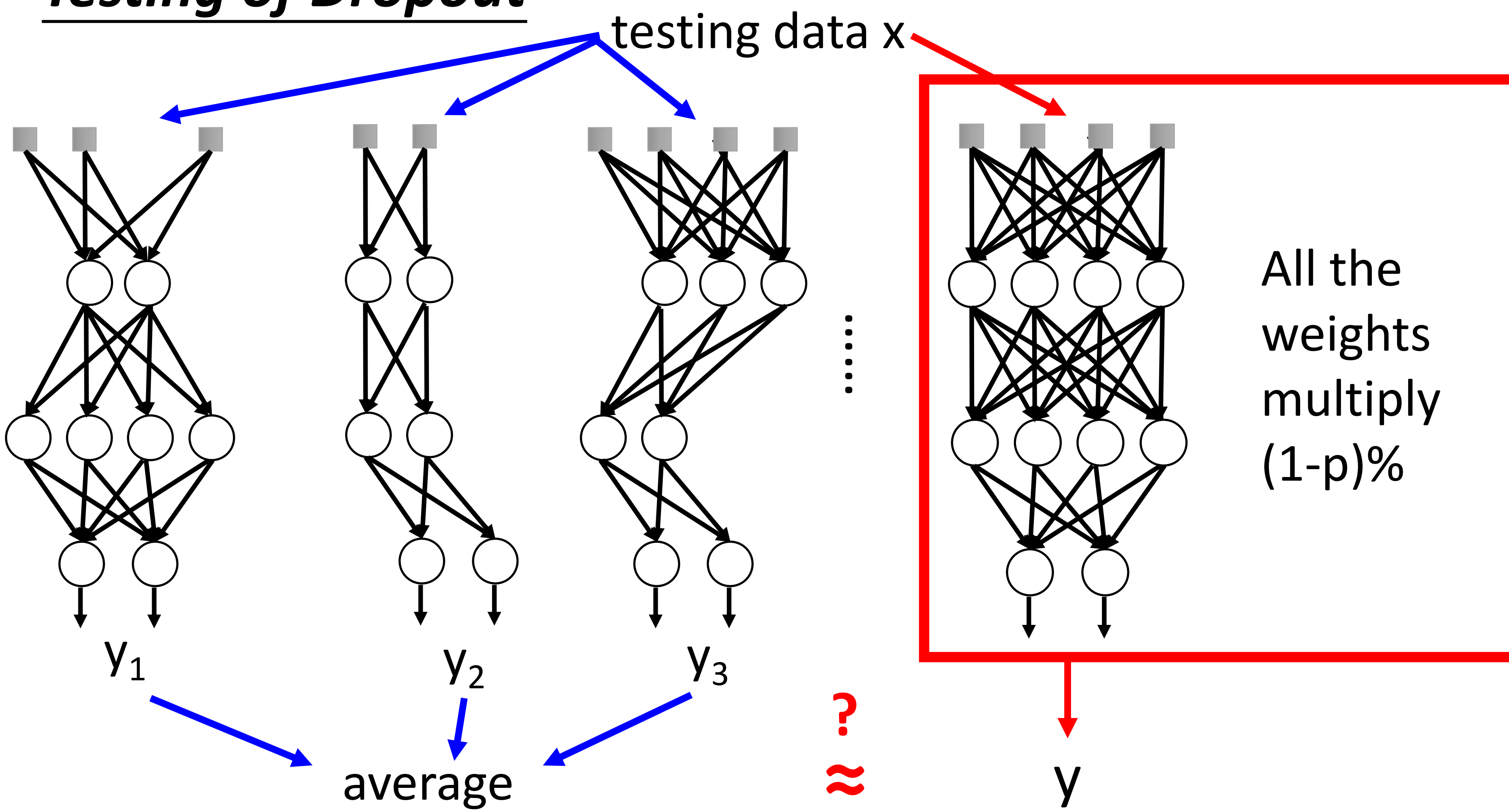
2^M possible networks

- ➢ Using one data to train one network
- ➢ Some parameters in the network are shared

