

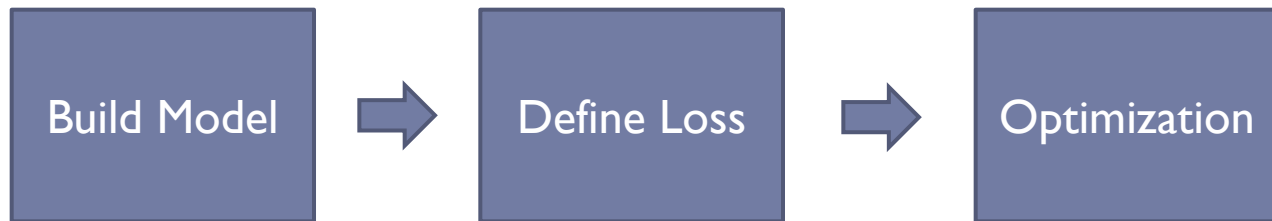
DNN Introduction

講者：Isaac

Outline

- ▶ Build DNN Model
- ▶ Define Loss Function
 - ▶ Mean square
 - ▶ Cross entropy with softmax
- ▶ Optimization
 - ▶ Gradient decent with moment
 - ▶ Adagrad, RMS, and Adam
- ▶ Predict/Validate Result

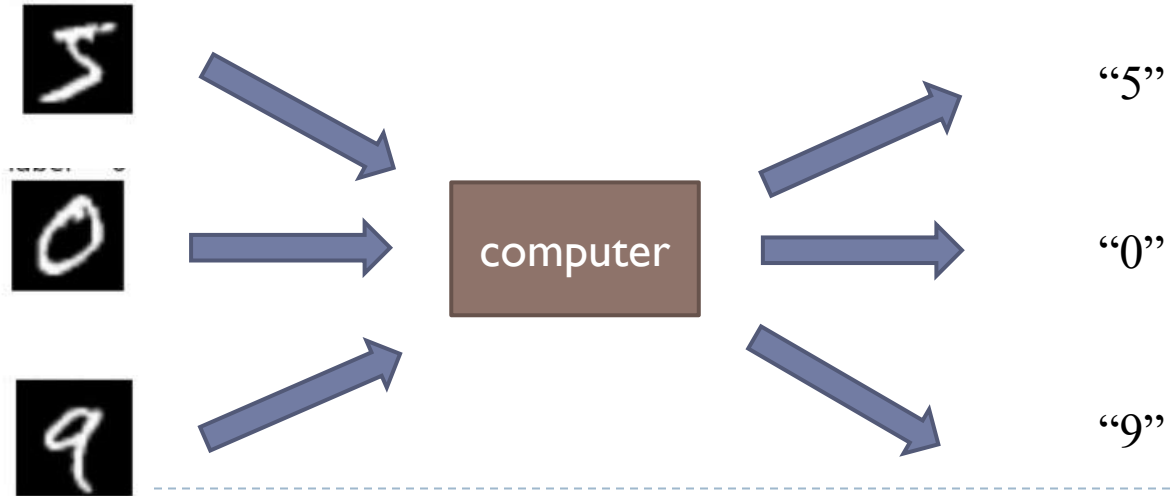
Big Picture



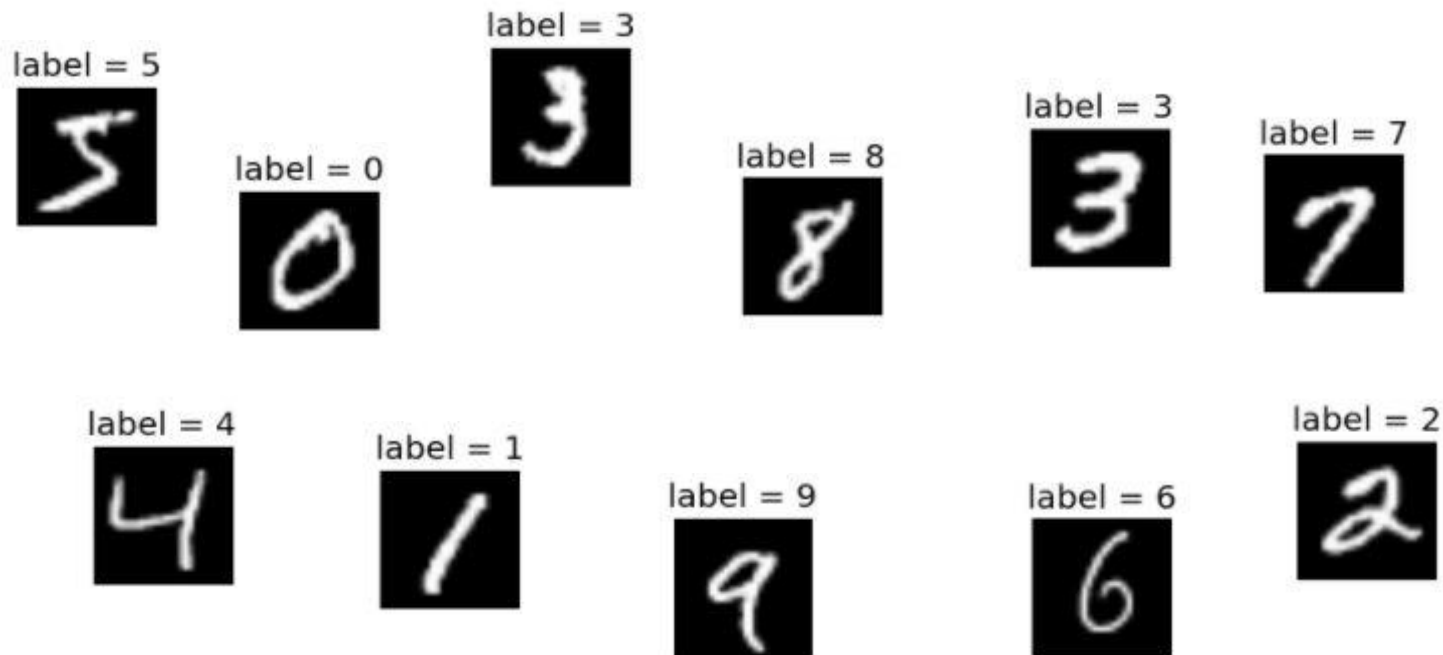
Same logic when implementation in TensorFlow



