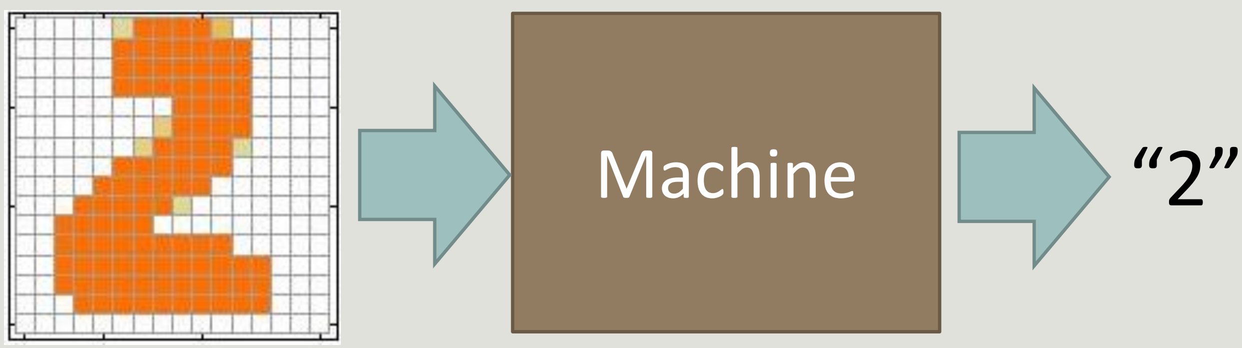
XAI ES, Course 3

Neurons and neural networks

Example Application

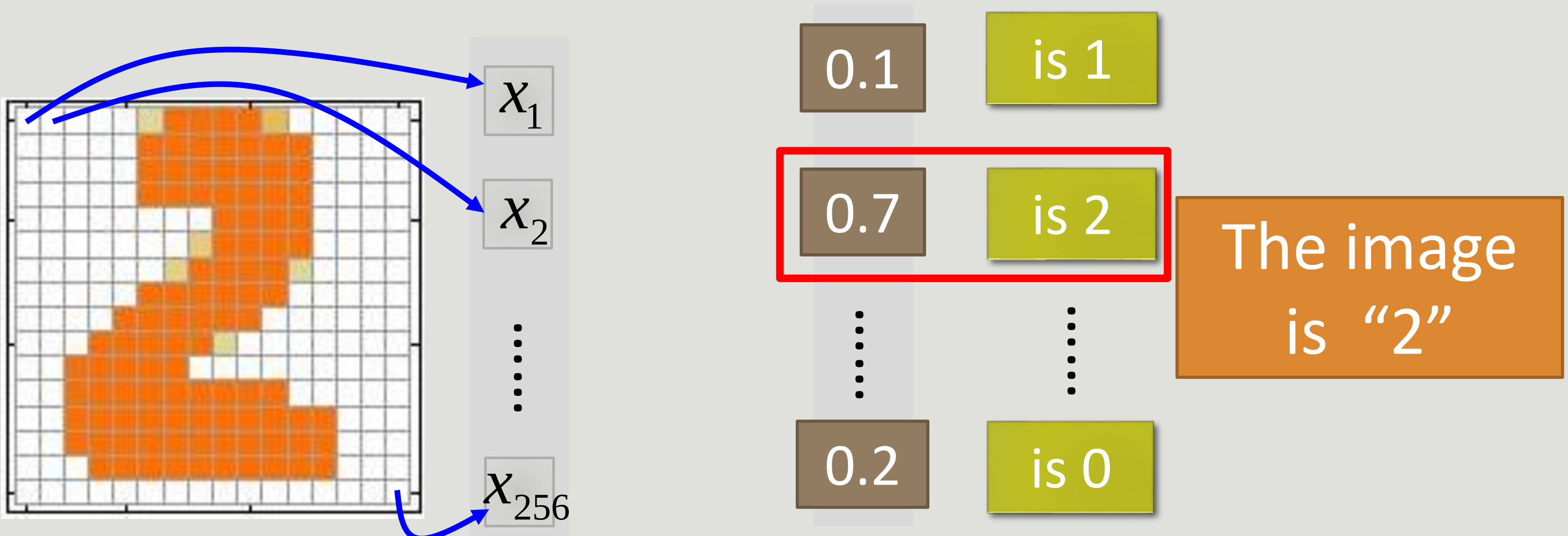
Handwriting Digit Recognition



Handwriting Digit Recognition

INPUT

OUTPUT



16 x 16 = 256

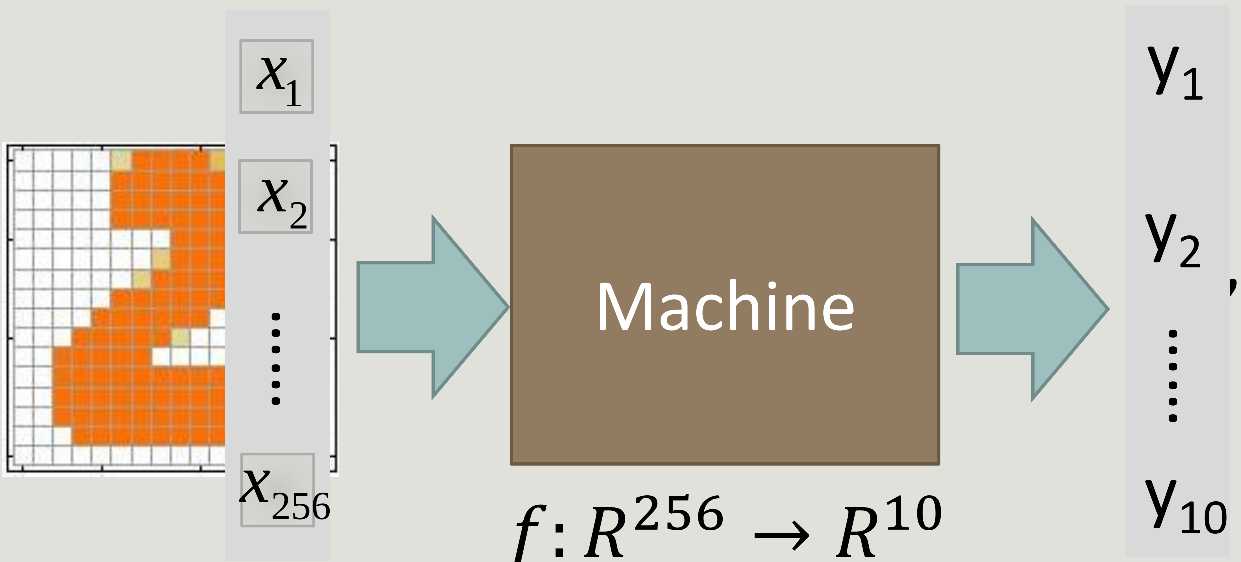
Ink → 1

No ink → 0

Each dimension represents the confidence of a digit.