Dropout
- Ensemble

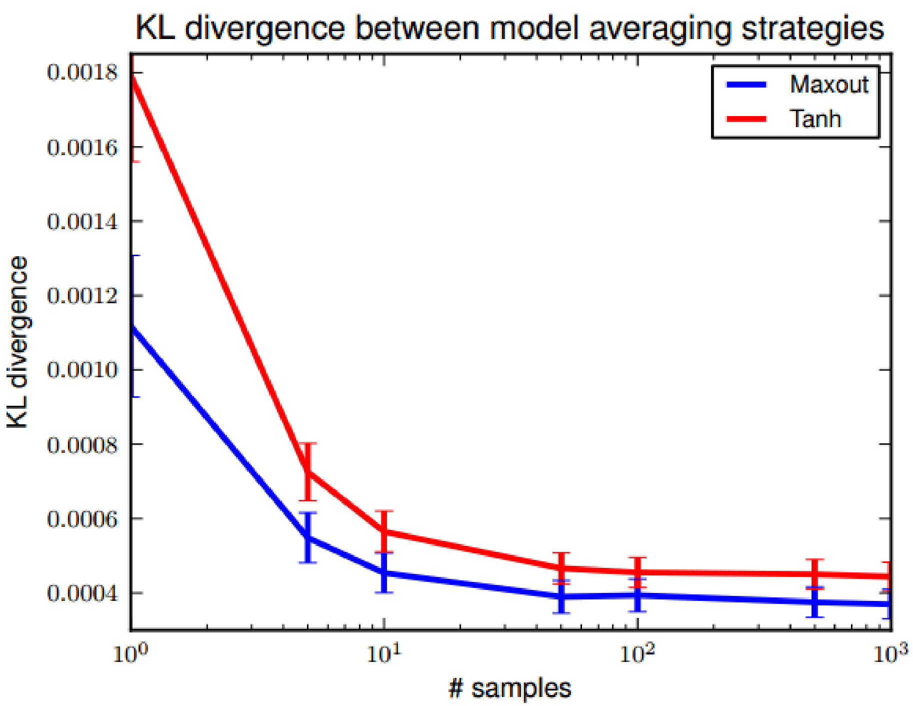
***Dropout* ≈ *Ensemble*.**

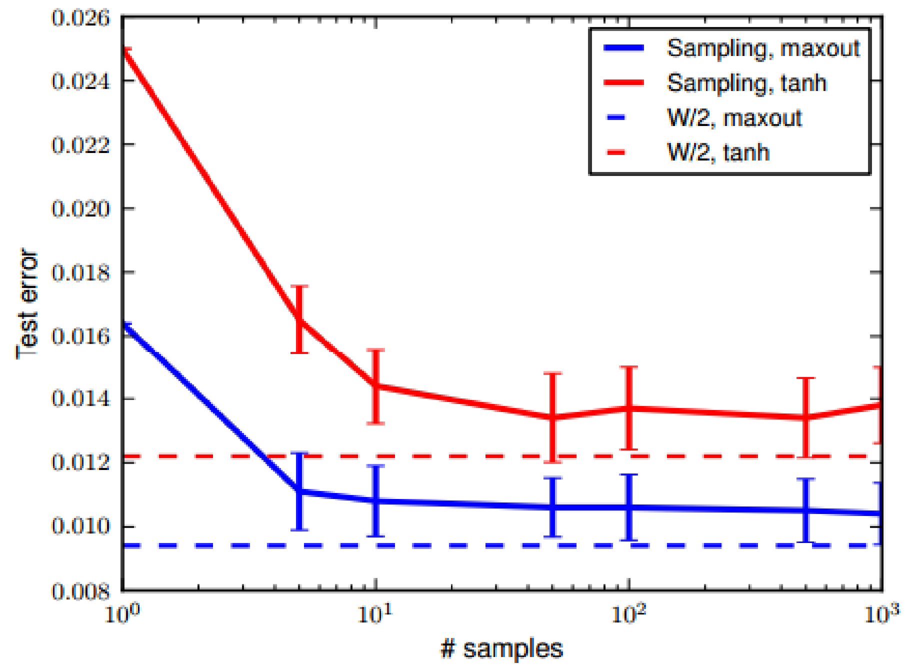
Testing of Dropout



Dropout
- Ensemble

- Experiments on hand writing digital classification





Ref: http://arxiv.org/pdf/1302.4389.pdf

Practical Suggestion for Dropout

- Larger network
  - If you know your task need ***n*** neurons, for dropout rate ***p***, your network need ***n/(1-p)*** neurons.
- Longer training time
- Higher learning rate
- Larger momentum

Concluding Remarks

Not covered today: Parameters Initialization

http://neuralnetworksanddeeplearning.com/chap3.html#weight_initialization

- **Activation Function** — ReLU, Maxout
- **Cost Function** — Softmax + Cross Entropy
- **Data Preprocessing** — Mean=0, Variance=1
- **Optimization** — Adagrad, Momentum
- **Generalization** — Early Stopping, Weight decay, Dropout