Assume we want to build a handwritten system to recognize image from 0 to 9



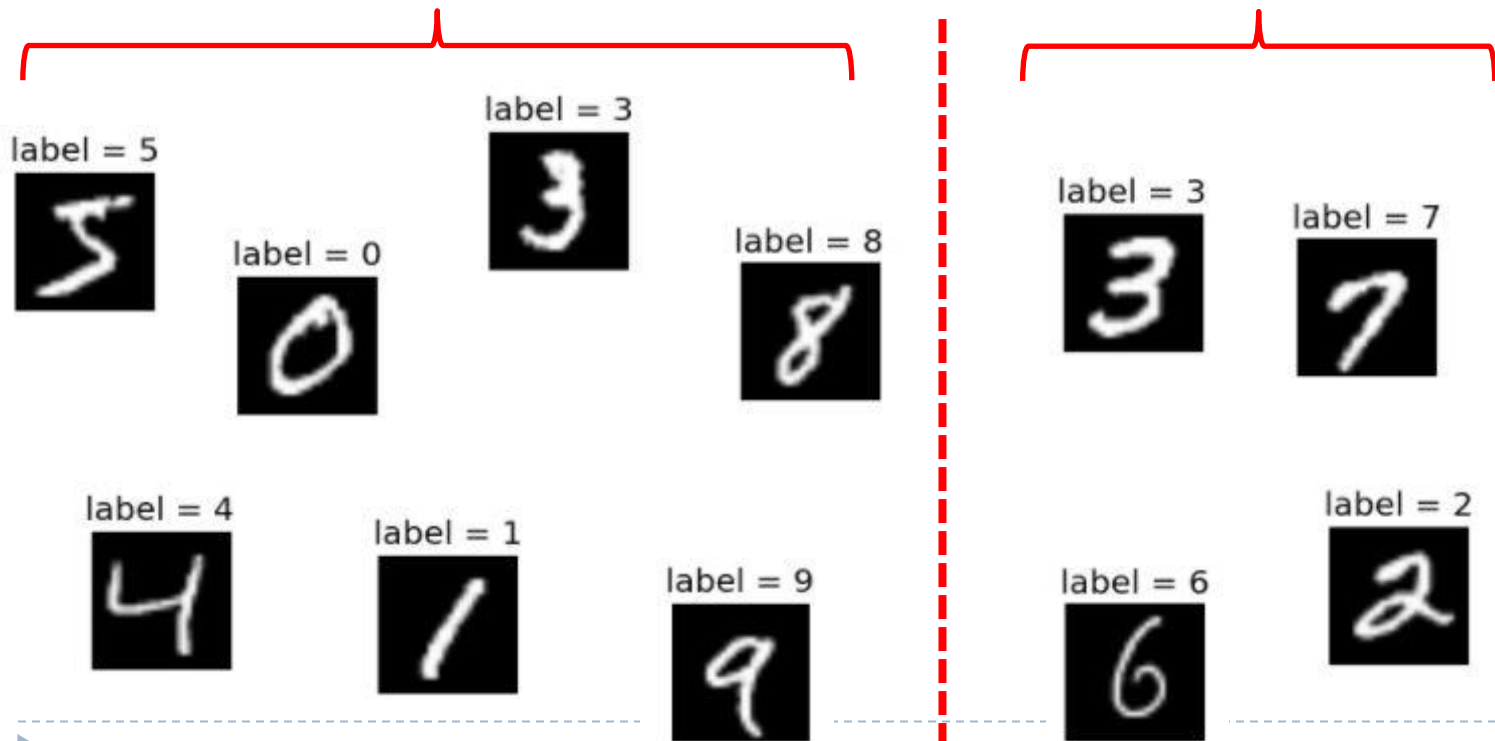
Total 10000 Images with labels



Split the data

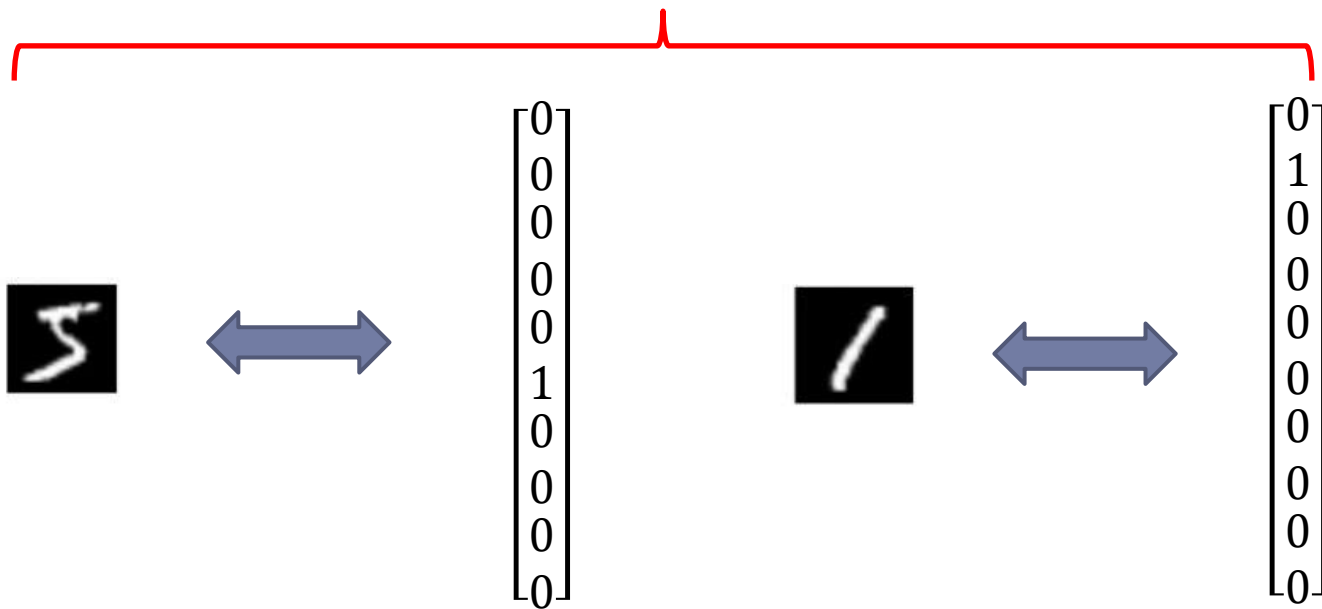
8000 images as training data

2000 images as testing data



Encode labels

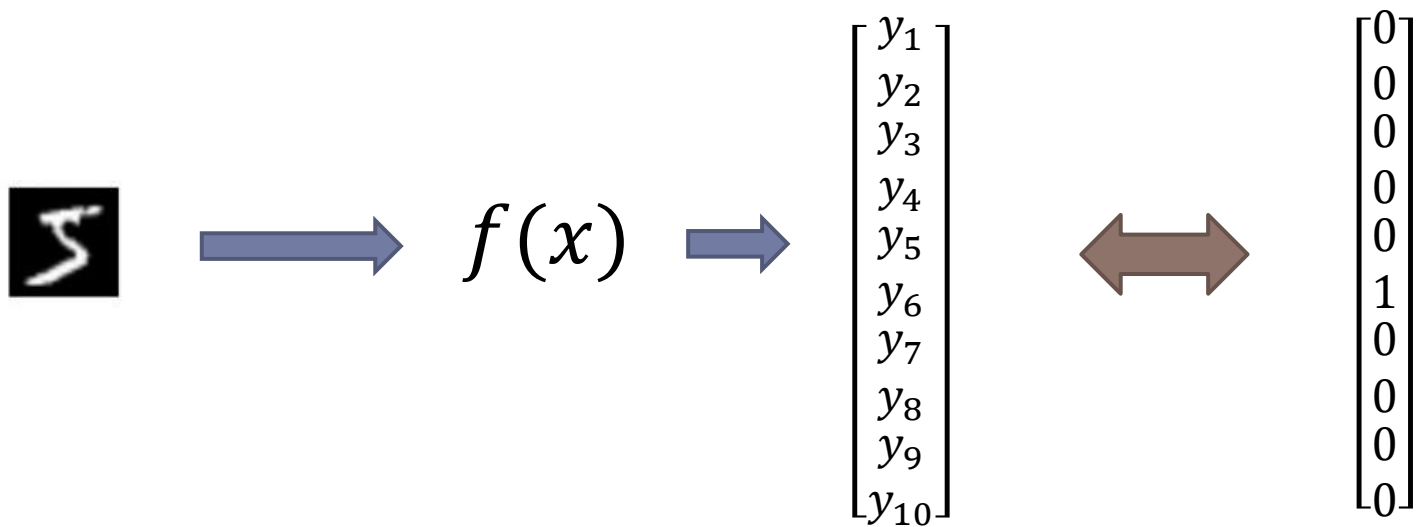
8000 images as training data



One-hot encoding

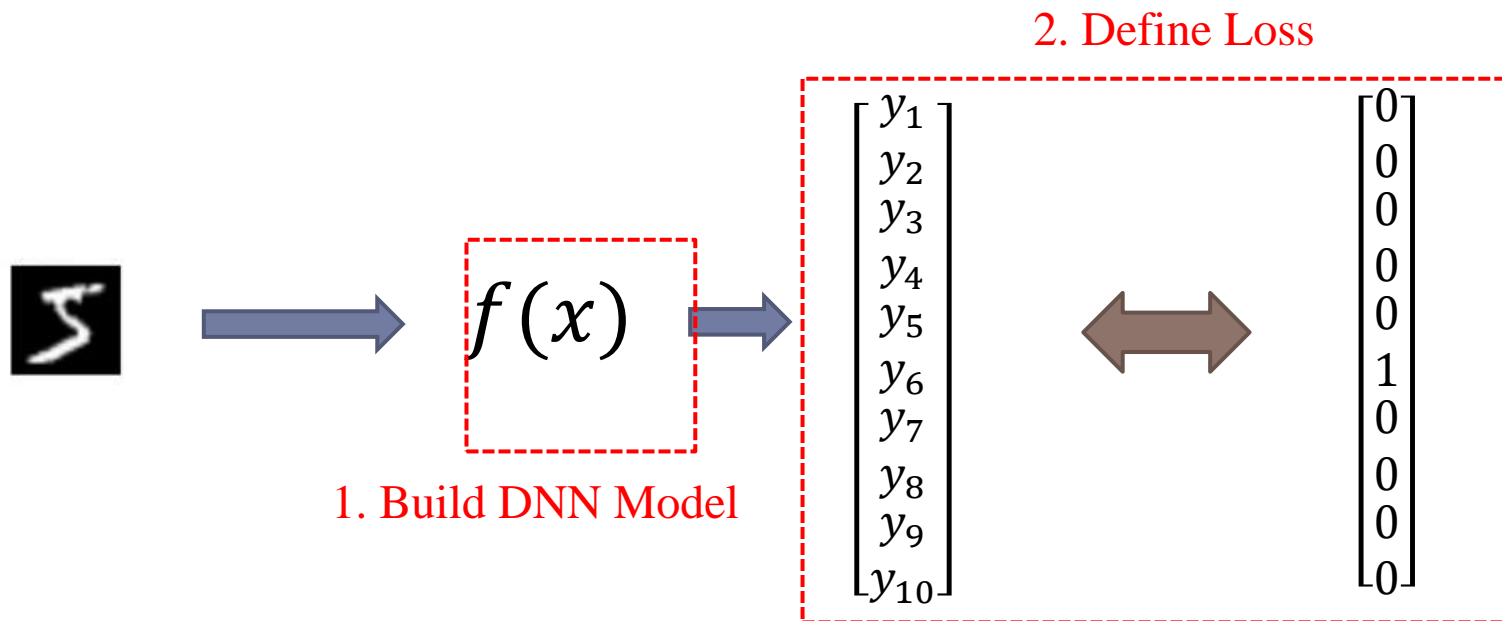
One-hot encoding

What we want

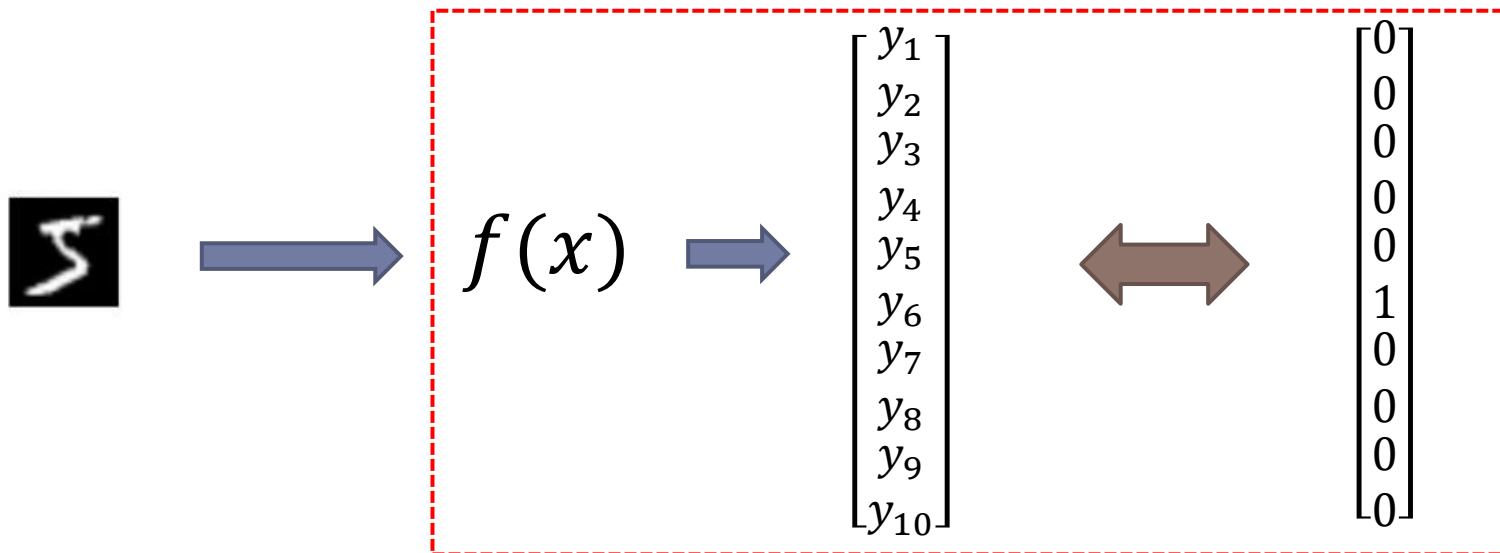


We want this two as close as possible

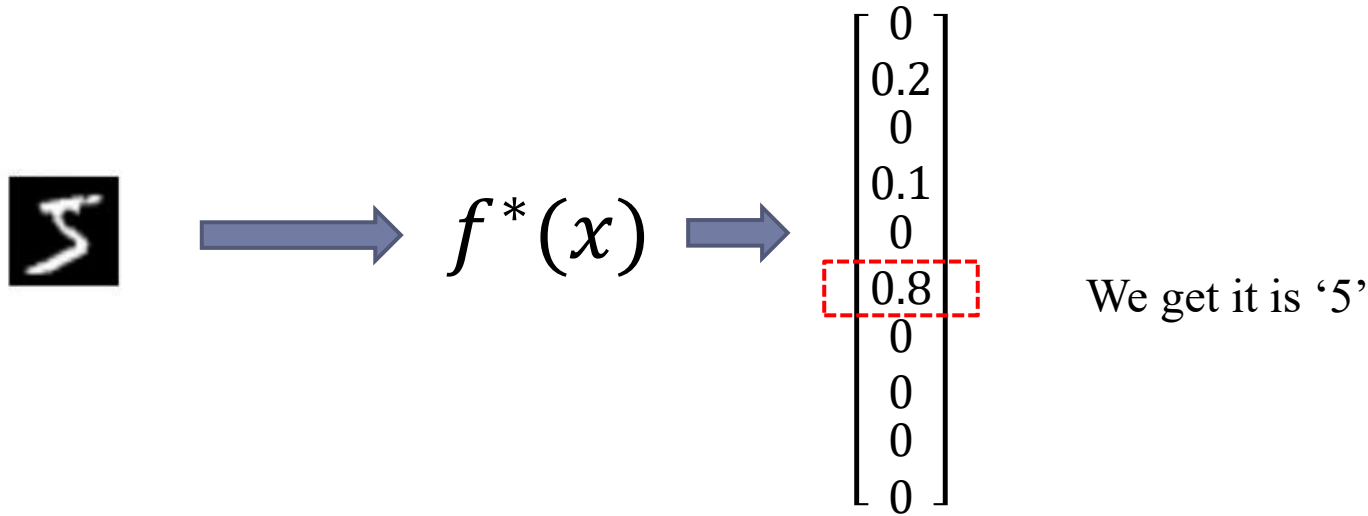
What we want



3. Optimization

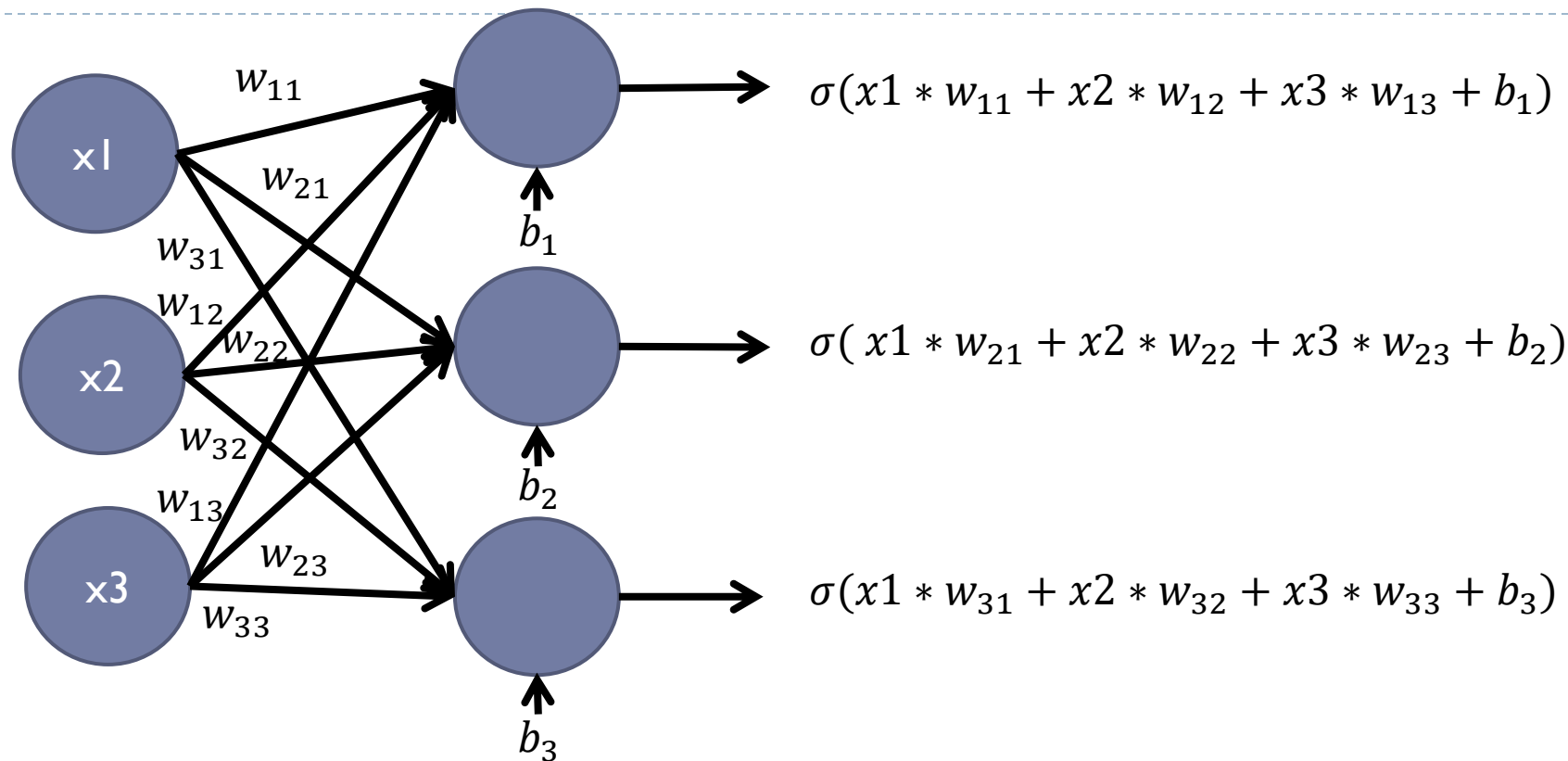


Finally, we get

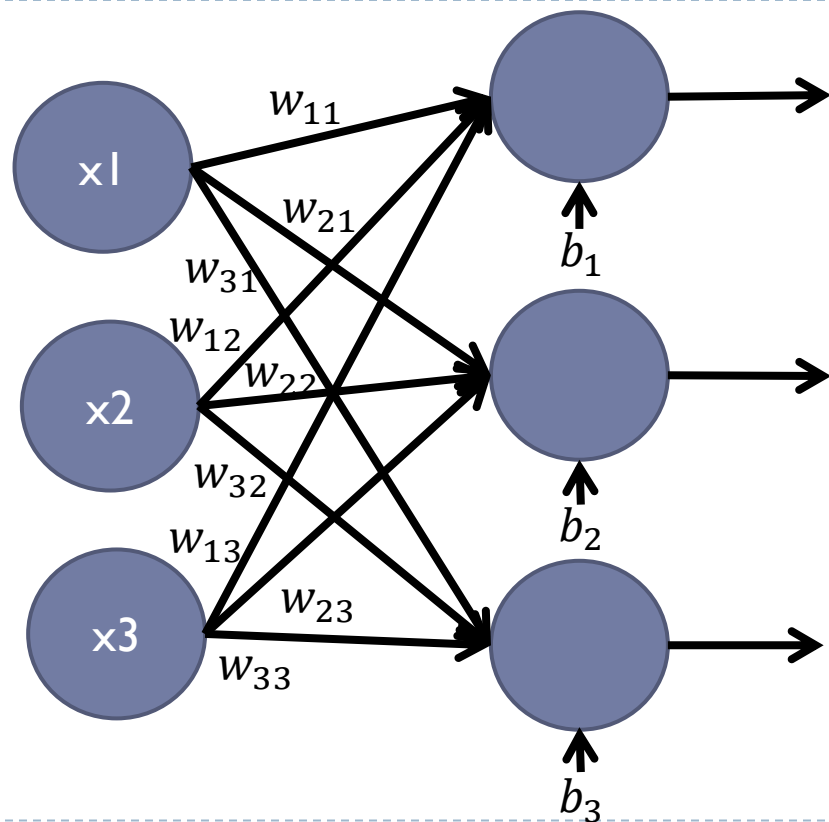


Build DNN Model

Model Overview



Model Overview



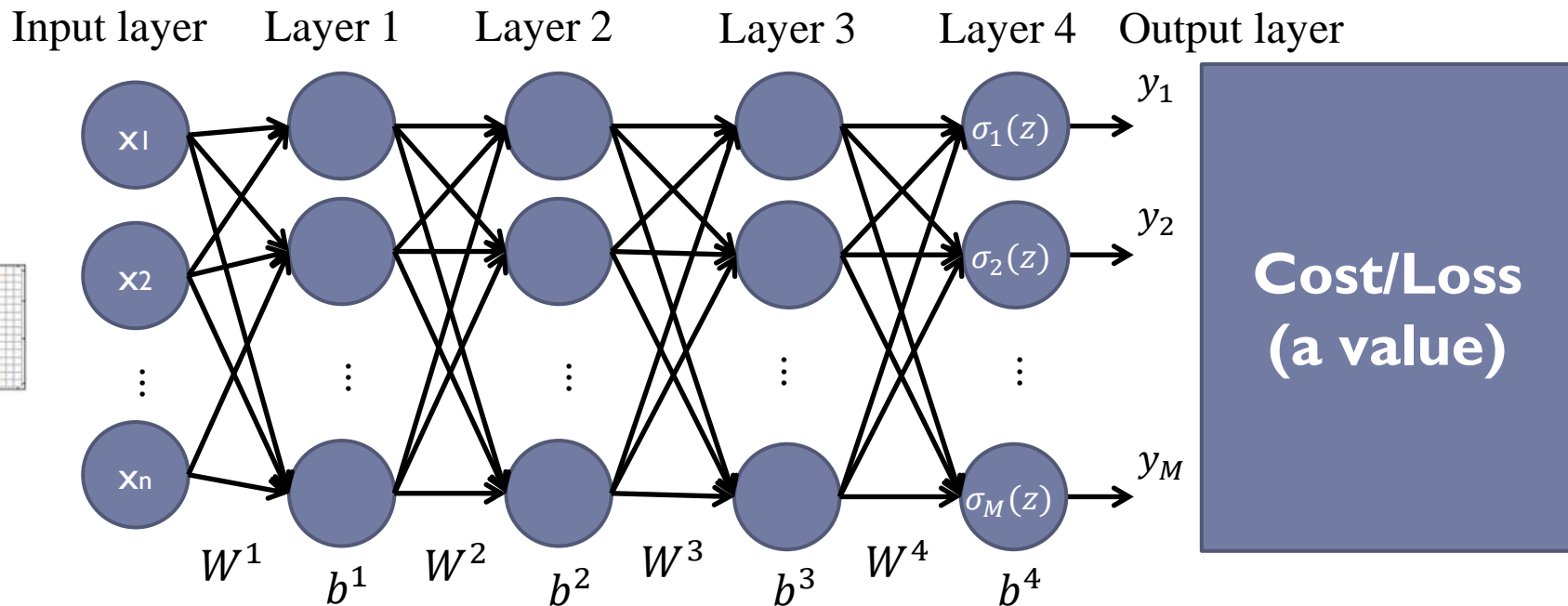
$$\sigma(W * X + b)$$

$$X = \begin{bmatrix} x1 \\ x2 \\ x3 \end{bmatrix}$$