Example Application

Handwriting Digit Recognition



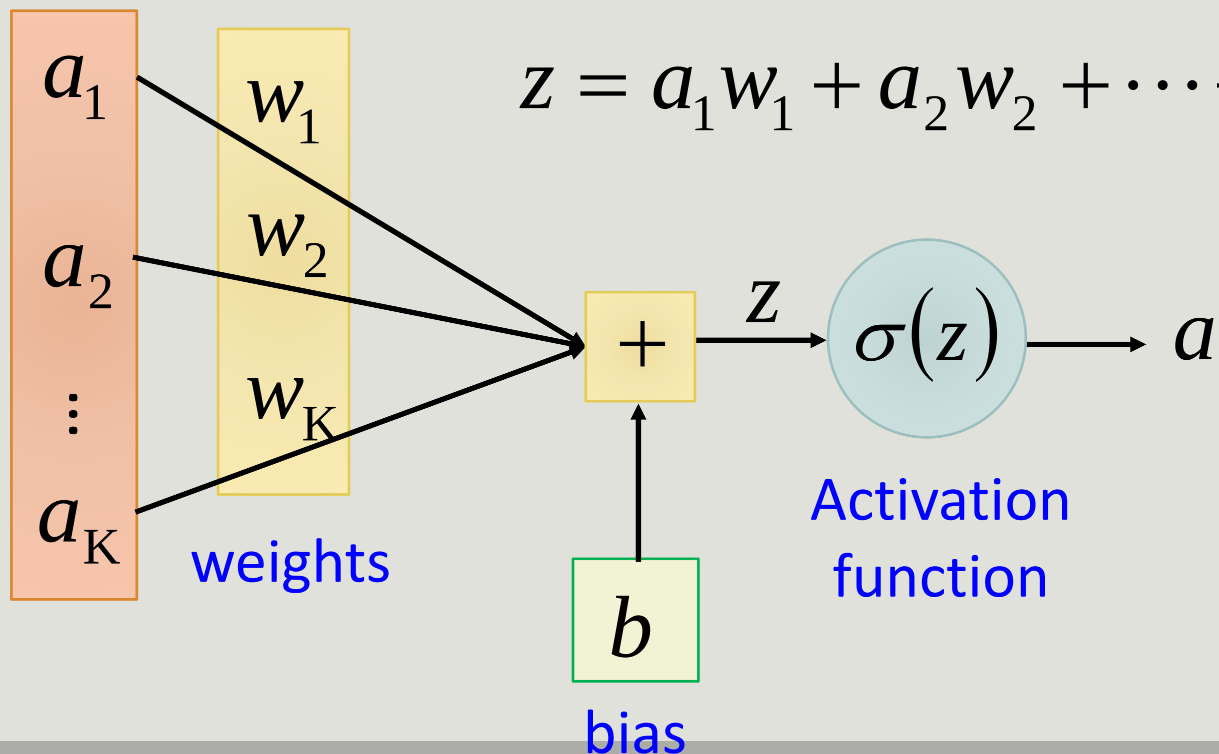
$$f: R^{256} \rightarrow R^{10}$$

In deep learning, the function f is represented by neural network

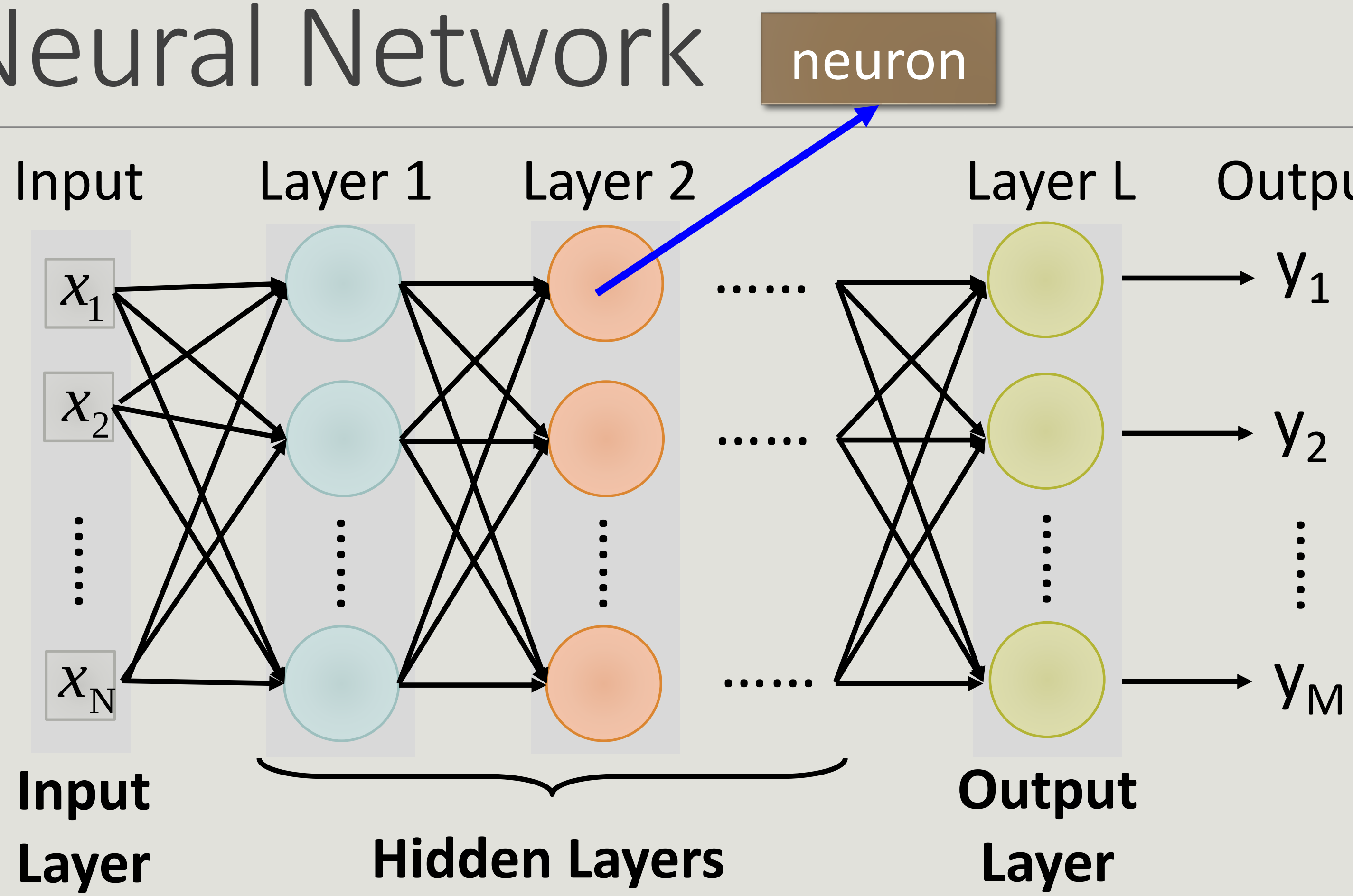
Element of Neural Network

Neuron $f: R^K \to R$

$$z = a_1 w_1 + a_2 w_2 + \cdots + a_K w_K + b$$

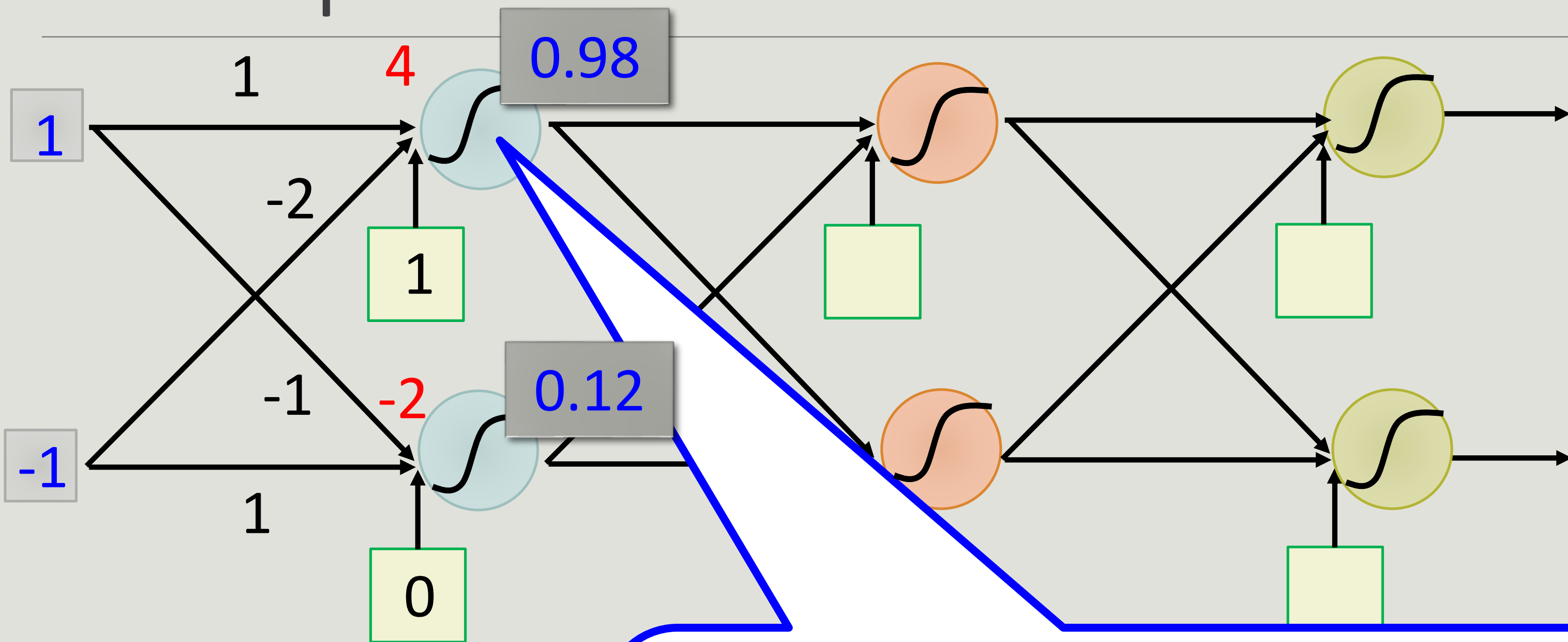


Neural Network



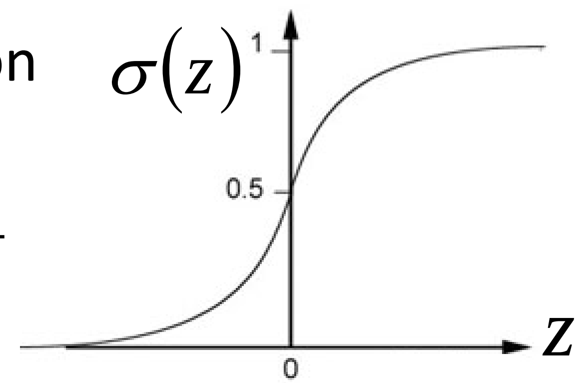
Deep means many hidden layers

Example of Neural Network

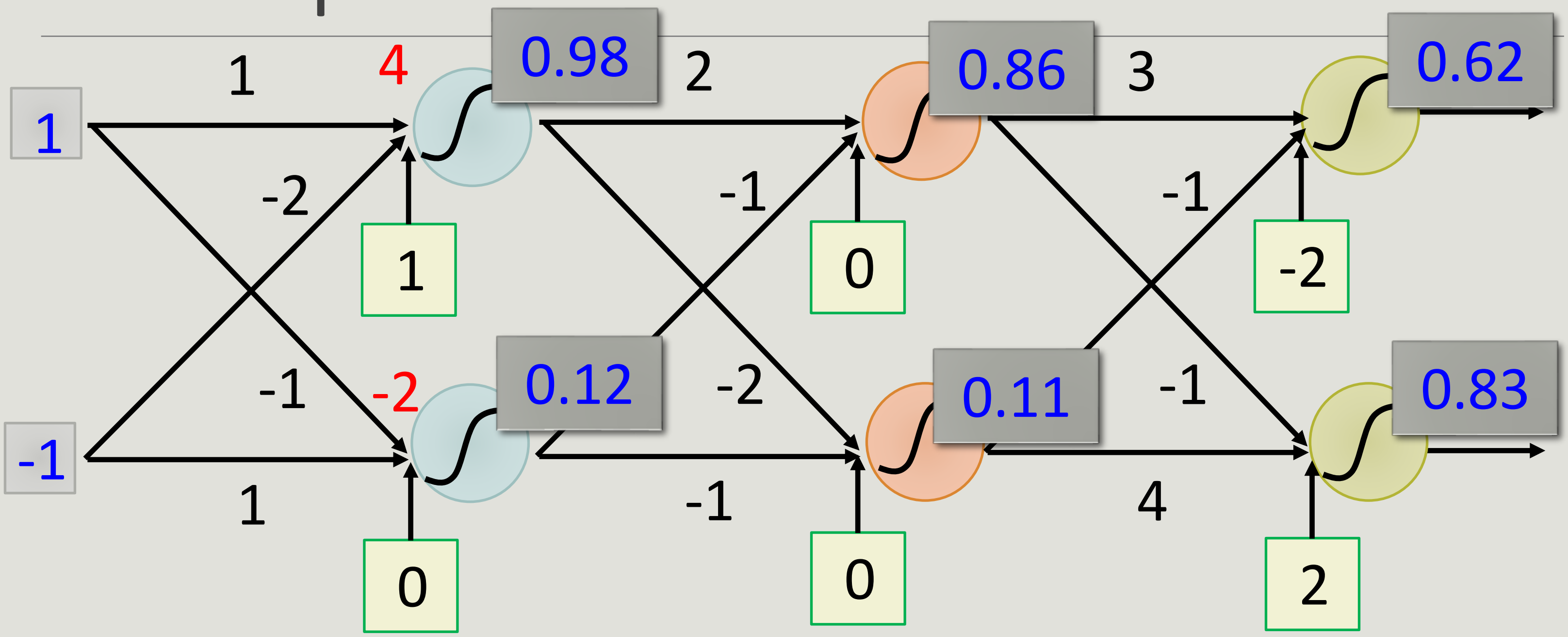


Sigmoid Function

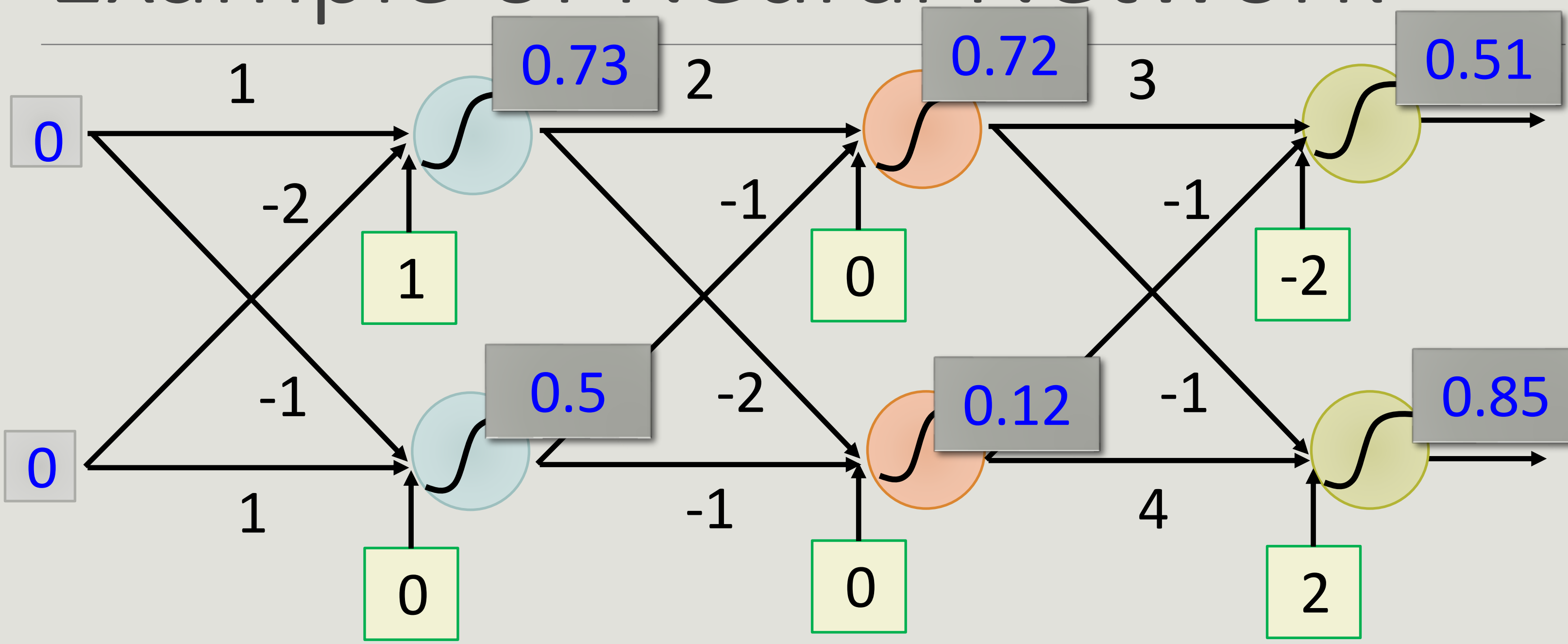
$$\sigma(z) = \frac{1}{1+e^{-z}}$$



Example of Neural Network



Example of Neural Network

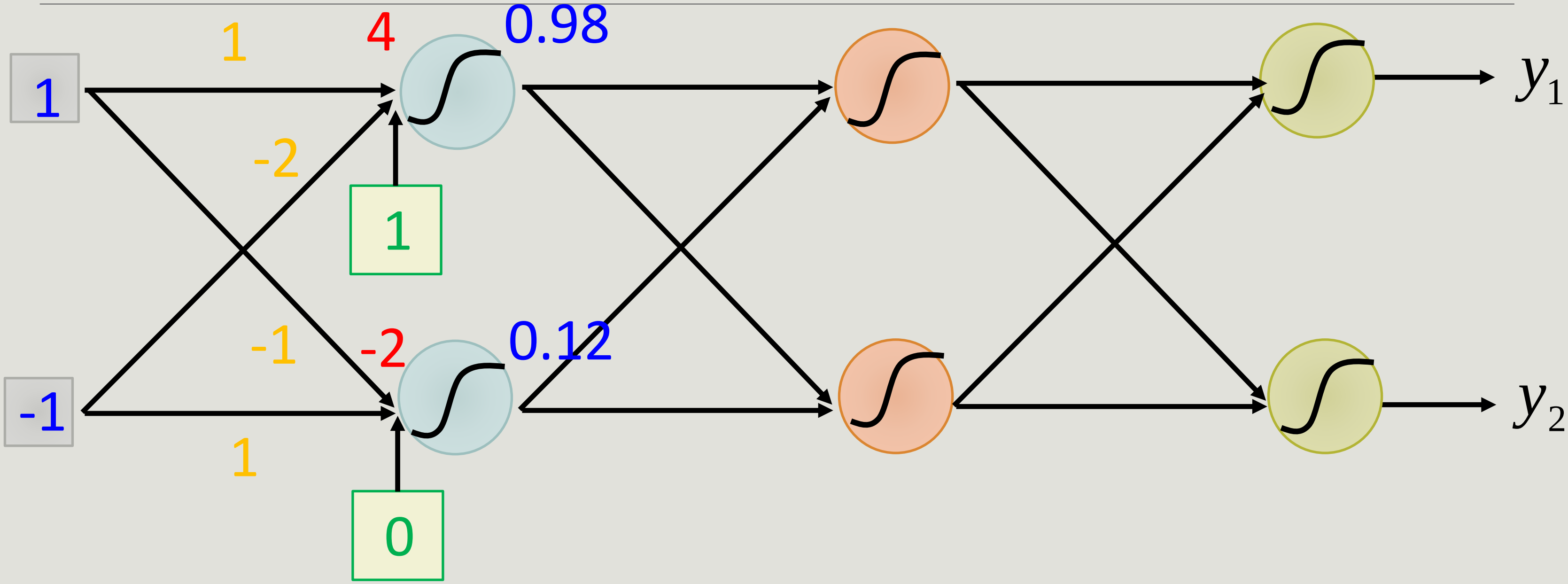


$f: R^2 \rightarrow R^2$

$$f\left(\begin{bmatrix} 1 \\ -1 \end{bmatrix}\right) = \begin{bmatrix} 0.62 \\ 0.83 \end{bmatrix} \quad f\left(\begin{bmatrix} 0 \\ 0 \end{bmatrix}\right) = \begin{bmatrix} 0.51 \\ 0.85 \end{bmatrix}$$

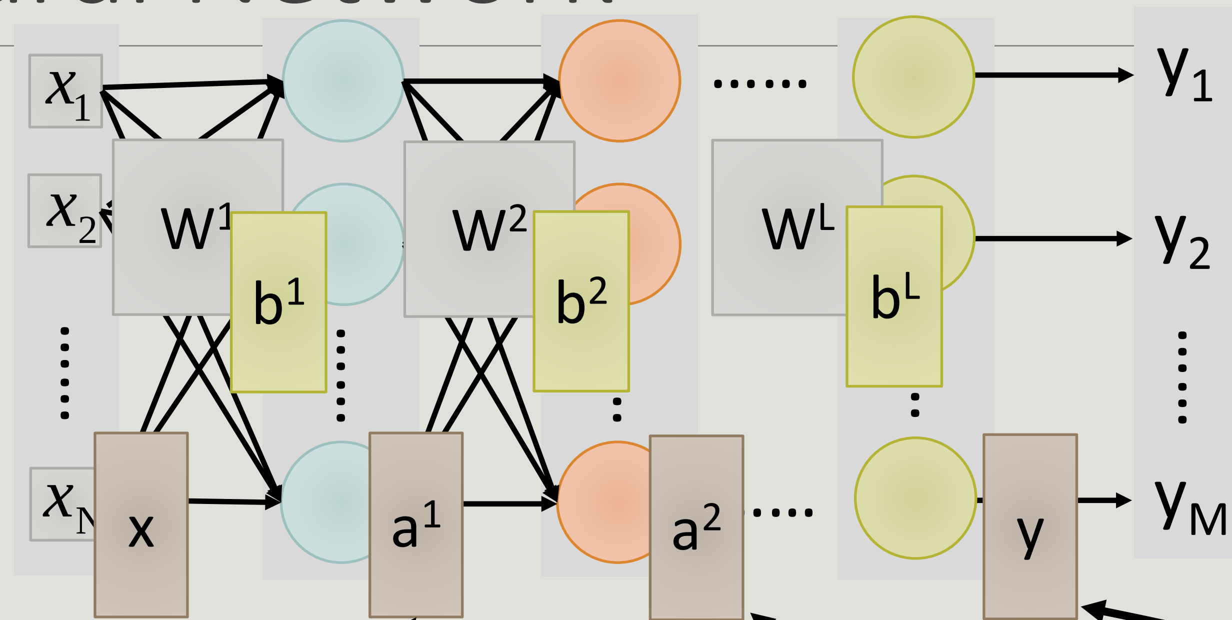
Different parameters define different function

Matrix Operation



$$\sigma\left(\underbrace{\begin{bmatrix}1 & -2\\ -1 & 1\end{bmatrix}\begin{bmatrix}1\\ -1\end{bmatrix}+\begin{bmatrix}1\\ 0\end{bmatrix}}_{\begin{bmatrix}4\\ -2\end{bmatrix}}\right)=\begin{bmatrix}0.98\\ 0.12\end{bmatrix}$$

Neural Network

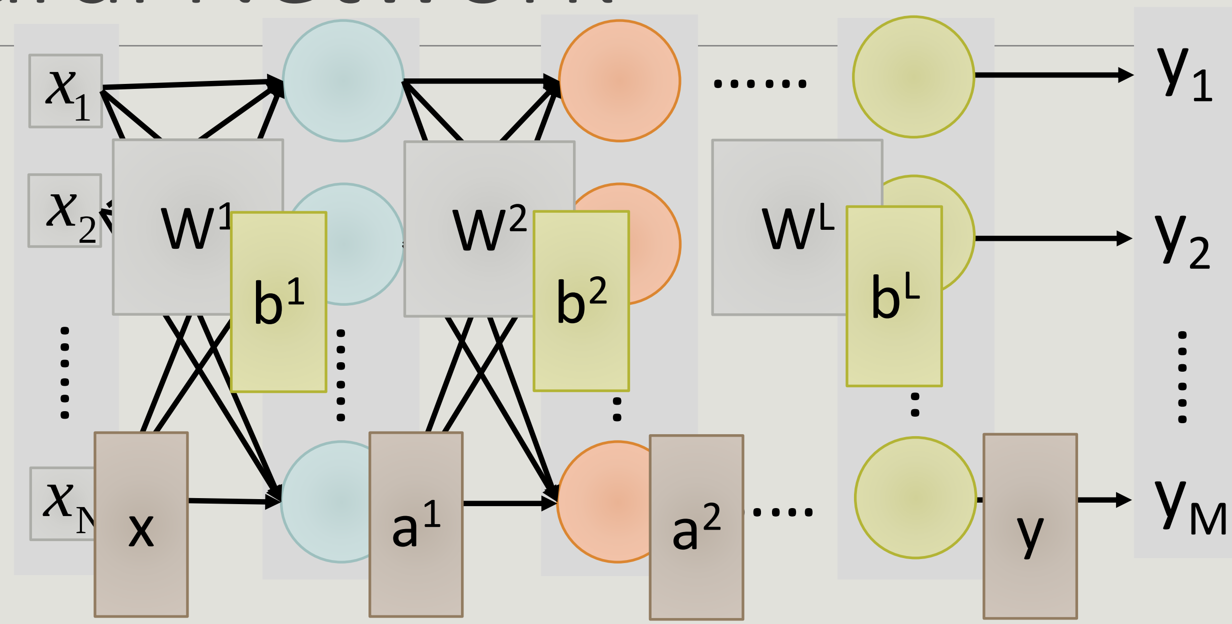


$$\sigma(W^1 x + b^1) \rightarrow a^1$$

$$\sigma(W^2 a^1 + b^2) \rightarrow a^2$$

$$\sigma(W^L a^{L-1} + b^L) \rightarrow y$$

Neural Network



$$\mathrm{y} = f(\mathrm{x})$$

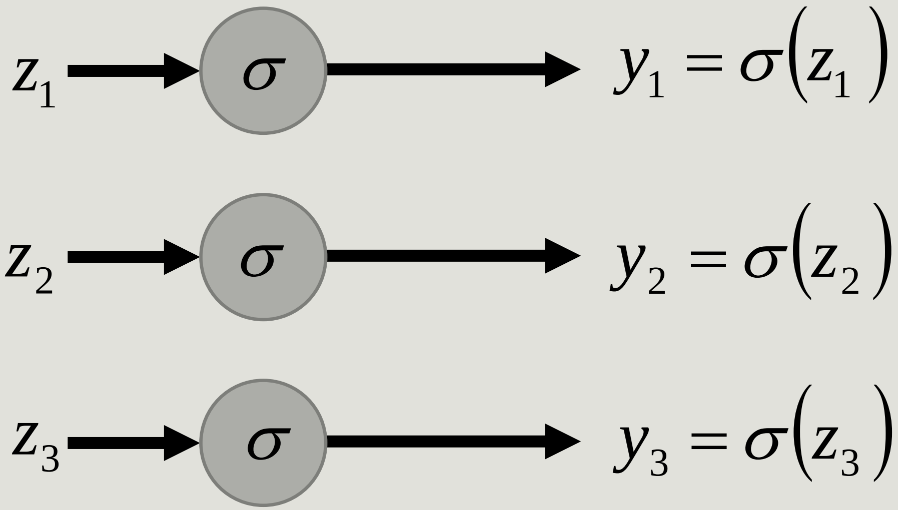
Using parallel computing techniques to speed up matrix operation

$$= \sigma(W^L \cdots \sigma(W^2\, \sigma(W^1 \mathrm{x} + b^1) + b^2) \cdots + b^L)$$

Softmax

Softmax layer as the output layer

Ordinary Layer



In general, the output of network can be any value.

May not be easy to interpret

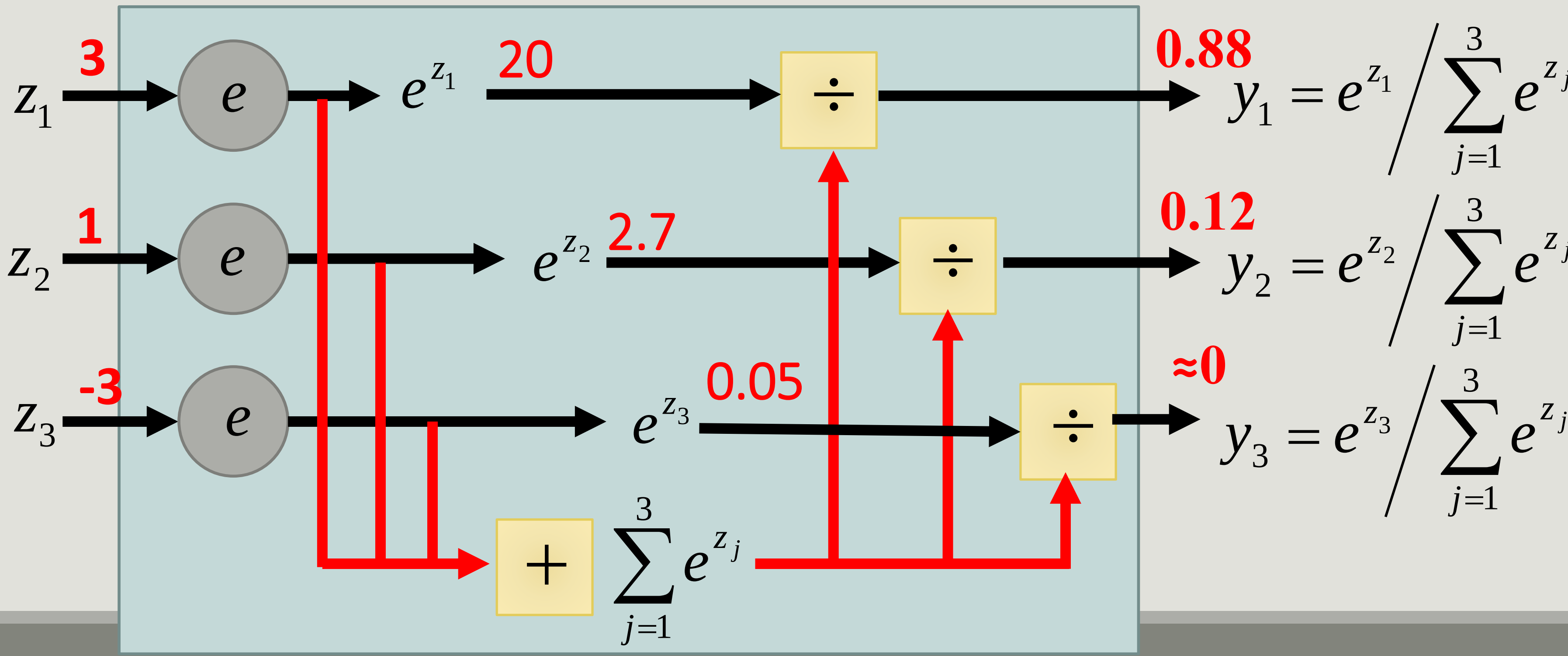
Softmax

Softmax layer as the output layer

Probability:

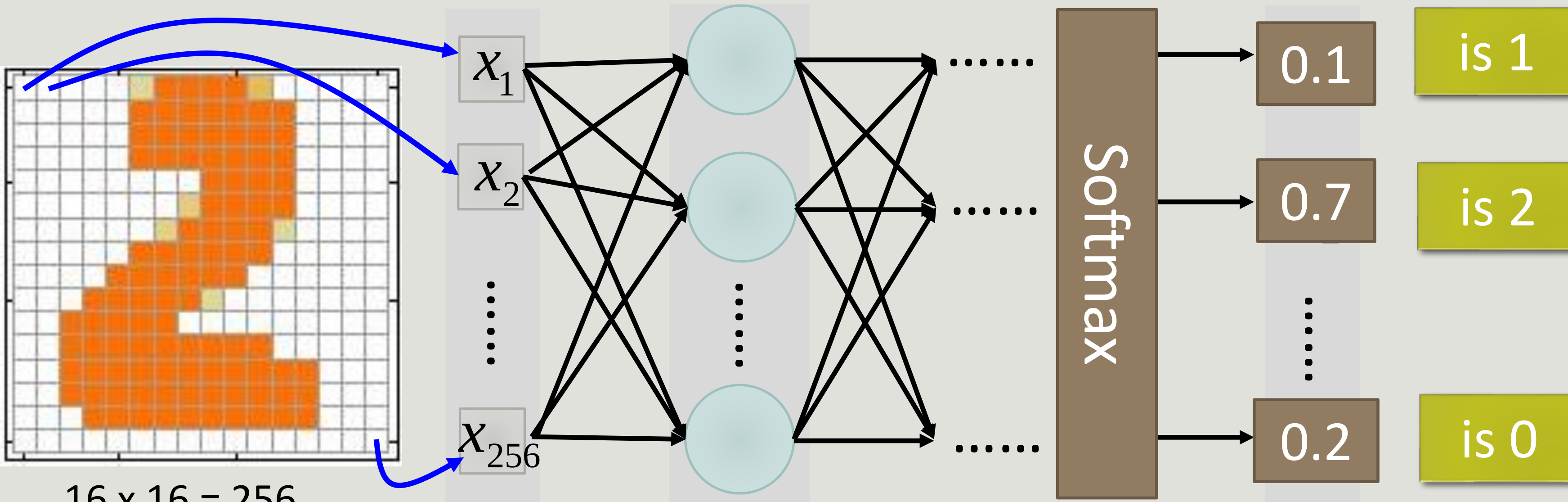
- $1 > y_i > 0$
- $\sum_i y_i = 1$

Softmax Layer



How to set network parameters

$$\theta = \{W^1, b^1, W^2, b^2, \cdots W^L, b^L\}$$

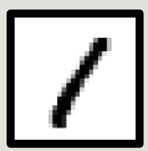


16 x 16 = 256

Ink → 1

No ink → 0

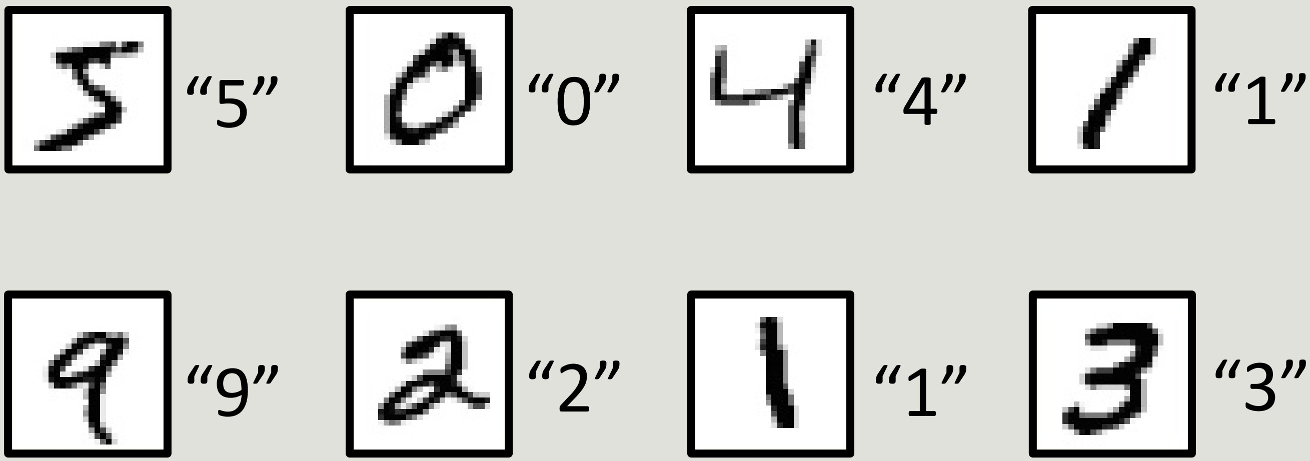
Set the network parameters θ such that ……

Input:  y_1 has the maximum value

Input:  y_2 has the maximum value

Training Data

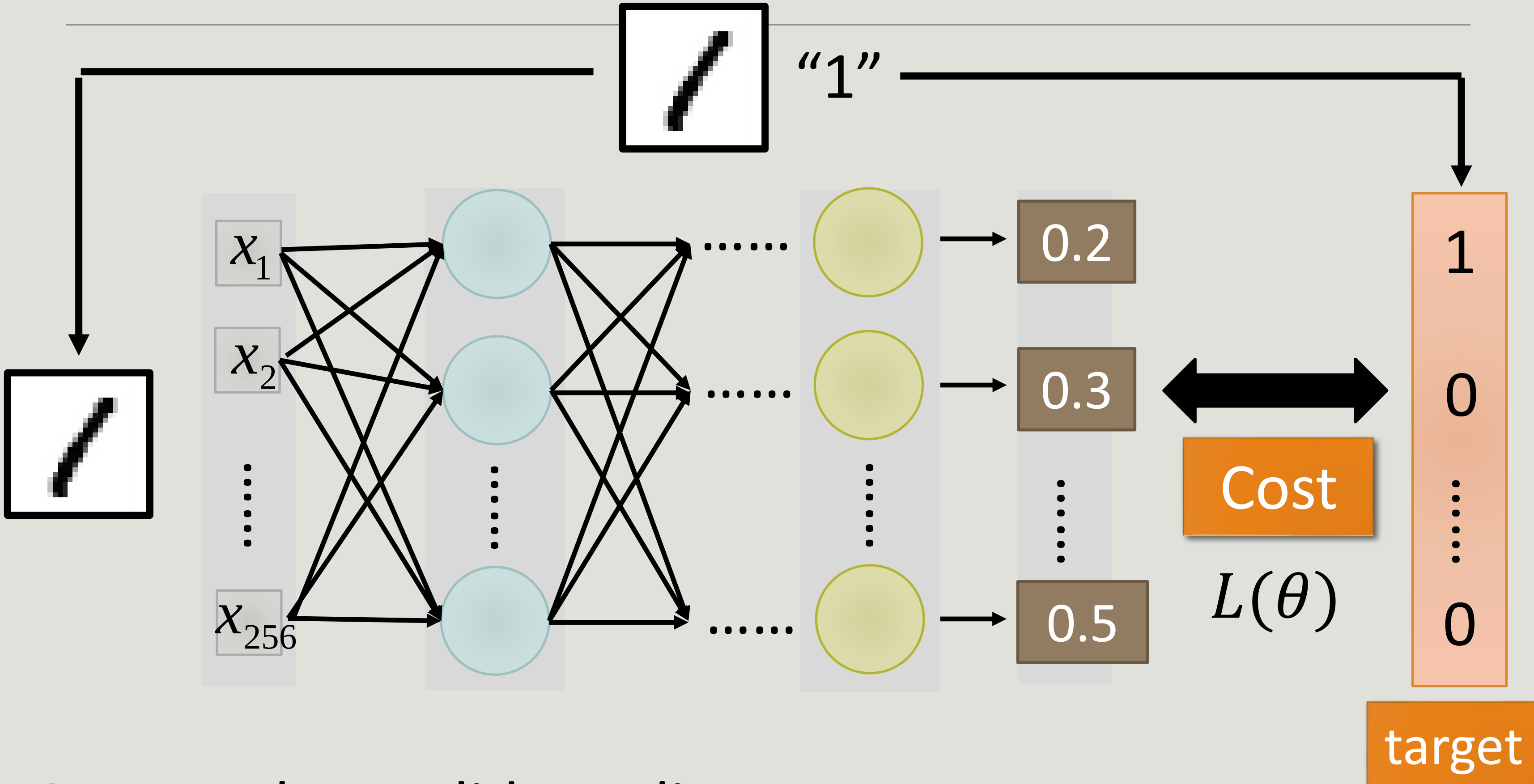
Preparing training data: images and their labels



Using the training data to find the network parameters.

