

## BIG DATA and AI for business

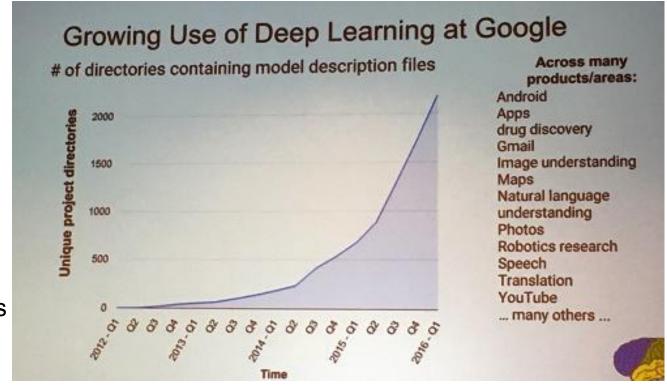
Deep Learning (1)

Decisions, Operations & Information Technologies Robert H. Smith School of Business Fall, 2020

# Deep learning attracts lots of attention.

I believe you have seen lots of exciting results

before.



Deep learning trends at Google. Source: SIGMOD/Jeff Dean

We mainly focus on the basic techniques.

# Introduction to Deep Learning

### Outline

Introduction of Deep Learning

"Hello World" for Deep Learning

Tips for Deep Learning

# Machine Learning ≈ Looking for a Function

Speech Recognition

$$f($$
 )= "How are you"

• Image Recognition

• Playing Go $^{f(}$ 

• Dialogue System 
$$f(\text{"Hi"})=\text{"Hello"}$$
  
(what the user said) (system response)

#### Image Recognition:

## Framewor



A set of function

## Model

$$f_1, f_2 \cdots$$

$$f_1($$

$$f_2($$



$$f_1$$



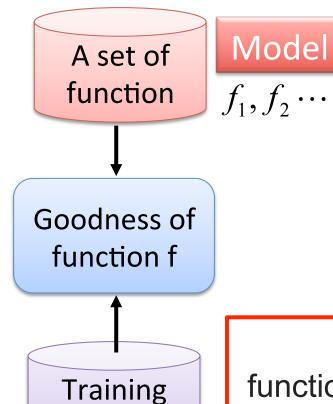
$$f_2($$



#### Image Recognition:

## Framewor





Data

$$f_1($$
  $)=$  "cat"  $f_2($   $)=$  "money"  $f_1($   $)=$  "dog"  $f_2($   $)=$  "snake"

#### Supervised Learning

function input:







function

Ulithlit.

"monkey"

"cat

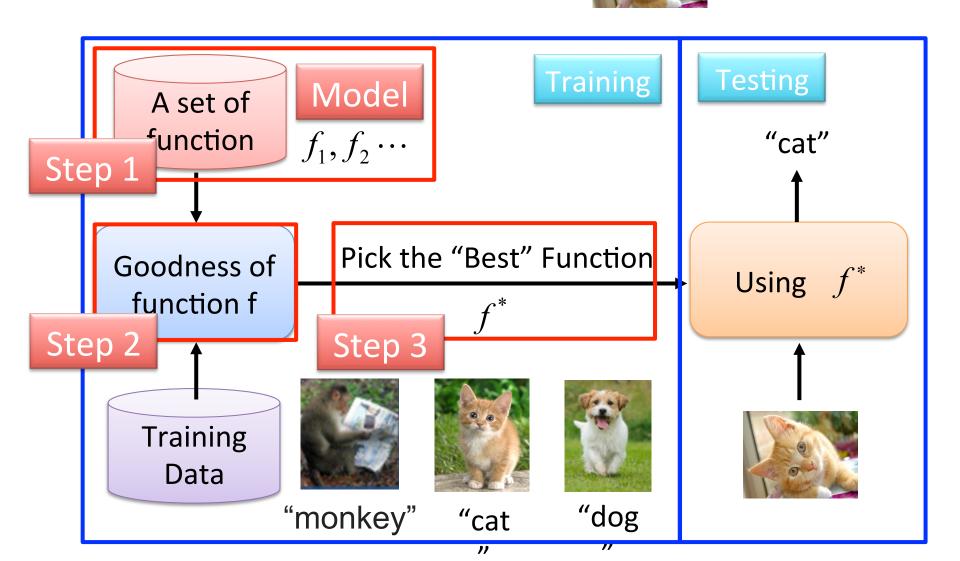
"dog

"

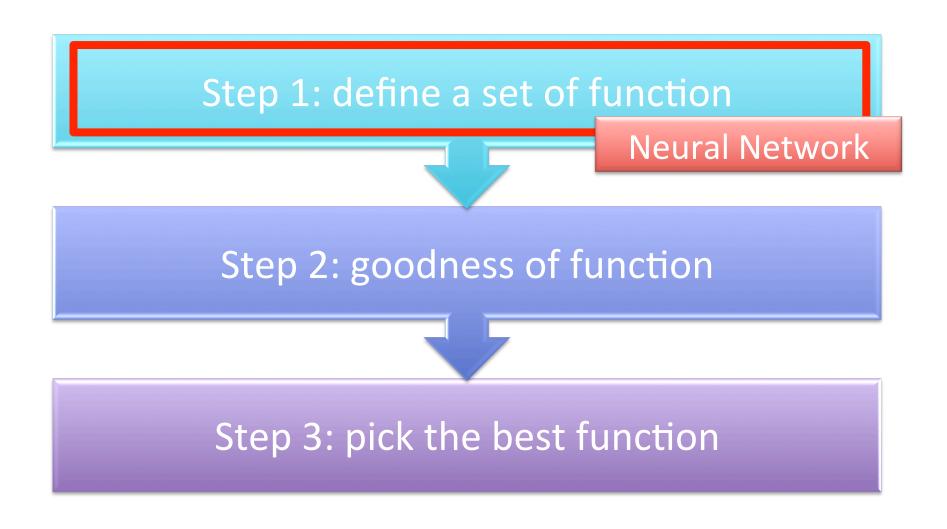
#### Image Recognition:

### Framework

$$f($$
  $)=$  "cat"



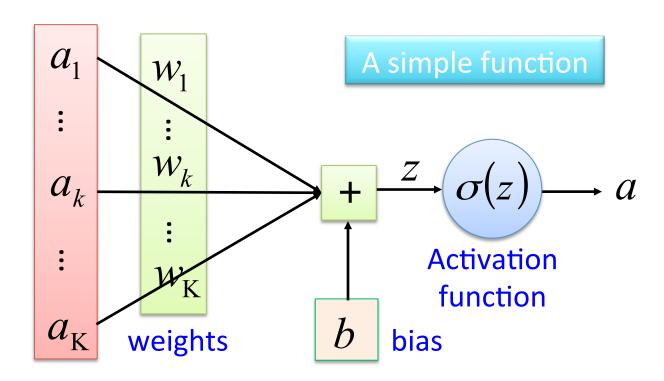
## Three Steps for Deep Learning



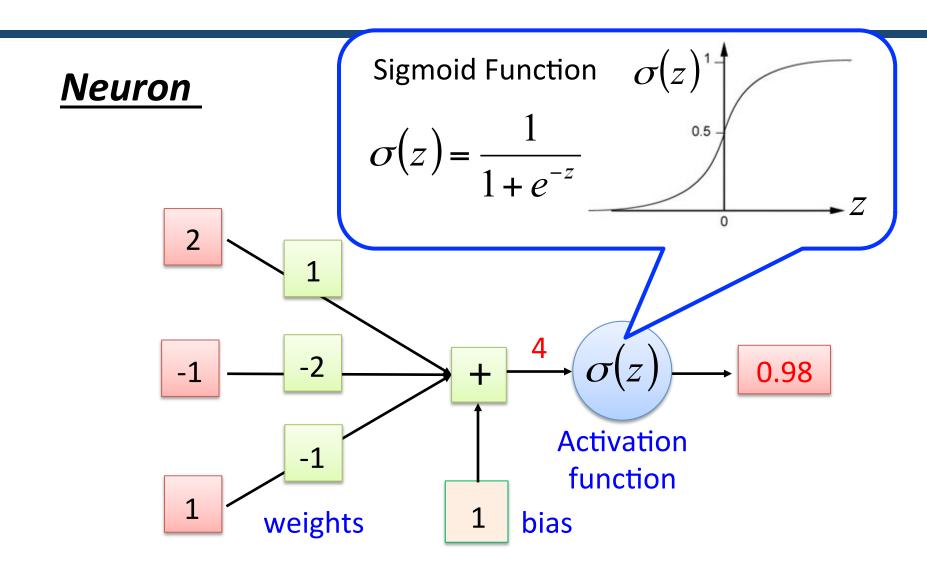
## **Neural Network**

#### Neuron

$$z = a_1 w_1 + \dots + a_k w_k + \dots + a_K w_K + b$$

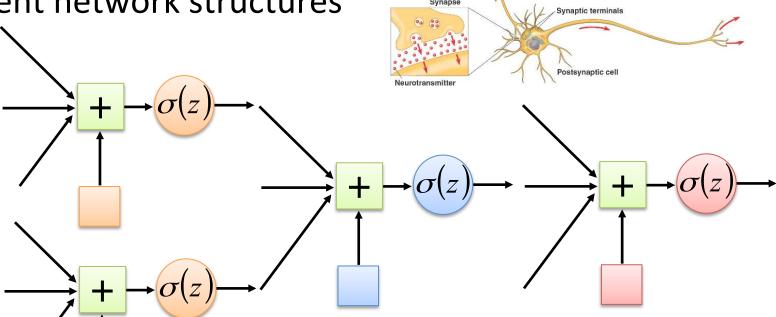


## **Neural Network**



## **Neural Network**

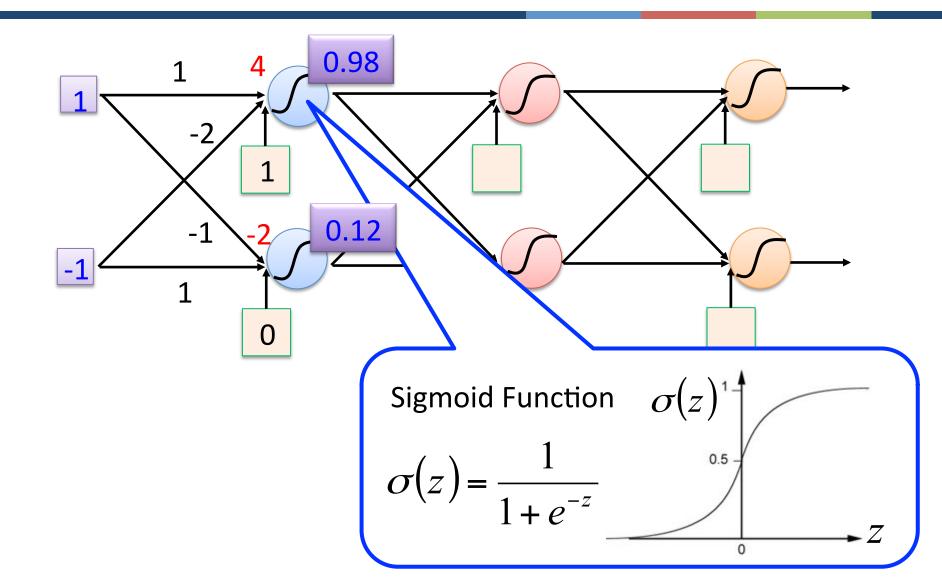
Different connections lead to different network structures

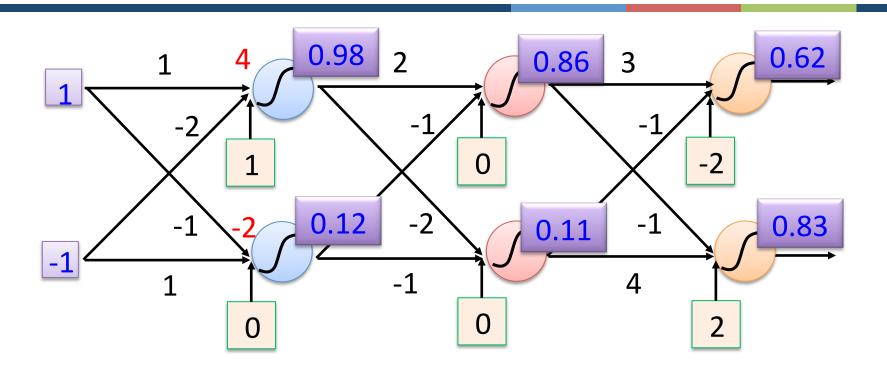


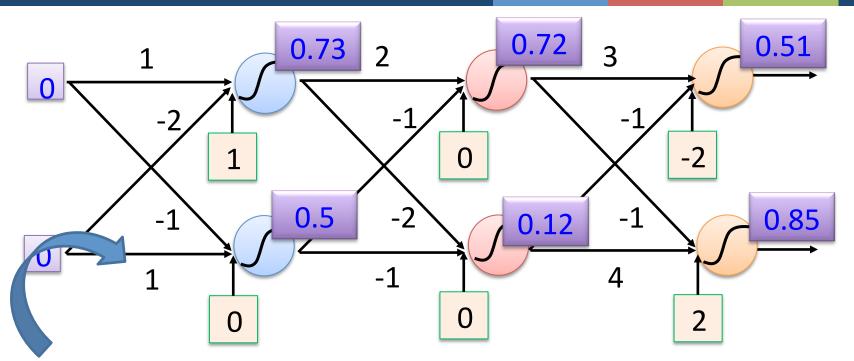
The neurons have different values of weights and biases.