$$W = \begin{bmatrix} w_{11} & w_{12} & w_{13} \\ w_{21} & w_{22} & w_{23} \\ w_{31} & w_{32} & w_{33} \end{bmatrix}$$

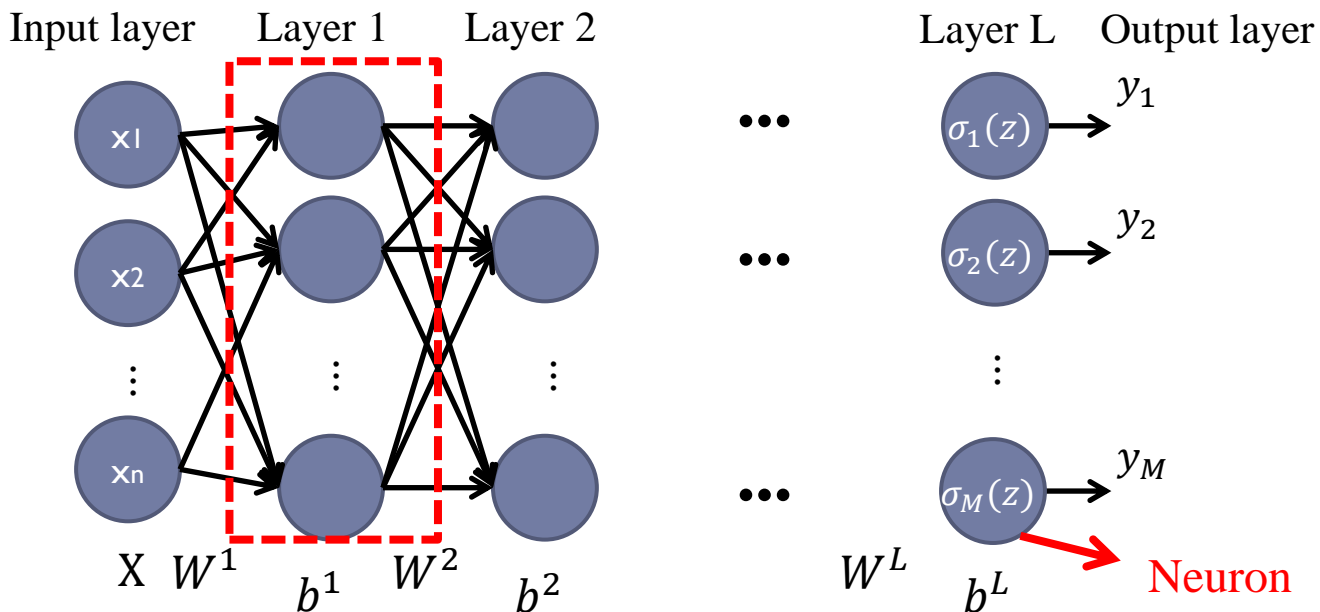
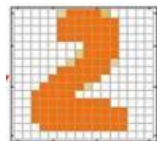
$$b = \begin{bmatrix} b1 \\ b2 \\ b3 \end{bmatrix}$$

Model Overview



DNN also called “Multilayer perceptron”

Model Overview

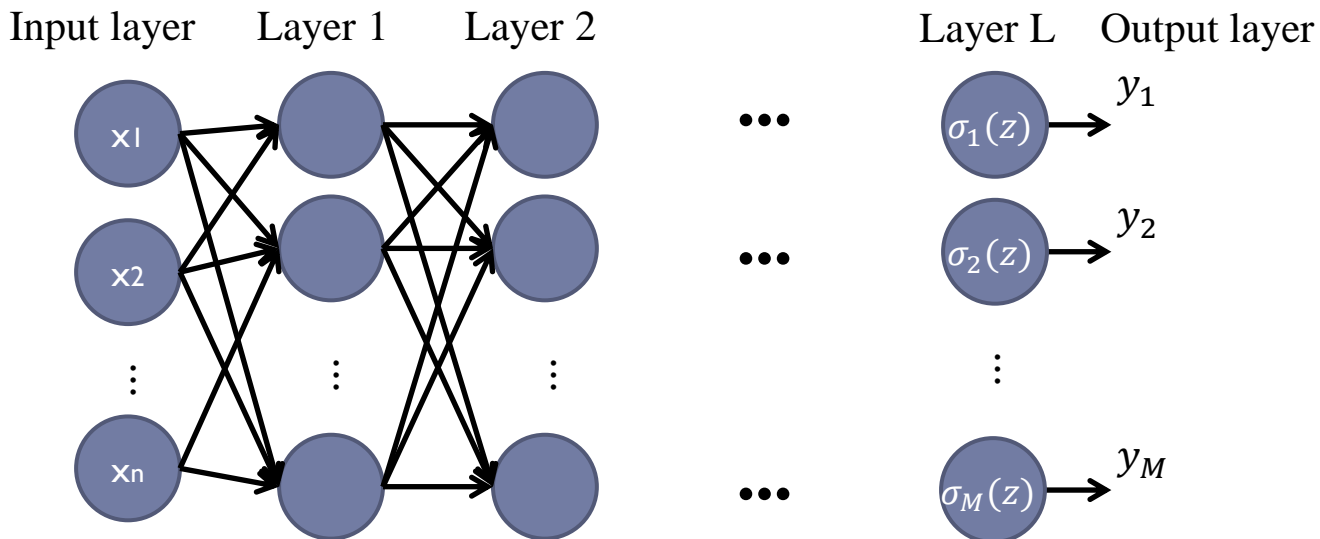


Hidden Layer

Activation function

$$y = f(x) = \sigma(W^L \dots \sigma(W^2 \sigma(W^1 X + b^1) + b^2) \dots + b^L)$$

Model Overview

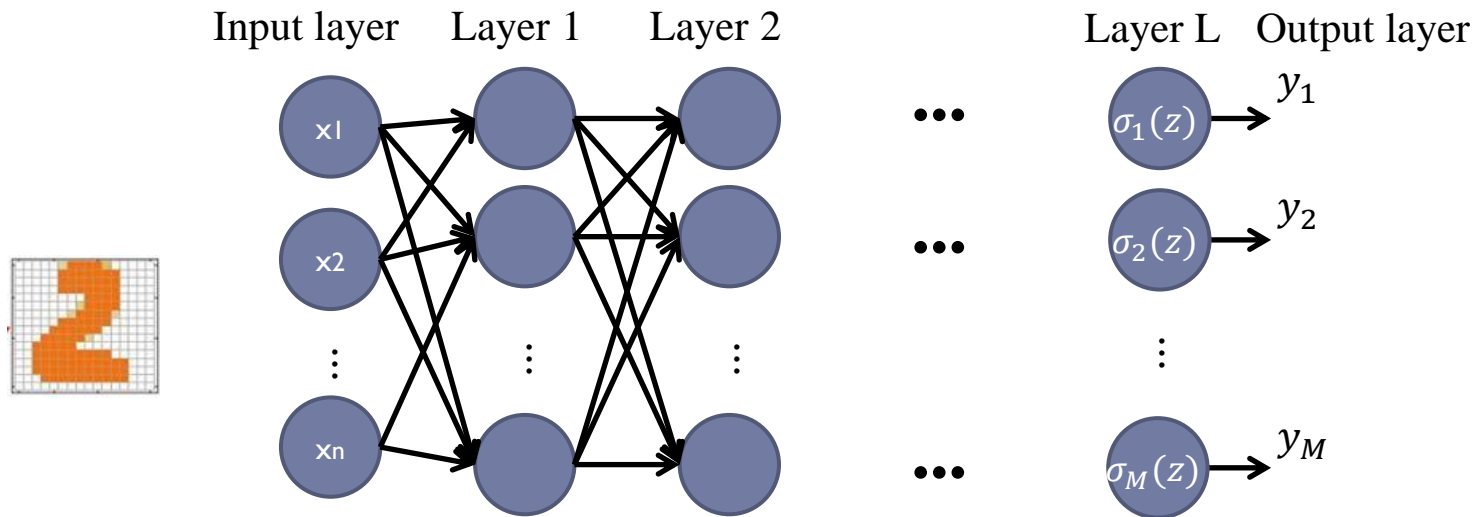


$$y = f(x) = \sigma(W^L \dots \sigma(W^2 \sigma(W^1 X + b^1) + b^2) \dots + b^L)$$

Weight (variable)

Bias (variable)

Model Overview



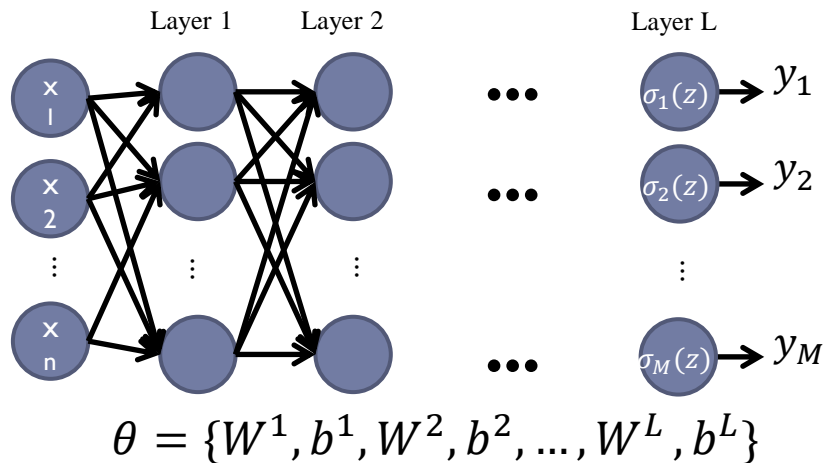
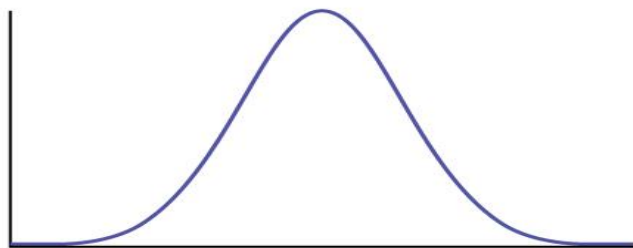
$$y = f(x) = \sigma(W^L \dots \sigma(W^2 \sigma(W^1 X + b^1) + b^2) \dots + b^L)$$

We want to find the best parameter set :