Cost

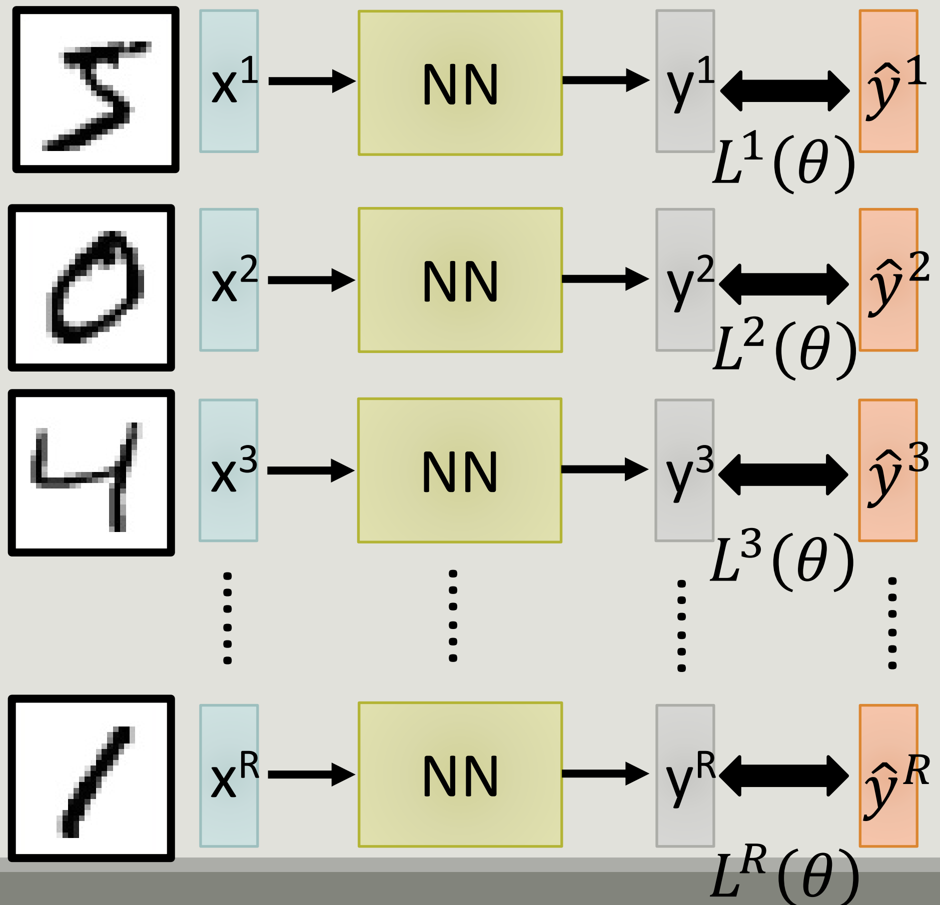
Given a set of network parameters θ, each example has a cost value.



Cost can be Euclidean distance or cross entropy of the network output and target

Total Cost

For all training data …



Total Cost:

$$C(\theta) = \sum_{r=1}^{R} L^r(\theta)$$

How bad the network parameters θ is on this task

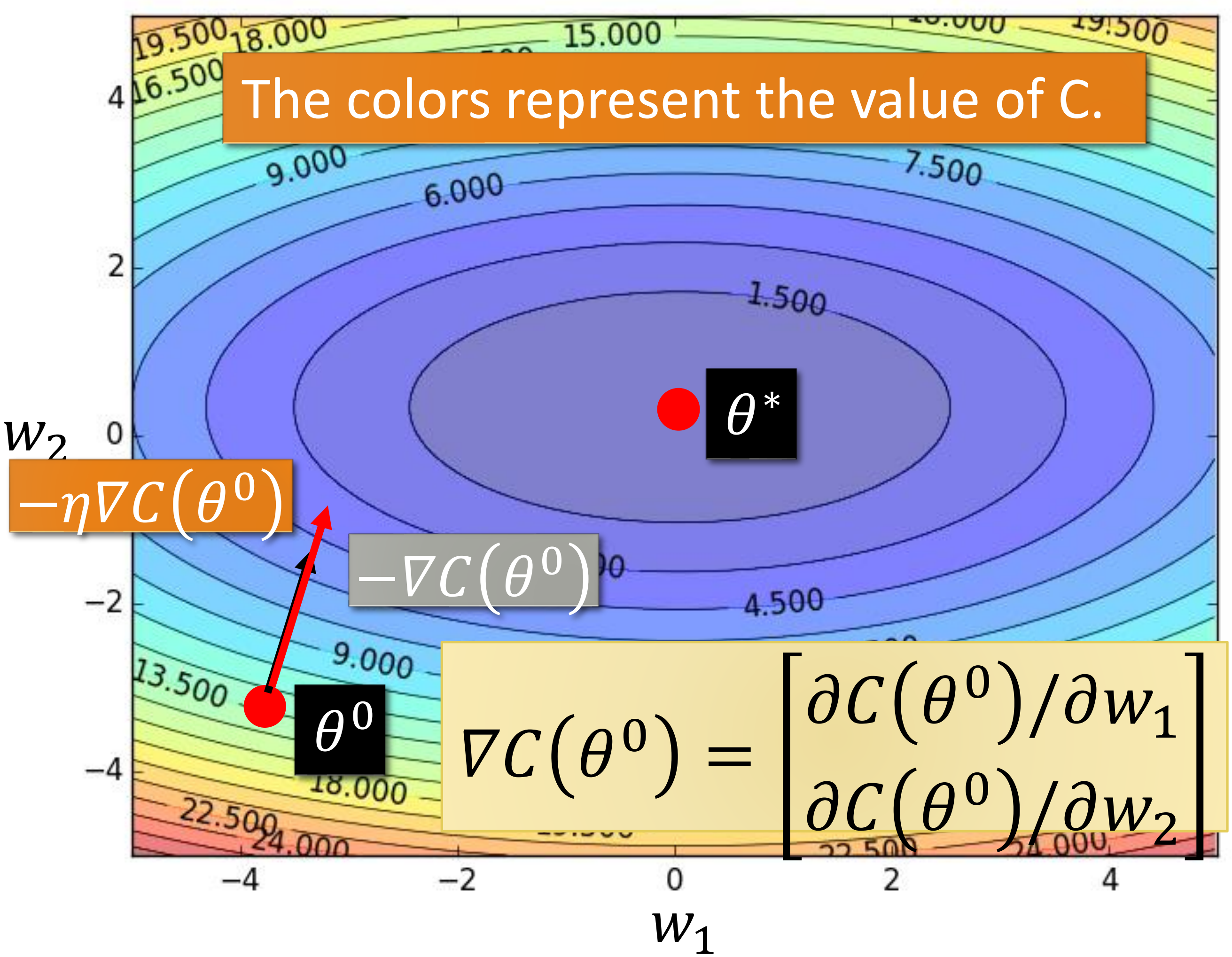
Find the network parameters θ^* that minimize this value

Gradient Descent

Assume there are only two parameters w_1 and w_2 in a network.

$$\theta = \{w_1, w_2\}$$

Error Surface



Randomly pick a starting point θ^0

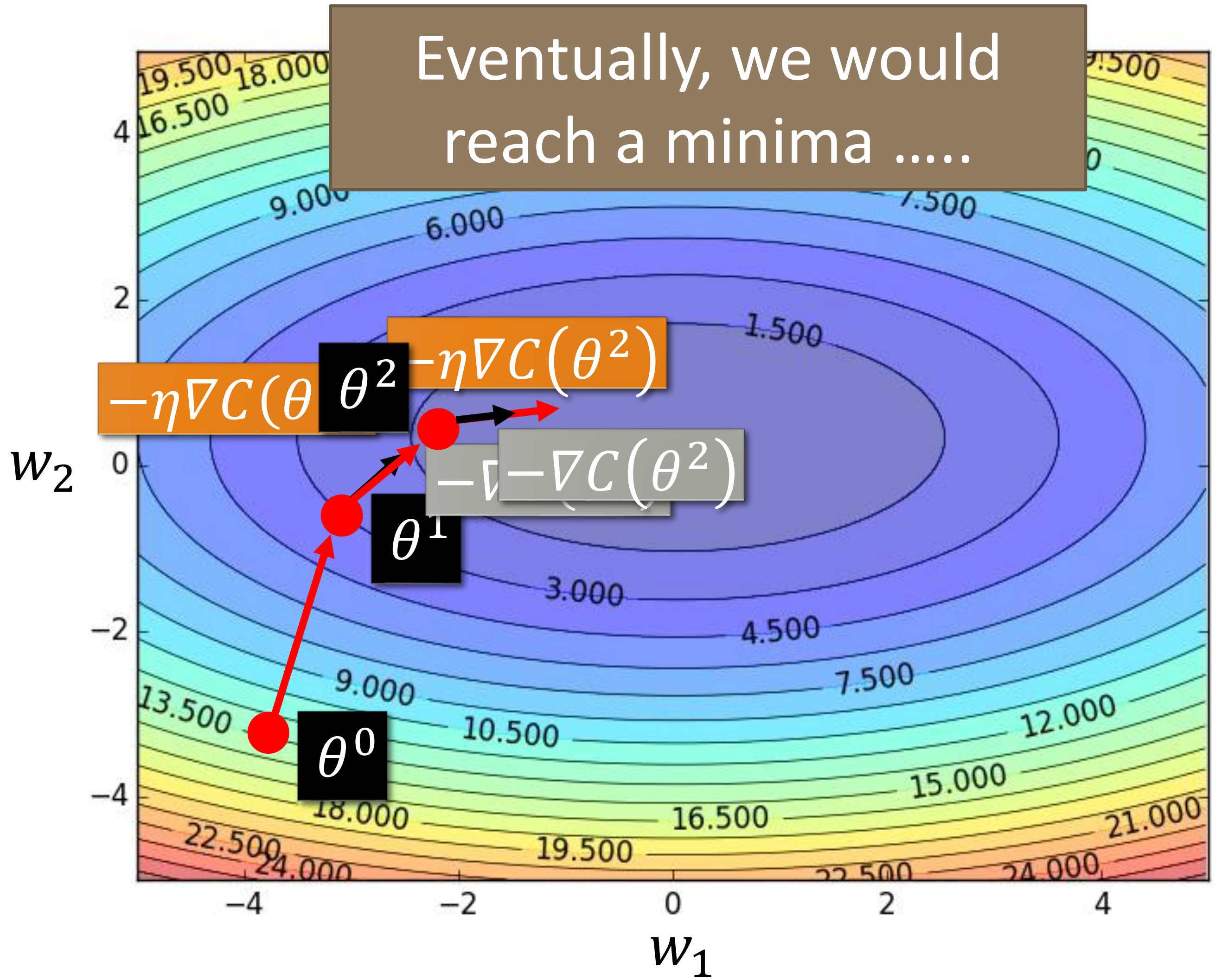
Compute the negative gradient at θ^0

$\Rightarrow -\nabla C(\theta^0)$

Times the learning rate η

$\Rightarrow -\eta \nabla C(\theta^0)$

Gradient Descent



Randomly pick a starting point θ^0

Compute the negative gradient at θ^0

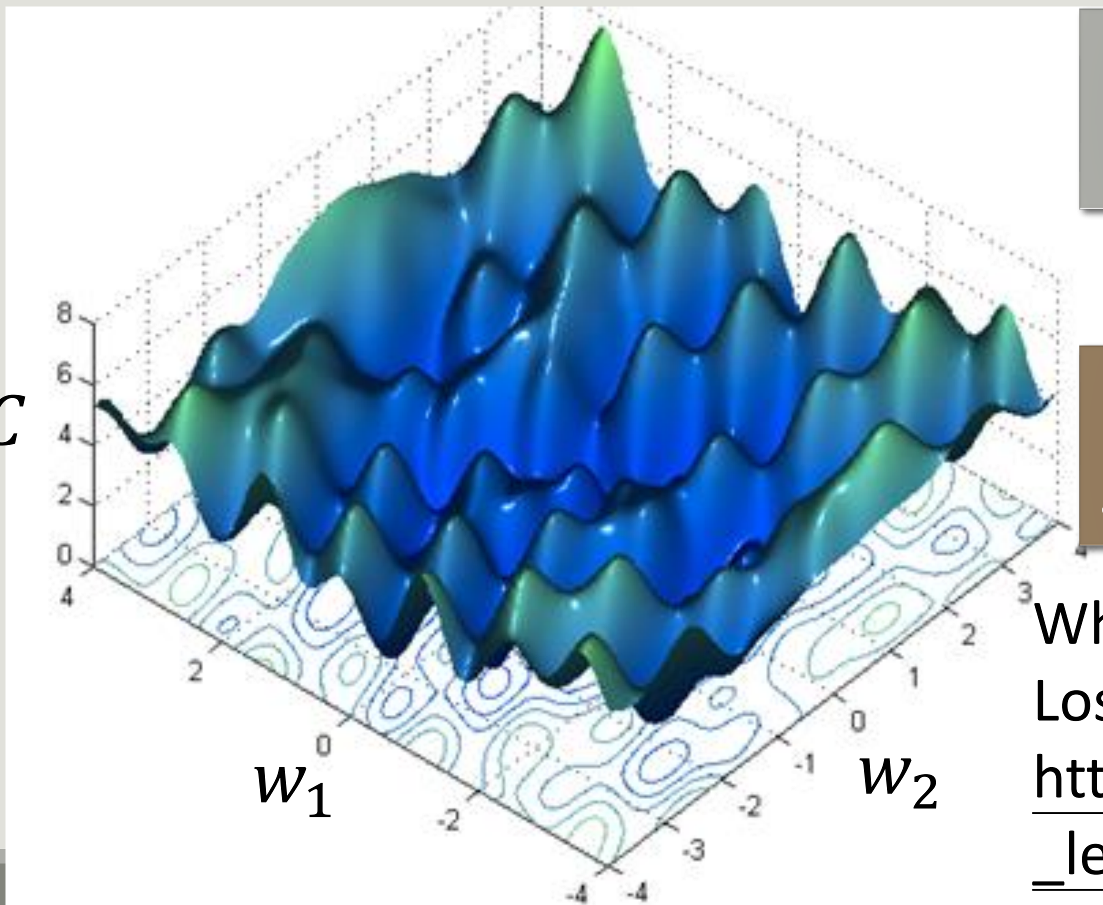
$\rightarrow -\nabla C(\theta^0)$

Times the learning rate η

$\rightarrow -\eta\nabla C(\theta^0)$

Local Minima

Gradient descent never guarantee global minima

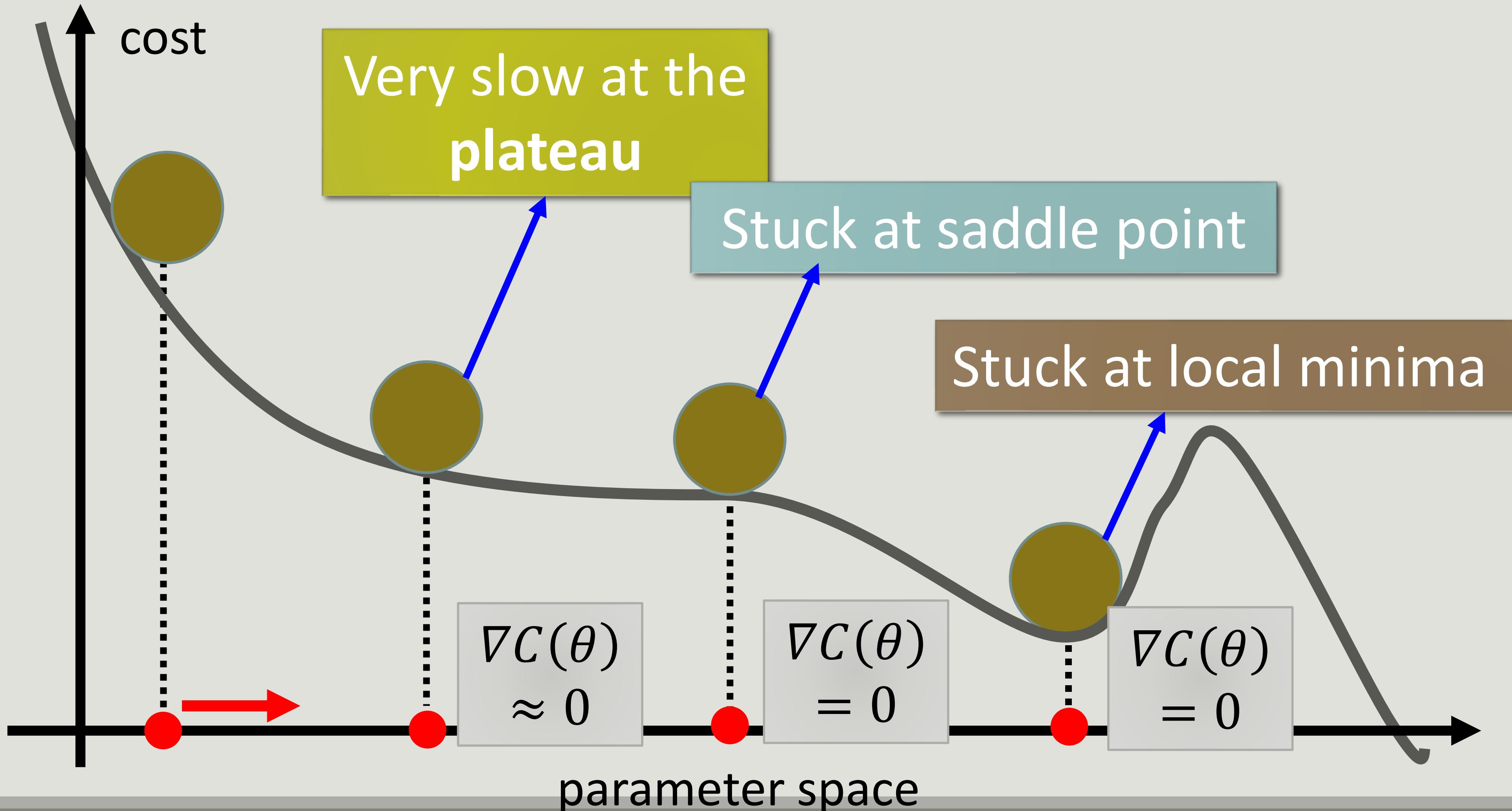


Different initial point θ^0

Reach different minima, so different results

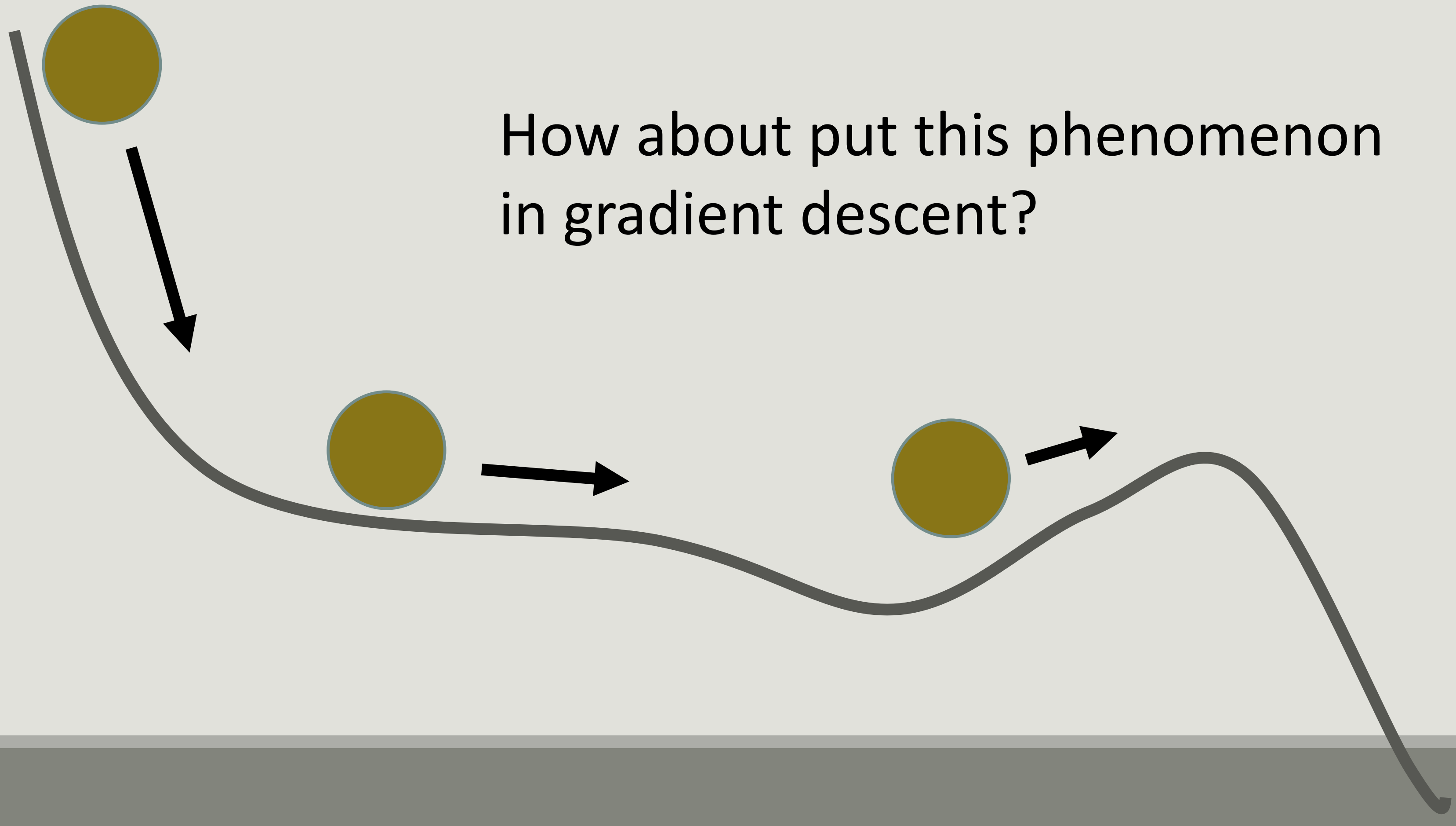
Who is Afraid of Non-Convex Loss Functions?
http://videolectures.net/eml07_lecun_wia/