Presynaptic

Weights and biases are network parameters  $\theta$ 







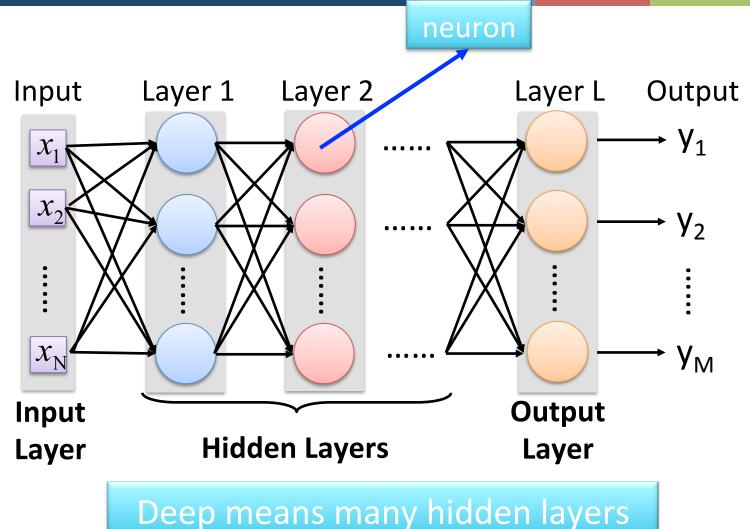
This is a function.

$$f([\blacksquare 1@-1]) = [\blacksquare 0.62@0.88] \blacksquare 0.00] = [\blacksquare 0.51@0.88]$$

Input vector, output vector

Given parameters  $\theta$ , define a function

Given network structure, define *a function set* 



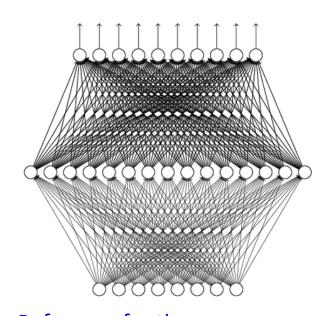
## Why Deep? Universality Theorem

Any continuous function f

$$f: \mathbb{R}^N \to \mathbb{R}^M$$

Can be realized by a network with one hidden layer

(given **enough** hidden neurons)



Reference for the reason:
<a href="http://">http://</a>
<a href="neuralnetworksanddeeplearning.com/chap4.html">neuralnetworksanddeeplearning.com/chap4.html</a>

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

#### Why Deep? Analogy

#### Logic circuits

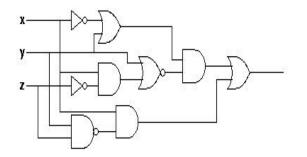
- Logic circuits consists of gates
- A two layers of logic gates can represent any Boolean function.
- Using multiple layers of logic gates to build some functions are much simpler

#### Neural network

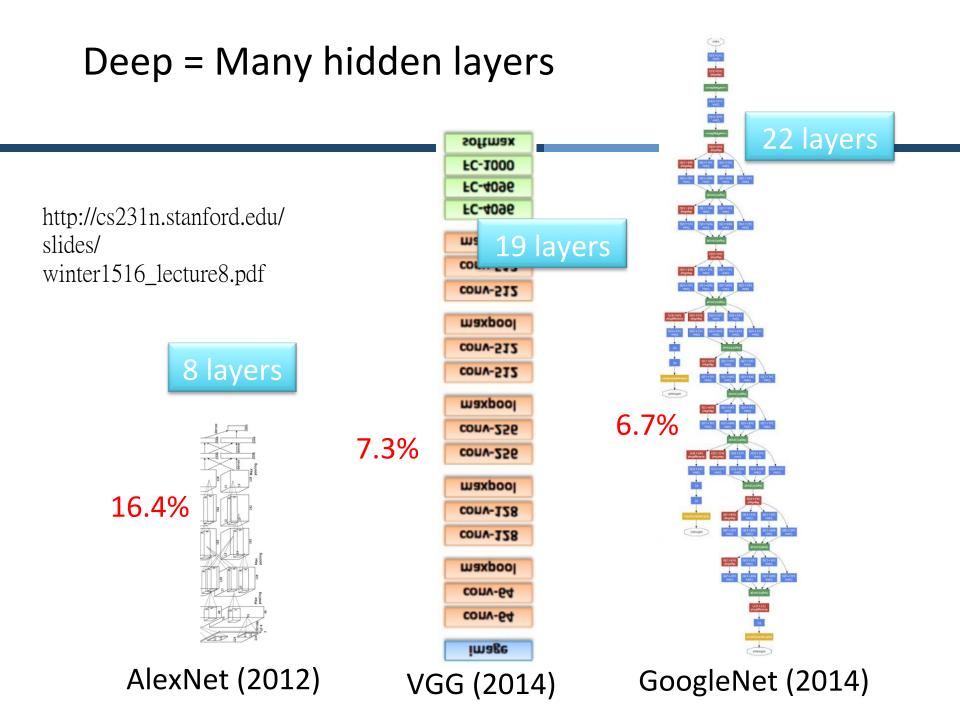
- Neural network consists of neurons
- A hidden layer network can represent any continuous function.
- Using multiple layers of neurons to represent some functions are much simpler



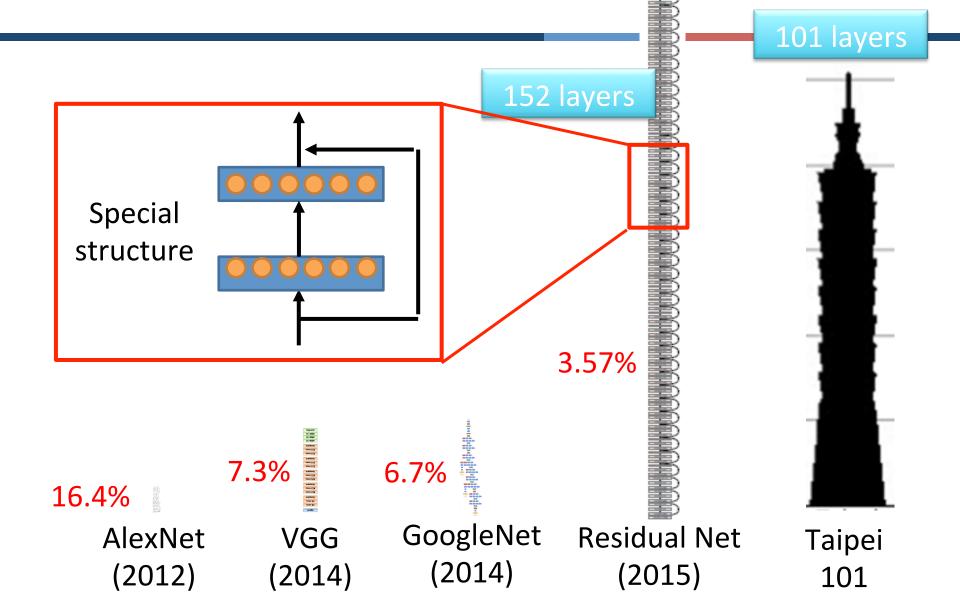




More reason: https://www.youtube.com/watch? v=XsC9byQkUH8&list=PLJV\_el3uVTsPy9oCRY3 0oBPNLCo89yu49&index=13



### Deep = Many hidden layers



## **Output Layer**

Softmax layer as the output layer

#### **Ordinary Layer**

$$z_1 \longrightarrow \sigma \longrightarrow y_1 = \sigma(z_1)$$

$$z_2 \longrightarrow \sigma \longrightarrow y_2 = \sigma(z_2)$$

$$z_3 \longrightarrow \sigma \longrightarrow y_3 = \sigma(z_3)$$

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

May not be easy to interpret

## **Output Layer**

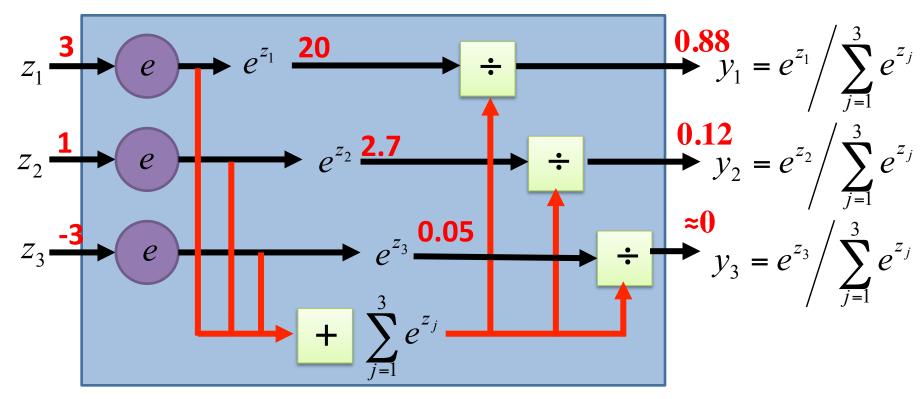
Softmax layer as the output layer

#### **Probability**:

■  $1 > y_i > 0$ 

$$\blacksquare \sum_i y_i = 1$$

#### Softmax Layer

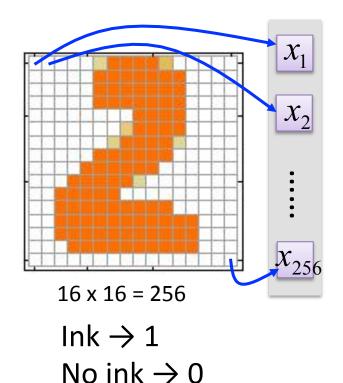


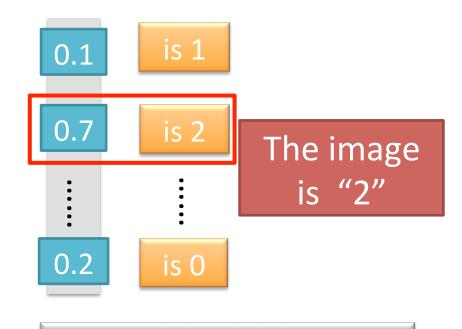
## **Example Application**



#### Input

## Output

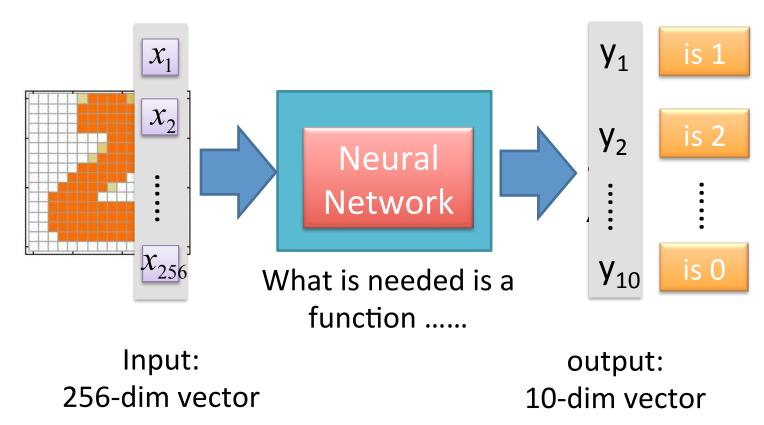




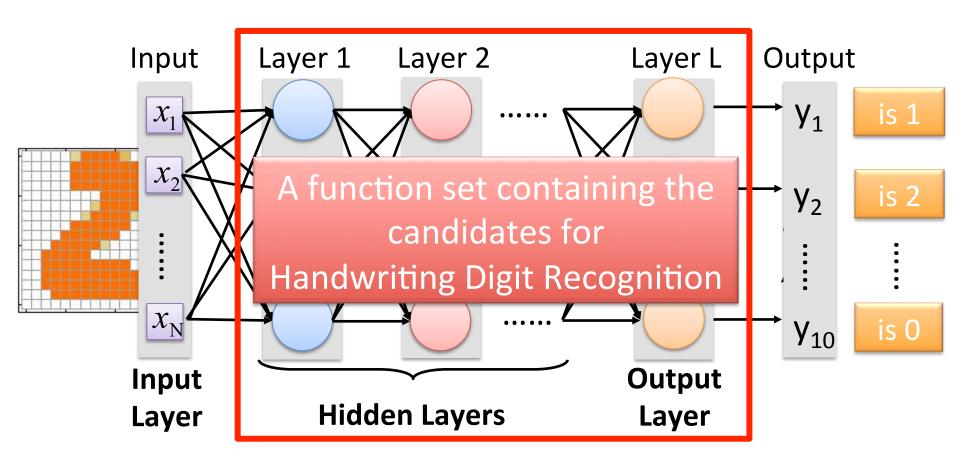
Each dimension represents the confidence of a digit.

## **Example Application**

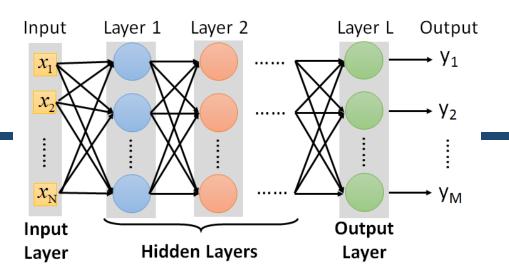
Handwriting Digit Recognition



## **Example Application**



You need to decide the network structure to let a good function in your function set.



 Q: How many layers? How many neurons for each layer?

Trial and Error

Intuition

Q: Can we design the network structure?

Convolutional Neural Network (CNN) in the next lecture

+

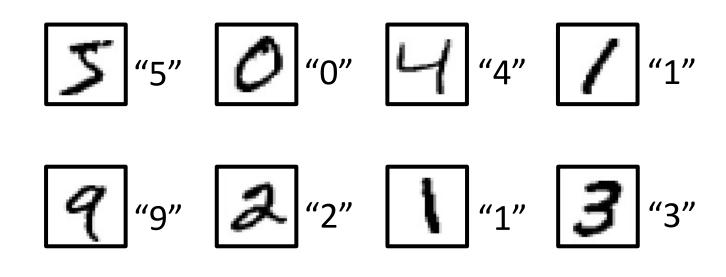
- Q: Can the structure be automatically determined?
  - Yes, but not widely studied yet.

## Three Steps for Deep Learning

Step 1: define a set of function Step 2: goodness of function Step 3: pick the best function

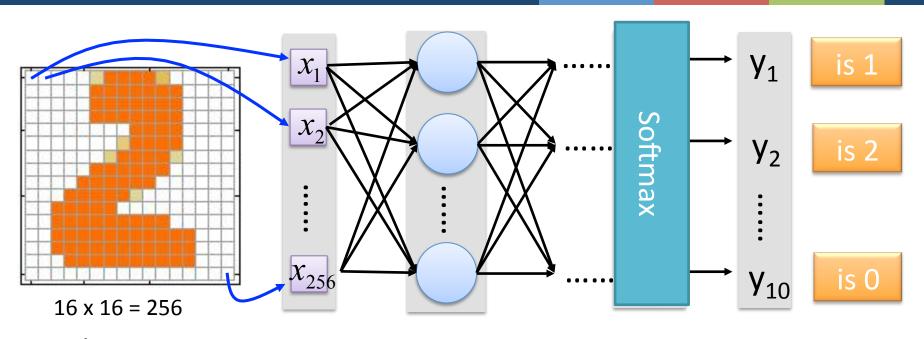
## **Training Data**

Preparing training data: images and their labels



The learning target is defined on the training data.