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

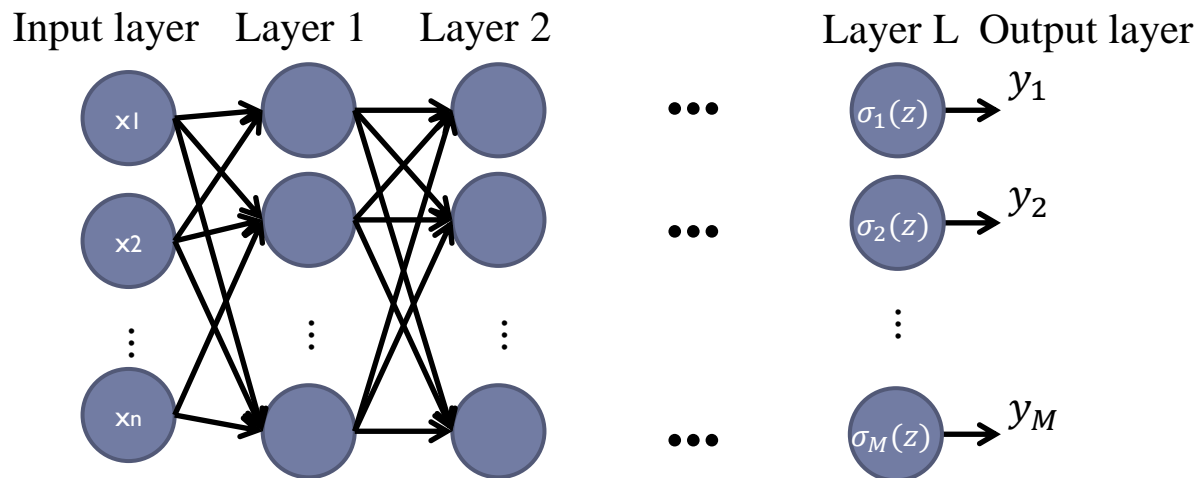
Parameters Initialization

- ▶ The most common way are
 - ▶ Use random normal distribution with zero mean and small standard deviation
- ▶ In complex model, it is very important to find better way to initialize the parameters



Activation Function

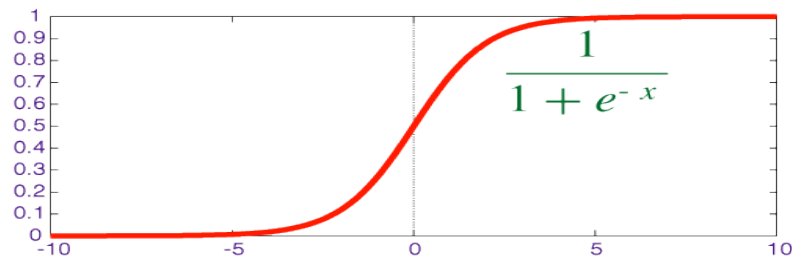
- ▶ Give NN nonlinearity property
- ▶ Can be regarded as "ON" (1) or "OFF" (0)



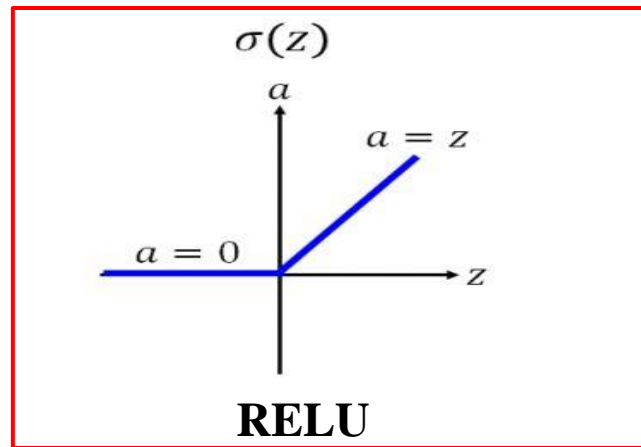
$$y = f(x) = \sigma(W^L \dots \sigma(W^2 \sigma(W^1 X + b^1) + b^2) \dots + b^L)$$

Activation Function

- ▶ There are many kinds of activation
 - ▶ relu, sigmoid, elu, etc.....
- ▶ Usually, we use relu as first try on building neural network

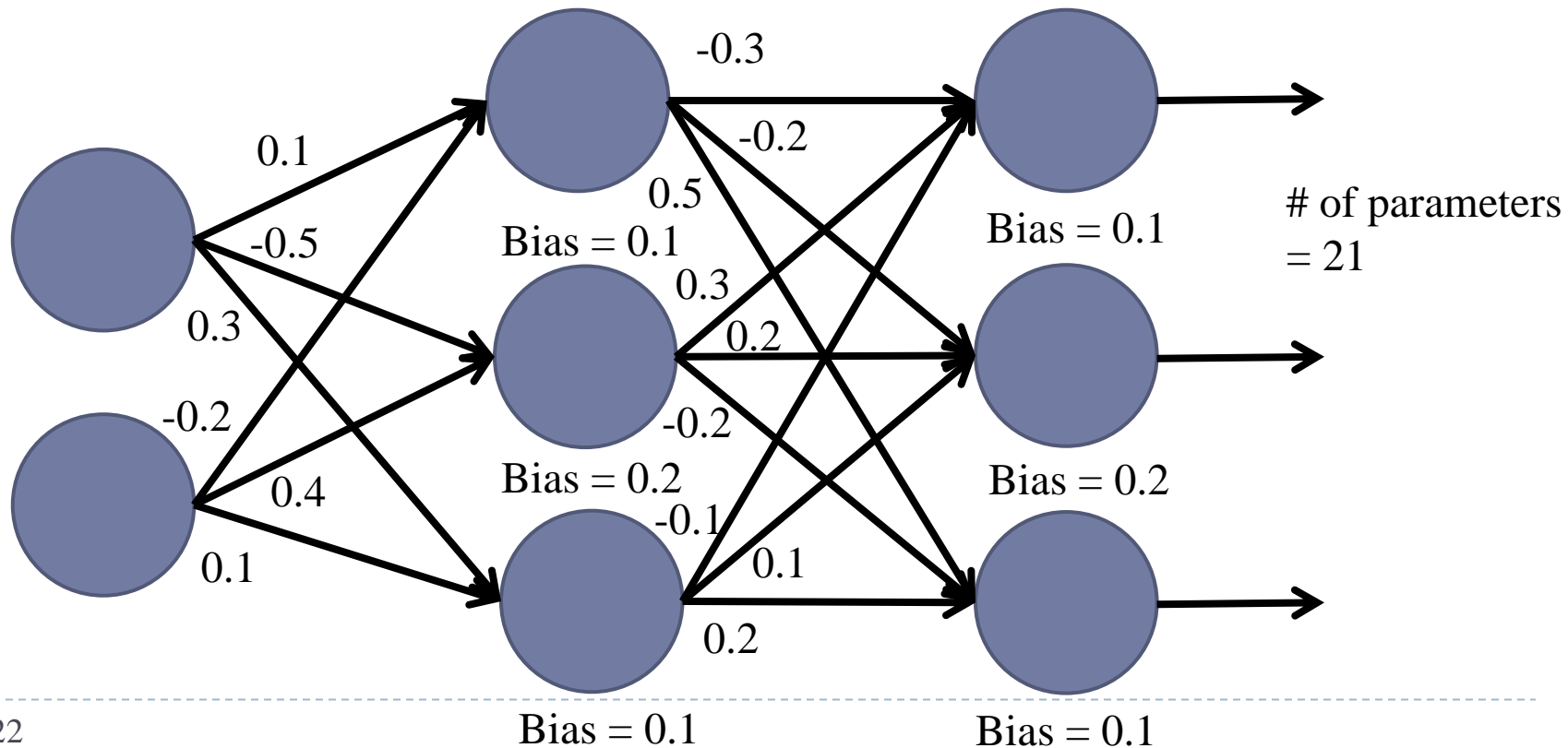


Sigmoid function

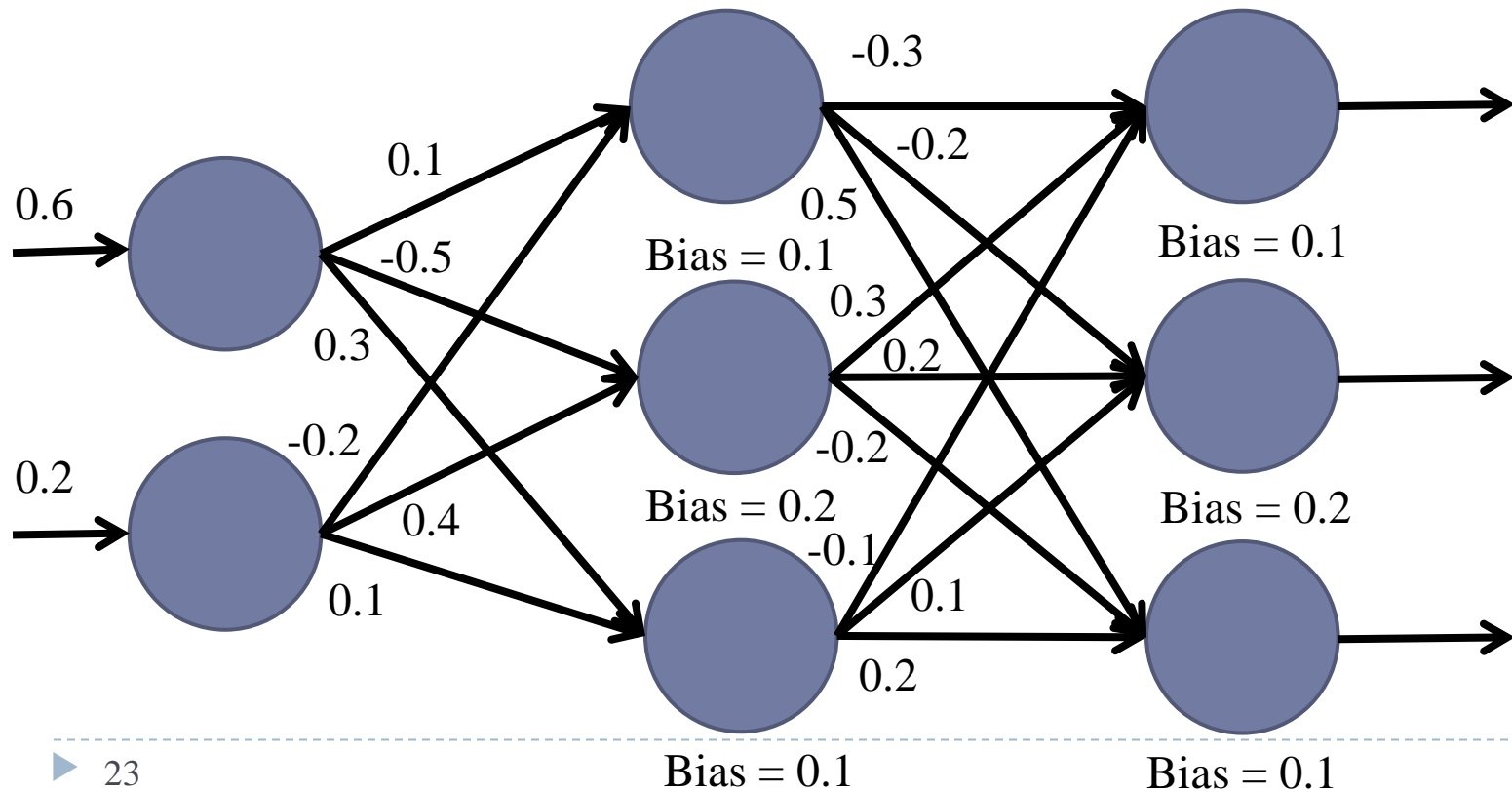


We usually use this now !