Besides local minima ……



In physical world ……

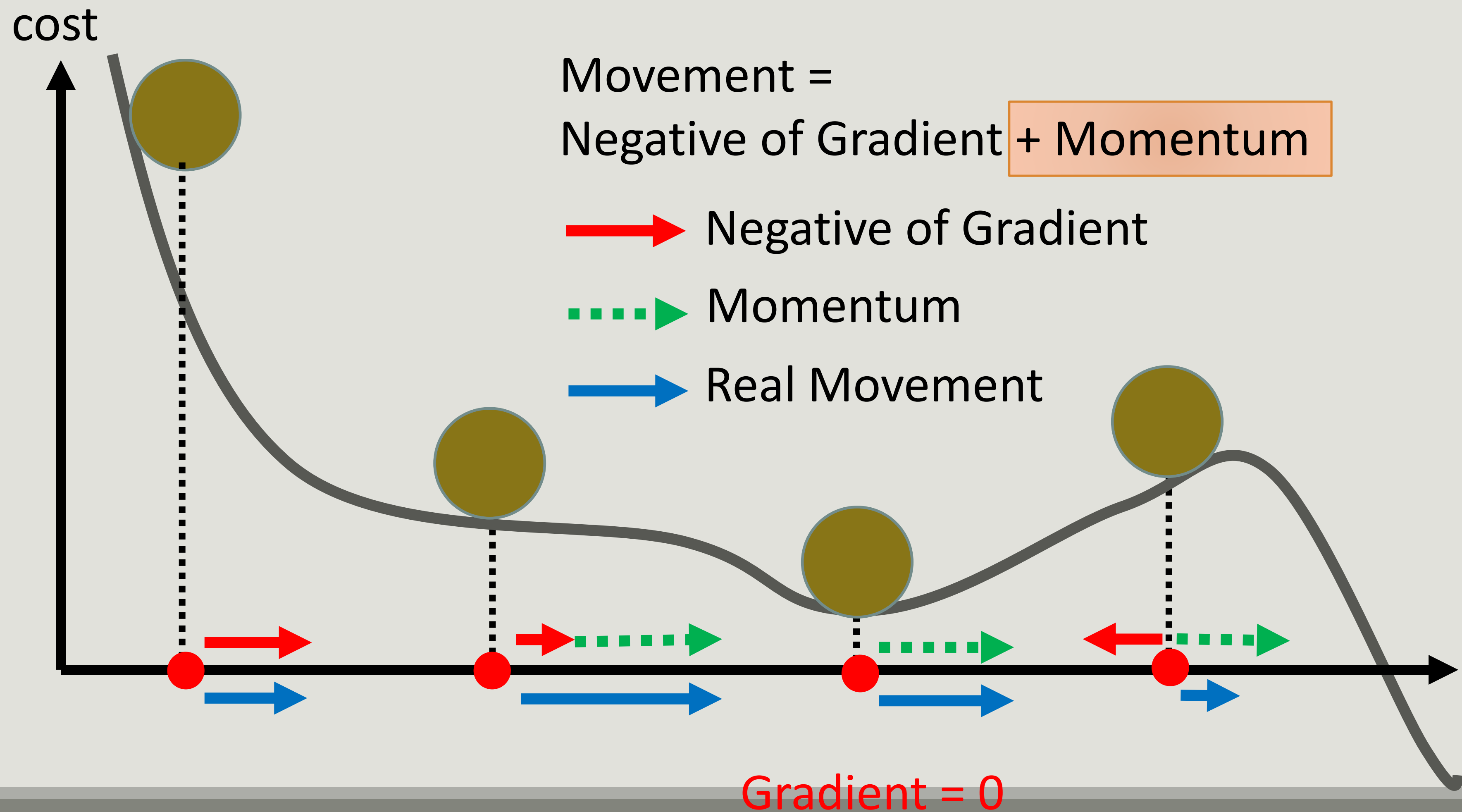
Momentum



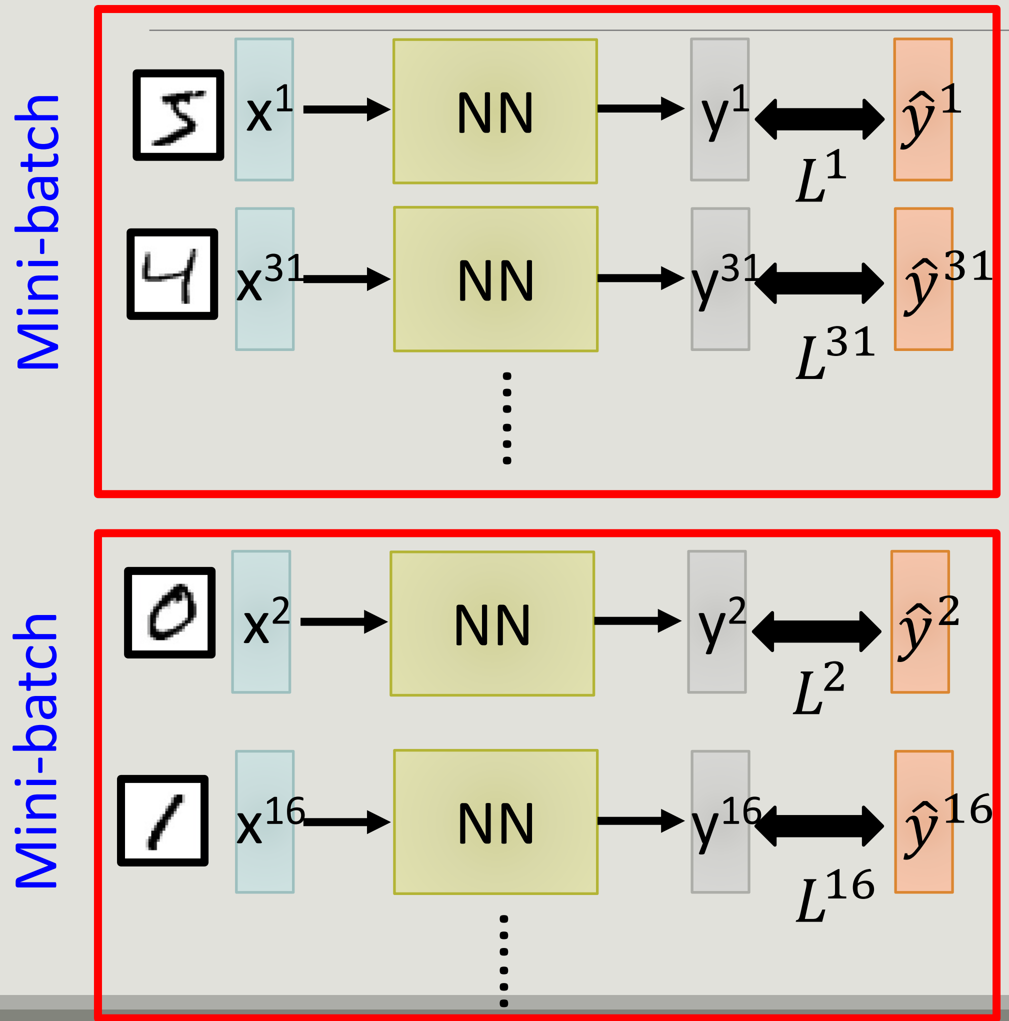
How about put this phenomenon in gradient descent?

Momentum

Still not guarantee reaching global minima, but give some hope ……



Mini-batch



- Randomly initialize θ^0
- Pick the 1st batch

$$C = L^1 + L^{31} + \cdots$$

$$\theta^1 \leftarrow \theta^0 - \eta \nabla C\left(\theta^0\right)$$

- Pick the 2nd batch

$$C = L^2 + L^{16} + \cdots$$

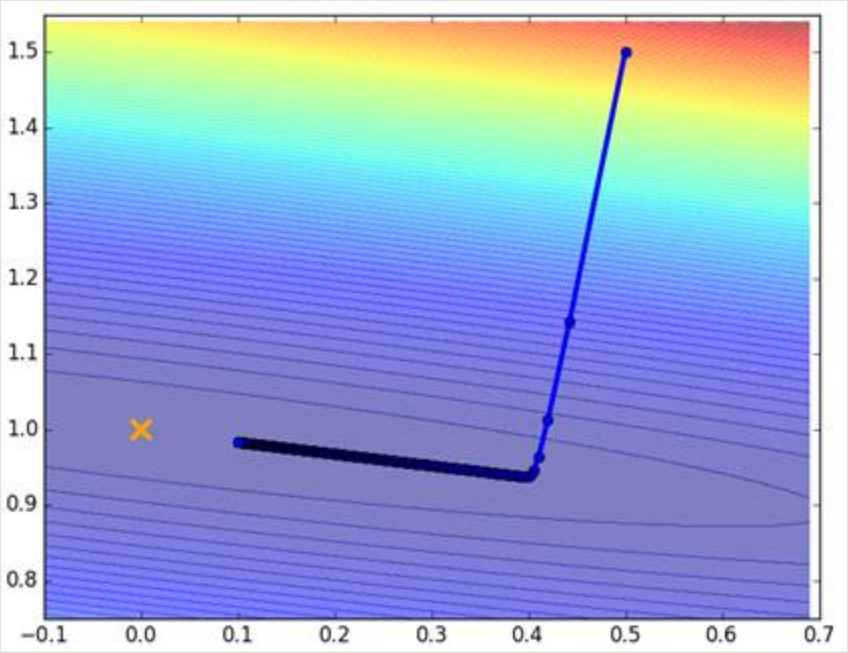
$$\theta^2 \leftarrow \theta^1 - \eta \nabla C(\theta^1)$$

$$\vdots$$

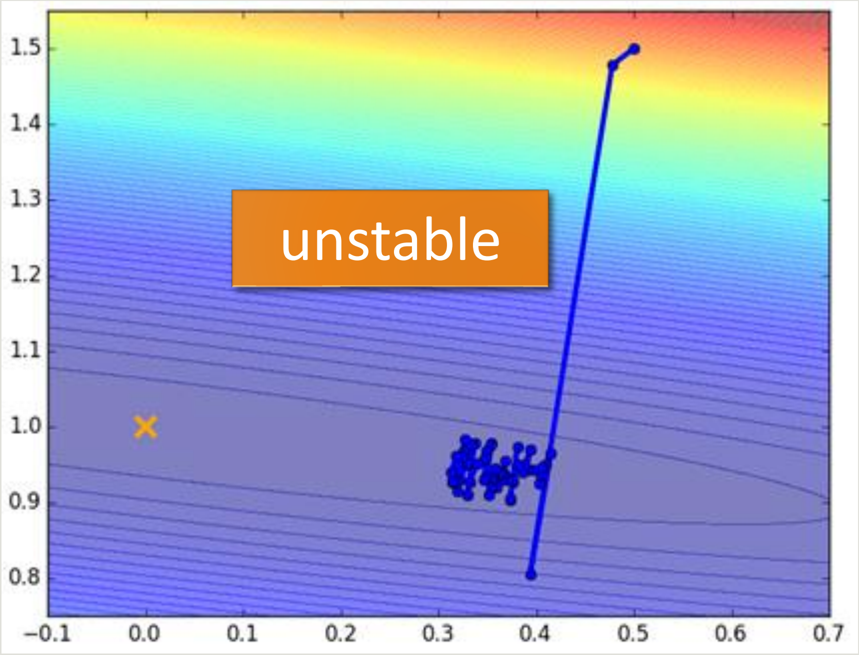
C is different each time when we update parameters!

Mini-batch

Original Gradient Descent



With Mini-batch

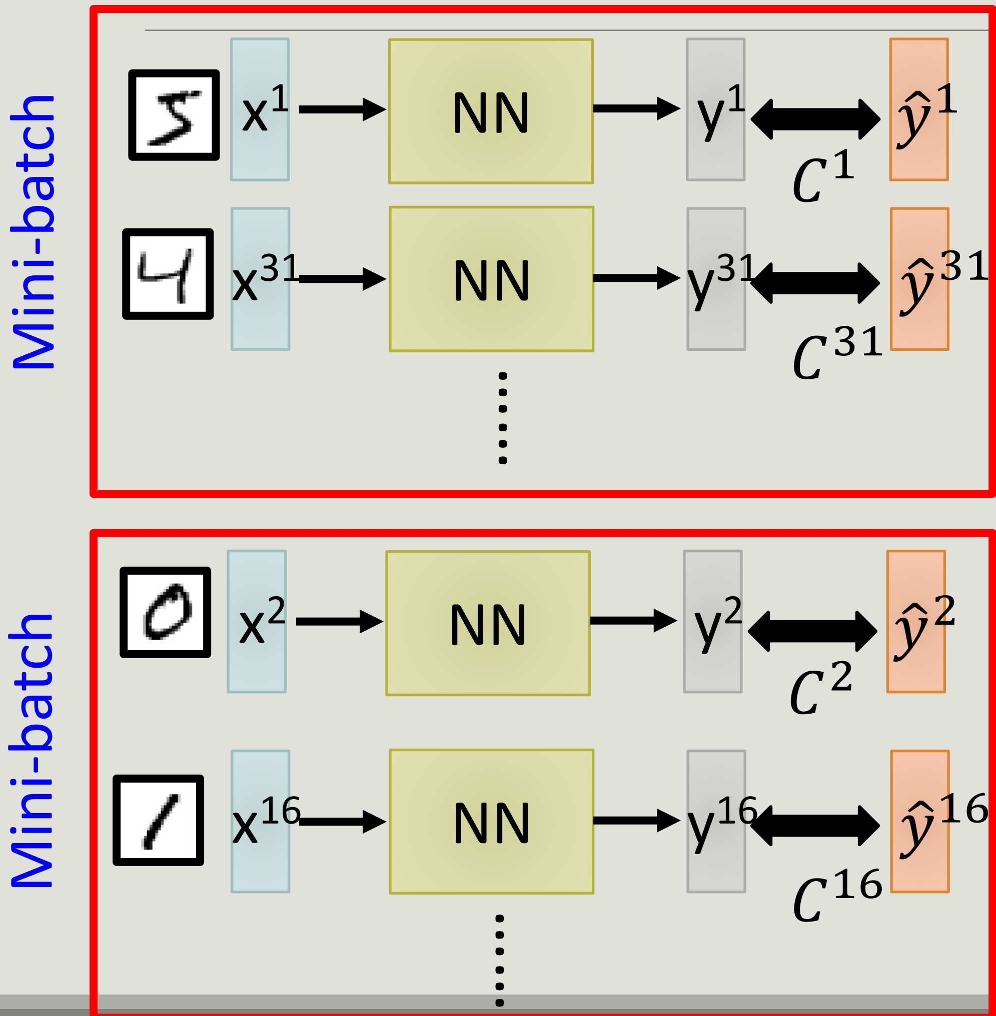


The colors represent the total C on all training data.

Mini-batch

Faster

Better!



- Randomly initialize θ^0
- Pick the 1st batch

$$C = C^1 + C^{31} + \cdots$$

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

- Pick the 2nd batch

$$C = C^2 + C^{16} + \cdots$$

$$\theta^2 \leftarrow \theta^1 - \eta \nabla C(\theta^1)$$

$$\vdots$$

- Until all mini-batches have been picked

one epoch

Repeat the above process

Backpropagation

A network can have millions of parameters.

- Backpropagation is the way to compute the gradients efficiently (not today)
- Ref: http://speech.ee.ntu.edu.tw/~tlkagk/courses/MLDS_2015_2/Lecture/DNN%20backprop.ecm.mp4/index.html

Many toolkits can compute the gradients automatically

Ref: http://speech.ee.ntu.edu.tw/~tlkagk/courses/MLDS_2015_2/Lecture/Theano%20DNN.ecm.mp4/index.html

Deeper is Better?

Layer X Size	Word Error Rate (%)	Layer X Size	Word Error Rate (%)
1 X 2k	24.2		
2 X 2k	20.4		
3 X 2k	18.4		
4 X 2k	17.8		
5 X 2k	17.2	1 X 3772	22.5
7 X 2k	17.1	1 X 4634	22.6
		1 X 16k	22.1

Not surprised, more parameters, better performance

Seide, Frank, Gang Li, and Dong Yu. "Conversational Speech Transcription Using Context-Dependent Deep Neural Networks." *Interspeech*. 2011.

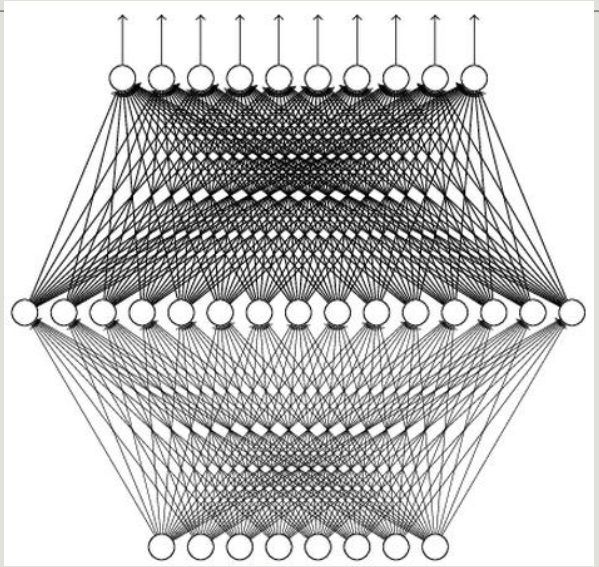
Universality Theorem

Any continuous function f

$$f : R^N \rightarrow R^M$$

Can be realized by a network with one hidden layer

(given **enough** hidden neurons)

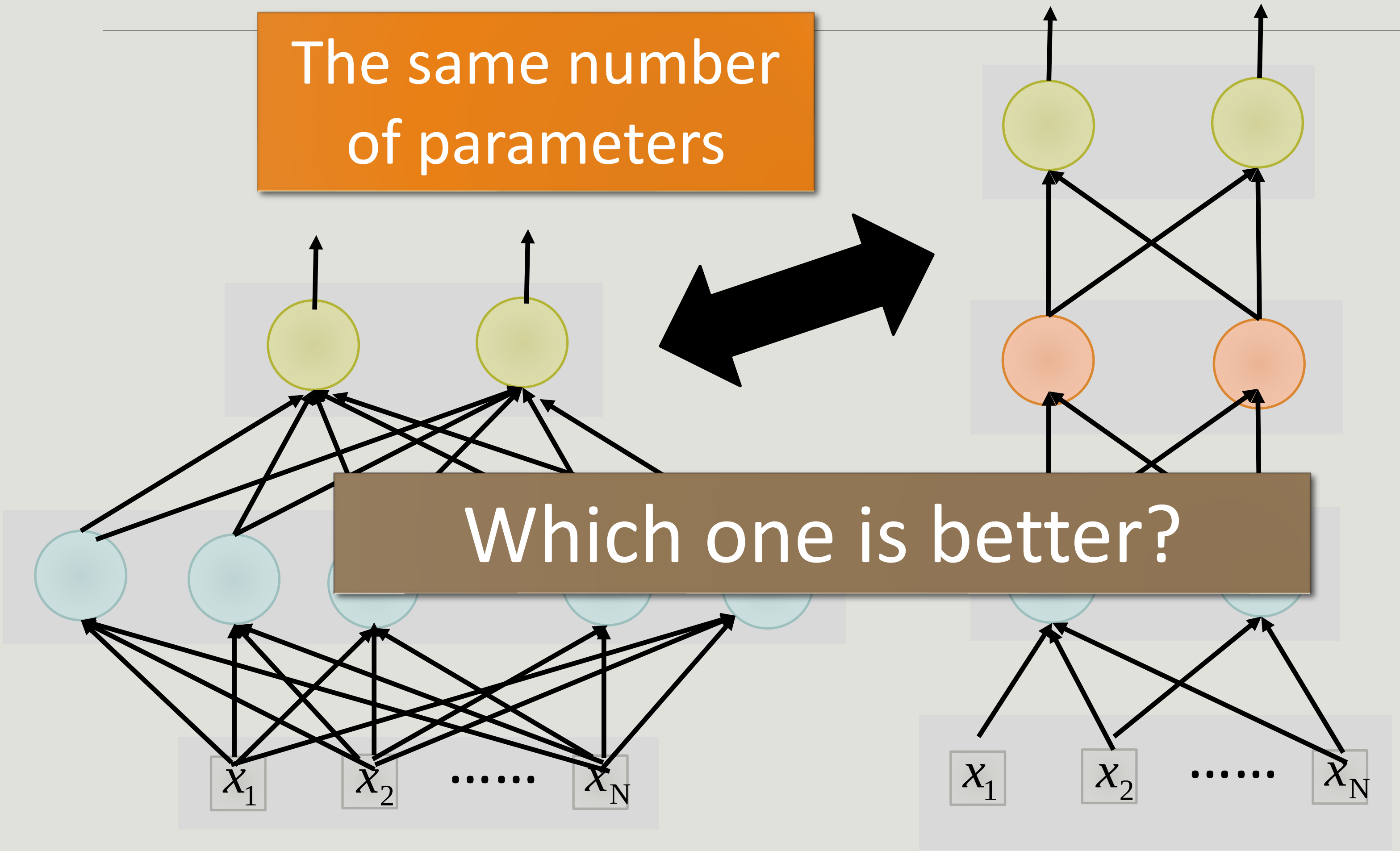


Reference for the reason: http://neuralnetworksanddeeplearning.com/chap4.html

Why "Deep" neural network not "Fat" neural network?

Fat + Short v.s. Thin + Tall

The same number of parameters



Which one is better?

Shallow

Deep

Fat + Short v.s. Thin + Tall

Layer X Size	Word Error Rate (%)	Layer X Size	Word Error Rate (%)
1 X 2k	24.2		
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		1 X 16k	22.1

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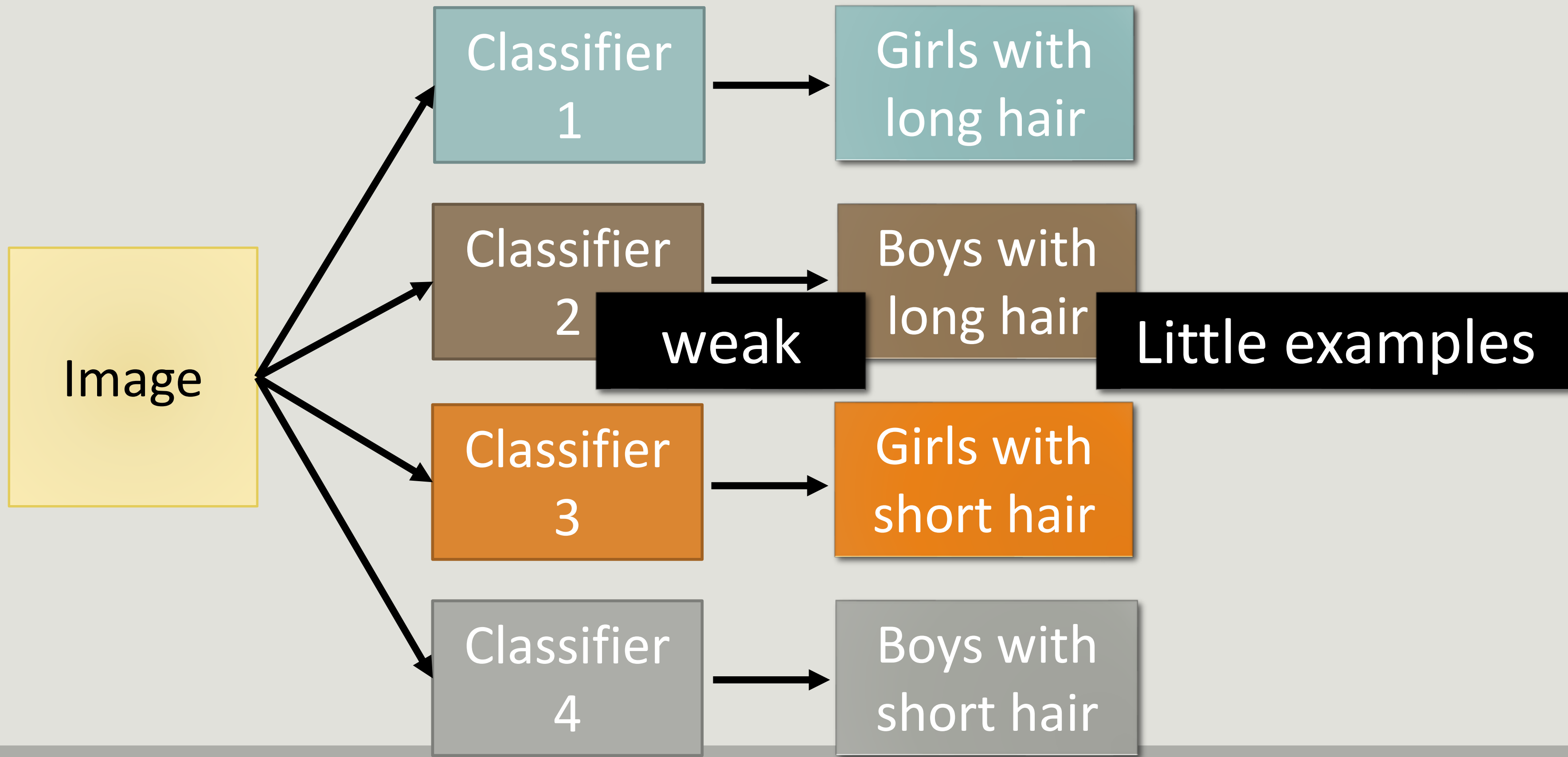
Why Deep?