## **Learning Target**



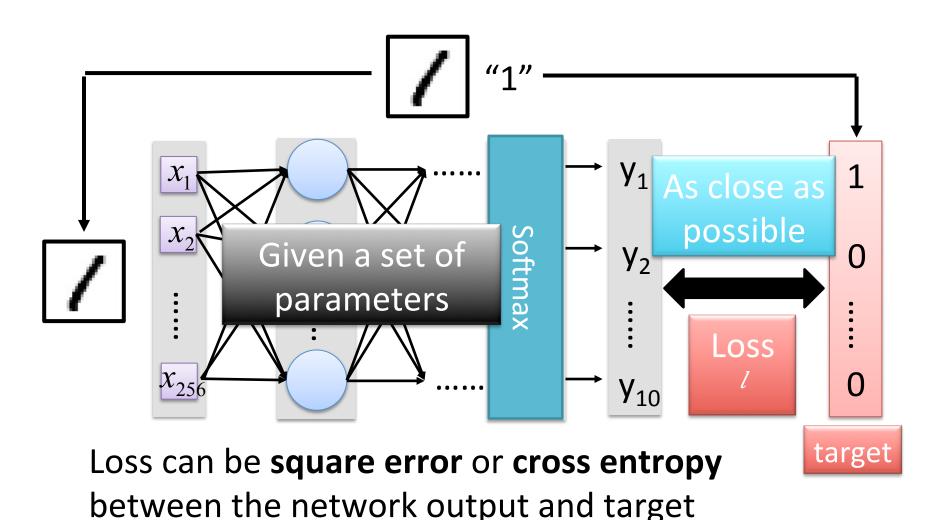
Ink  $\rightarrow$  1 No ink  $\rightarrow$  0

The learning target is ......

Input:  $y_1$  has the maximum value

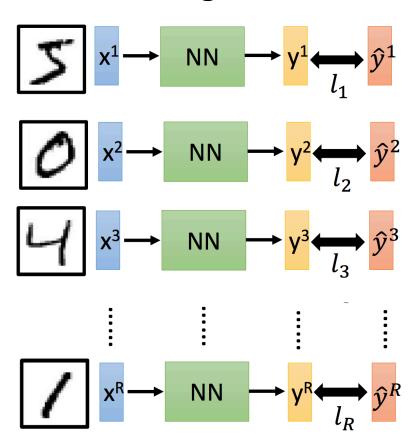
Input:  $|\mathbf{A}| \Rightarrow y_2$  has the maximum value

## A good function should make the loss of all examples as small as possible.



## **Total Loss**

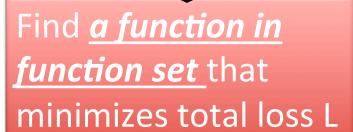
For all training data ...



Total Loss:

$$L = \sum_{r=1}^{R} l_r$$

As small as possible



Find <u>the network</u>

parameters en that

minimize total loss L

## Three Steps for Deep Learning

Step 1: define a set of function Step 2: goodness of function Step 3: pick the best function

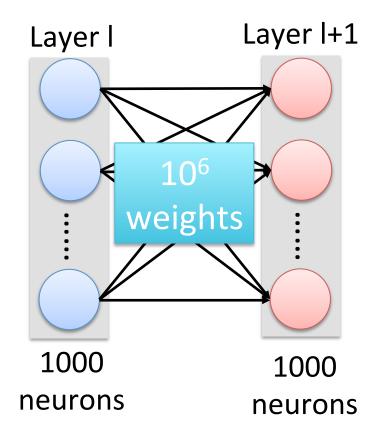
## How to pick the best function

#### Find network parameters of that minimize total loss L

#### Enumerate all possible values



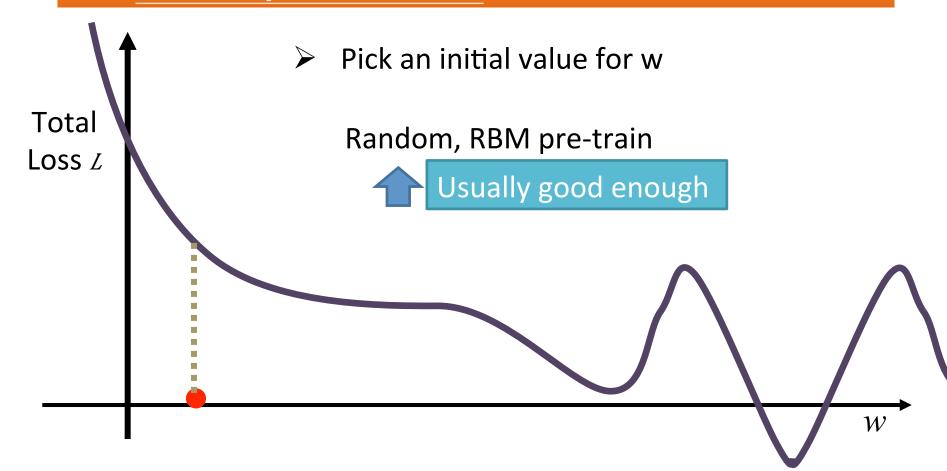
E.g. speech recognition: 8 layers and 1000 neurons each layer



### **Gradient Descent**

Network parameters  $\theta = \{w_1, w_2, ..., b_1, b_2, ...\}$ 

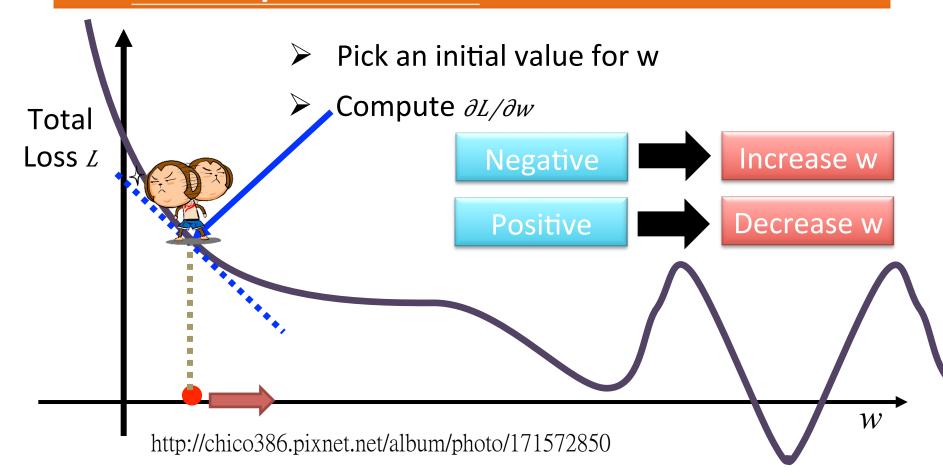
#### Find *network parameters* $\theta^*$ that minimize total loss L



## **Gradient Descent**

Network parameters  $\theta = \{w_1, w_2, ..., b_1, b_2, ...\}$ 

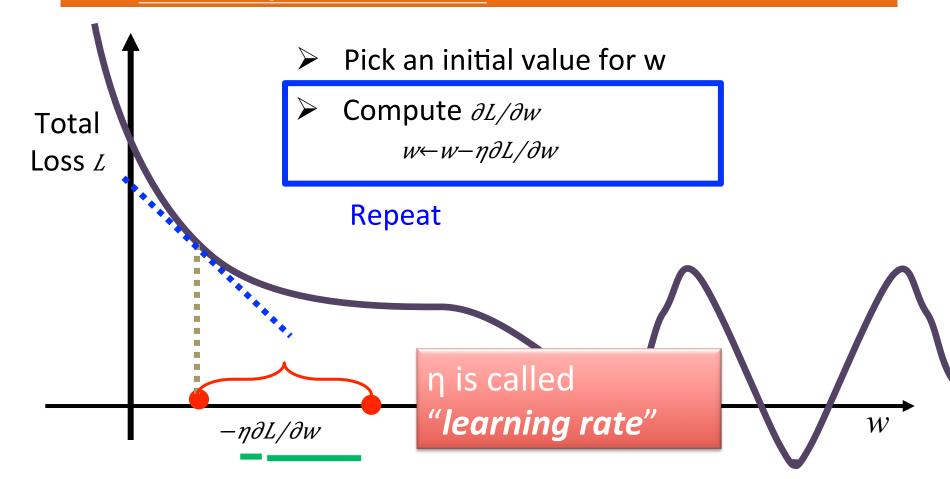
#### Find *network parameters* $\theta^*$ that minimize total loss L



## **Gradient Descent**

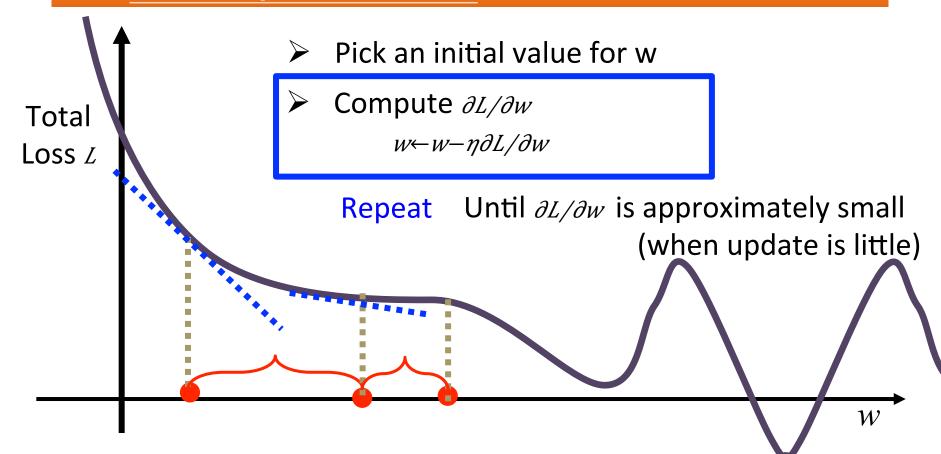
Network parameters  $\theta = \{w_1, w_2, ..., b_1, b_2, ...\}$ 

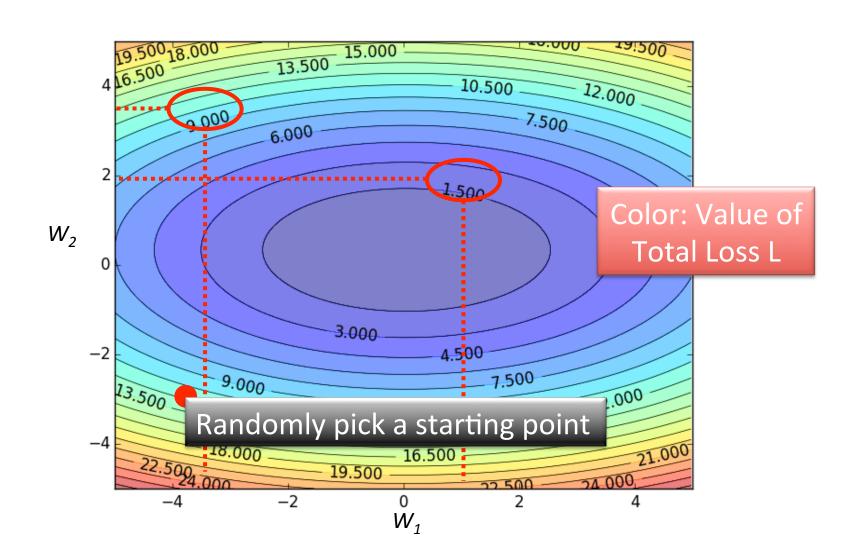
#### Find *network parameters* $\theta^*$ that minimize total loss L



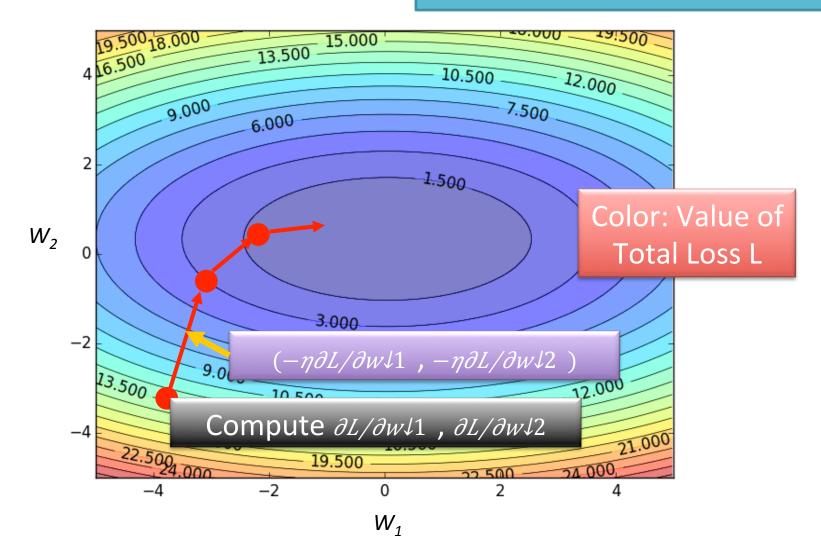
Network parameters  $\theta = \{w_1, w_2, ..., b_1, b_2, ...\}$ 