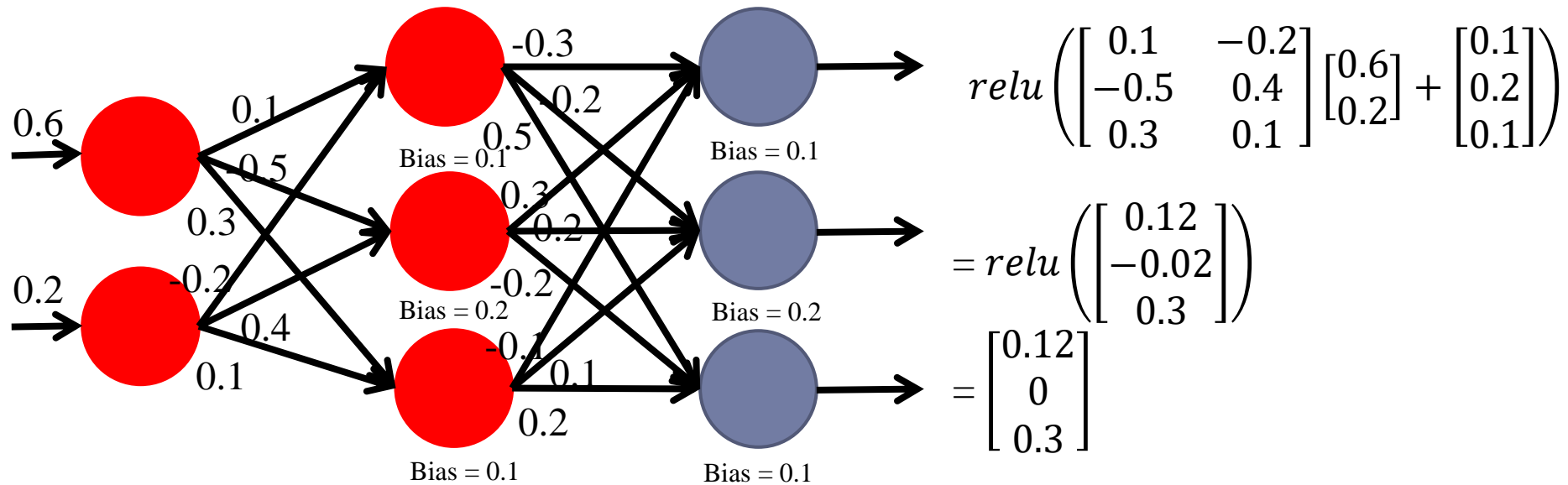
Example-initialization



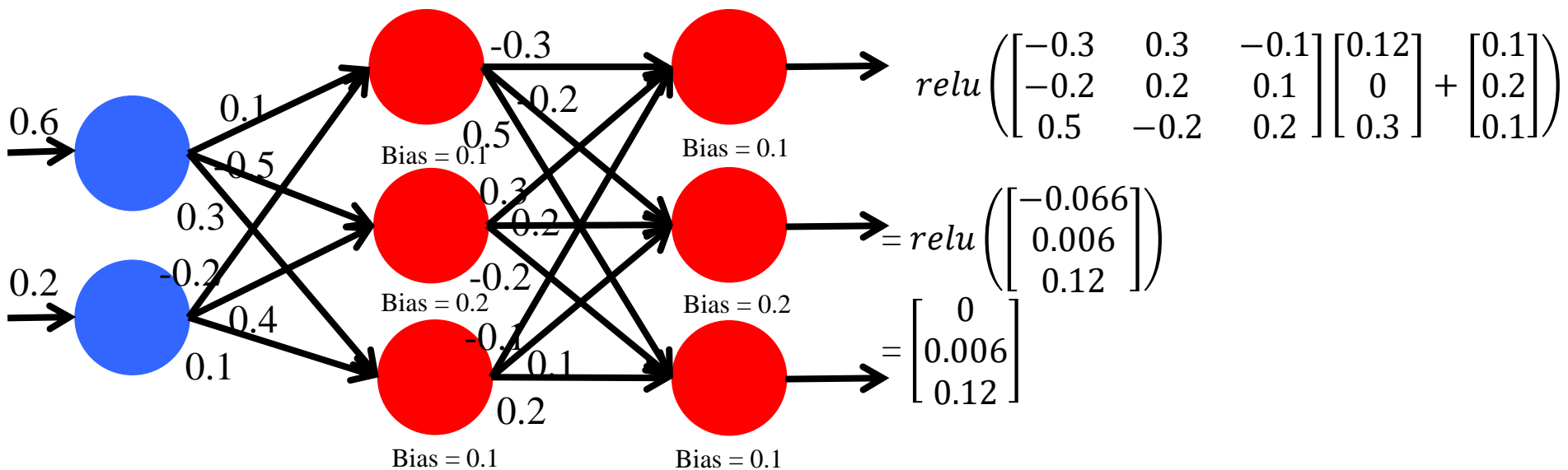
Example-feed data



Example-forward pass



Example-forward pass

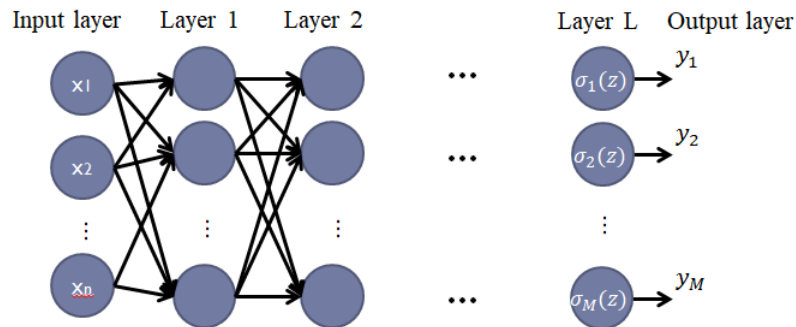


Define Loss Function

Loss Function

- ▶ There are many kinds of loss function
- ▶ Usually, it is a function that map multi-variables to a single value
- ▶ We will introduce two loss function in DNN
 - ▶ Mean square
 - ▶ Cross-entropy

What is one-hot encode



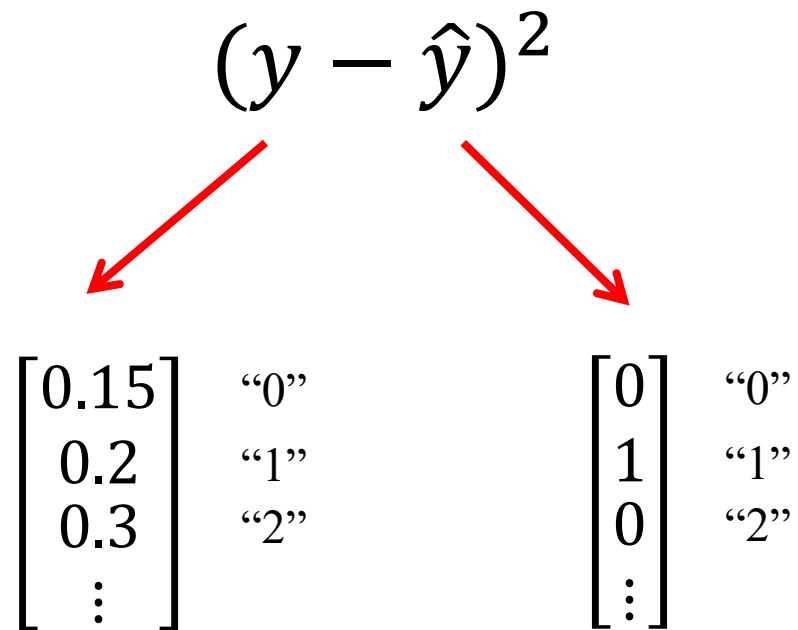
$$\begin{bmatrix} 0.15 \\ 0.2 \\ 0.3 \\ \vdots \end{bmatrix} \quad \begin{array}{l} \text{"0"} \\ \text{"1"} \\ \text{"2"} \\ \end{array}$$

Output of NN look like this

$$\begin{bmatrix} 0 \\ 1 \\ 0 \\ \vdots \end{bmatrix} \quad \begin{array}{l} \text{"0"} \\ \text{"1"} \\ \text{"2"} \\ \end{array}$$

What we want (one hot encode)

Mean Square



Cross-entropy with Softmax

► Information

- $\log\left(\frac{1}{p_i}\right)$ where p_i is probability of an event

Sun rises in the east tomorrow

It will rain tomorrow in Taiwan

Which is more informative?



Cross-entropy with Softmax

- ▶ Entropy
 - ▶ Expected value(mean) of information contained in each message
- ▶ Entropy can be seen as index of uncertainty
 - ▶ Bigger mean more chaos
- ▶ Cross-entropy
 - ▶ Measurement on the difference between two probability distribution
 - ▶ Different distribution apply on entropy
 - ▶ Cross-entropy is greater than entropy

$$H(y) = \sum_i y_i \log \frac{1}{y_i} = - \sum_i y_i \log y_i$$

Entropy

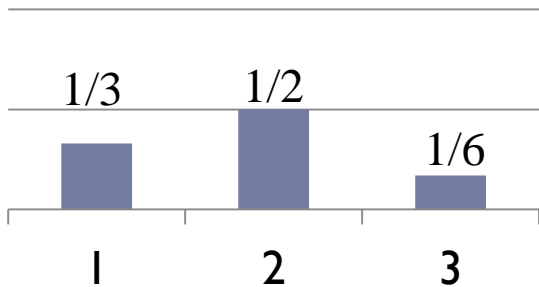
$$H(y) = - \sum_i y_i \log \hat{y}_i$$

Cross-entropy

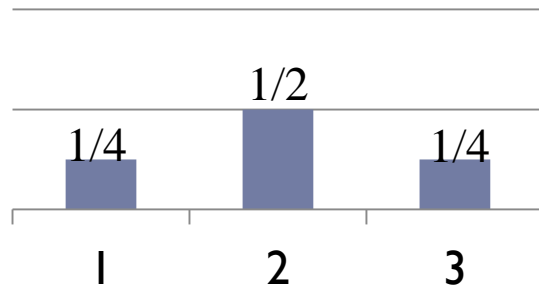


Example

Probability distribution 1



Probability distribution 2



Entropy on distribution 1

$$= 1/3 * \log(3) + 1/2 * \log(2) + 1/6 * \log(6)$$

Entropy on distribution 2

$$= 1/4 * \log(4) + 1/2 * \log(2) + 1/4 * \log(4)$$

Cross-entropy on distribution 1 over distribution 2

$$= 1/3 * \log(4) + 1/2 * \log(2) + 1/6 * \log(4)$$

Cross-entropy on distribution 2 over distribution 1

$$= 1/4 * \log(3) + 1/2 * \log(2) + 1/4 * \log(6)$$

Example

Entropy on distribution 1

$$= 1/3 * \log(3) + 1/2 * \log(2) + 1/6 * \log(6) \\ = 0.439$$

Entropy on distribution 2

$$= 1/4 * \log(4) + 1/2 * \log(2) + 1/4 * \log(4) \\ = 0.452$$

Cross-entropy on distribution 1 over distribution 2

$$= 1/3 * \log(4) + 1/2 * \log(2) + 1/6 * \log(4) = 0.456$$

Cross-entropy on distribution 2 over distribution 1

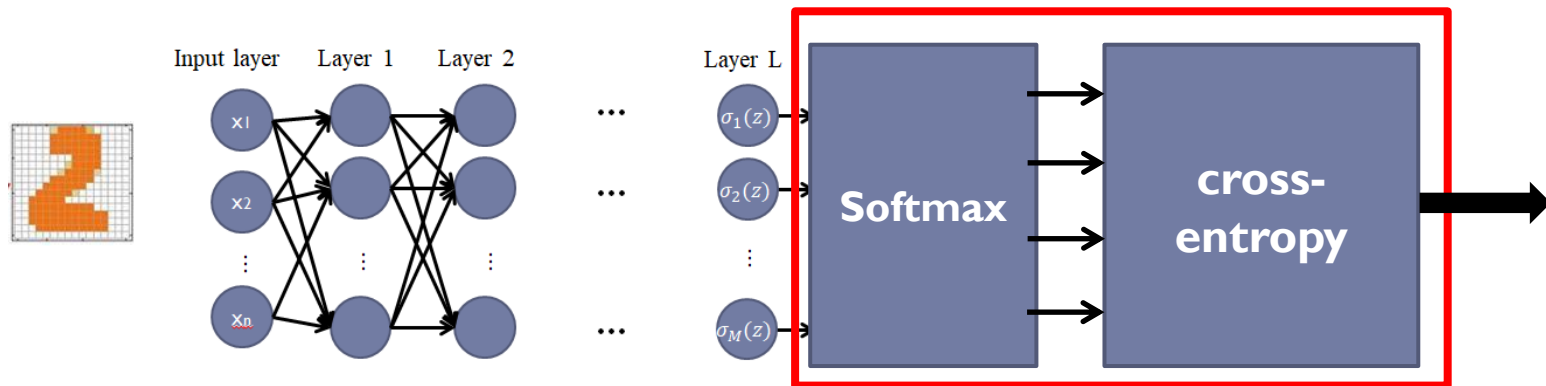
$$= 1/4 * \log(3) + 1/2 * \log(2) + 1/4 * \log(6) = 0.464$$

- Cross-entropy is greater than entropy
 - Cross-entropy on distribution 1 over 2 > Entropy on distribution 1
 - Cross-entropy on distribution 2 over 1 > Entropy on distribution 2
- If two distribution become closer
 - Value of cross-entropy is closer to entropy

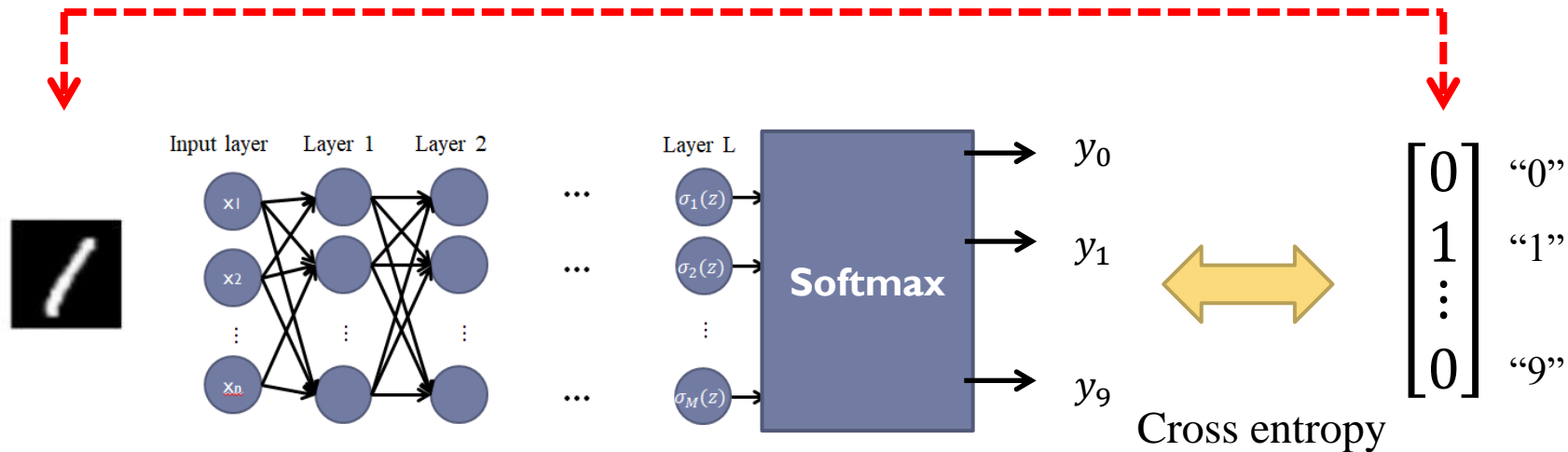
Cross-entropy with Softmax

- ▶ Cross-entropy usually come with softmax layer in NN
- ▶ Softmax function squash all of elements in vector to $[0, 1]$

$$\sigma(\mathbf{z})_j = \frac{e^{z_j}}{\sum_{k=1}^K e^{z_k}} \quad \text{for } j = 1, \dots, K.$$



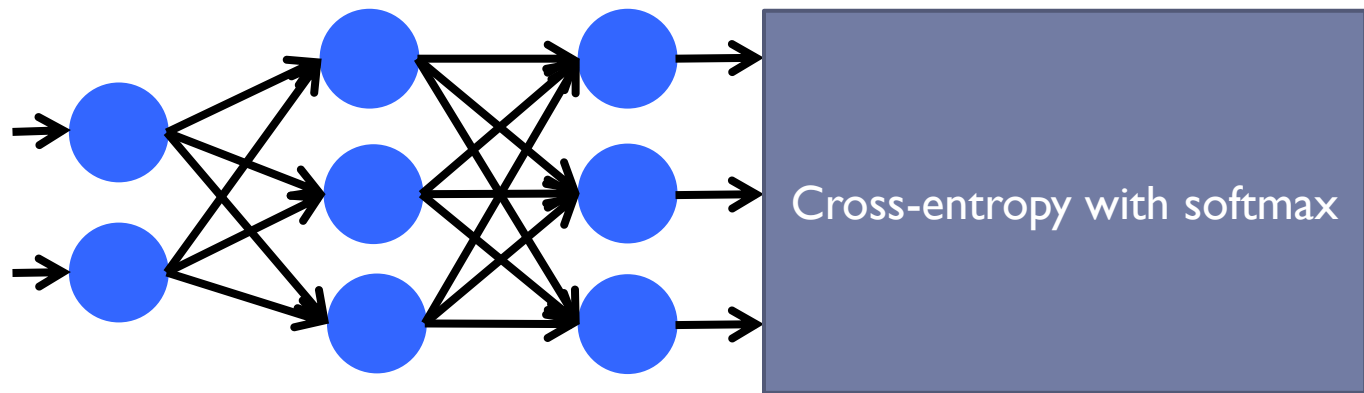
Cross-entropy with Softmax



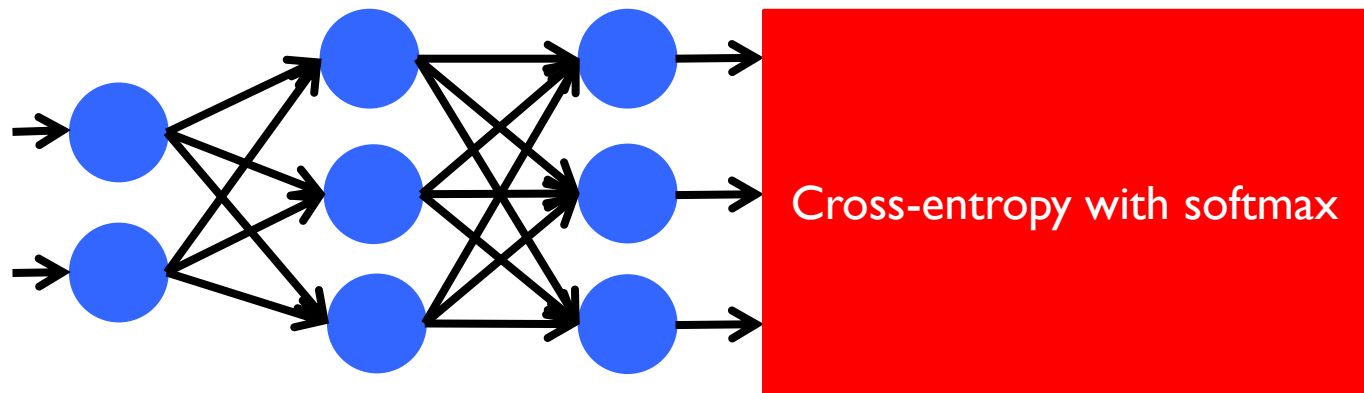
$$H(y) = - \sum_i y_i \log \hat{y}_i$$

$$Cost = -(0 * \log(y_0) + 1 * \log(y_1) + 0 * \log(y_2) + \dots + 0 * \log(y_9))$$