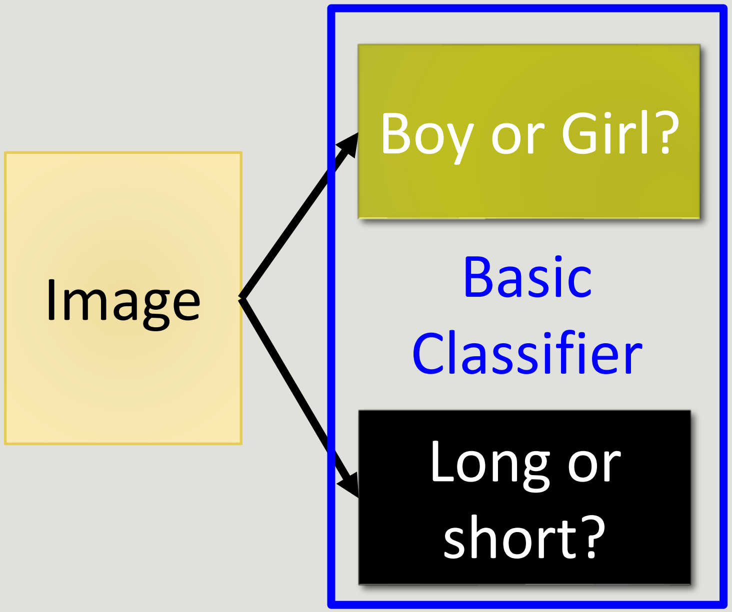
Deep → Modularization



Why Deep?

Each basic classifier can have sufficient training examples.

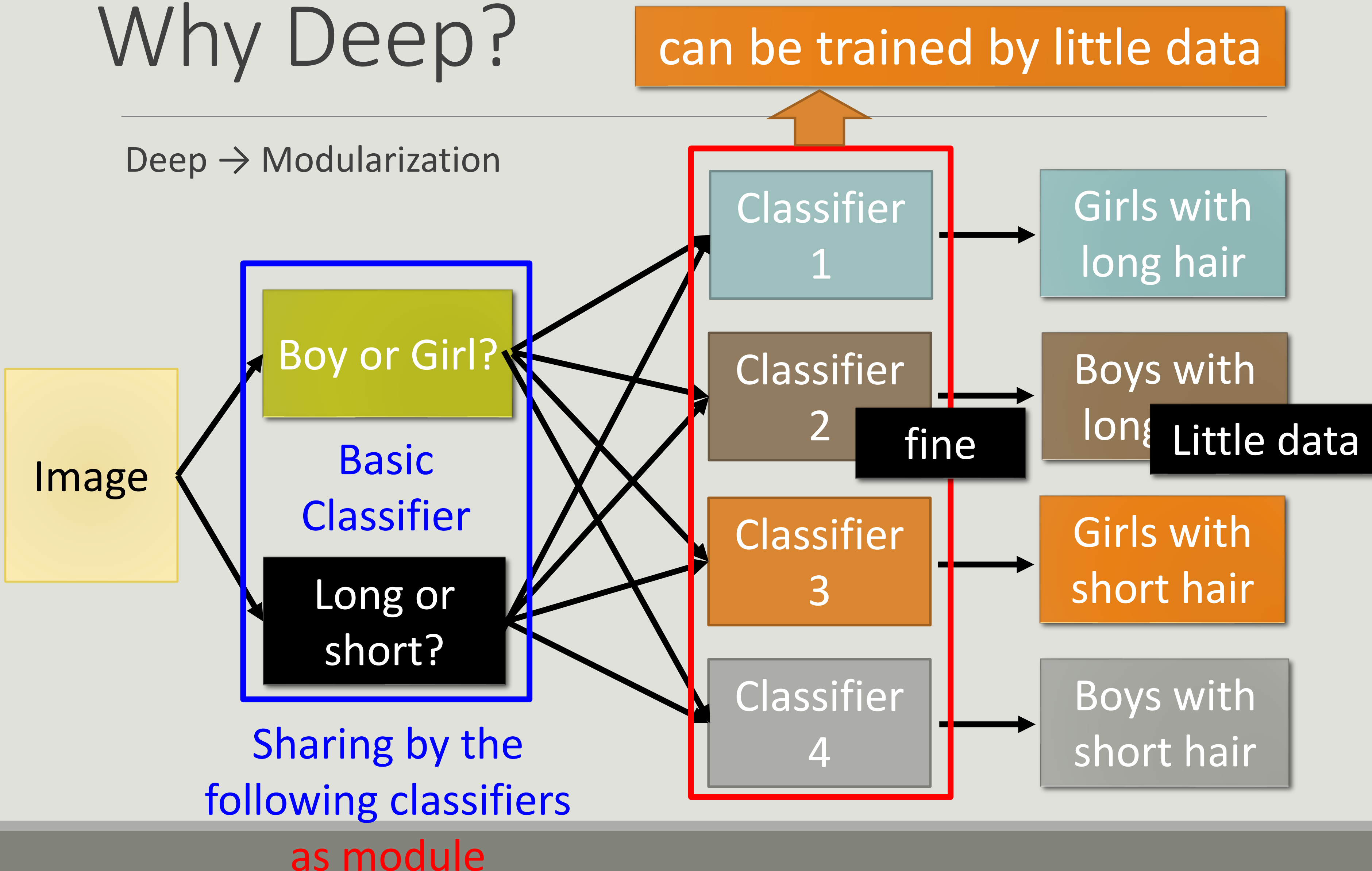
Deep → Modularization



Classifiers for the attributes

Why Deep?

Deep → Modularization

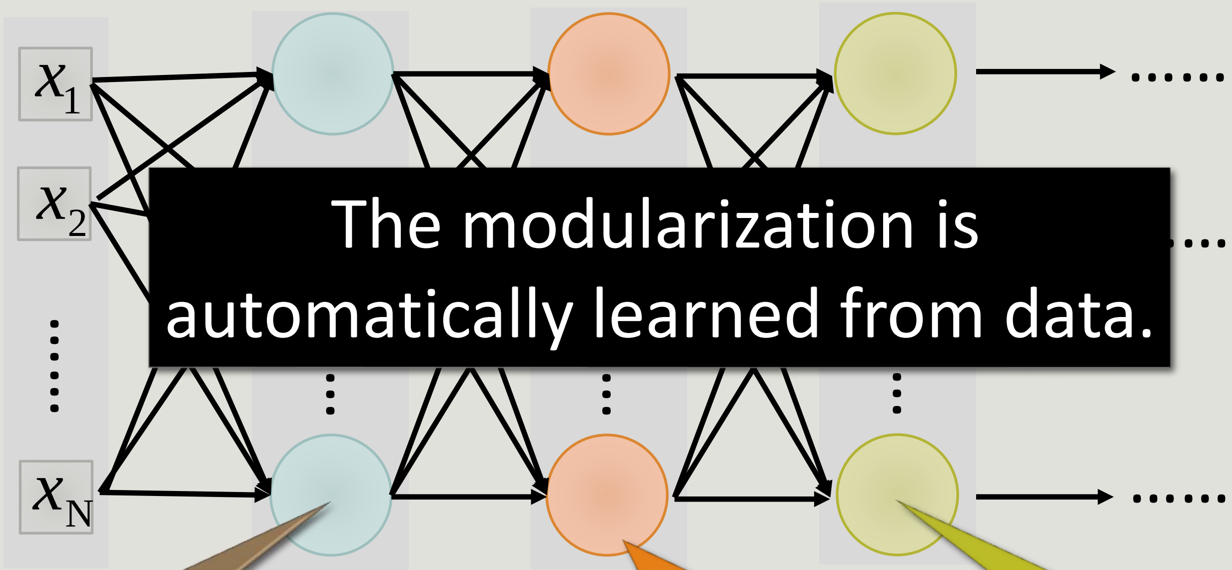


Why Deep?

Deep Learning also works on small data set like TIMIT.

Deep → Modularization

→ Less training data?



The modularization is automatically learned from data.

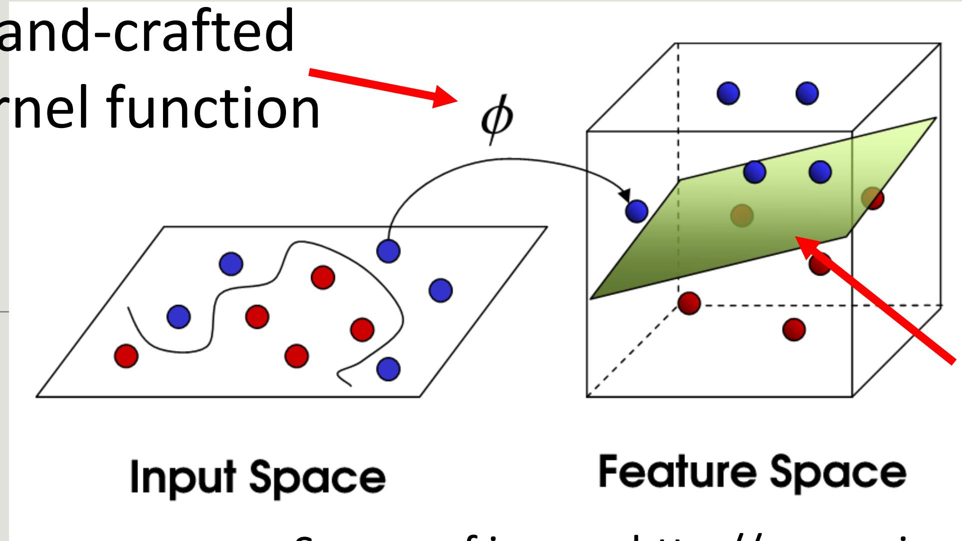
The most basic classifiers

Use 1st layer as module to build classifiers

Use 2nd layer as module ......

SVM

Hand-crafted kernel function



Apply simple classifier

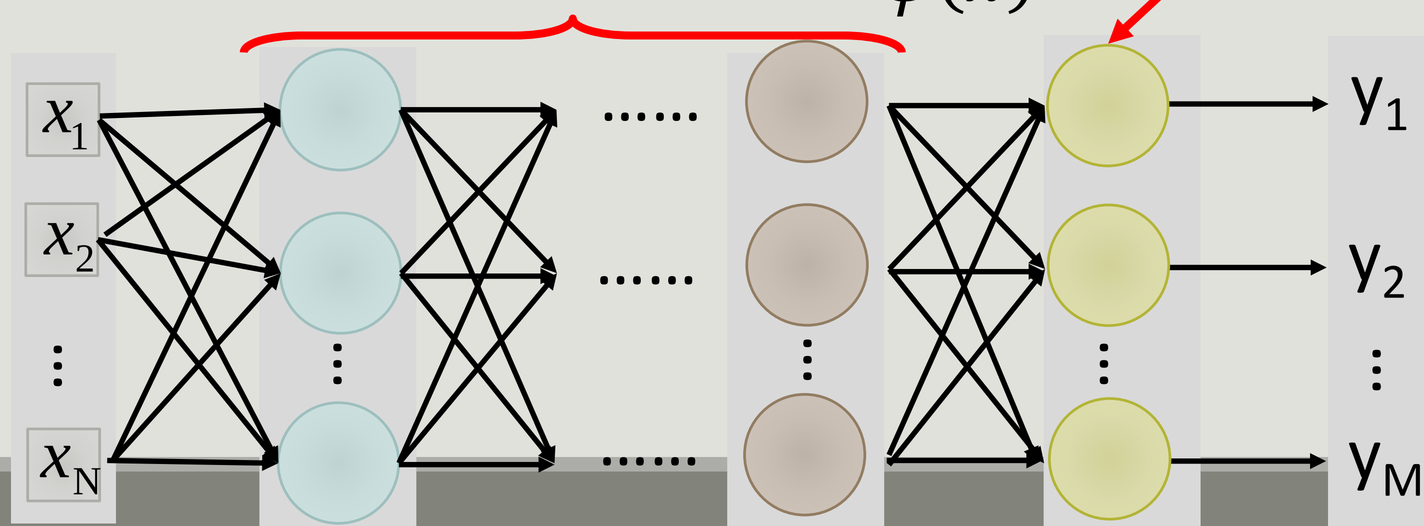
Source of image: http://www.gipsa-lab.grenoble-inp.fr/transfert/seminaire/455_Kadri2013Gipsa-lab.pdf

Deep Learning

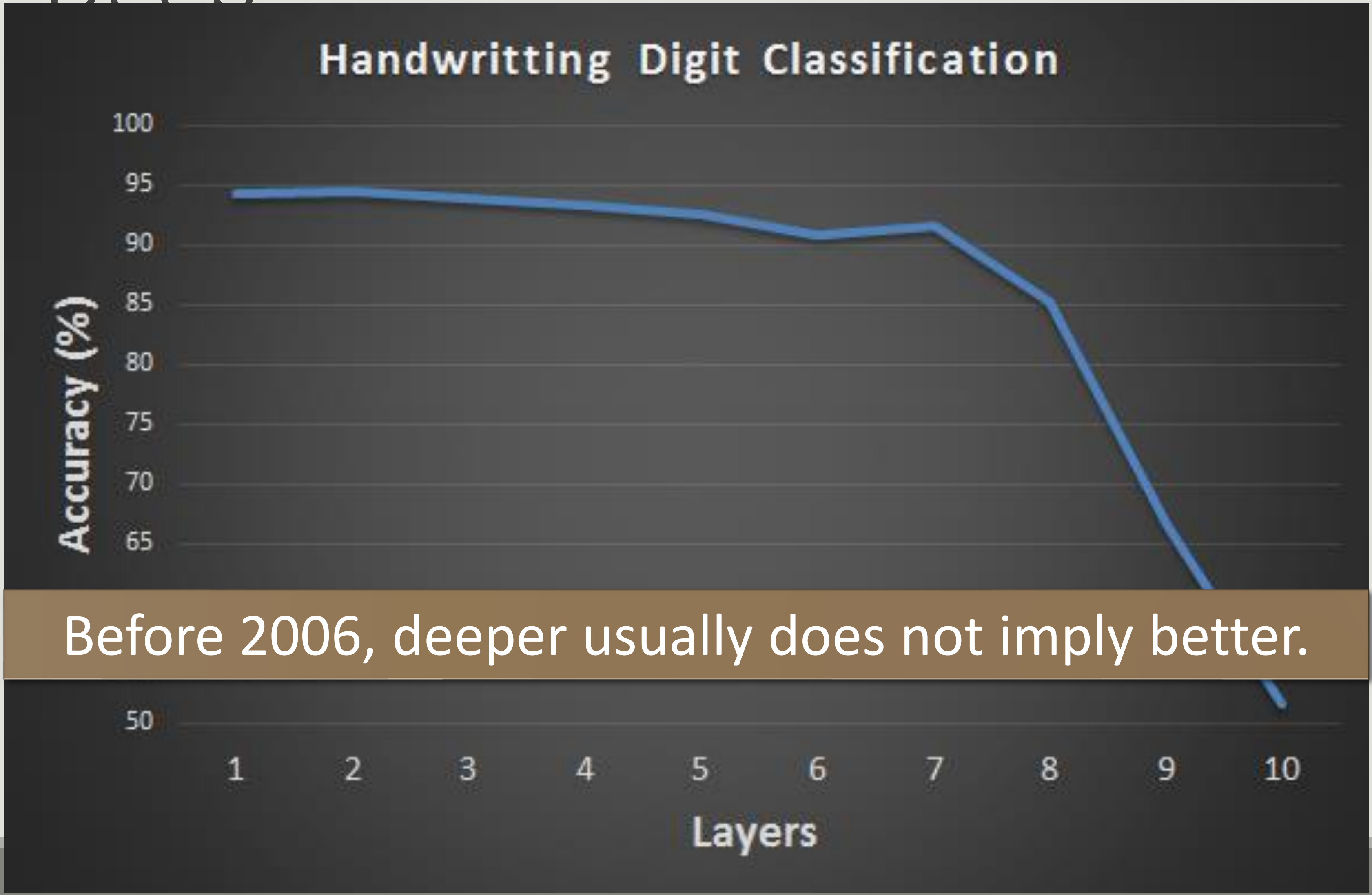
Learnable kernel

$\phi(x)$

simple classifier



Hard to get the power of Deep



Before 2006, deeper usually does not imply better.

Recipe for Learning

Modify the Network

- New activation functions, for example, ReLU or Maxout

Better optimization Strategy

- Adaptive learning rates

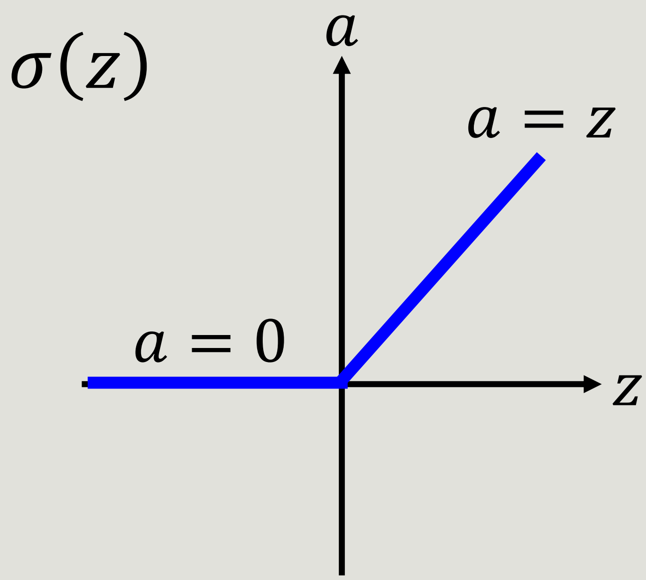
Prevent Overfitting

- Dropout

Only use this approach when you already obtained good results on the training data.

ReLU

Rectified Linear Unit (ReLU)

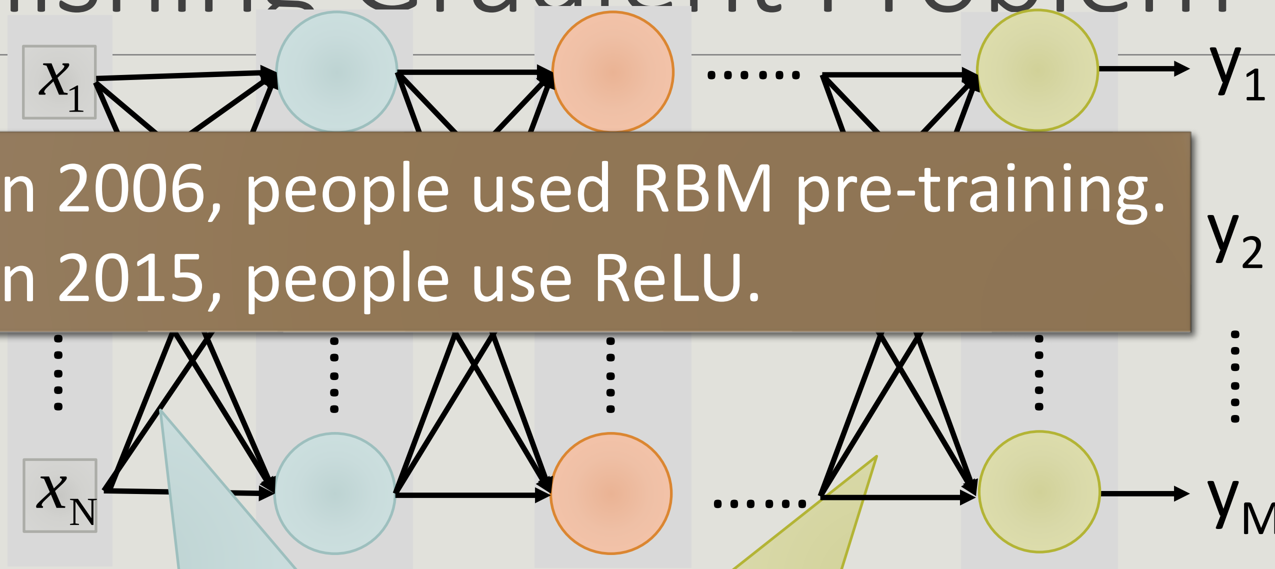


[Xavier Glorot, AISTATS'11]
[Andrew L. Maas, ICML'13]
[Kaiming He, arXiv'15]

Reason:

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

Vanishing Gradient Problem

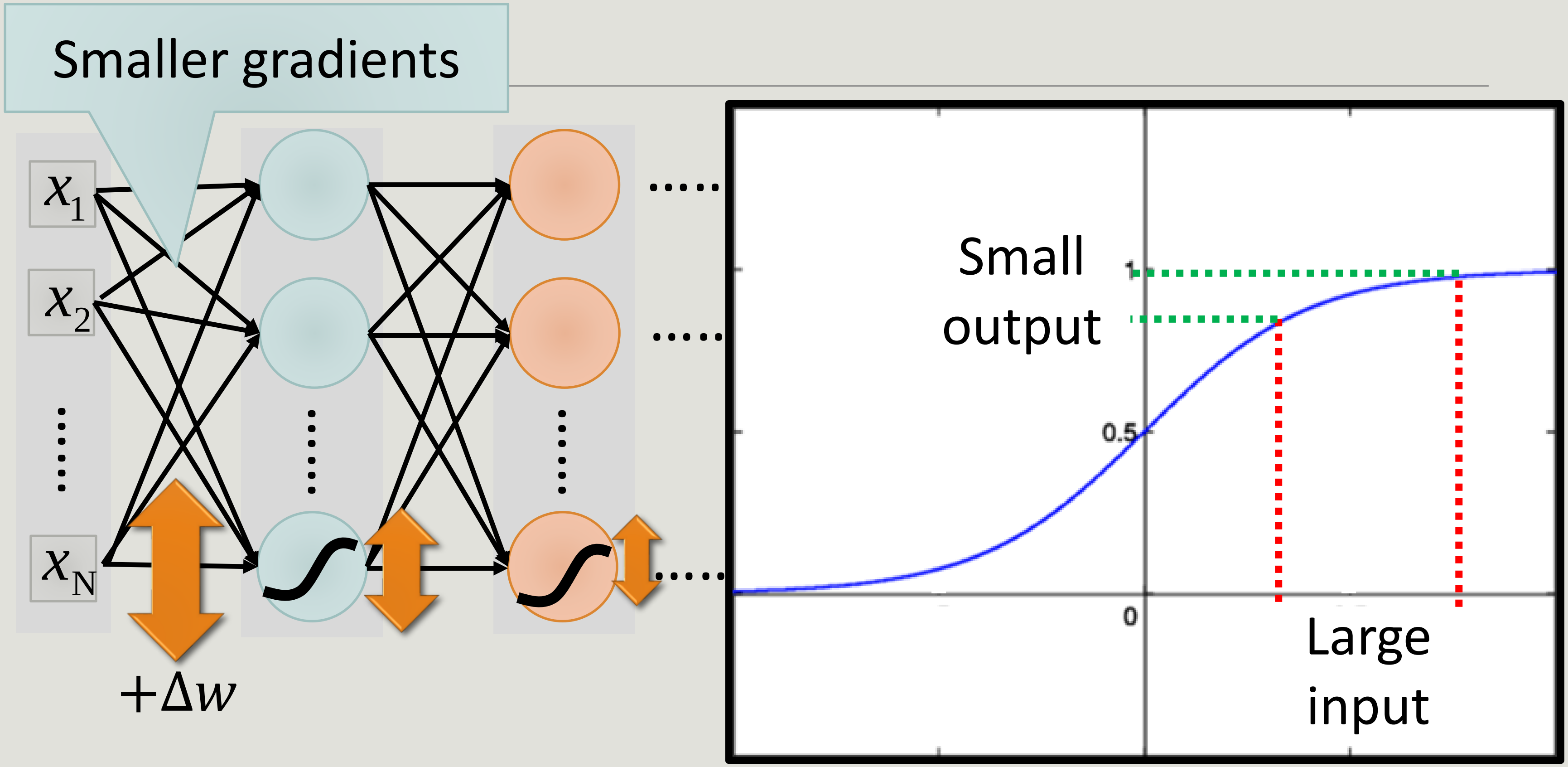


In 2006, people used RBM pre-training.
In 2015, people use ReLU.