#### Find *network parameters* $\theta^*$ that minimize total loss L

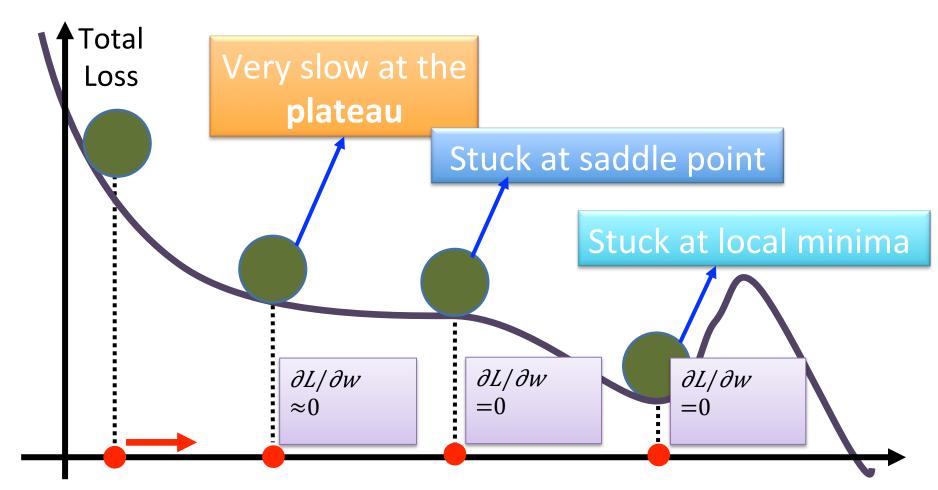




# Hopfully, we would reach a minima .....



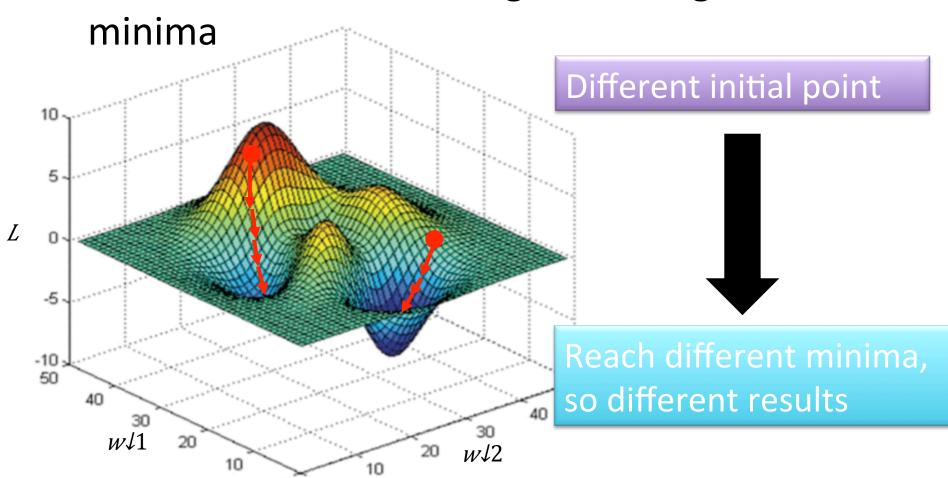
## **Local Minima**



The value of a network parameter w

## **Local Minima**

Gradient descent never guarantee global

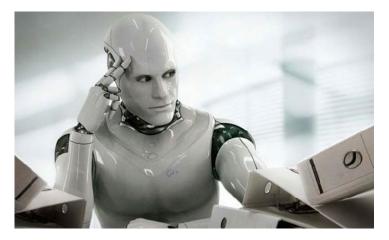


This is the "learning" of machines in deep learning ......



Even alpha go using this approach.

People image ......



Actually .....



I hope you are not too disappointed :p

# Backpropagation

• Backpropagation: an efficient way to compute  $\partial L/\partial w$  in neural network

















# Three Steps for Deep Learning



Deep Learning is so simple .....

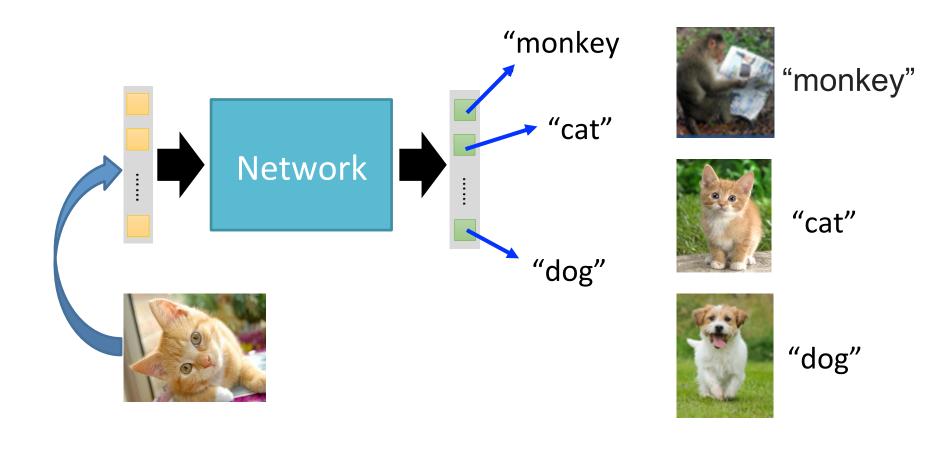
Now If you want to find a function

If you have lots of function input/output (?) as training data

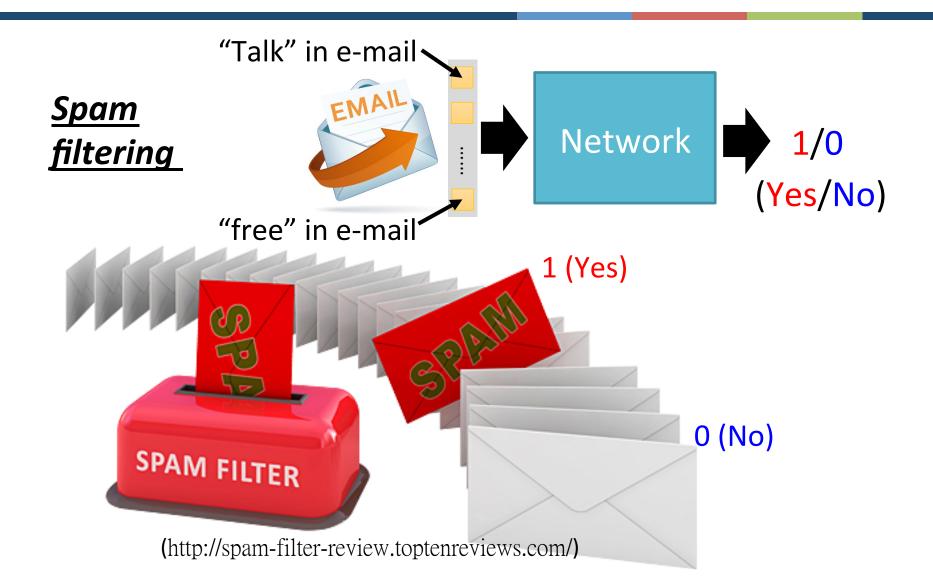


# For example, you can do ......

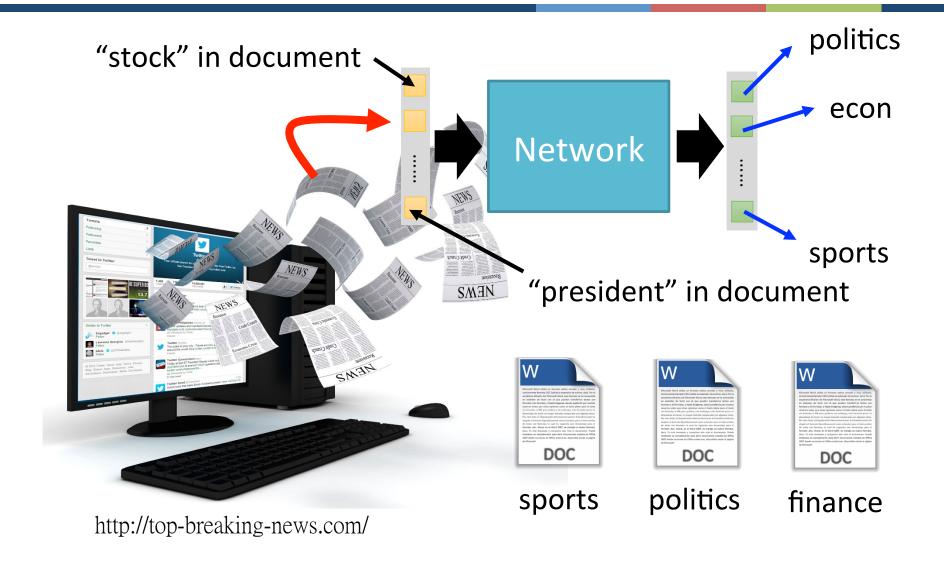
Image Recognition



# For example, you can do ......



# For example, you can do ......

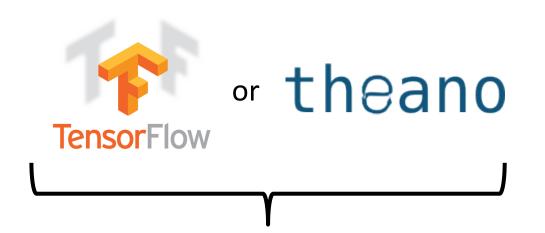


## Outline

Introduction of Deep Learning

"Hello World" for Deep Learning

Tips for Deep Learning



Very flexible

Need some effort to learn

Interface of TensorFlow or Theano



Easy to learn and use (still have some flexibility)

You can modify it if you can write TensorFlow or Theano

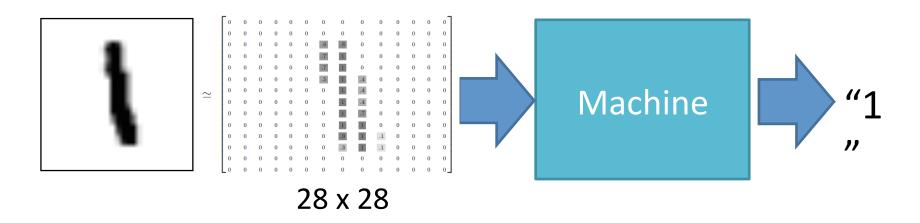
- François Chollet is the author of Keras.
- Keras means horn in Greek
- Documentation: <a href="http://keras.io/">http://keras.io/</a>
- Example: https://github.com/fchollet/keras/ tree/master/examples

Tutorial: <a href="https://pytorch.org/tutorials">https://pytorch.org/tutorials</a>



## **Example Application**

Handwriting Digit Recognition



MNIST Data: http://yann.lecun.com/exdb/mnist/ "Hello world" for deep learning

Keras provides data sets loading function: http://keras.io/datasets/

Step 1: define a set of function



Step 2: goodness of function



Step 3: pick the best function

```
28x28
   500
   500
             Softmax
          y_1
```

```
model = Sequential()
```

```
model.add( Dense( output_dim=500 ) )
model.add( Activation('sigmoid') )
```

```
model.add( Dense(output_dim=10 ) )
model.add( Activation('softmax') )
```

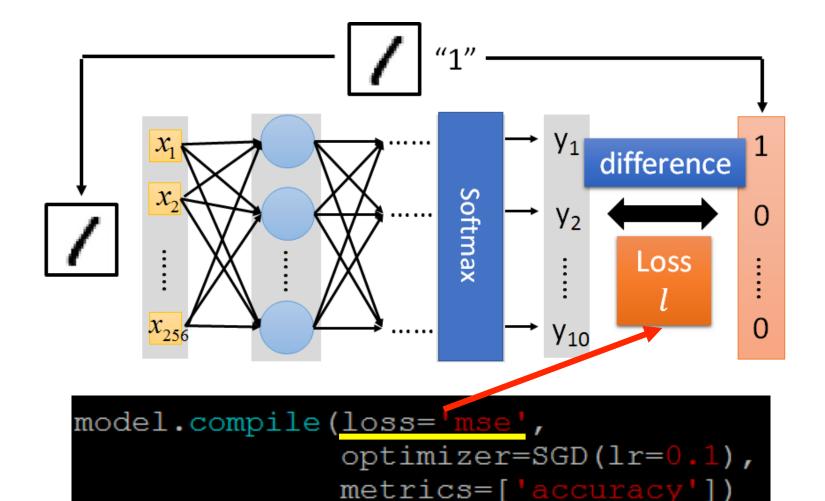
Step 1: define a set of function



Step 2: goodness of function



Step 3: pick the best function



Step 1: define a set of function



Step 2: goodness of function



Step 3: pick the best function

Step 3.1: Configuration

$$w \leftarrow w - \eta \partial L / \partial w$$

0.1

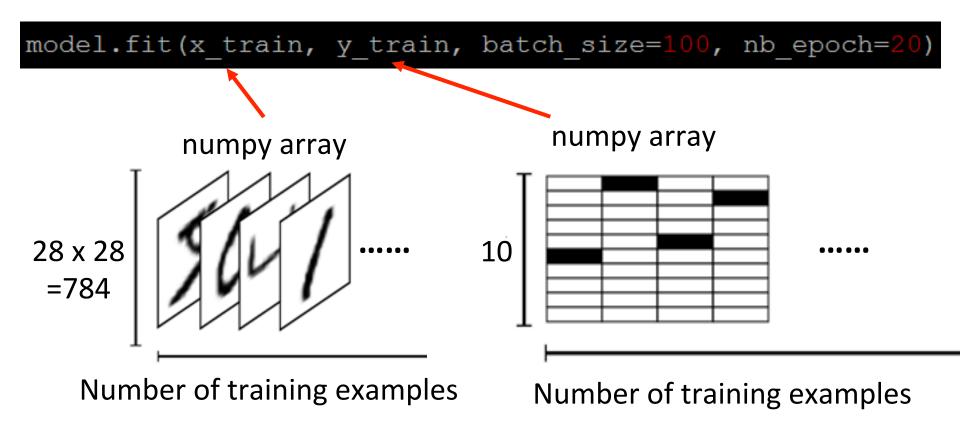
Step 3.2: Find the optimal network parameters

```
Training data (Images)

Labels (digits)
```

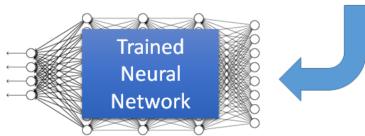
# Keras Step 1: define a set of function Step 2: goodness of function Step 3: pick the best function

Step 3.2: Find the optimal network parameters



https://www.tensorflow.org/versions/r0.8/tutorials/mnist/beginners/index.html





#### Save and load models

http://keras.io/getting-started/faq/#how-can-i-save-a-keras-model

How to use the neural network (testing):

```
case 1: print('Total loss on Testing Set:', score[0])
print('Accuracy of Testing Set:', score[1])
```

```
case 2: result = model.predict(x_test)
```

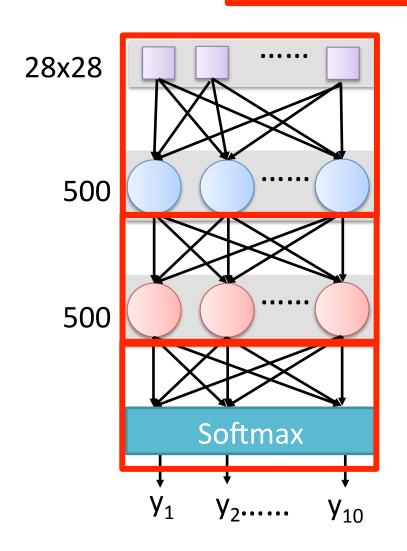
Step 1: define a set of function



Step 2: goodness of function



Step 3: pick the best function



```
import torch.nn as nn
import torch.nn.functional as F
class MyNetwork(nn.Module):
  def init (self):
     super(MyNetwork, self). init ()
    self.fc1 = nn.Linear(28 * 28, 500)
     self.fc2 = nn.Linear(500, 500)
    self.fc3 = nn.Linear(500, 10)
  def forward(self, x):
    x = F.sigmoid(self.fc1(x))
    x = F.sigmoid(self.fc2(x))
    x = self.fc3(x)
    return F.log softmax(x)
```