Example-forward pass



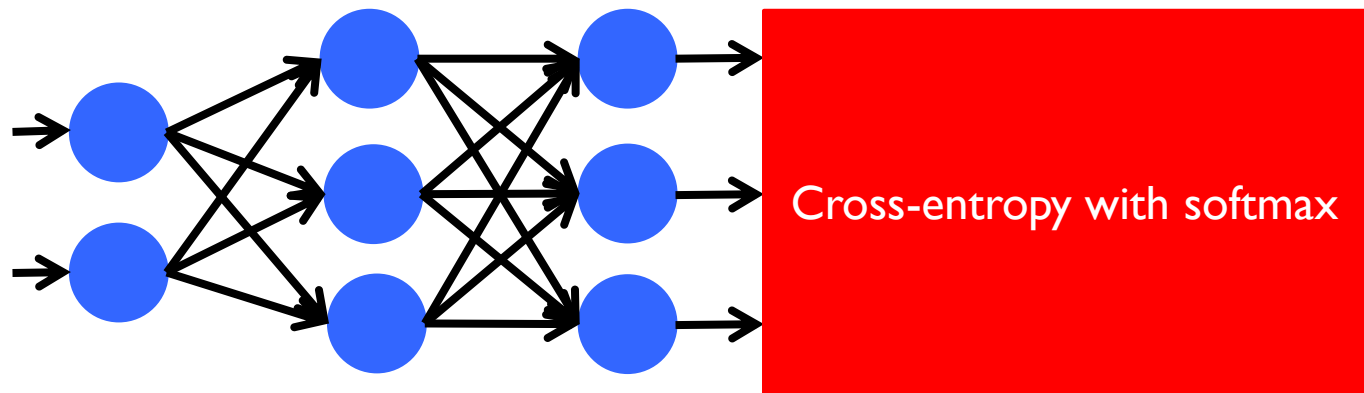
Example-forward pass



$$\text{Softmax}\left(\begin{bmatrix} 0 \\ 0.006 \\ 0.12 \end{bmatrix}\right) = \begin{bmatrix} 0.319 \\ 0.321 \\ 0.36 \end{bmatrix}$$

$$\sigma(\mathbf{z})_j = \frac{e^{z_j}}{\sum_{k=1}^K e^{z_k}} \quad \text{for } j = 1, \dots, K.$$

Example-forward pass



What we expect
(label)

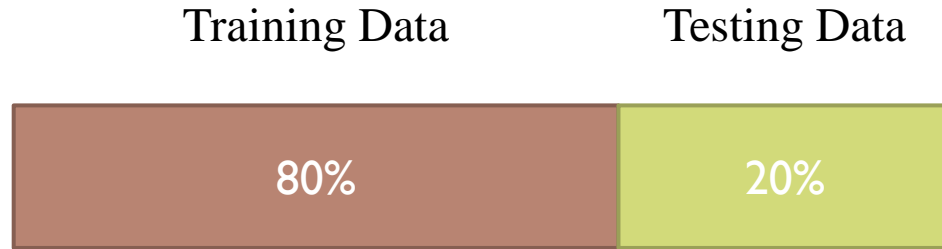
$$\begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix}$$


$$\begin{aligned} & - 0 * \ln(0.319) - 1 * \ln(0.321) - 0 * \ln(0.36) \\ & = 1.1363 \end{aligned}$$

$$- \sum_{i=0}^{class \#} \hat{y}_i \ln(y_i)$$

This is large at the beginning. During training, this should decrease.

How to Feed data



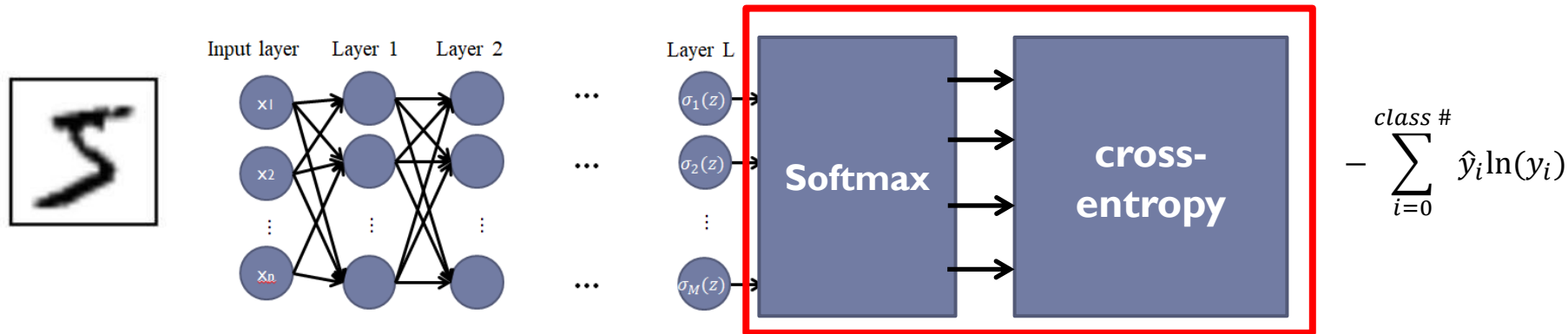
x:  **y: "2" (label)**

How to Feed data

How to feed data	Mean Square	Cross-entropy
All data at a time	$\frac{1}{N} \sum_{i=1}^N (y_i - \hat{y}_i)^2$	$\frac{1}{N} \sum_{j=1}^N \left(- \sum_{i=0}^{\text{class \#}} \hat{y}_i \ln(y_i) \right)$
One data at a time	$(y - \hat{y})$	$- \sum_{i=0}^{\text{class \#}} \hat{y}_i \ln(y_i)$
Batch of data a time ($B < N$)	$\frac{1}{B} \sum_{i=1}^B (y_i - \hat{y}_i)^2$	$\frac{1}{B} \sum_{j=1}^B \left(- \sum_{i=0}^{\text{class \#}} \hat{y}_i \ln(y_i) \right)$

How to Feed data

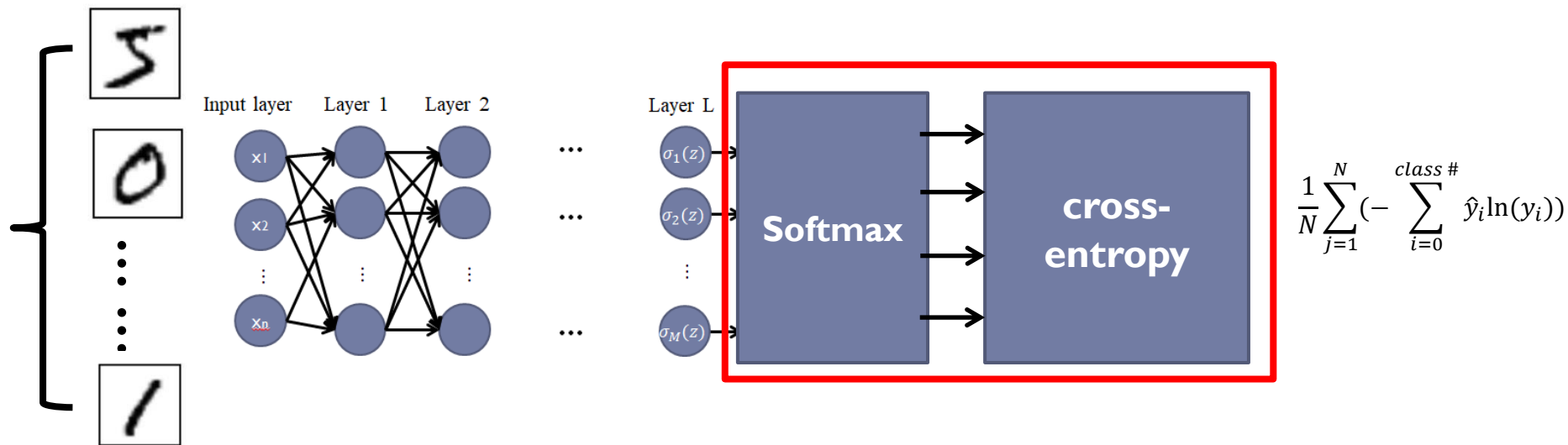
Pick one training data at a time



How to Feed data

Pick all training data at a time

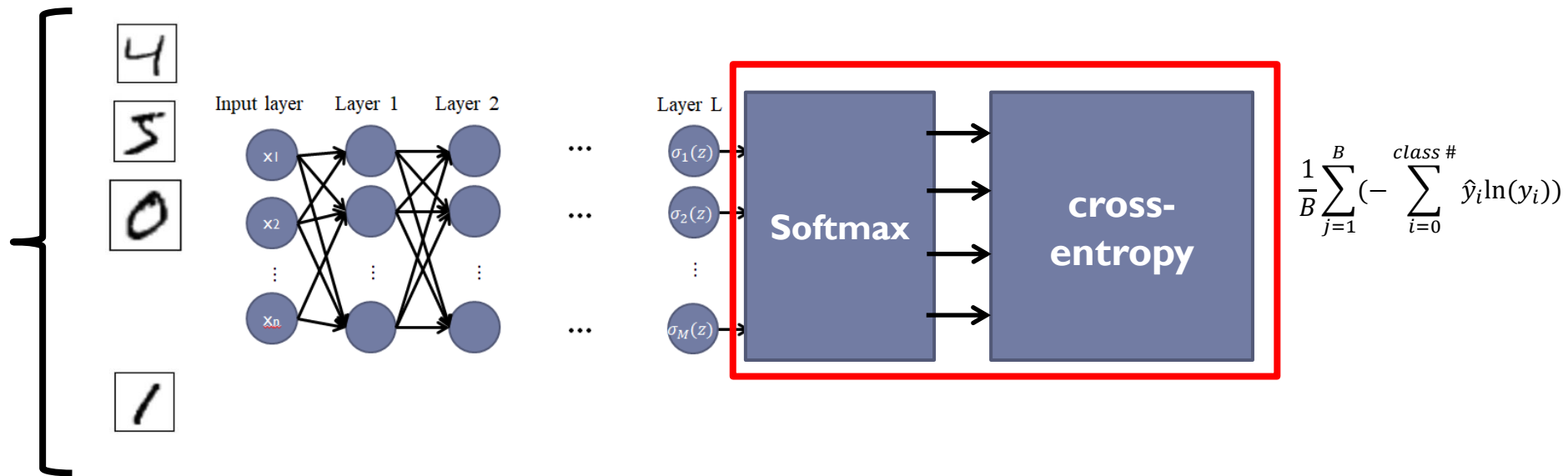
All training data



How to Feed data

A batch of data
(you can define)

Pick a batch of data at a time



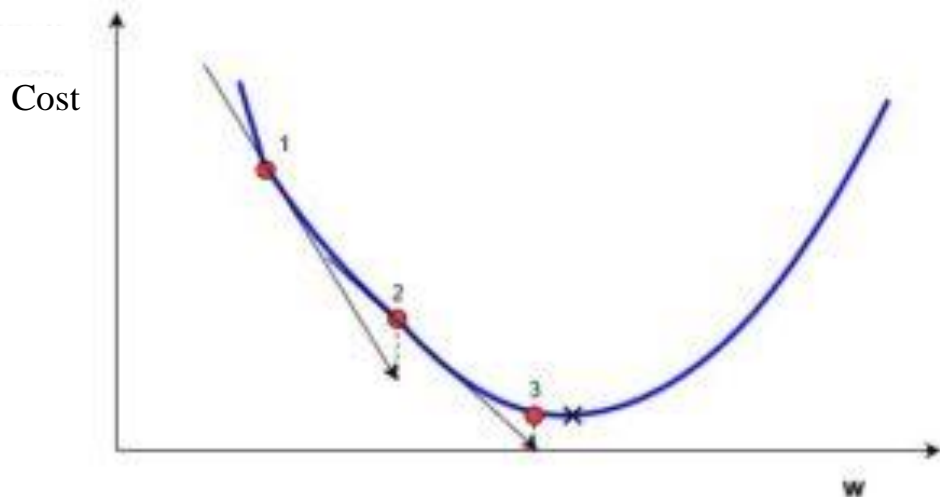
Optimization

Optimization

- ▶ We will introduce these Optimization methods
 - ▶ Gradient decent
 - ▶ Gradient decent with moment
 - ▶ Adagrad
 - ▶ RMSprop
 - ▶ Adam