Smaller gradients	Larger gradients
Learn very slow	Learn very fast
Almost random	Already converge

based on random!?

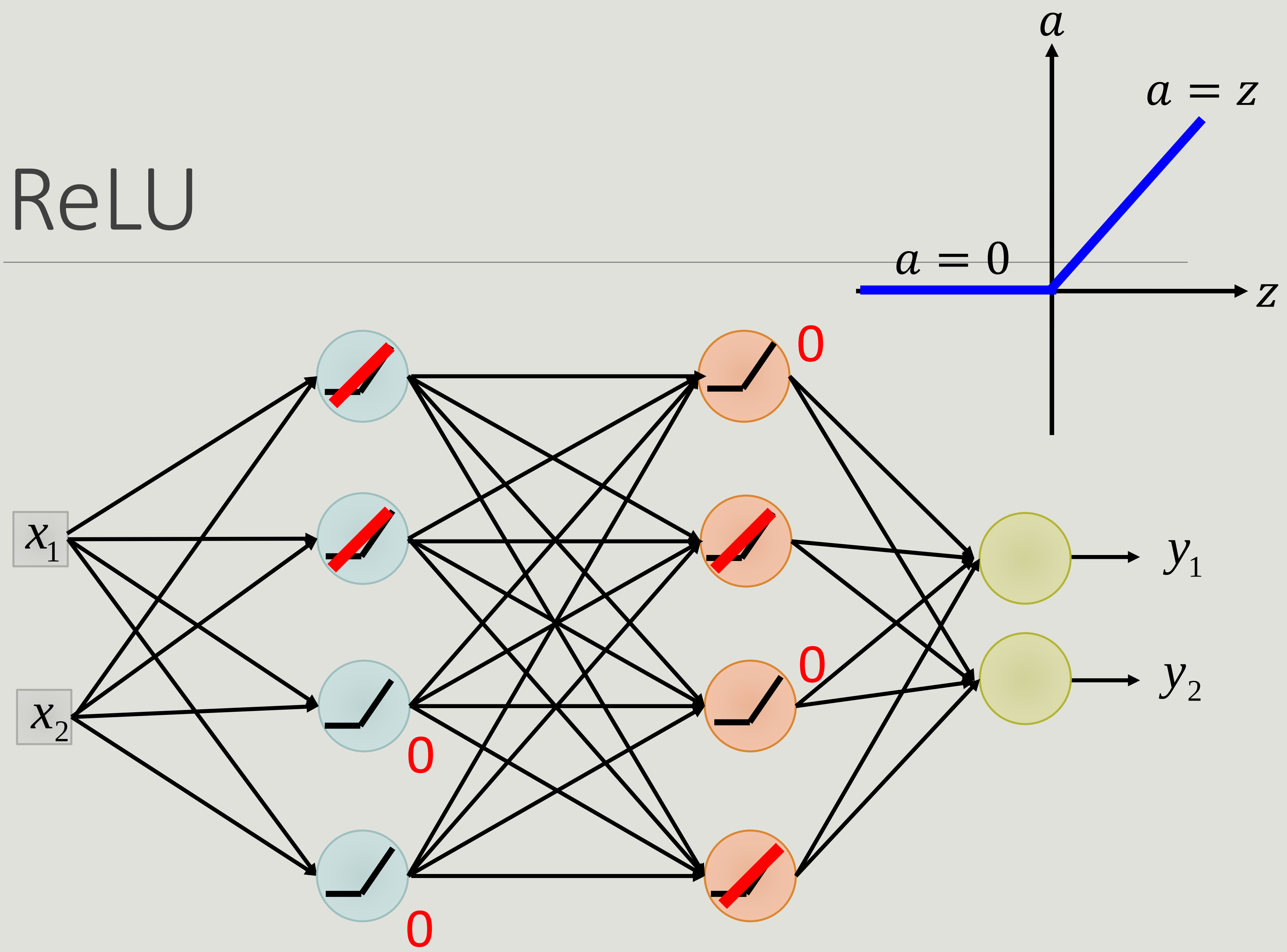
Vanishing Gradient Problem



Intuitive way to compute the gradient …

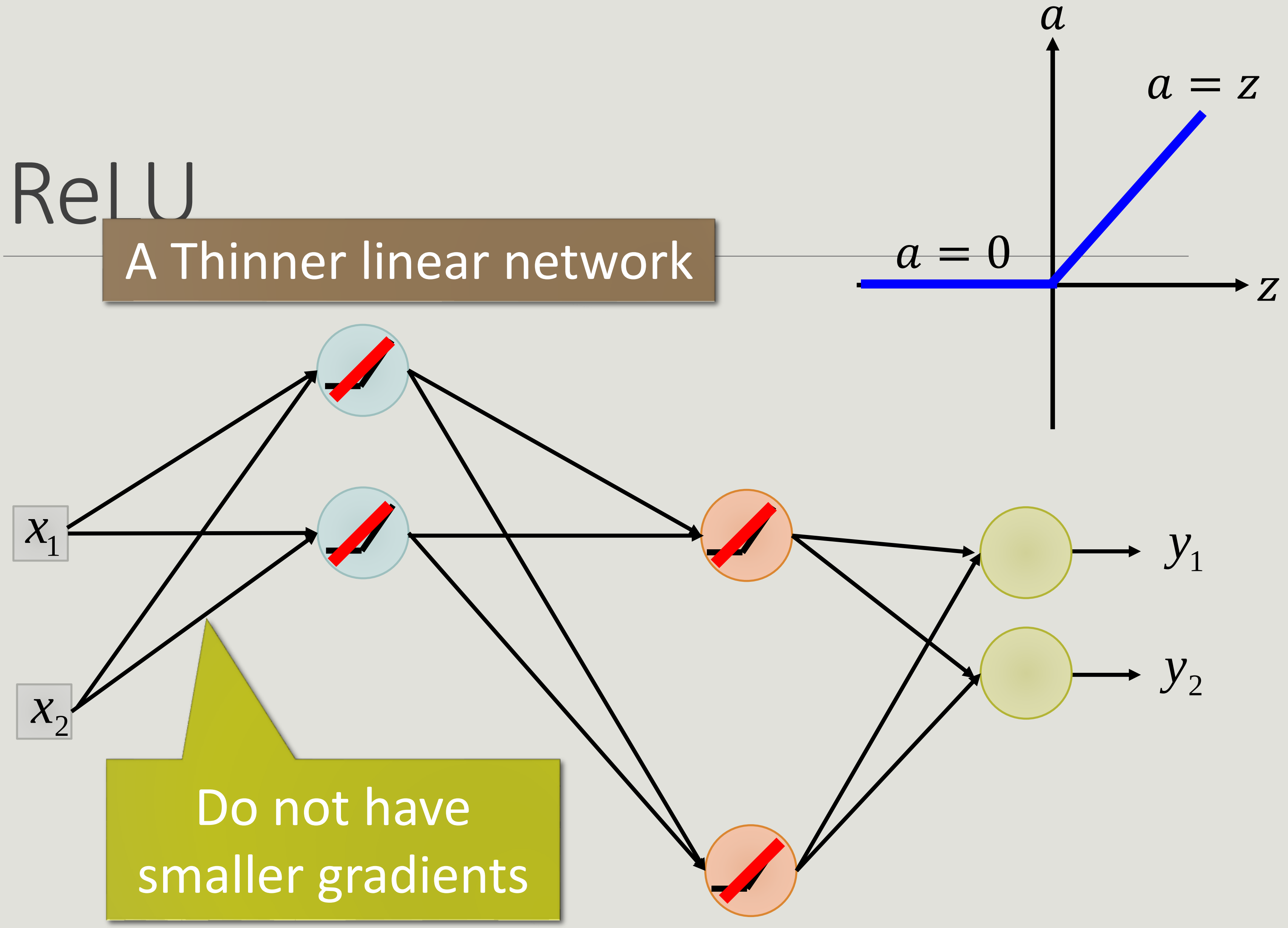
$$\frac{\partial C}{\partial w} =? \frac{\Delta C}{\Delta w}$$

ReLU



ReLU

A Thinner linear network

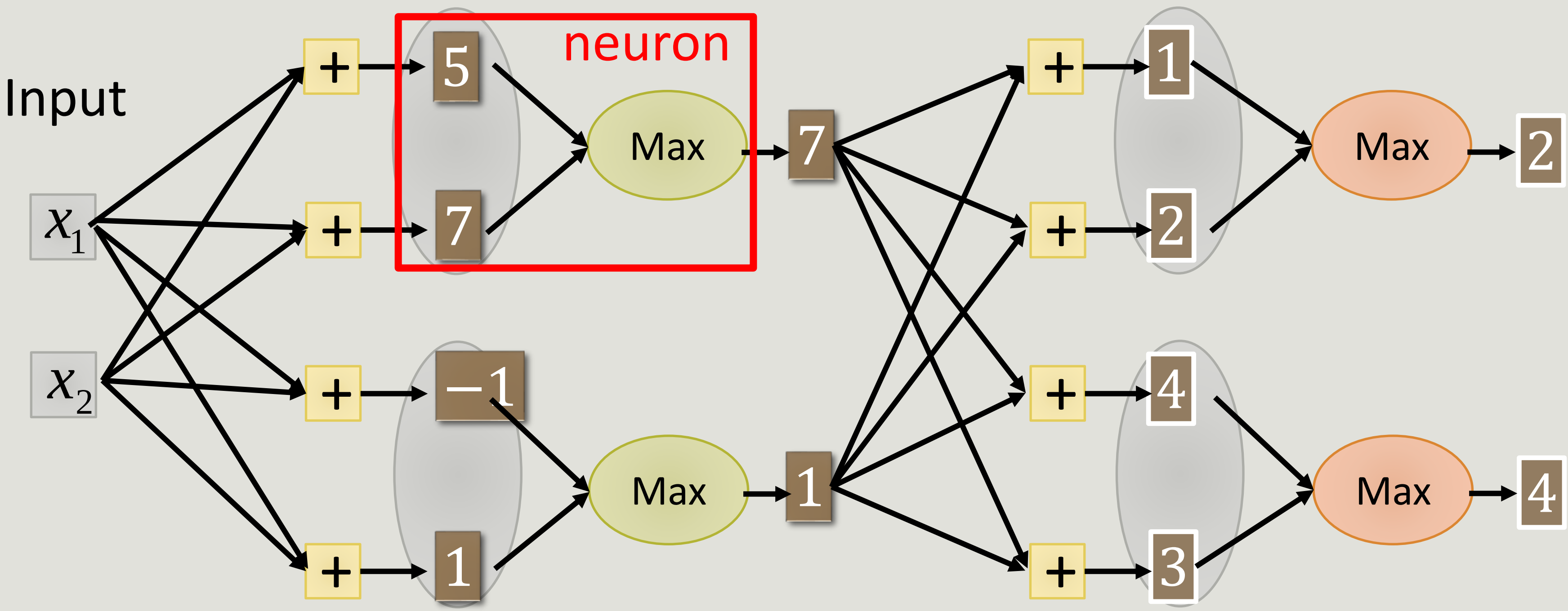


Do not have smaller gradients

Maxout

ReLU is a special cases of Maxout

Learnable activation function [Ian J. Goodfellow, ICML'13]



You can have more than 2 elements in a group.

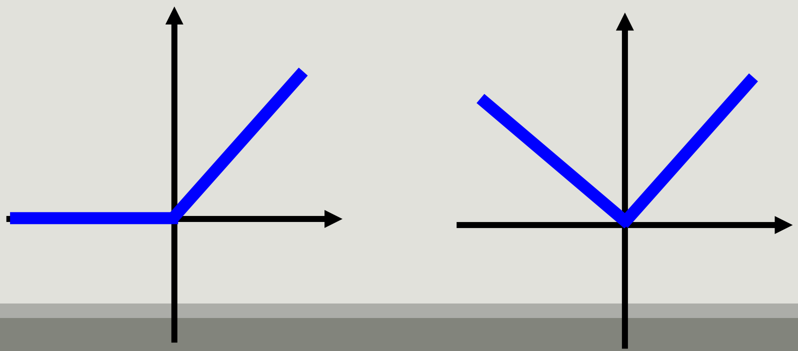
Maxout

ReLU is a special cases of Maxout

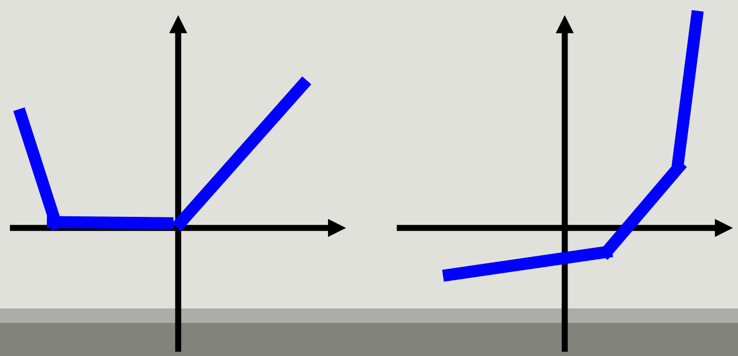
Learnable activation function [Ian J. Goodfellow, ICML'13]

- Activation function in maxout network can be any piecewise linear convex function
- How many pieces depending on how many elements in a group

2 elements in a group

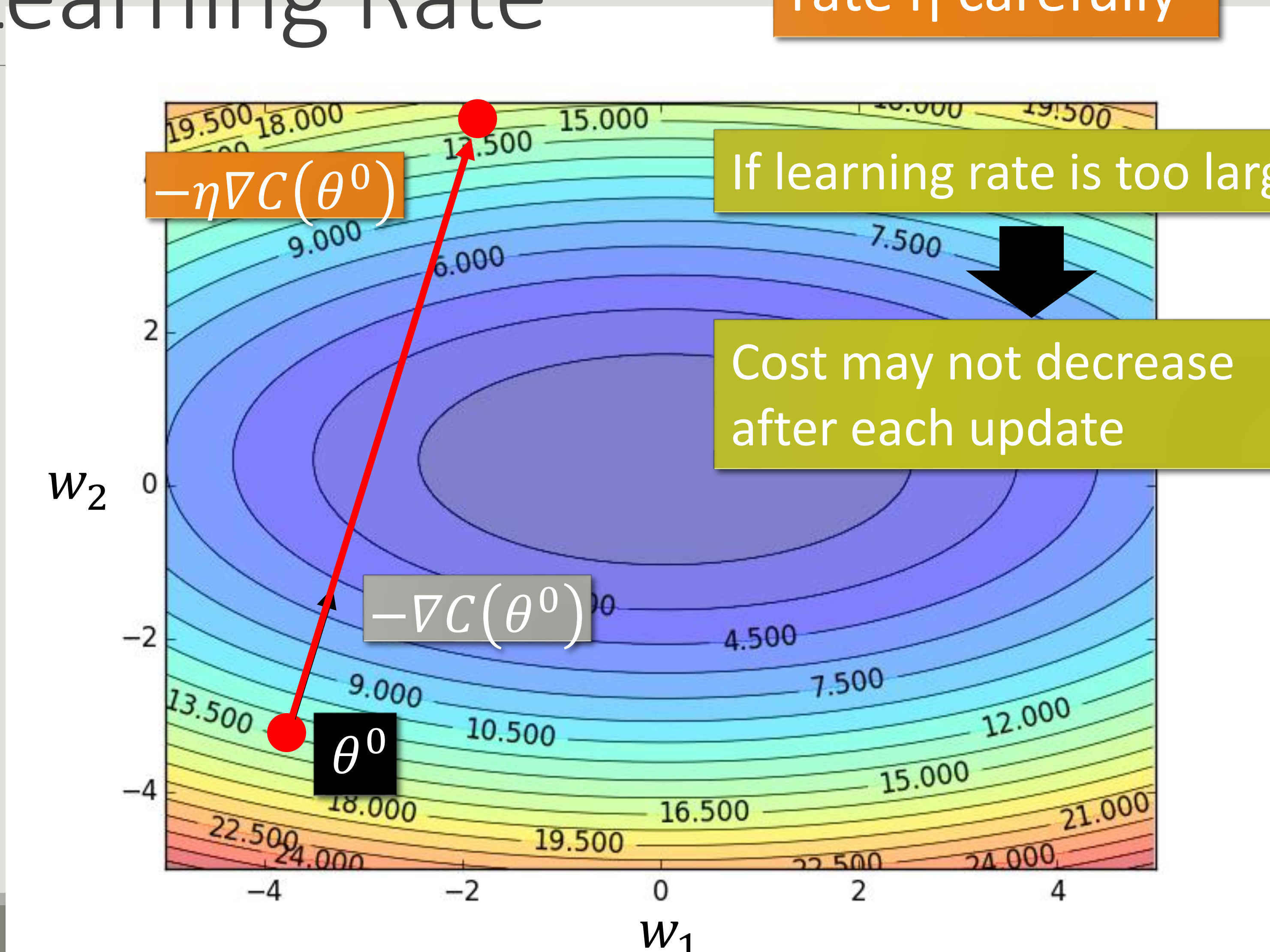


3 elements in a group



Learning Rate

Set the learning rate η carefully

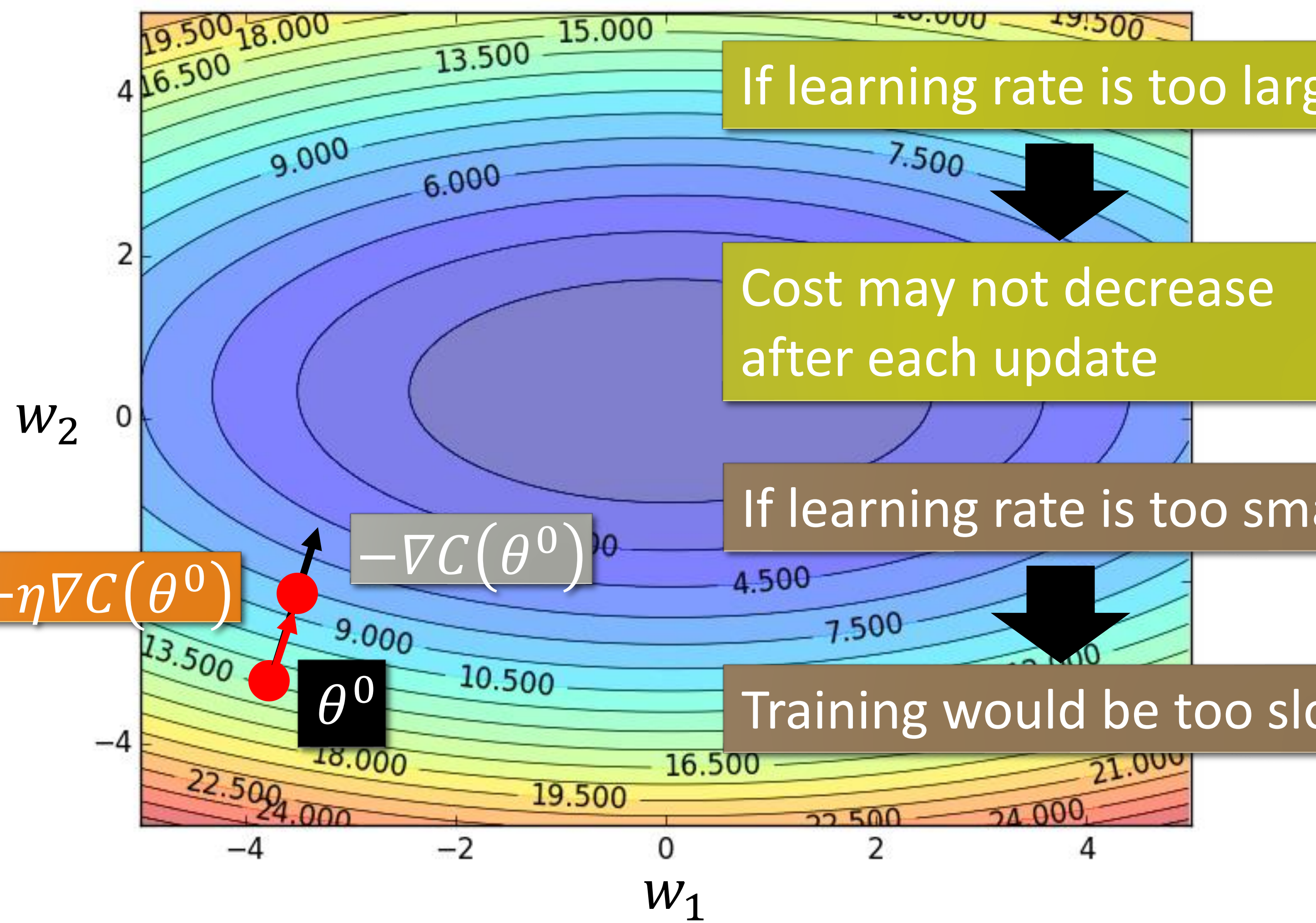


If learning rate is too large

Cost may not decrease after each update

Learning Rate

Can we give different parameters different learning rates?