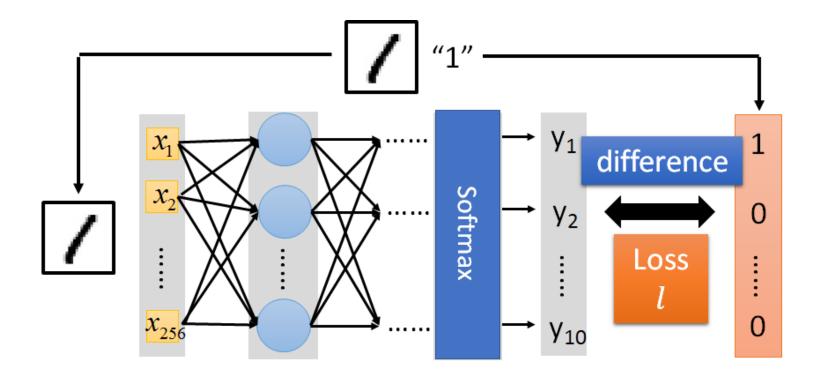
Step 1: define a set of function



Step 2: goodness of function



Step 3: pick the best function



```
net = MyNetwork()
optimizer = torch.optim.SGD(net.parameters(), lr=0.1, momentum=0.9)
criterion = nn.MSELoss()
```

Step 1: define a set of function



Step 2: goodness of function



Step 3: pick the best function

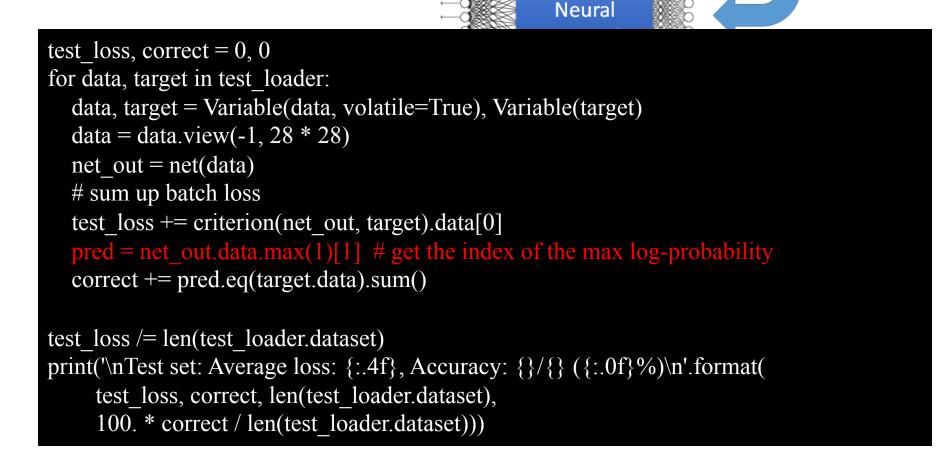
#### Step 3.1: Training

```
for epoch in range(epochs):
  for batch idx, (data, target) in enumerate(train loader):
     data, target = Variable(data), Variable(target)
     # resize data from (batch size, 1, 28, 28) to (batch size, 28*28)
     data = data.view(-1, 28*28)
    optimizer.zero grad()
    net out = net(data)
     loss = criterion(net out, target)
     loss.backward()
    optimizer.step()
     if batch idx \% \log \text{ interval} == 0:
       print('Train Epoch: {} [{}/{} ({:.0f}%)]\tLoss: {:.6f}'.format(
             epoch, batch idx * len(data), len(train loader.dataset),
                 100. * batch idx / len(train loader), loss.data[0]))
```



Trained

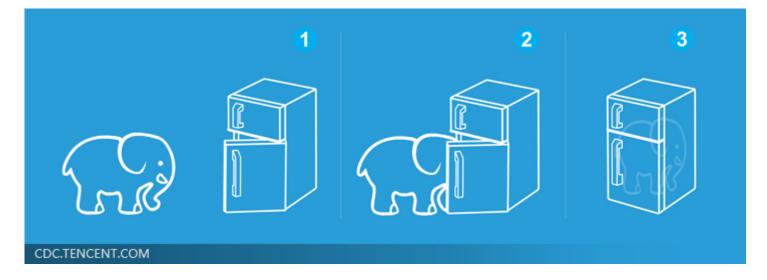
Step 3.2: Performance report



# Three Steps for Deep Learning



Deep Learning is so simple ......



## Outline

Introduction of Deep Learning

"Hello World" for Deep Learning

Tips for Deep Learning

## Recipe of Deep Learning





Step 1: define a set of function

Step 2: goodness of function

Step 3: pick the best function

Overfitting!

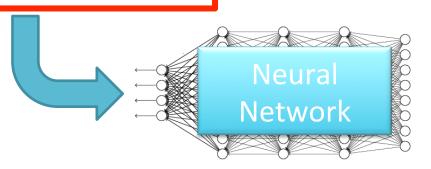
NO

Good Results on Testing Data?

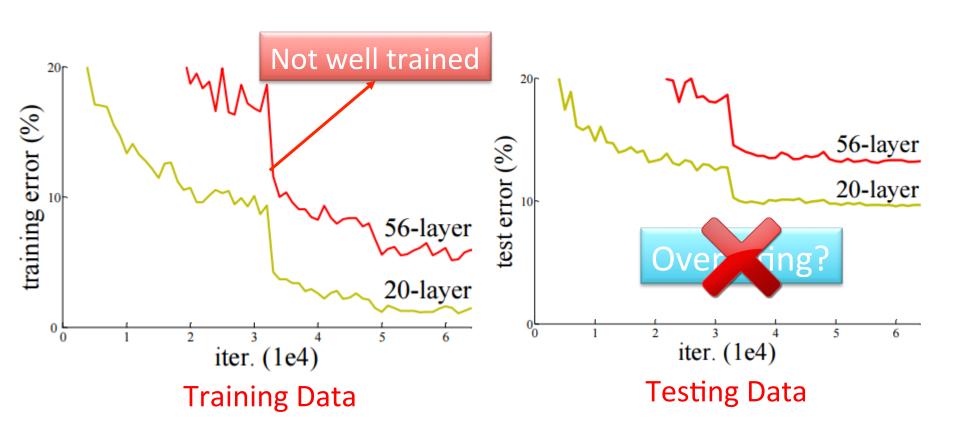


NO

Good Results on Training Data?



# Do not always blame Overfitting



Deep Residual Learning for Image Recognition http://arxiv.org/abs/1512.03385

## Recipe of Deep Learning





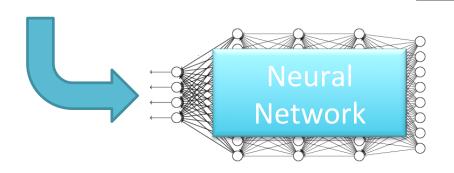
Different approaches for different problems.

e.g. dropout for good results on testing data

Good Results on Testing Data?



Good Results on Training Data?



## Recipe of Deep Learning



YES

Choosing proper loss

Mini-batch

New activation function

Adaptive Learning Rate

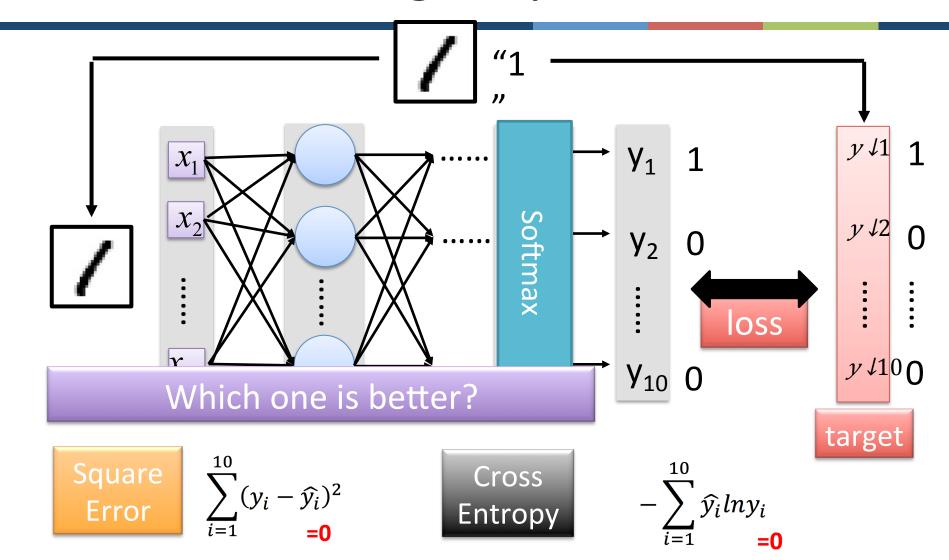
Momentum

Good Results on Testing Data?

YES

Good Results on Training Data?

# **Choosing Proper Loss**



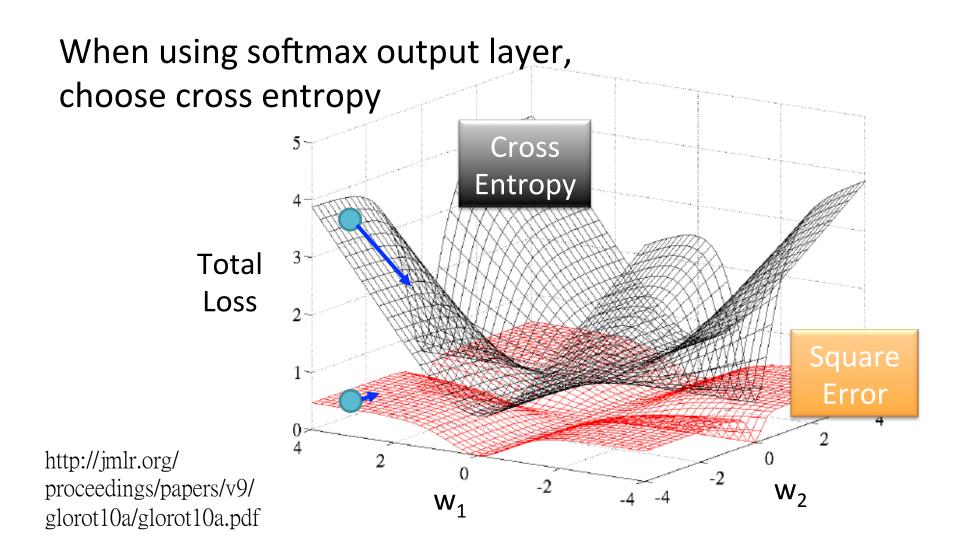
## Demo

#### Square Error

#### **Cross Entropy**

Several alternatives: https://keras.io/objectives/

# **Choosing Proper Loss**



## Recipe of Deep Learning

YES

Choosing proper loss

Mini-batch

New activation function

Adaptive Learning Rate

Momentum

Good Results on Testing Data?

YES

Good Results on Training Data?

model.fit(x\_train, y\_train, batch\_size=100, nb\_epoch=20)

#### We do not really minimize total loss!

# Mini-batch,

Randomly initialize

network parameters

Mini-batch

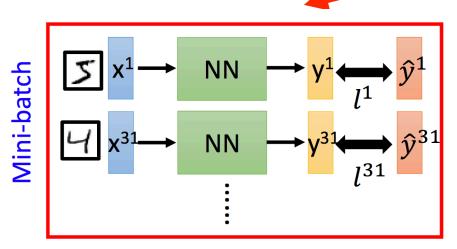
- Pick the 1<sup>st</sup> batch  $L' = l^1 + l^{31} + \cdots$  Update parameters once
- Pick the  $2^{nd}$  batch  $L'' = l^2 + l^{16} + \cdots$  Update parameters once  $\vdots$
- Until all mini-batches have been picked

one epoch

Repeat the above process

### Mini-batch

model.fit(x train, y train, batch size=100, nb epoch=20



100 examples in a mini-batch

Pick the 1st batch  $L' = l^1 + l^{31} + \cdots$ Update parameters once

- Pick the 2<sup>nd</sup> batch  $L'' = l^2 + l^{16} + \cdots$ Update parameters once
- Until all mini-batches have been picked

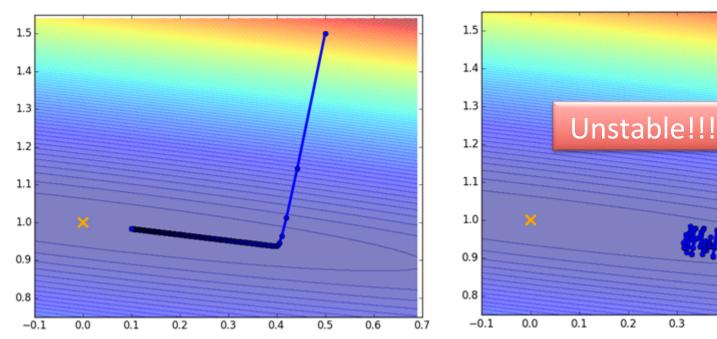
Repeat 20 times

## Mini-batch

### **Original Gradient Descent**

### With Mini-batch

0.6



The colors represent the total loss.

## Mini-batch is Faster

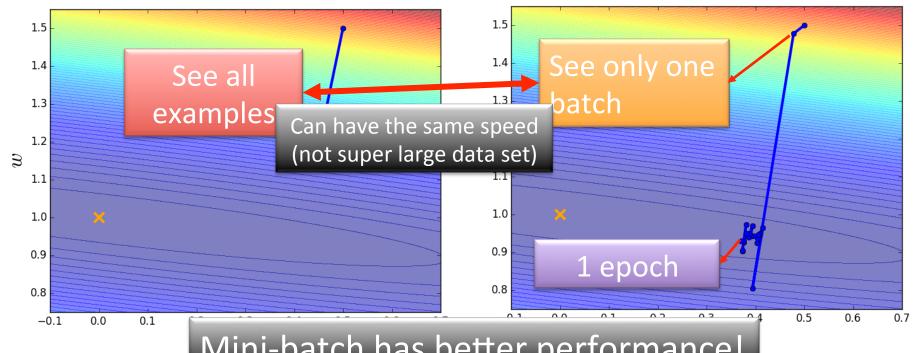
parallel computing.