Gradient Descent

- An algorithm that find the minimum of a function



Randomly select θ_1 as start point

$$\text{Compute } \frac{dC(\theta_1)}{d\theta}$$

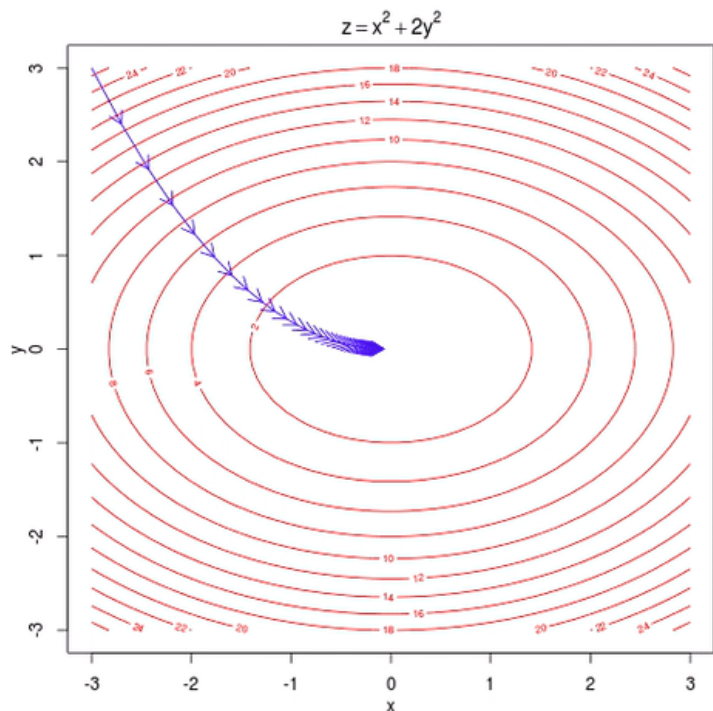
$$\theta_2 \leftarrow \theta_1 - \eta \frac{dC(\theta_1)}{d\theta}$$

$$\text{Compute } \frac{dC(\theta_2)}{d\theta}$$

$$\theta_3 \leftarrow \theta_2 - \boxed{\eta} \frac{dC(\theta_2)}{d\theta}$$

Learning rate

Gradient Descent



$$\theta = \begin{bmatrix} x \\ y \end{bmatrix} \quad \nabla C(\theta) = \begin{bmatrix} dz/dx \\ dz/dy \end{bmatrix}$$

Randomly select θ_1 as start point

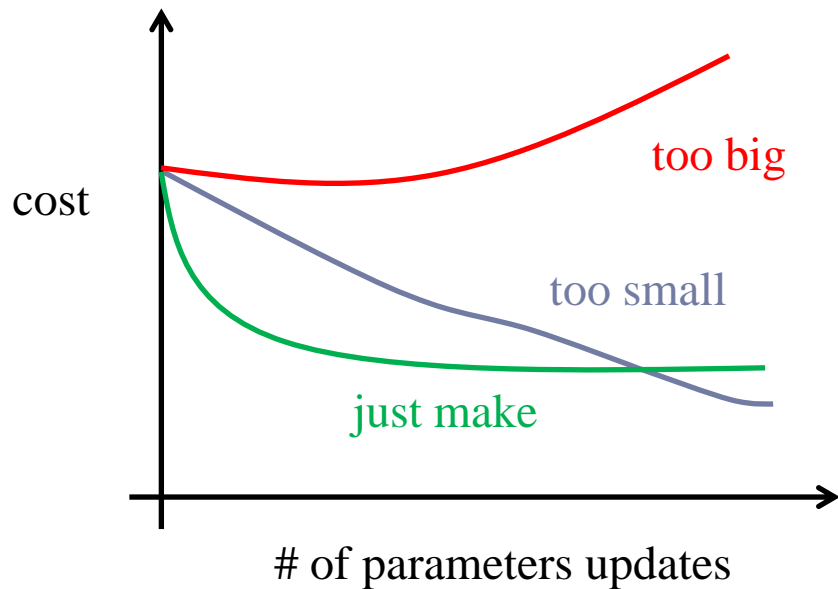
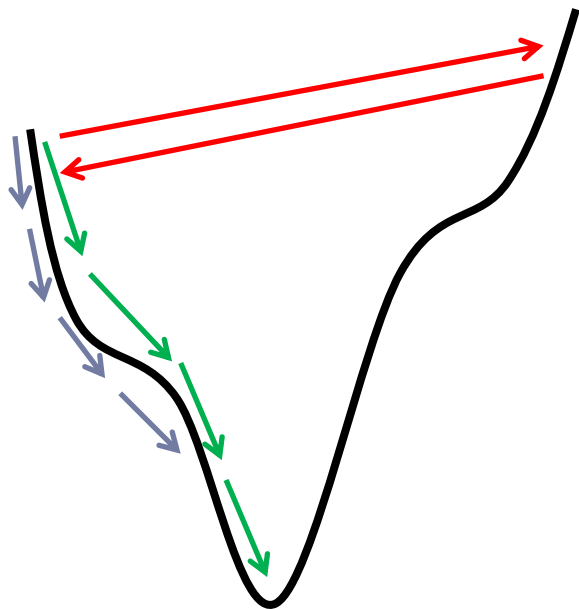
Compute $\nabla C(\theta_1)$

$$\theta_2 \leftarrow \theta_1 - \eta \nabla C(\theta_1)$$

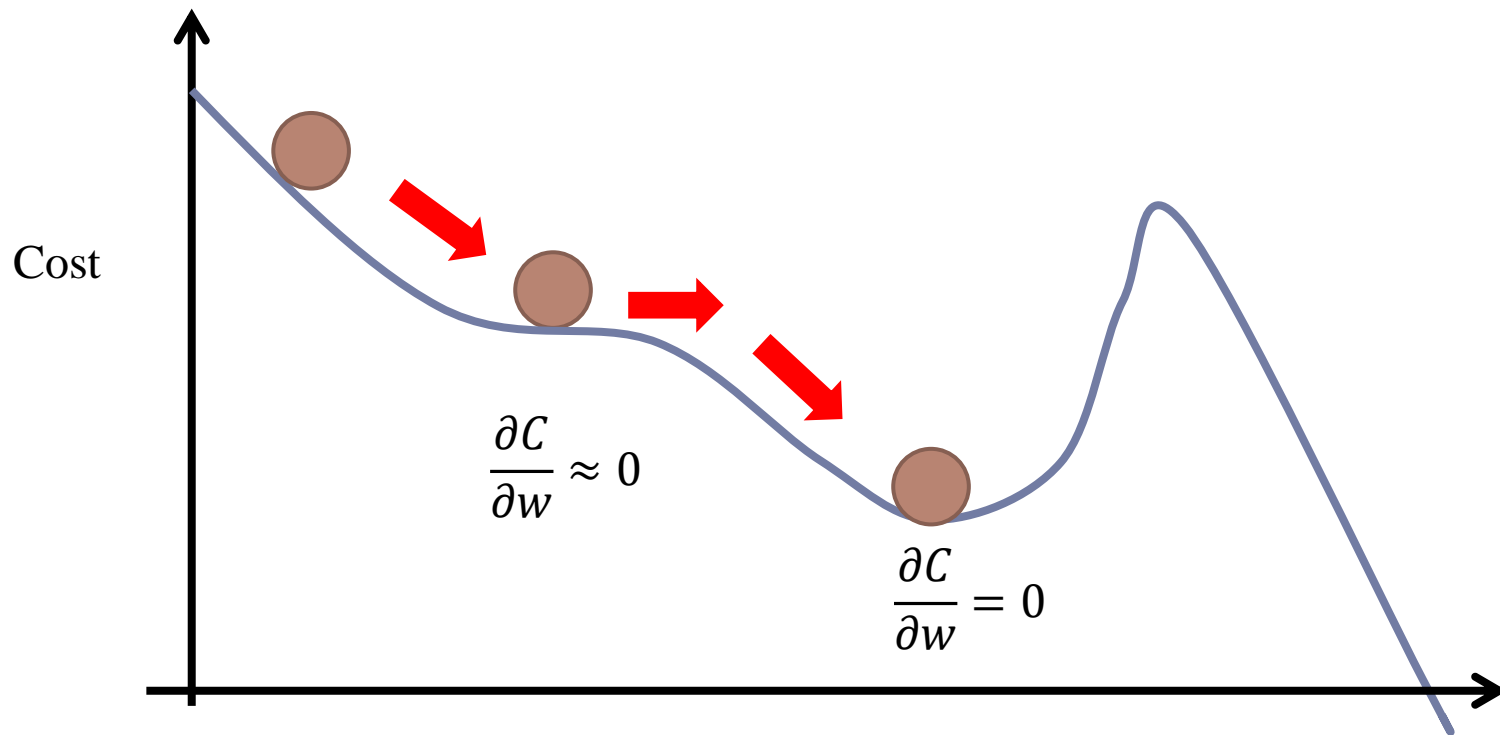
Compute $\nabla C(\theta_2)$

$$\theta_3 \leftarrow \theta_2 - \eta \nabla C(\theta_2)$$

Gradient Descent



Gradient Descent



Gradient Descent with Momentum

Randomly select θ_1 as start point

Compute $\nabla\theta_1$

$$\theta_2 \leftarrow \theta_1 - \eta \nabla\theta_1$$

Compute $\nabla\theta_2$

$$\theta_3 \leftarrow \theta_2 - \eta \nabla\theta_2$$

\vdots

Without momentum

*Randomly select θ_1 as start point
, initialize $v_1 = 0$*

Compute $\nabla\theta_1, v_2 = \lambda v_1 - \eta \nabla\theta_1$

$$\theta_2 \leftarrow \theta_1 + v_2$$

Compute $\nabla\theta_2, v_3 = \lambda v_2 - \eta \nabla\theta_2$

$$\theta_3 \leftarrow \theta_2 + v_3$$

\vdots

With momentum

Gradient Descent

- ▶ Drawback of gradient descent
 - ▶ Learning rate would not decay over time
 - ▶ Direction of learning rate is fixed
- ▶ Adaptive learning rate is needed

Adagrad

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

$$\sigma^0 = \sqrt{(g^0)^2}$$

$$w^2 \leftarrow w^1 - \frac{\eta^1}{\sigma^1} g^1$$

$$\sigma^1 = \sqrt{\frac{1}{2} [(g^0)^2 + (g^1)^2]}$$

$$w^3 \leftarrow w^2 - \frac{\eta^2}{\sigma^2} g^2$$

$$\sigma^2 = \sqrt{\frac{1}{3} [(g^0)^2 + (g^1)^2 + (g^2)^2]}$$

\vdots

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

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

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

RMSProp

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

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

$$w^3 \leftarrow w^2 - \frac{\eta}{\sigma^2} g^2 \quad \sigma^2 = \sqrt{\alpha(\sigma^1)^2 + (1 - \alpha)(g^2)^2}$$

\vdots

$$w^{t+1} \leftarrow w^t - \frac{\eta}{\sigma^t} g^t \quad \underline{\sigma^t = \sqrt{\alpha(\sigma^{t-1})^2 + (1 - \alpha)(g^t)^2}}$$

Adam

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. g_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 β_1^t and β_2^t we denote β_1 and β_2 to the power t .

Require: α : Stepsize

Require: $\beta_1, \beta_2 \in [0, 1)$: Exponential decay rates for the moment estimates

Require: $f(\theta)$: Stochastic objective function with parameters θ

Require: θ_0 : Initial parameter vector

$m_0 \leftarrow 0$ (Initialize 1st moment vector) \rightarrow for momentum

$v_0 \leftarrow 0$ (Initialize 2nd moment vector) \rightarrow for RMSprop

$t \leftarrow 0$ (Initialize timestep)

while θ_t not converged **do**

$t \leftarrow t + 1$

$g_t \leftarrow \nabla_{\theta} f_t(\theta_{t-1})$ (Get gradients w.r.t. stochastic objective at timestep t)

$m_t \leftarrow \beta_1 \cdot m_{t-1} + (1 - \beta_1) \cdot g_t$ (Update biased first moment estimate)

$v_t \leftarrow \beta_2 \cdot v_{t-1} + (1 - \beta_2) \cdot g_t^2$ (Update biased second raw moment estimate)

$\hat{m}_t \leftarrow m_t / (1 - \beta_1^t)$ (Compute bias-corrected first moment estimate)

$\hat{v}_t \leftarrow v_t / (1 - \beta_2^t)$ (Compute bias-corrected second raw moment estimate)

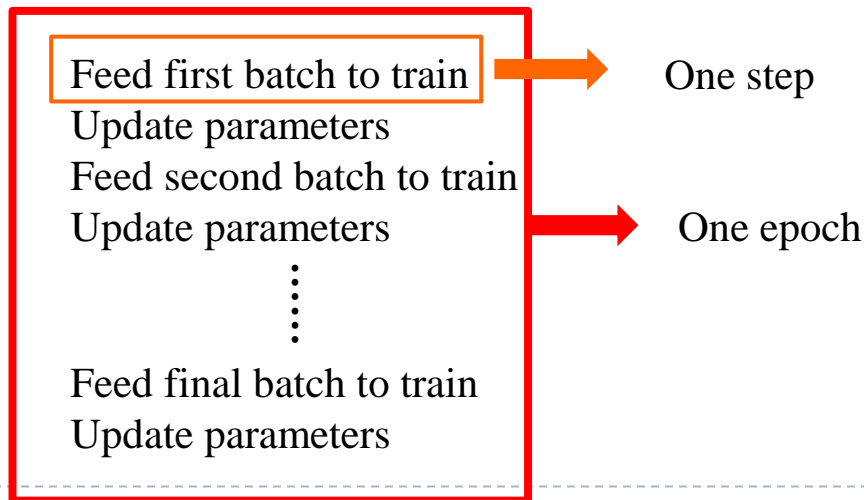
$\theta_t \leftarrow \theta_{t-1} - \alpha \cdot \hat{m}_t / (\sqrt{\hat{v}_t} + \epsilon)$ (Update parameters)

end while

return θ_t (Resulting parameters)

What is one epoch/step

- ▶ One epoch
 - ▶ One pass of all the training data
- ▶ One step
 - ▶ Pass a batch of training data (batch size is user defined)



Backpropagation

- ▶ An efficient way to compute gradient given a set of variable

$$\frac{\partial \mathcal{C}}{\partial w_{ij}^l} \quad ?$$

Backpropagation

$$y = f(x) = \sigma(W^L \dots \sigma(W^2 \sigma(W^1 X + b^1) + b^2) \dots + b^L)$$