If learning rate is too large

Cost may not decrease after each update

If learning rate is too small

Training would be too slow

Adagrad

Original Gradient Descent

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

Each parameter w are considered separately

$$w^{t+1} \leftarrow w^t - \boxed{\eta_w} \underline{g^t} \qquad \underline{g^t} = \frac{\partial C(\theta^t)}{\partial w}$$

Parameter dependent learning rate

$$\eta_w = \frac{\eta}{\sqrt{\boxed{\sum_{i=0}^{t} (g^i)^2}}}$$

constant

Summation of the square of the previous derivatives

Adagrad

$$\eta_w = \boxed{\frac{\eta}{\sqrt{\sum_{i=0}^{t}(g^i)^2}}}$$

w_1

g^0
0.1

w_2

g^0
20.0

Learning rate:

$$\frac{\eta}{\sqrt{0.1^2}} = \frac{\eta}{0.1}$$

$$\frac{\eta}{\sqrt{0.1^2 + 0.2^2}} = \frac{\eta}{0.22}$$

Learning rate:

$$\frac{\eta}{\sqrt{20^2}} = \frac{\eta}{20}$$

$$\frac{\eta}{\sqrt{20^2 + 10^2}} = \frac{\eta}{22}$$

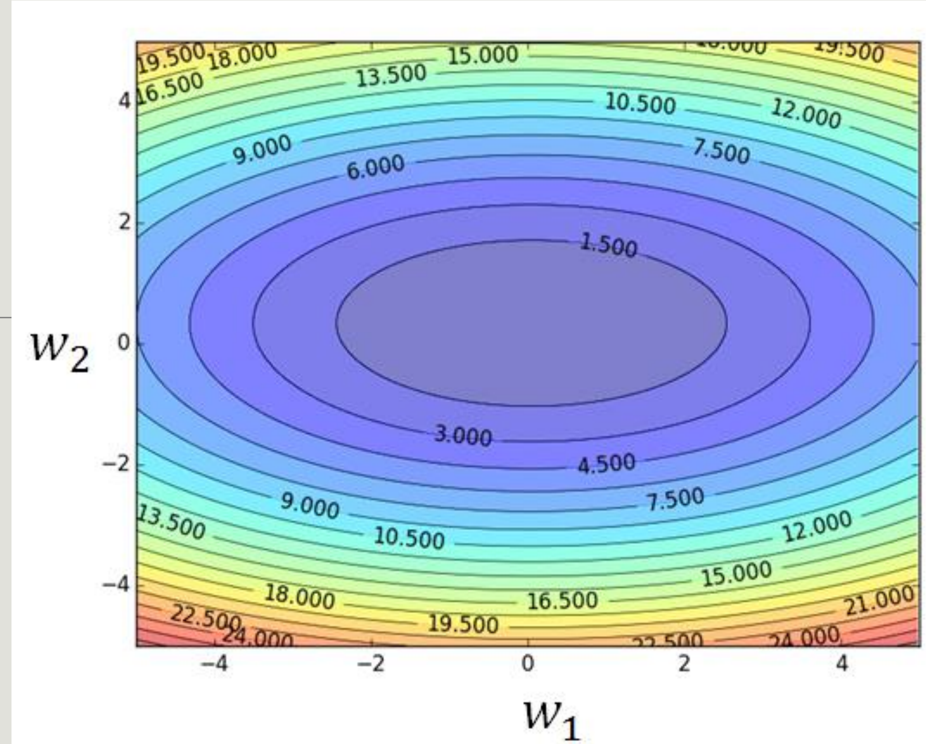
Observation: 1. Learning rate is smaller and smaller for all parameters

2. Smaller derivatives, larger learning rate, and vice versa

Why?

Larger derivatives

Smaller Learning Rate



Smaller Derivatives

Larger Learning Rate

2. Smaller derivatives, larger learning rate, and vice versa

Why?

Not the whole story ……

Adagrad [John Duchi, JMLR'11]

RMSprop

- https://www.youtube.com/watch?v=O3sxAc4hxZU

Adadelta [Matthew D. Zeiler, arXiv'12]

Adam [Diederik P. Kingma, ICLR'15]

AdaSecant [Caglar Gulcehre, arXiv'14]

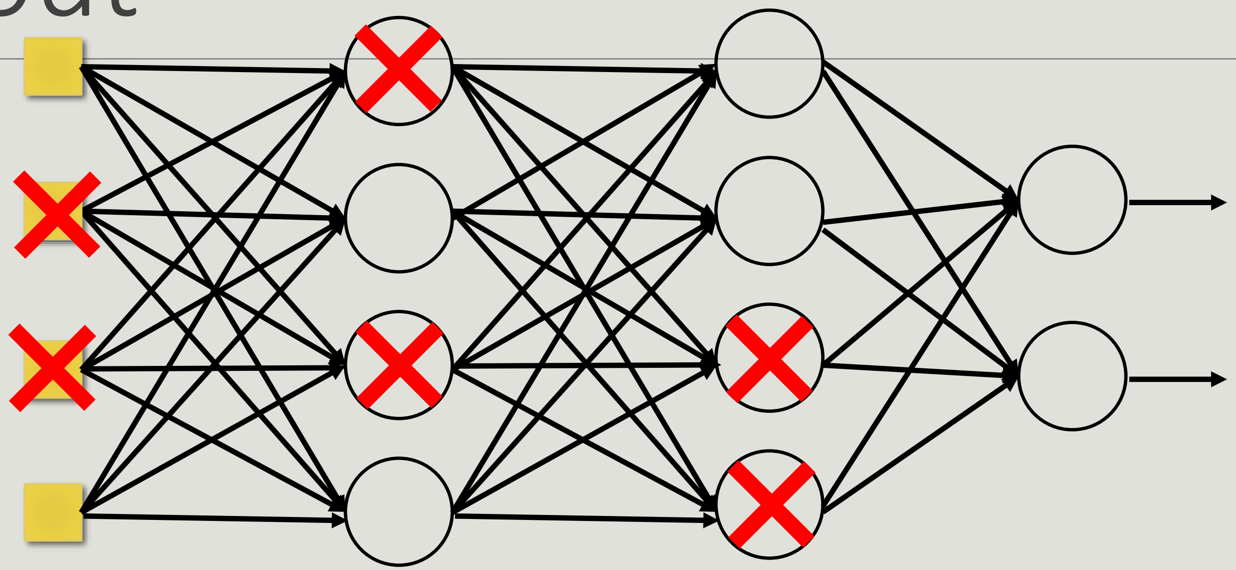
"No more pesky learning rates" [Tom Schaul, arXiv'12]

Pick a mini-batch

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

Dropout

Training:



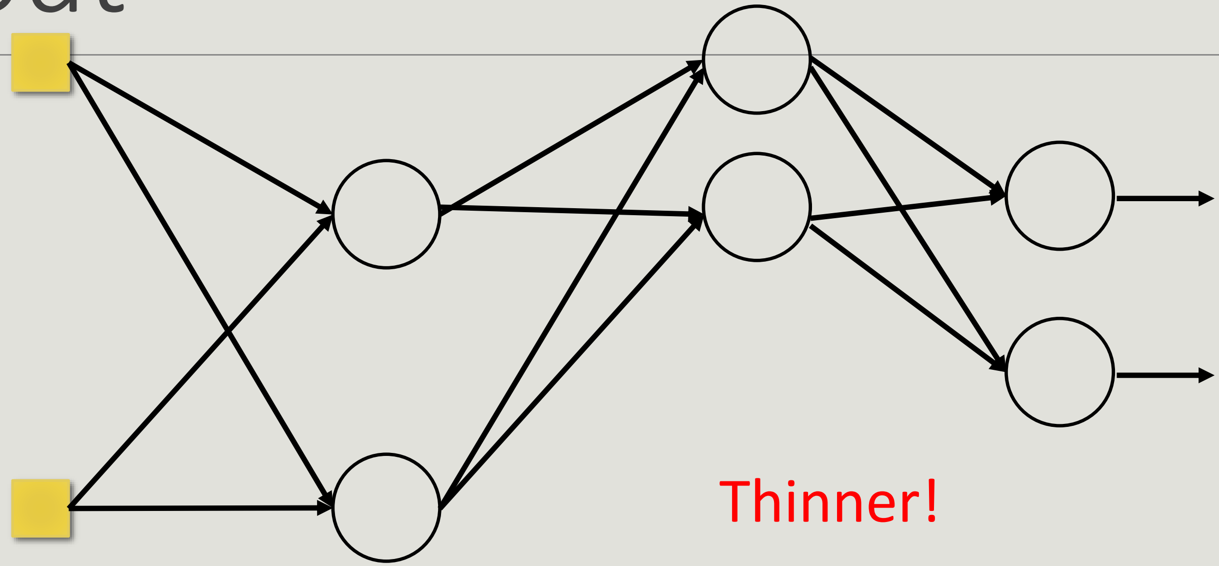
- **Each time before computing the gradients**
  - Each neuron has p% to dropout

Pick a mini-batch

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

Dropout

Training:



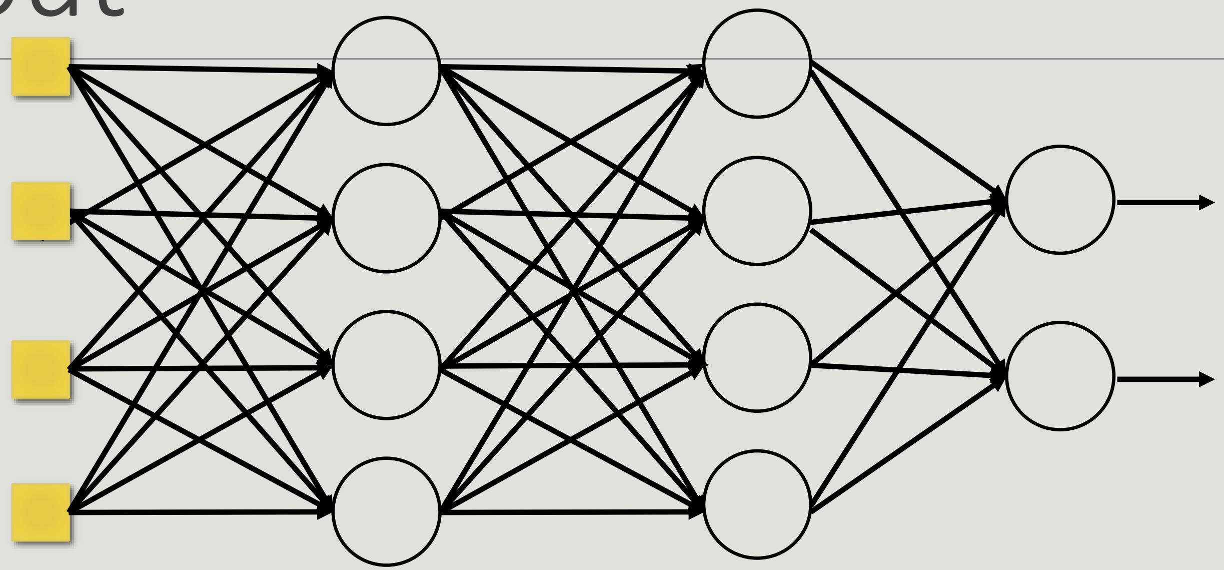
- **Each time before computing the gradients**
  - Each neuron has p% to dropout

    ⇒ **The structure of the network is changed.**
  - Using the new network for training

For each mini-batch, we resample the dropout neurons

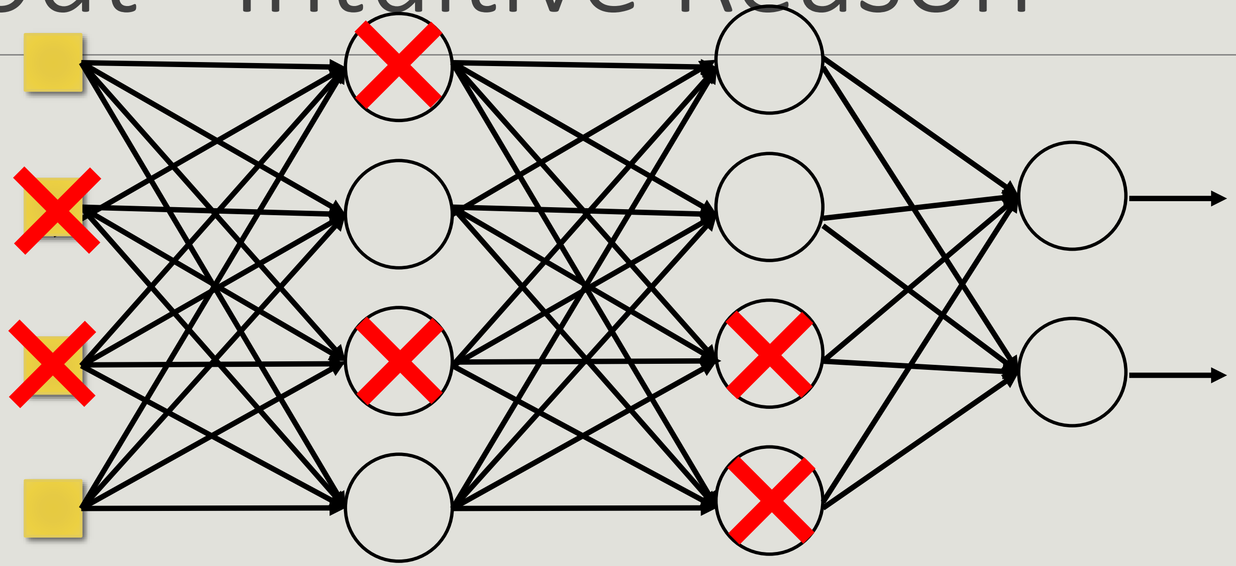
Dropout

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 a weight $w = 1$ by training, set $w = 0.5$ for testing.

Dropout - Intuitive Reason



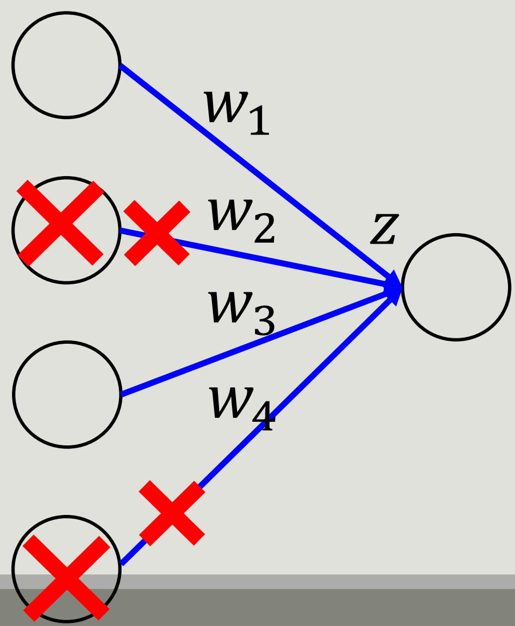
- When teams up, if everyone expect the partner will do the work, nothing will be done finally.
- However, if you know your partner will dropout, you will do better.
- When testing, no one dropout actually, so obtaining good results eventually.

Dropout - Intuitive Reason

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

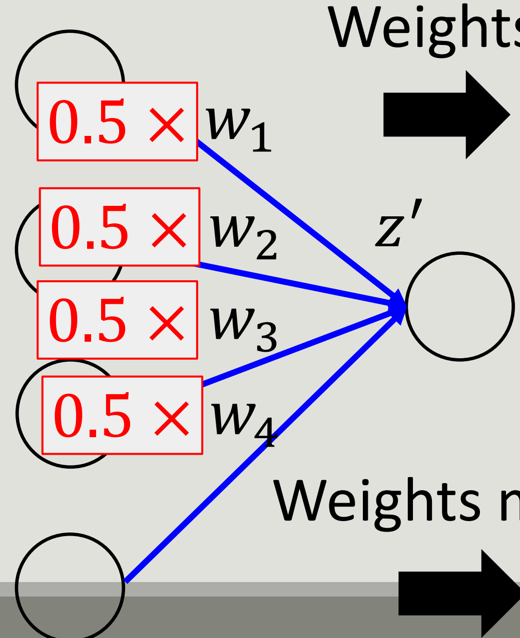
<u>Training of Dropout</u>

Assume dropout rate is 50%



<u>Testing of Dropout</u>

No dropout



Weights from training

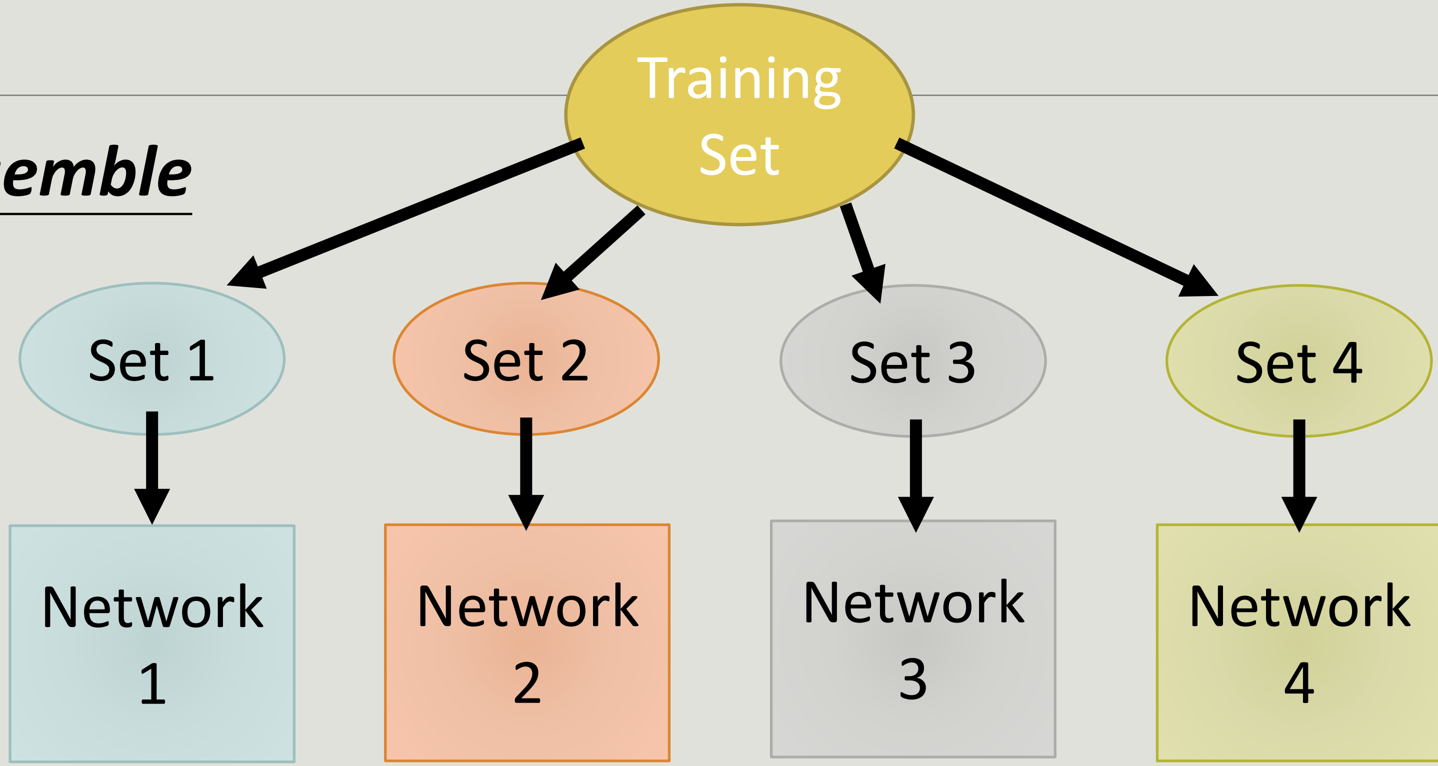
$\Rightarrow z' \approx 2z$

Weights multiply (1-p)%

$\Rightarrow z' \approx z$

Dropout is a kind of ensemble.