### **Original Gradient Descent**

Update after seeing all examples

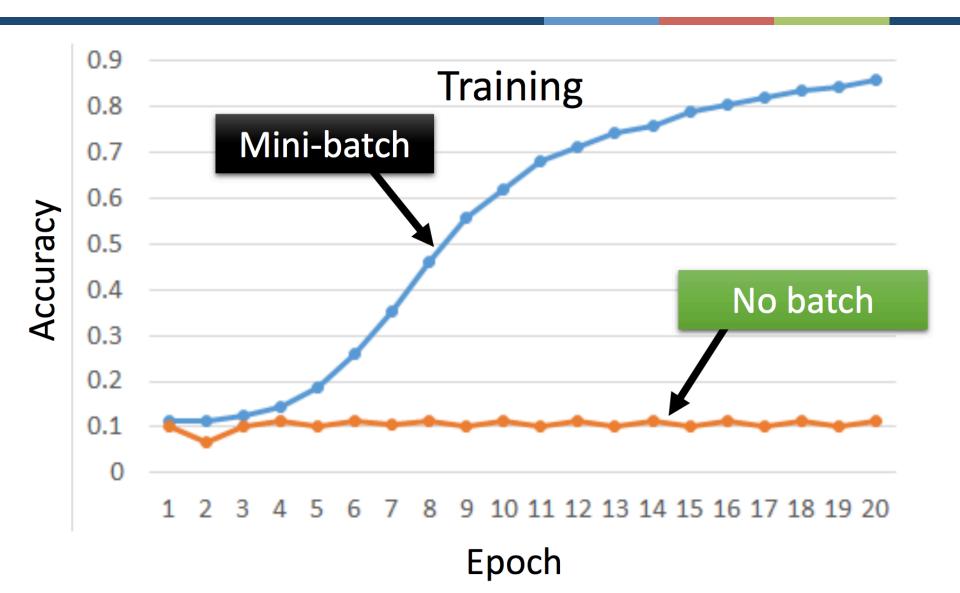
### With Mini-batch

If there are 20 batches, update 20 times in one epoch.

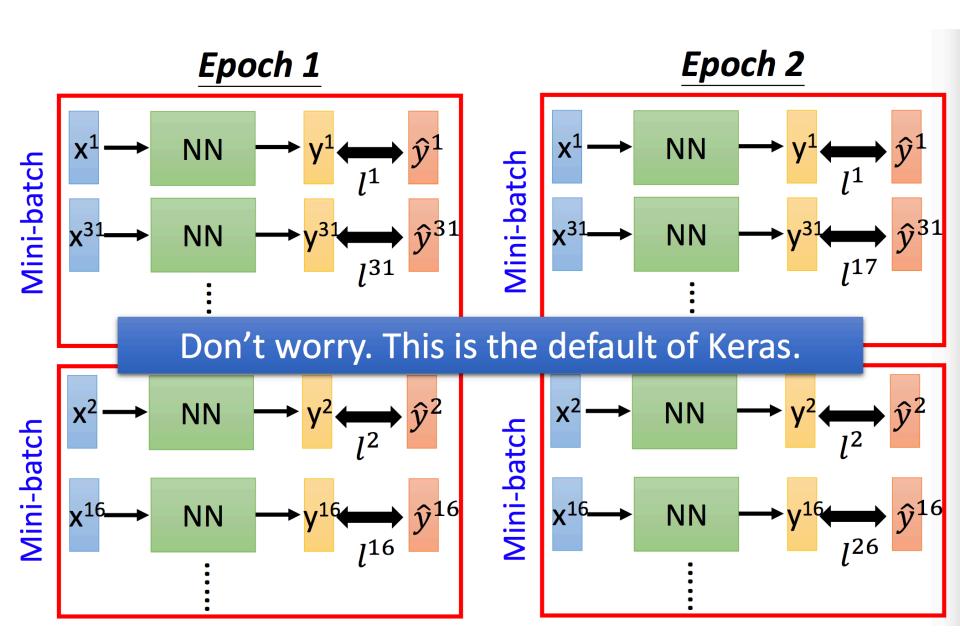


Mini-batch has better performance!

### Mini-batch is Faster



### Shuffle the training examples for each epoch



### Recipe of Deep Learning



YES

Choosing proper loss

Mini-batch

New activation function

Adaptive Learning Rate

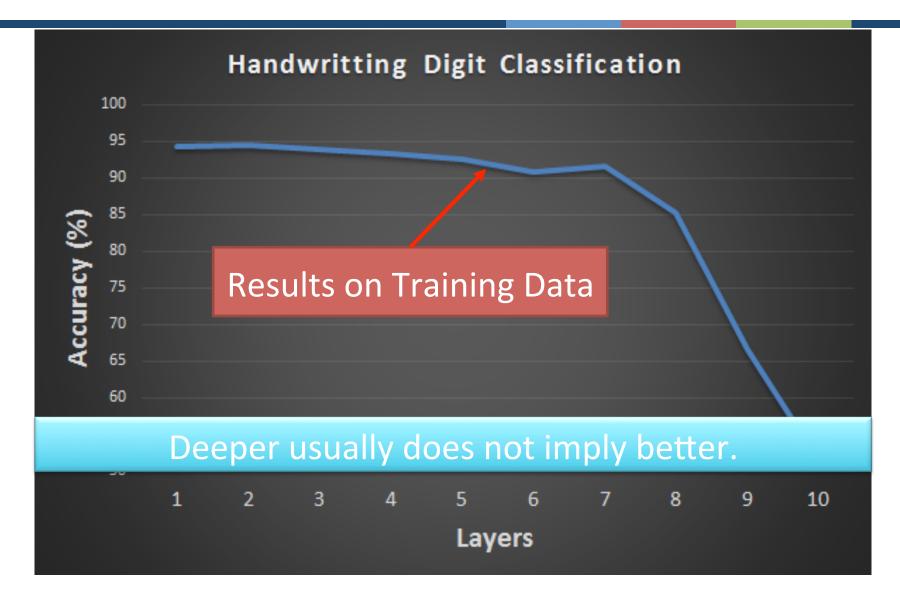
Momentum

Good Results on Testing Data?

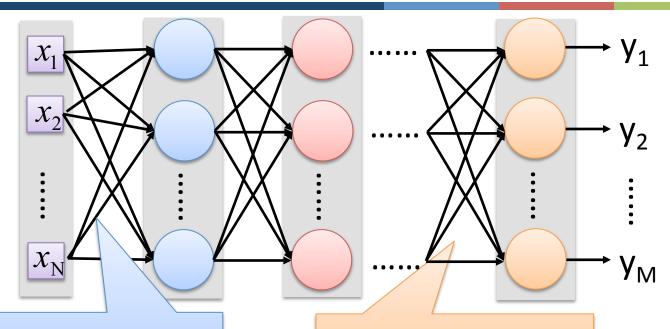
YES

Good Results on Training Data?

## Hard to get the power of Deep ...



## Vanishing Gradient Problem



**Smaller gradients** 

Learn very slow

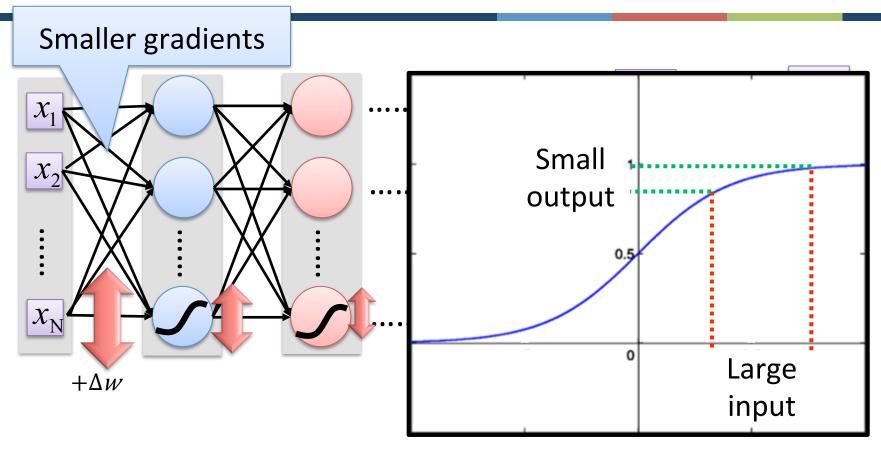
Almost random

Larger gradients

Learn very fast

Already converge

## Vanishing Gradient Problem

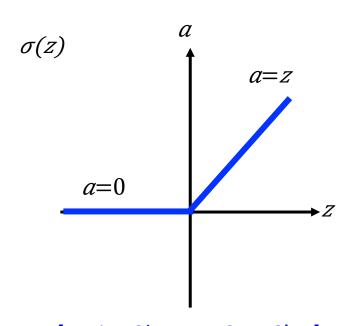


Intuitive way to compute the derivatives ...

 $\partial l/\partial w = ? \Delta l/\Delta w$ 

### ReLU

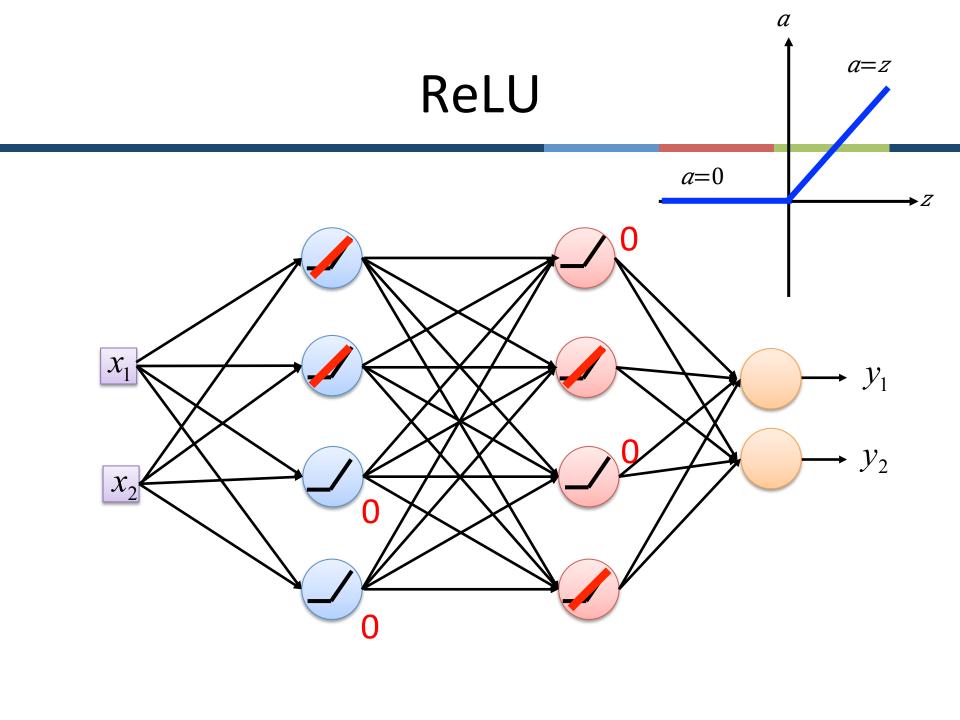
Rectified Linear Unit (ReLU)

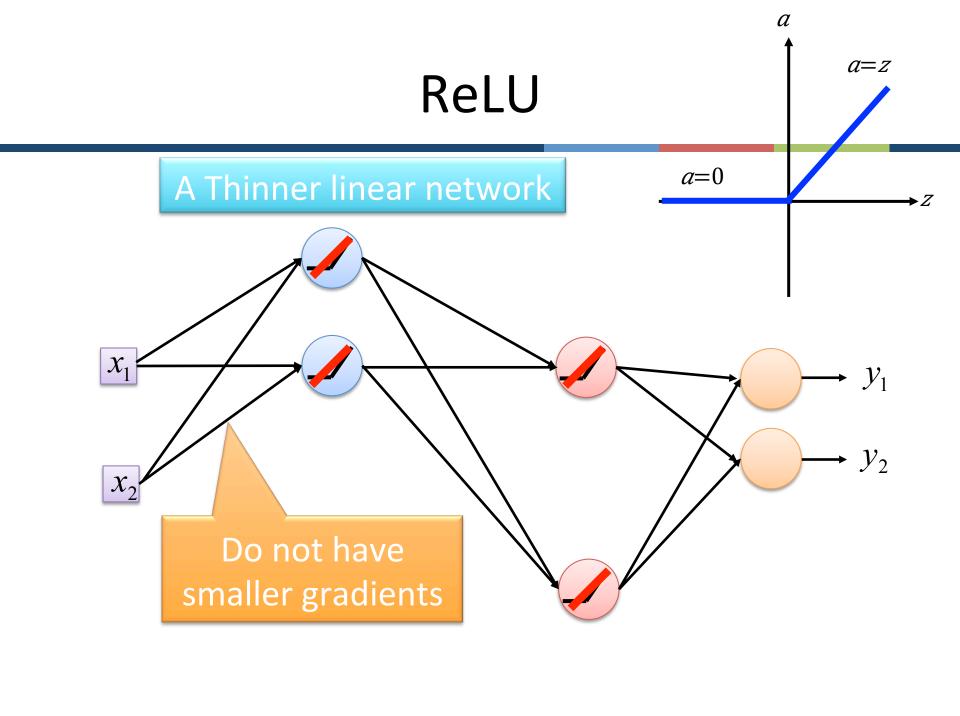


[Xavier Glorot, AISTATS'11] [Andrew L. Maas, ICML'13] [Kaiming He, arXiv'15]

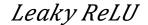
### Reason:

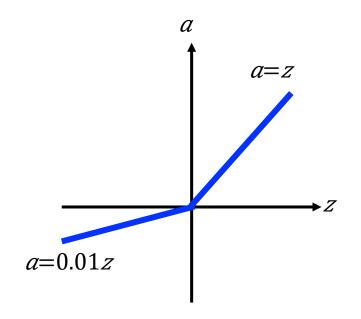
- 1. Fast to compute
- 2. Sparsity
- 3. Vanishing gradient problem



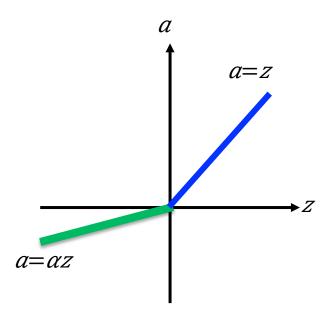


## ReLU - variant





### Parametric ReLU

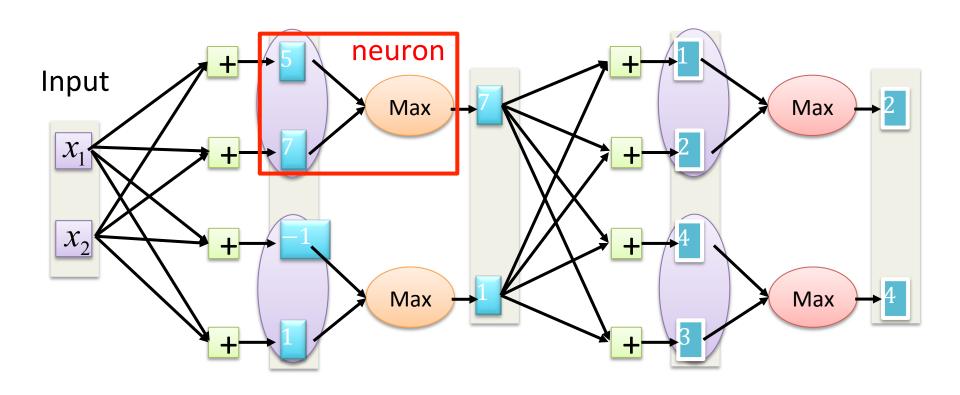


α also learned by gradient descent

## Maxout

### ReLU is a special cases of Maxout

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



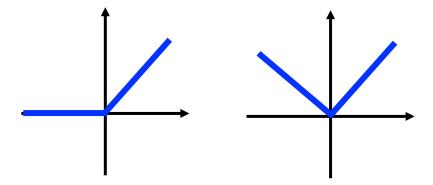
You can have more than 2 elements in a group.

## Maxout

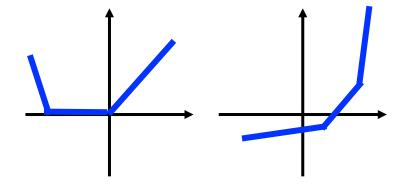
### ReLU is a special cases of Maxout

- Learnable activation function [lan 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



### Recipe of Deep Learning



YES

Choosing proper loss

Mini-batch

New activation function

Adaptive Learning Rate

Momentum

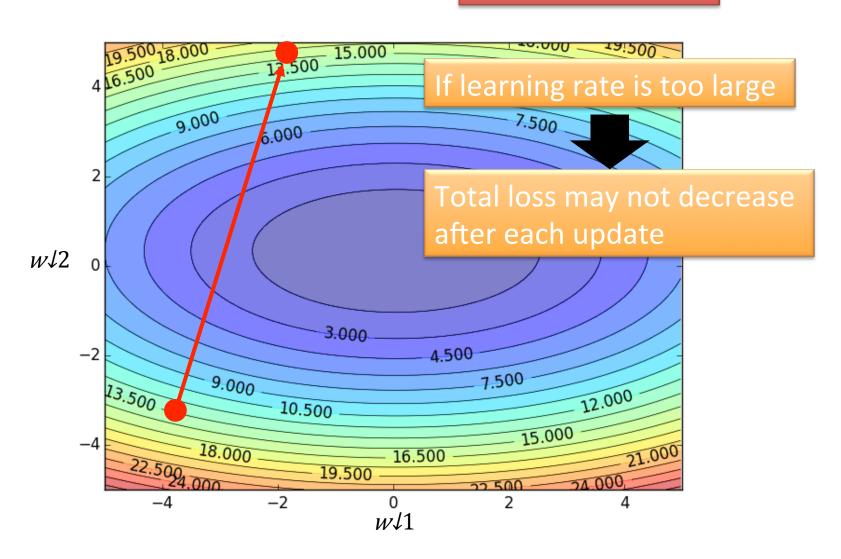
Good Results on Testing Data?

YES

Good Results on Training Data?

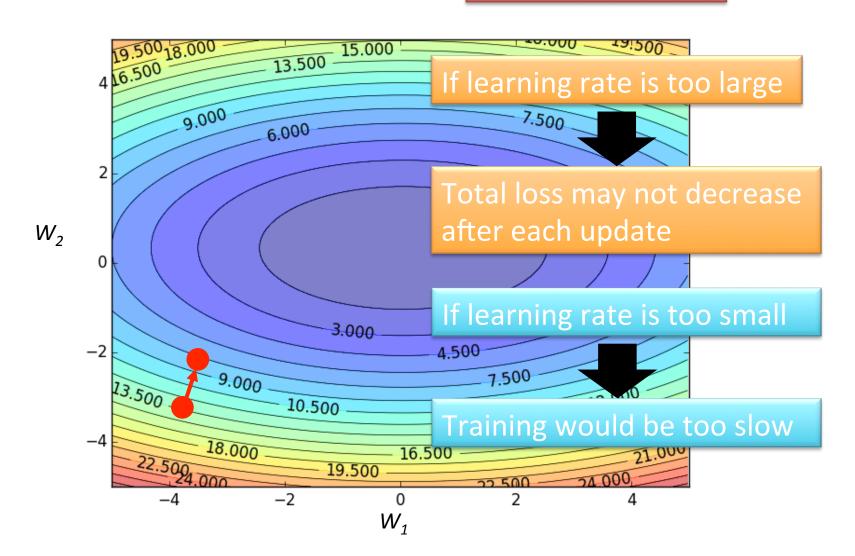
## Learning Rates

Set the learning rate η carefully



## **Learning Rates**

Set the learning rate η carefully



## **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
  - Giving different parameters different learning rates

## Adagrad

Original: 
$$w \leftarrow w - \eta \partial L / \partial w$$

Adagrad:  $w \leftarrow w - \eta_w \partial L / \partial w$ 

Parameter dependent learning rate

$$\eta_w = \frac{\eta}{\sqrt{\sum_{i=0}^t (g^i)^2}}$$
constant
$$g^i \text{ is } \partial L / \partial w \text{ obtained at the i-th update}$$

Summation of the square of the previous derivatives

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

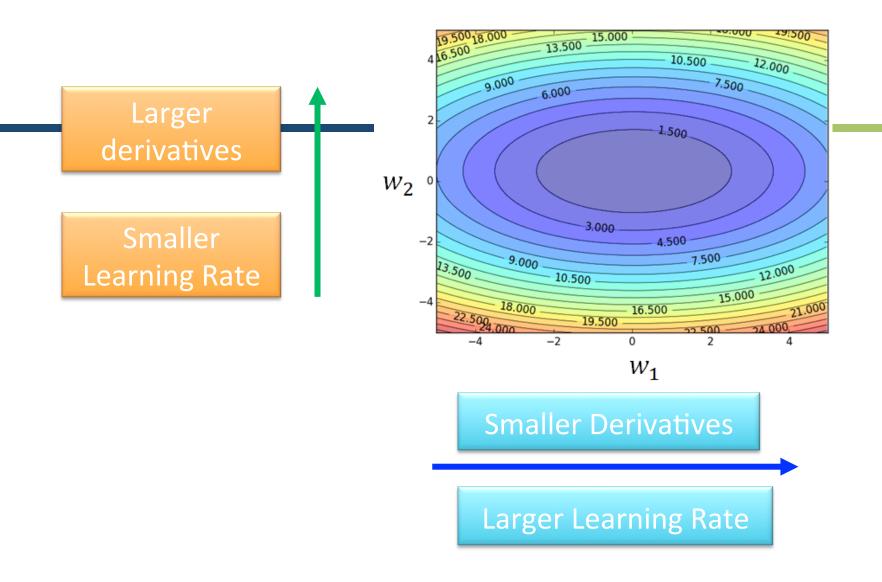
# Adagrad



Learning rate:

Learning rate: 
$$\frac{\eta}{\sqrt{0.1^2}} = \frac{\eta}{0.1} \qquad \frac{\eta}{\sqrt{20^2}} = \frac{\eta}{20}$$
 
$$\frac{\eta}{\sqrt{0.1^2 + 0.2^2}} = \frac{\eta}{0.22} \qquad \frac{\eta}{\sqrt{20^2 + 10^2}} = \frac{\eta}{22}$$

- **Observation:** 1. Learning rate is smaller and smaller for all parameters
  - 2. Smaller derivatives, larger learning rate, and vice versa



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



## Not the whole story .....

- Adagrad [John Duchi, JMLR'11]
- RMSprop
  - https://www.youtube.com/watch?v=O3sxAc4hxZU
- Adadelta [Matthew D. Zeiler, arXiv'12]
- "No more pesky learning rates" [Tom Schaul, arXiv'12]
- AdaSecant [Caglar Gulcehre, arXiv'14]
- Adam [Diederik P. Kingma, ICLR'15]
- Nadam
  - http://cs229.stanford.edu/proj2015/054\_report.pdf

### Recipe of Deep Learning



YES

Choosing proper loss

Mini-batch

New activation function

Adaptive Learning Rate

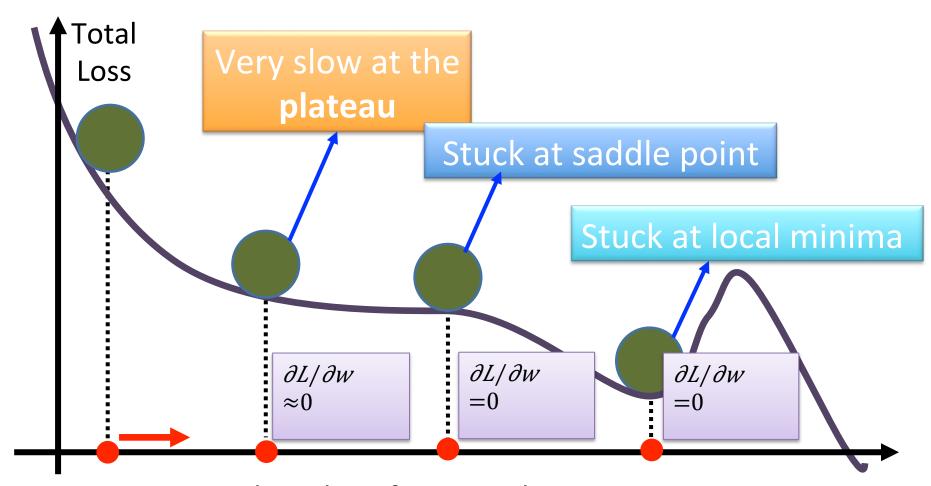
Momentum

Good Results on Testing Data?

YES

Good Results on Training Data?

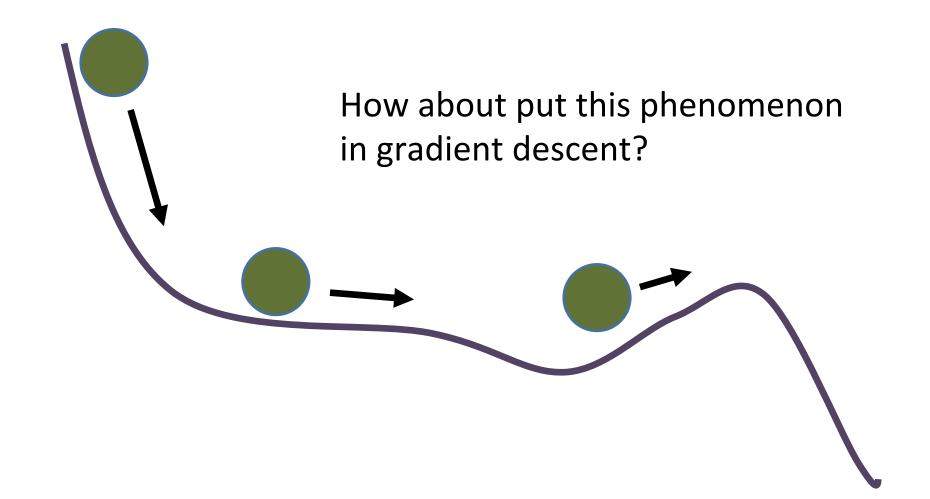
# Hard to find optimal network parameters



The value of a network parameter w

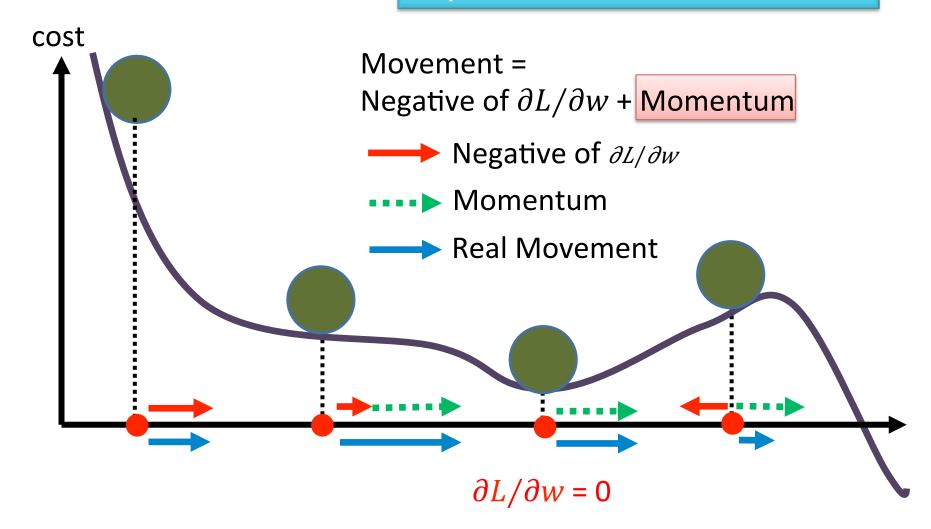
## In physical world .....