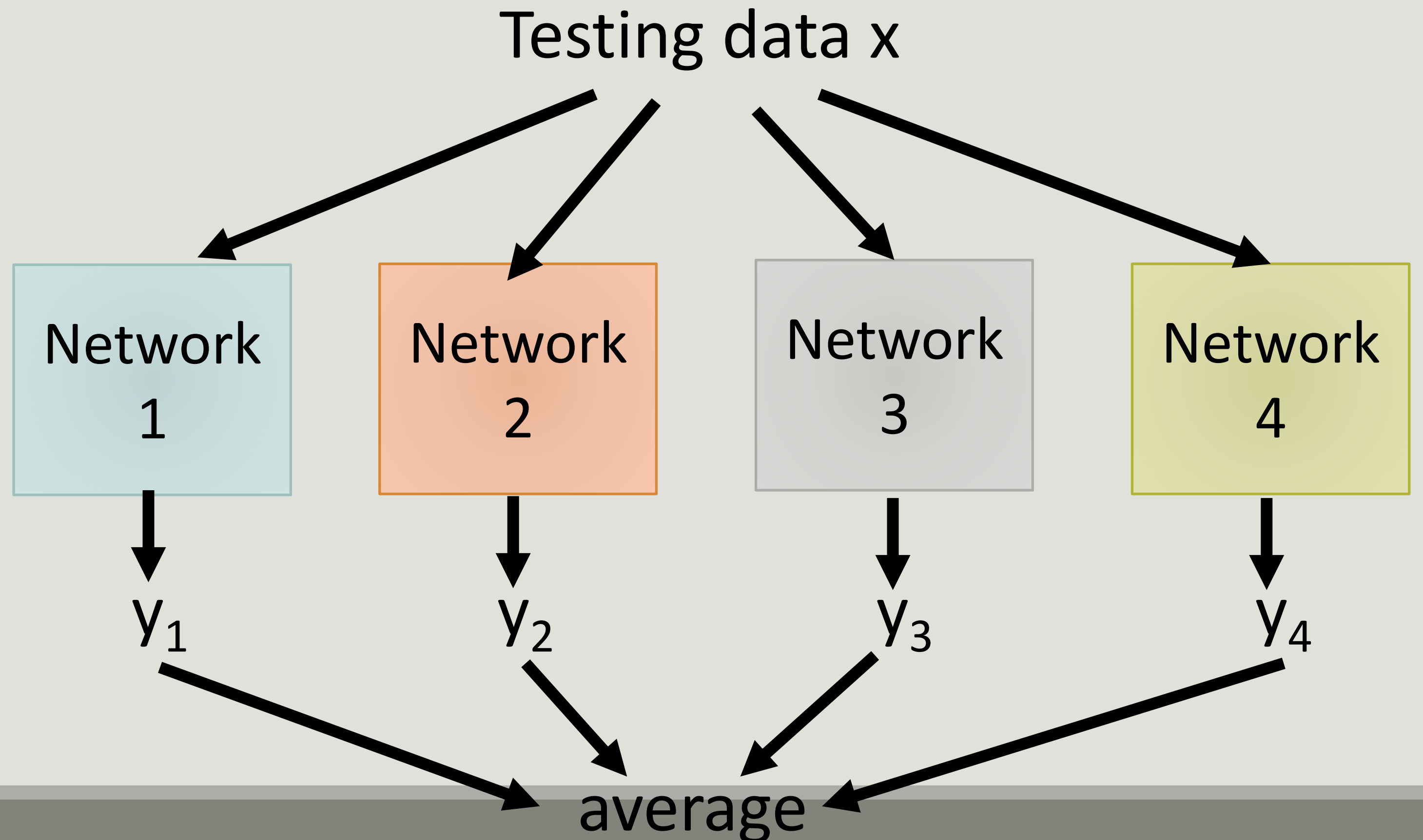
Ensemble



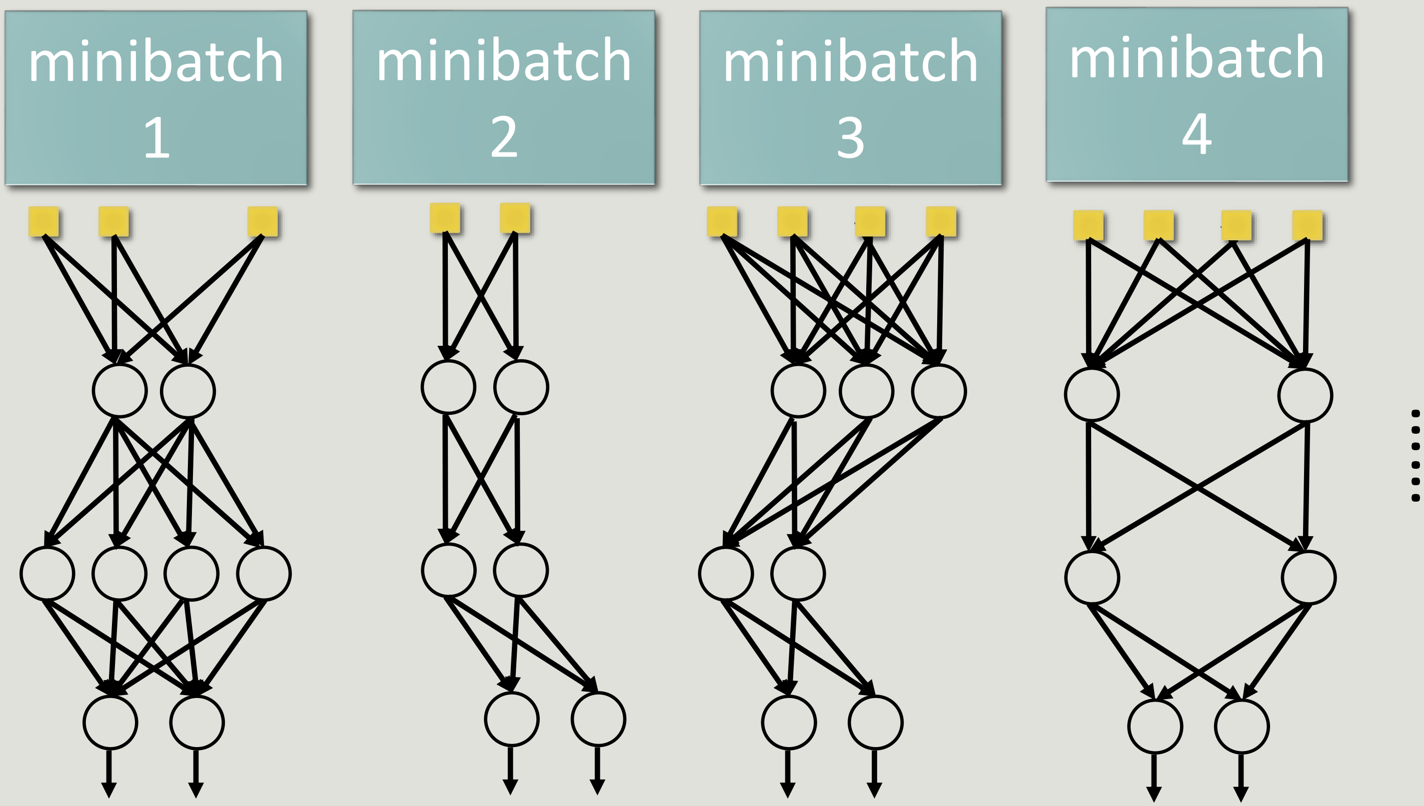
Train a bunch of networks with different structures

Dropout is a kind of ensemble.

Ensemble



Dropout is a kind of ensemble.



<u>Training of Dropout</u>

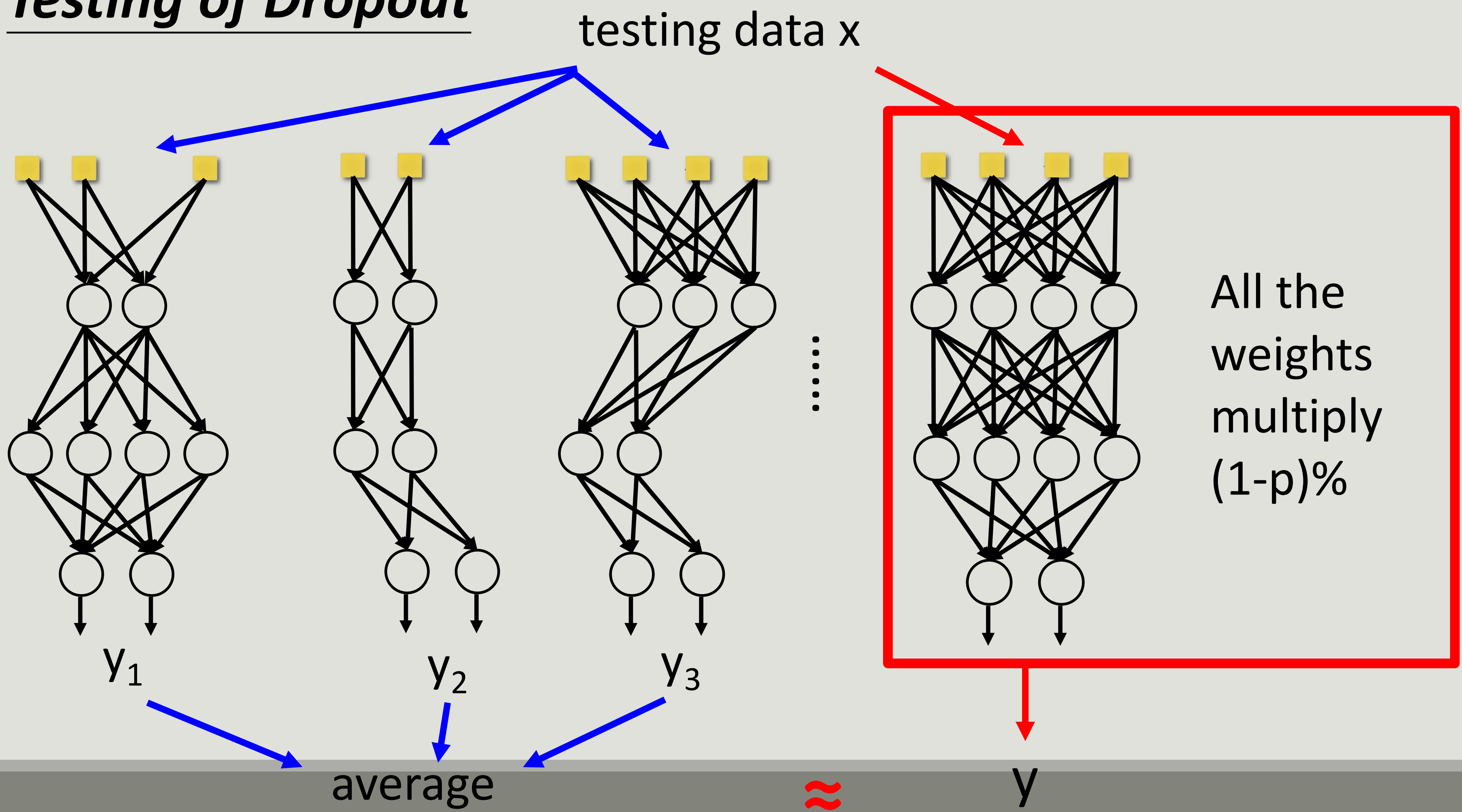
M neurons

2^M possible networks

- Using one mini-batch to train one network
- Some parameters in the network are shared

Dropout is a kind of ensemble.

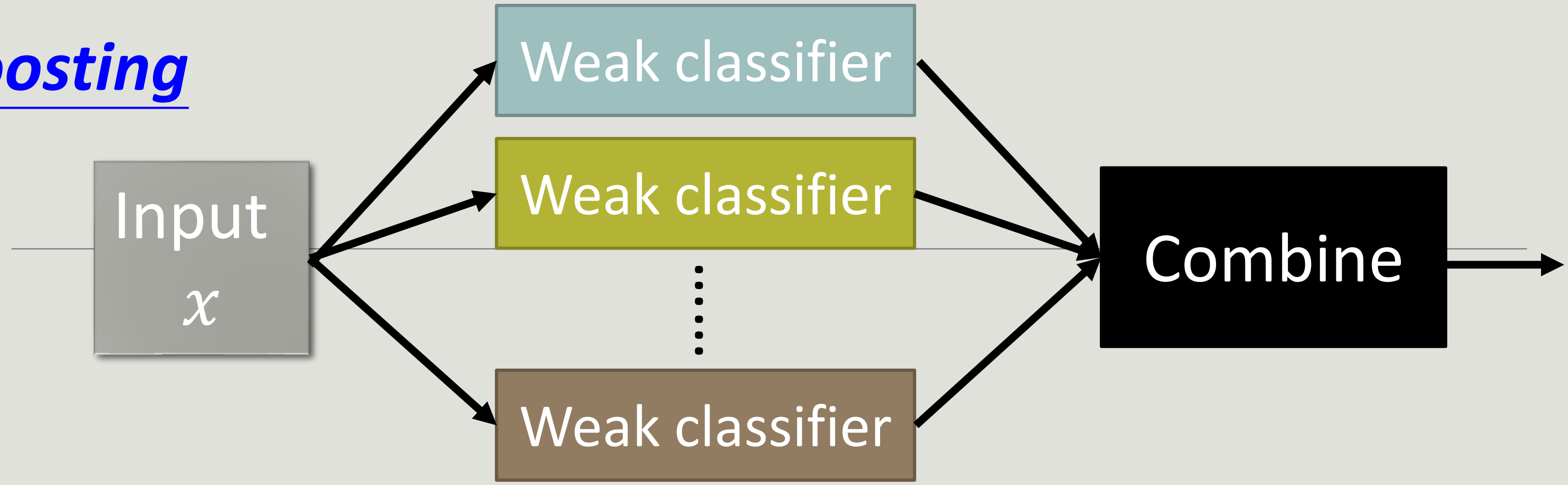
Testing of Dropout



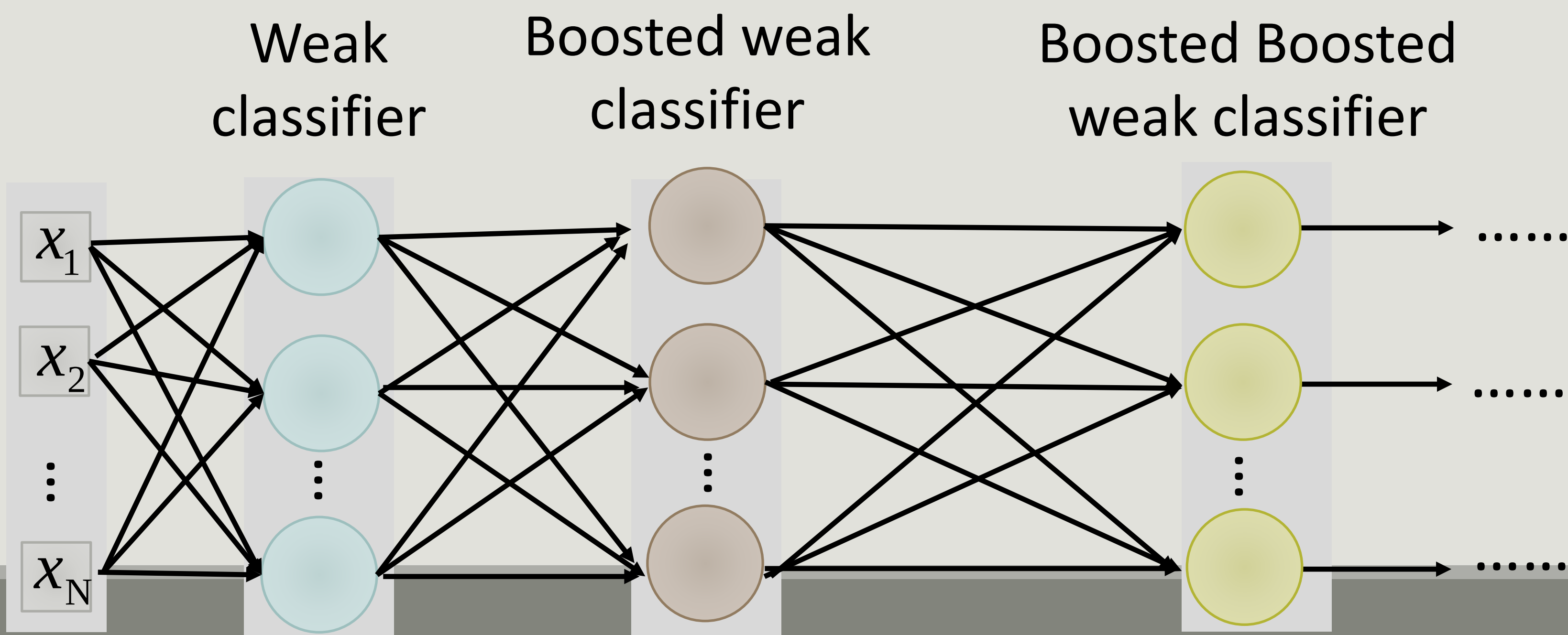
More about dropout

- More reference for dropout [Nitish Srivastava, JMLR'14] [Pierre Baldi, NIPS'13][Geoffrey E. Hinton, arXiv'12]
- Dropout works better with Maxout [Ian J. Goodfellow, ICML'13]
- Dropconnect [Li Wan, *ICML'13*]
  - Dropout delete neurons
  - Dropconnect deletes the connection between neurons
- Annealed dropout [S.J. Rennie, SLT'14]
  - Dropout rate decreases by epochs
- Standout [J. Ba, NISP'13]
  - Each neural has different dropout rate

Boosting

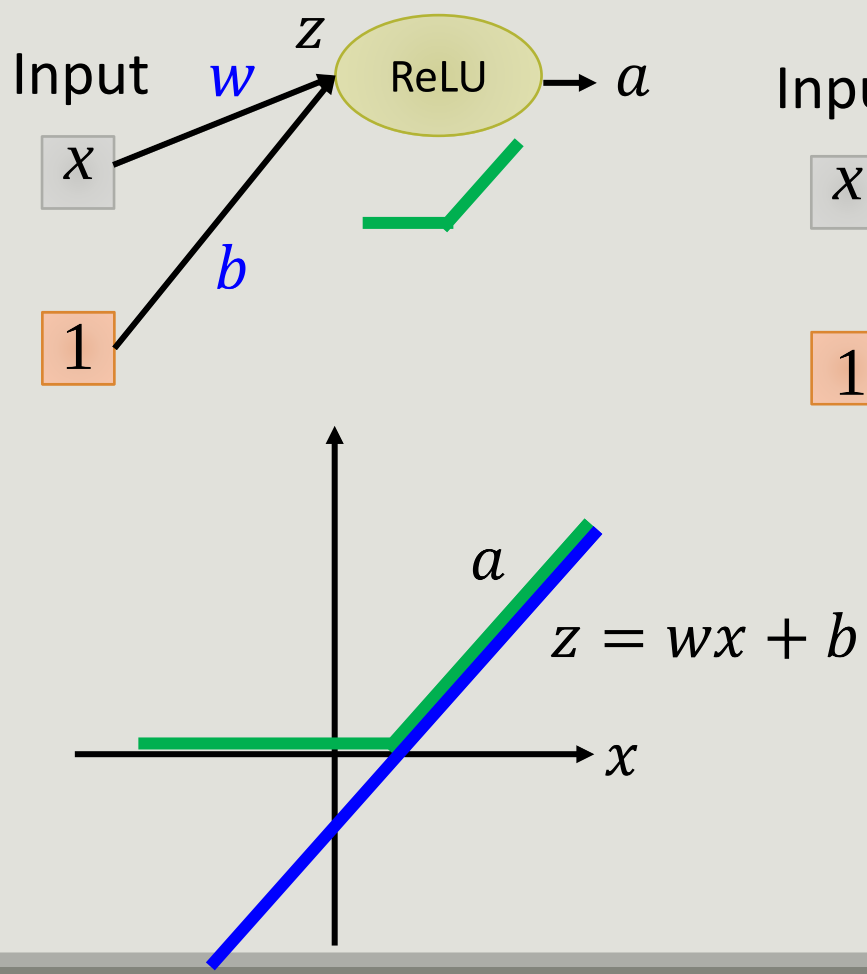


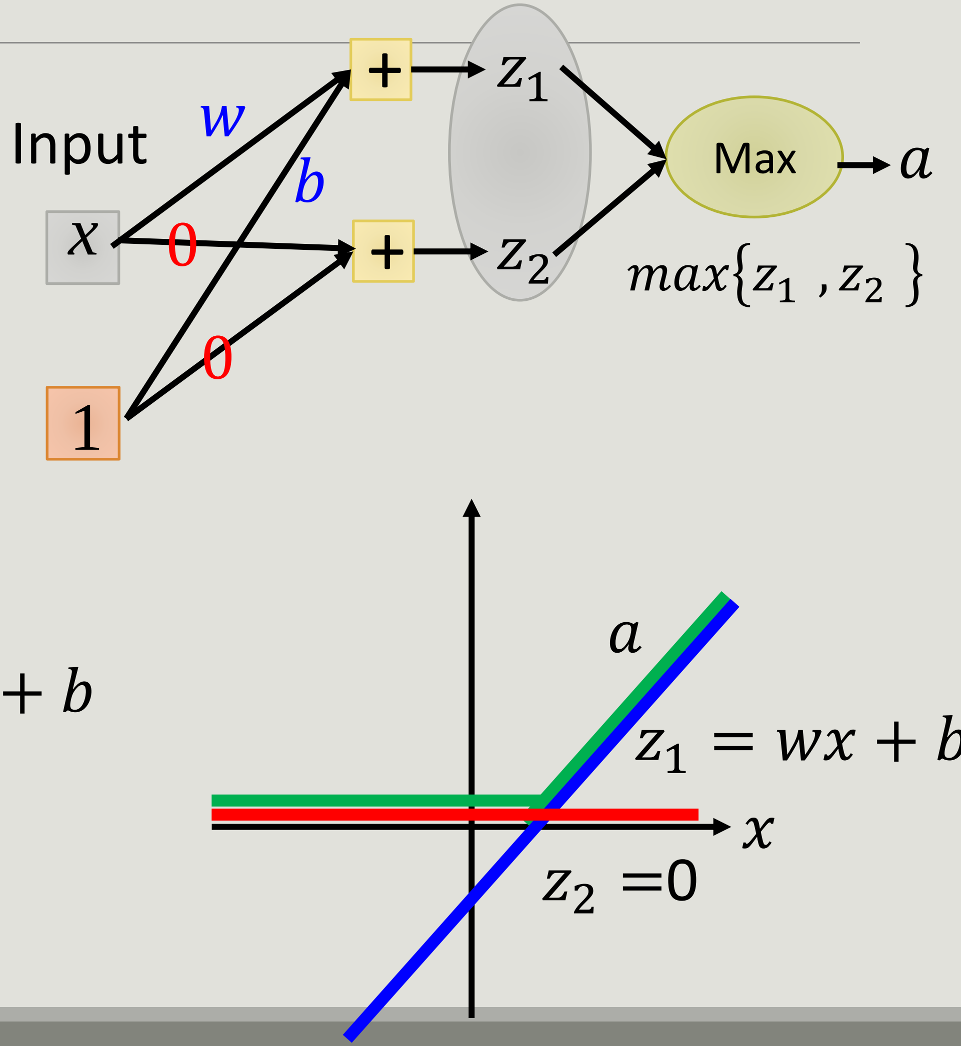
Deep Learning



Maxout

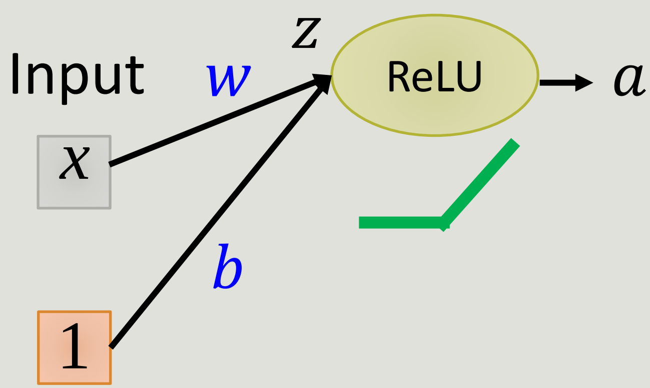
ReLU is a special cases of Maxout

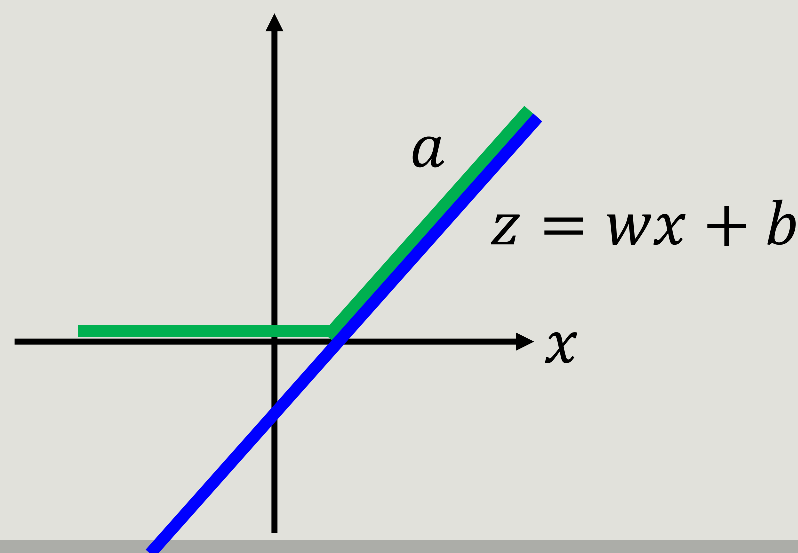


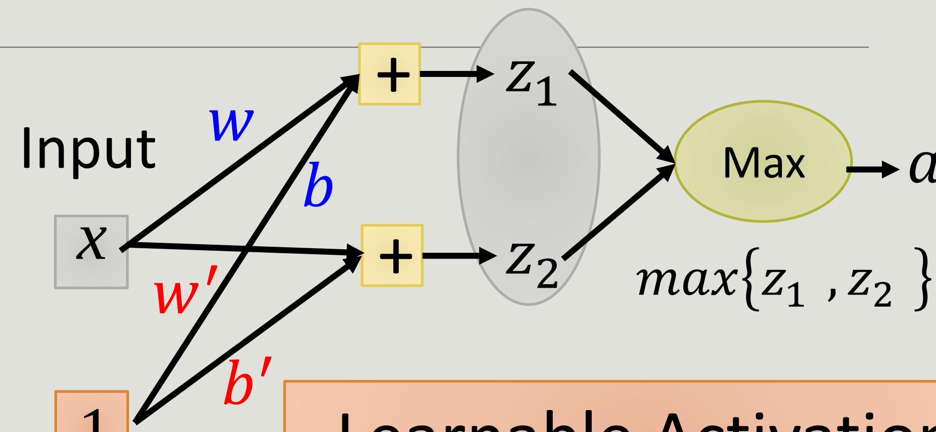


Maxout

ReLU is a special cases of Maxout







Learnable Activation Function