Momentum



## Momentum

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



### RMSProp (Advanced Adagrad) + Momentum

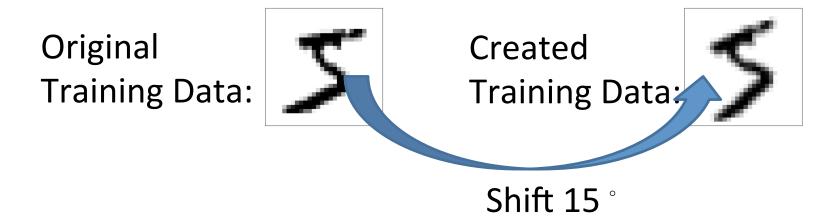
```
model.compile(loss='categorical crossentropy',
                                              optimizer=SGD(lr=0.1),
                                             metrics=['accuracy'])
model.compile(loss='categorical crossentropy',
                                              optimizer=Adam(),
                                             metrics=['accuracy'])
                                               Algorithm 1: Adam, our proposed algorithm for stochastic optimization. See section 2 for details,
                                                and for a slightly more efficient (but less clear) order of computation. q_t^2 indicates the elementwise
                                                square g_t \odot g_t. Good default settings for the tested machine learning problems are \alpha = 0.001,
                                                \beta_1 = 0.9, \beta_2 = 0.999 and \epsilon = 10^{-8}. All operations on vectors are element-wise. With \beta_1^t and \beta_2^t
                                                we denote \beta_1 and \beta_2 to the power t.
                                                Require: \alpha: Stepsize
                                                Require: \beta_1, \beta_2 \in [0, 1): Exponential decay rates for the moment estimates
                                                Require: f(\theta): Stochastic objective function with parameters \theta
                                                Require: \theta_0: Initial parameter vector
                                                  m_0 \leftarrow 0 (Initialize 1<sup>st</sup> moment vector)
                                                  v_0 \leftarrow 0 (Initialize 2<sup>nd</sup> moment vector)
                                                  t \leftarrow 0 (Initialize timestep)
 loss = nn.CrossEntropyLoss()
                                                                                                      at timestep t)
 optimizer = torch.optim.Adam(model.parameters(), lr=0.1)
                                                                                                      ent estimate)
                                                    \widehat{m}_t \leftarrow m_t/(1-\beta_1^t) (Compute bias-corrected first moment estimate)
                                                    \hat{v}_t \leftarrow v_t/(1-\beta_2^t) (Compute bias-corrected second raw moment estimate)
                                                    \theta_t \leftarrow \theta_{t-1} - \alpha \cdot \widehat{m}_t / (\sqrt{\widehat{v}_t} + \epsilon) (Update parameters)
                                                  return \theta_t (Resulting parameters)
```

## Recipe of Deep Learning YES **Early Stopping** Good Results on **Testing Data?** Regularization YES Dropout Good Results on **Training Data? Network Structure**

## Panacea for Overfitting

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

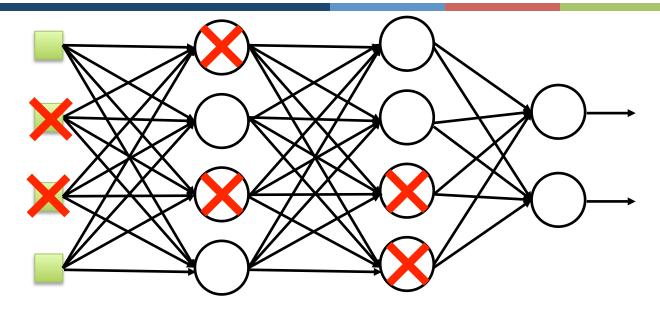
Handwriting recognition:



## Recipe of Deep Learning YES **Early Stopping** Good Results on Testing Data? Regularization YES Dropout Good Results on **Training Data? Network Structure**

## Dropout

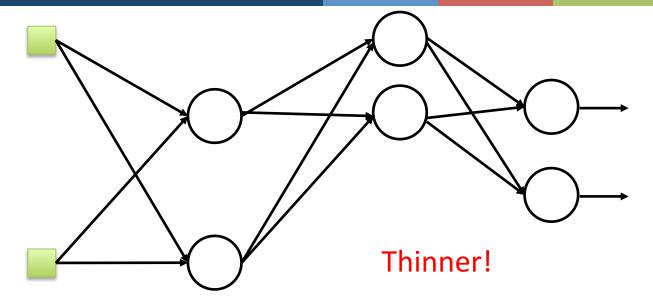
### **Training:**



- > Each time before updating the parameters
  - Each neuron has a probability of p to dropout

## Dropout

### **Training:**

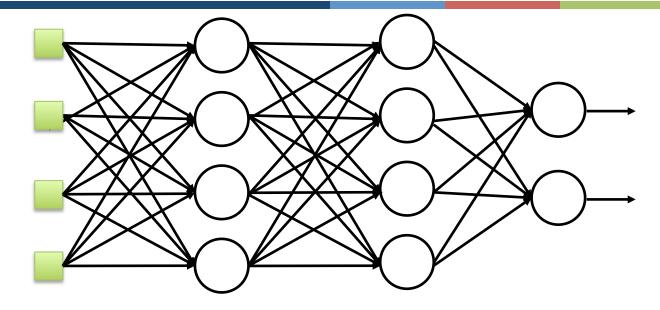


- > Each time before updating the parameters
  - Each neuron has a probability of p to dropout
    - The structure of the network is changed.
  - Using the new network for training

For each mini-batch, we resample the dropout neurons

## Dropout

### **Testing:**



### No dropout

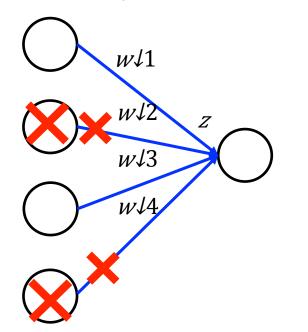
- If the dropout rate at training is p, all the weights times 1-p
- Assume that the dropout rate is 50%. If a weight w=1 by training, set w=0.5 for testing.

## **Dropout - Intuitive Reason**

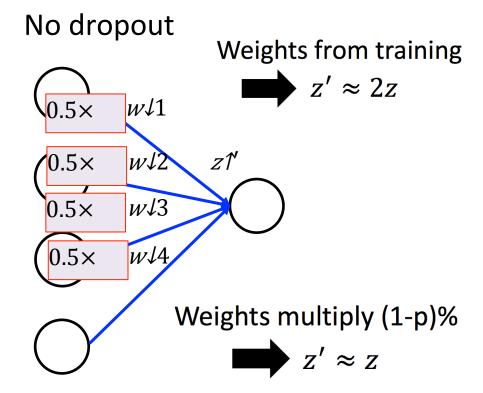
 Why the weights should multiply (1-p) when testing?

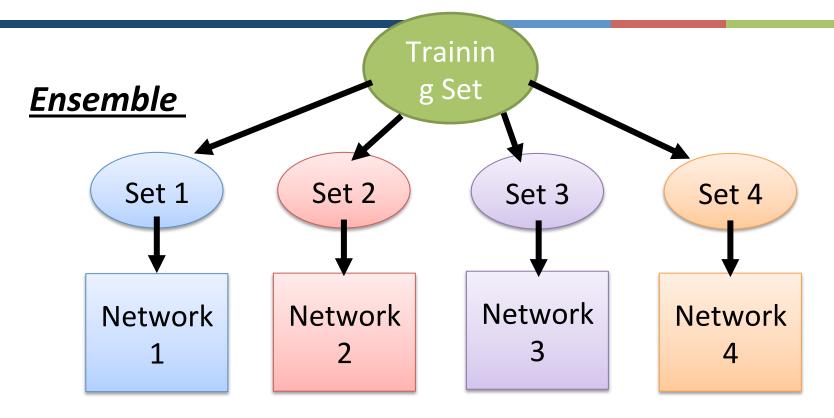
### **Training of Dropout**

Assume dropout rate is 0.5



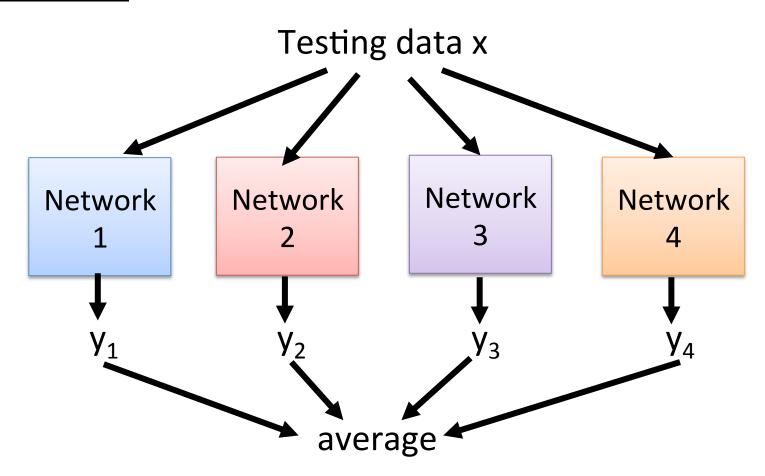


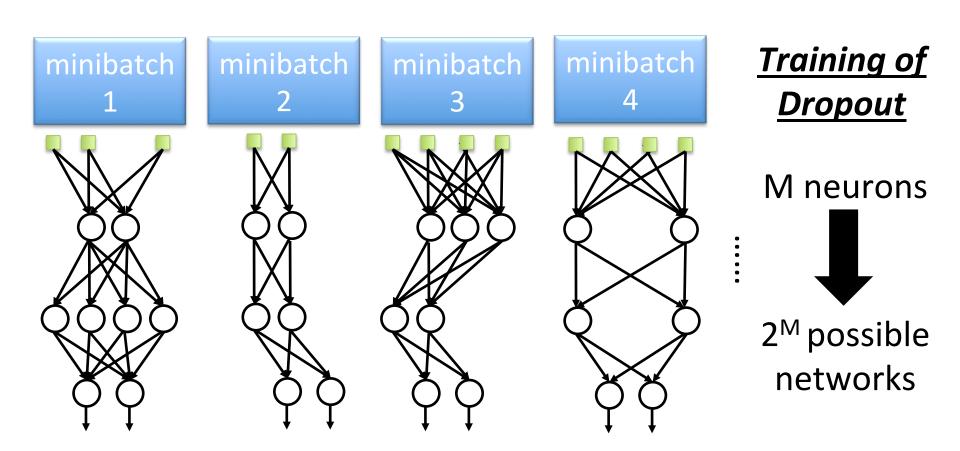




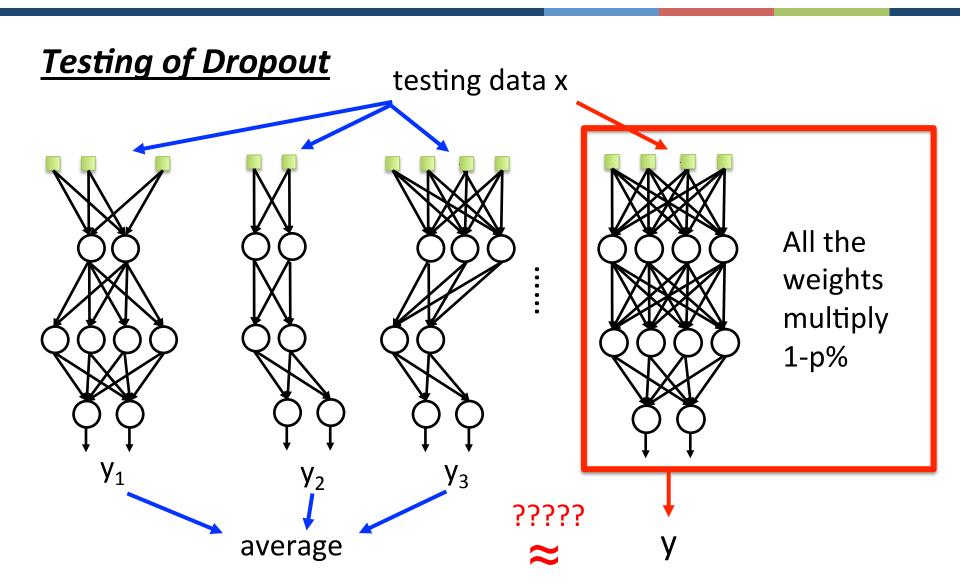
Train a bunch of networks with different structures

### **Ensemble**





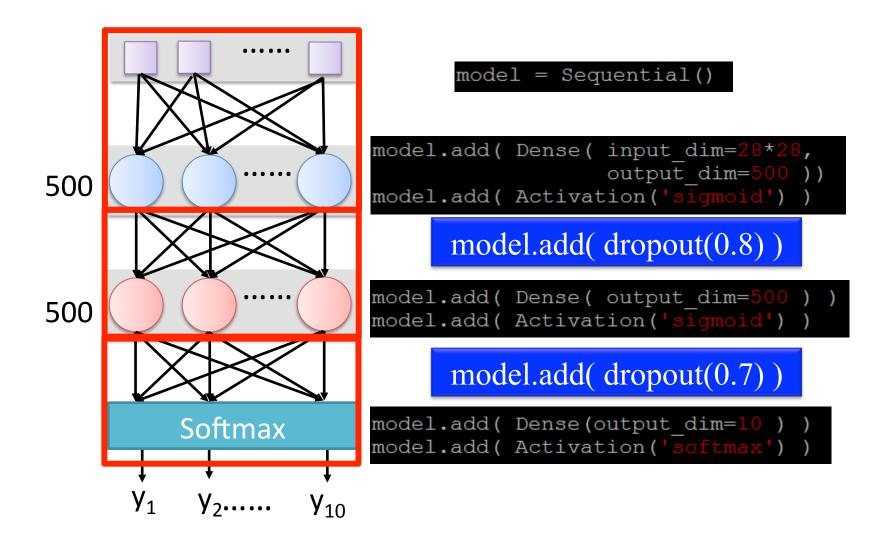
- >Using one mini-batch to train one network
- >Some parameters in the network are shared



## 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 [lan 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

### Demo



## PyTorch

28x28

500

500

Step 1: define a set of function

Softmax

 $y_1$ 





Step 2: goodness of function



Step 3: pick the best function

```
import torch.nn as nn
import torch.nn.functional as F
class MyNetwork(nn.Module):
  def init (self):
    super(MyNetwork, self). init ()
    self.fc1 = nn.Linear(28 * 28, 500)
    self.fc2 = nn.Linear(500, 500)
    self.fc3 = nn.Linear(500, 10)
  def forward(self, x):
    x = F.sigmoid(self.fc1(x))
    x = F.sigmoid(self.fc2(x))
    return F.log softmax(self.fc3(x))
```

## Recipe of Deep Learning YES **Early Stopping** Good Results on **Testing Data?** Regularization YES Dropout Good Results on **Training Data?** Network Structure CNN is a very good example! (next lecture)

# **Concluding Remarks**

### Recipe of Deep Learning





Step 1: define a set of function

Step 2: goodness of function

Step 3: pick the best function

NO

Good Results on Testing Data?



NO

Good Results on Training Data?