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

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

$$z^2 = W^2 a^1 + b^2$$

$$a^2 = \sigma(z^2)$$

\vdots

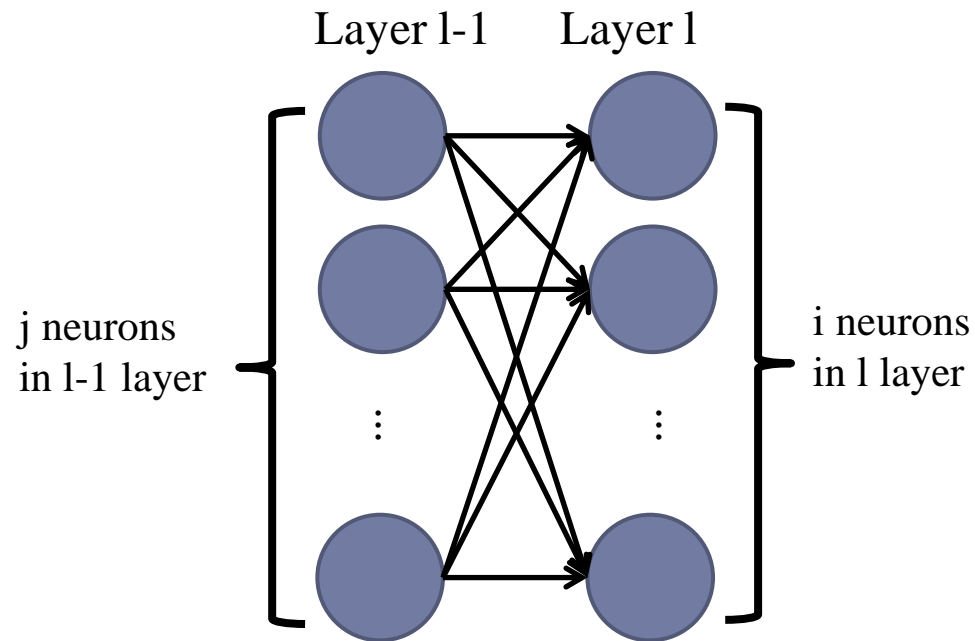
$$z^l = W^l a^{l-1} + b^l$$

$$a^l = \sigma(z^l)$$

$$\frac{\partial C}{\partial w_{ij}^l} = \frac{\partial C}{\partial z_i^l} * \frac{\partial z_i^l}{\partial w_{ij}^l}$$

1. Calculate $\frac{\partial z_i^l}{\partial w_{ij}^l}$
2. Calculate $\frac{\partial C}{\partial z_i^l}$ (**error signal** δ_i^l)

Backpropagation



$$\frac{\partial z_i^l}{\partial w_{ij}^l}$$

if $l = 1$ (input layer \rightarrow layer 1)

$$z_i^1 = \sum_j w_{ij}^1 x_j + b_i^1 \quad \frac{\partial z_i^1}{\partial w_{ij}^1} = x_j$$

if $l > 1$ (layer $l - 1 \rightarrow$ layer 1)

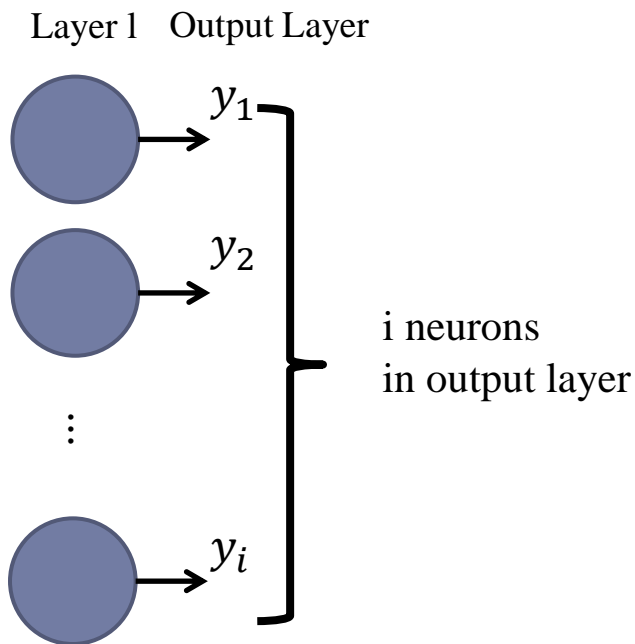
$$z_i^l = \sum_j w_{ij}^l a_j^{l-1} + b_i^l \quad \frac{\partial z_i^l}{\partial w_{ij}^l} = a_j^{l-1}$$

Backpropagation

$$\frac{\partial C}{\partial z_i^l} \quad (\text{error signal } \delta_i^l)$$

1. Compute δ^L (L layer error signal)
2. Compute relation between δ^l and δ^{l+1}

Backpropagation

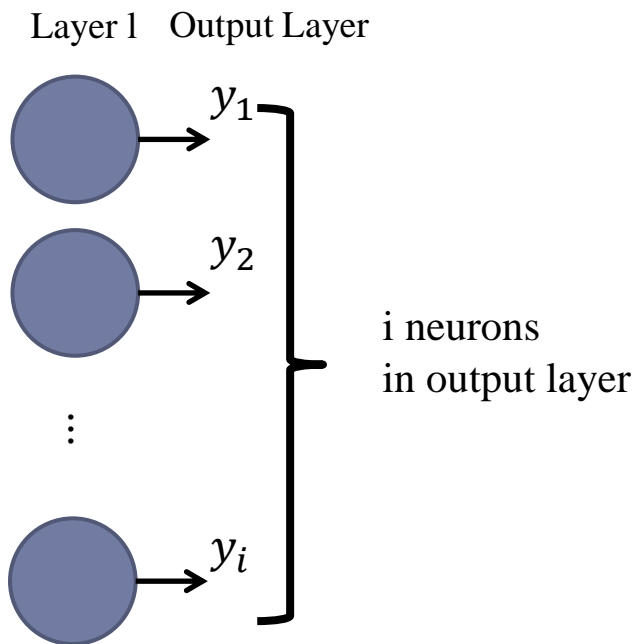


$$\frac{\partial C}{\partial z_i^l} \quad (\text{error signal } \delta_i^l)$$

1. Compute δ^L (L layer error signal)

$$\delta_i^L = \frac{\partial C}{\partial z_i^L} = \frac{\partial y_i}{\partial z_i^L} * \frac{\partial C}{\partial y_i} = \sigma'(z_i^L) * \frac{\partial C}{\partial y_i}$$

Backpropagation



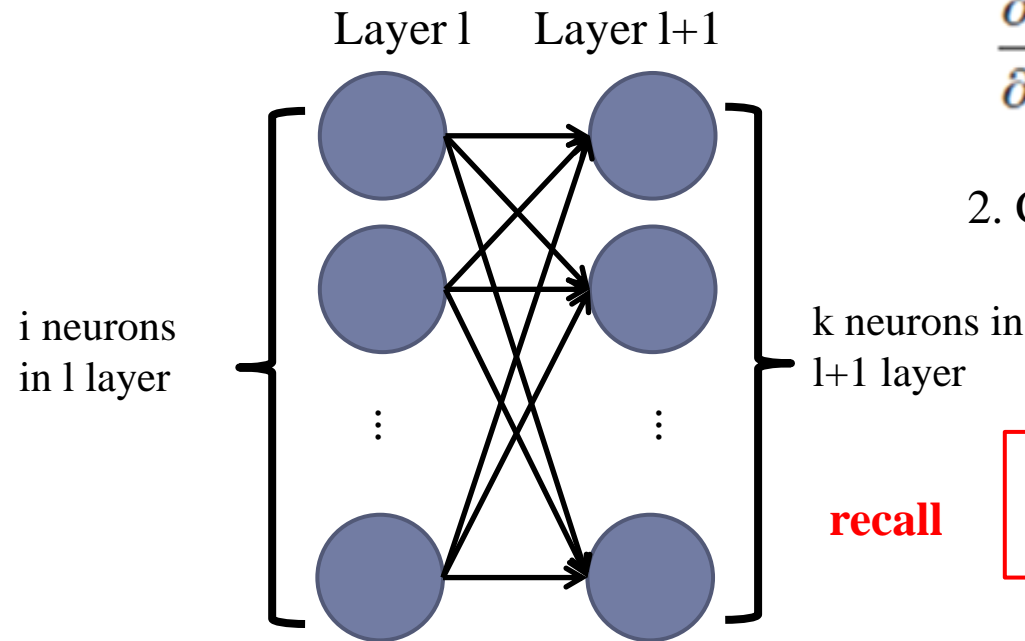
$$\frac{\partial C}{\partial z_i^l} \quad (\text{error signal } \delta_i^l)$$

1. Compute δ^L (L layer error signal)

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

$$\sigma'(z^L) = \begin{bmatrix} \sigma'(z_1^L) \\ \sigma'(z_2^L) \\ \vdots \\ \sigma'(z_n^L) \end{bmatrix} \quad \nabla C'(y) = \begin{bmatrix} \frac{\partial C}{\partial y_1} \\ \frac{\partial C}{\partial y_2} \\ \vdots \\ \frac{\partial C}{\partial y_n} \end{bmatrix}$$

Backpropagation



$$\frac{\partial C}{\partial z_i^l} \quad (\text{error signal } \delta_i^l)$$

2. Compute relation between δ^l and δ^{l+1}

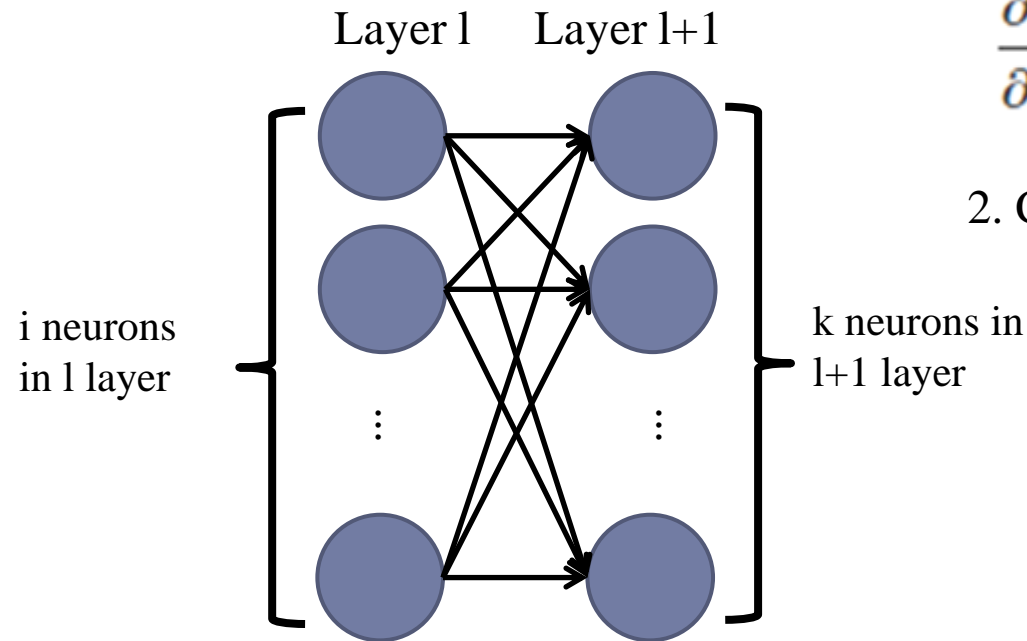
$$\delta_i^l = \frac{\partial C}{\partial z_i^l} = \frac{\partial a_i^l}{\partial z_i^l} \sum_k \frac{\partial z_k^{l+1}}{\partial a_i^l} \frac{\partial C}{\partial z_k^{l+1}}$$

recall

$$\frac{\partial a_i^l}{\partial z_i^l} = \sigma'(z_i^l), \quad \frac{\partial z_k^{l+1}}{\partial a_i^l} = w_{ki}^{l+1}, \quad \frac{\partial C}{\partial z_k^{l+1}} = \delta_k^{l+1}$$

$$\delta_i^l = \sigma'(z_i^l) \sum_k w_{ki}^{l+1} \delta_k^{l+1}$$

Backpropagation



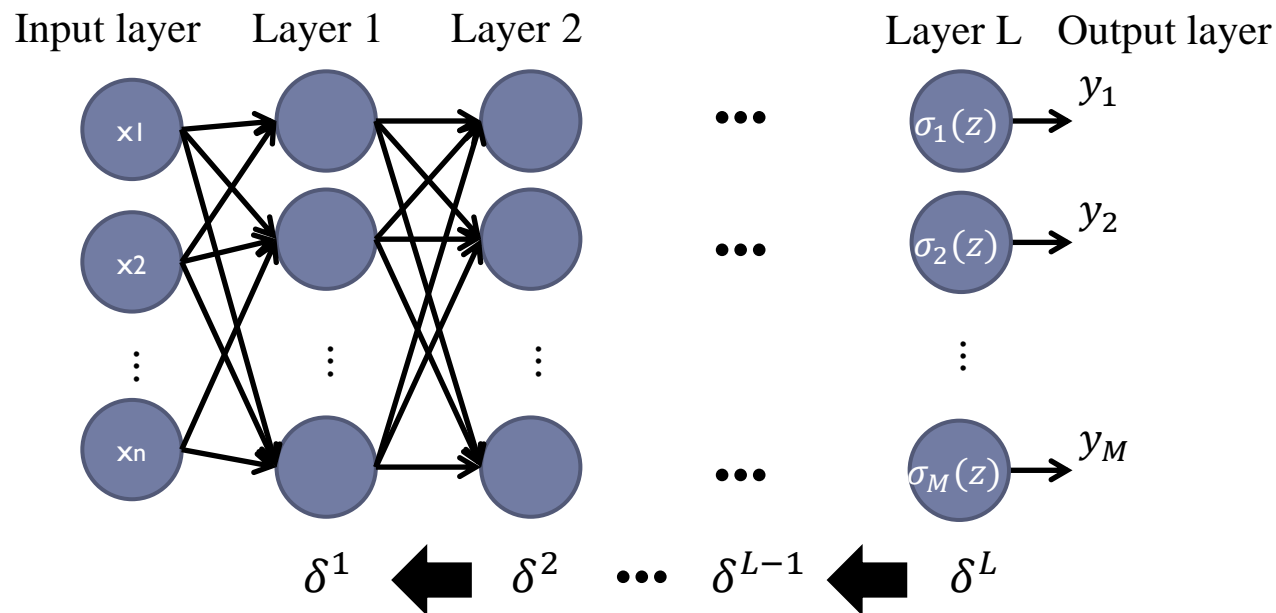
$$\frac{\partial C}{\partial z_i^l} \quad (\text{error signal } \delta_i^l)$$

2. Compute relation between δ^l and δ^{l+1}

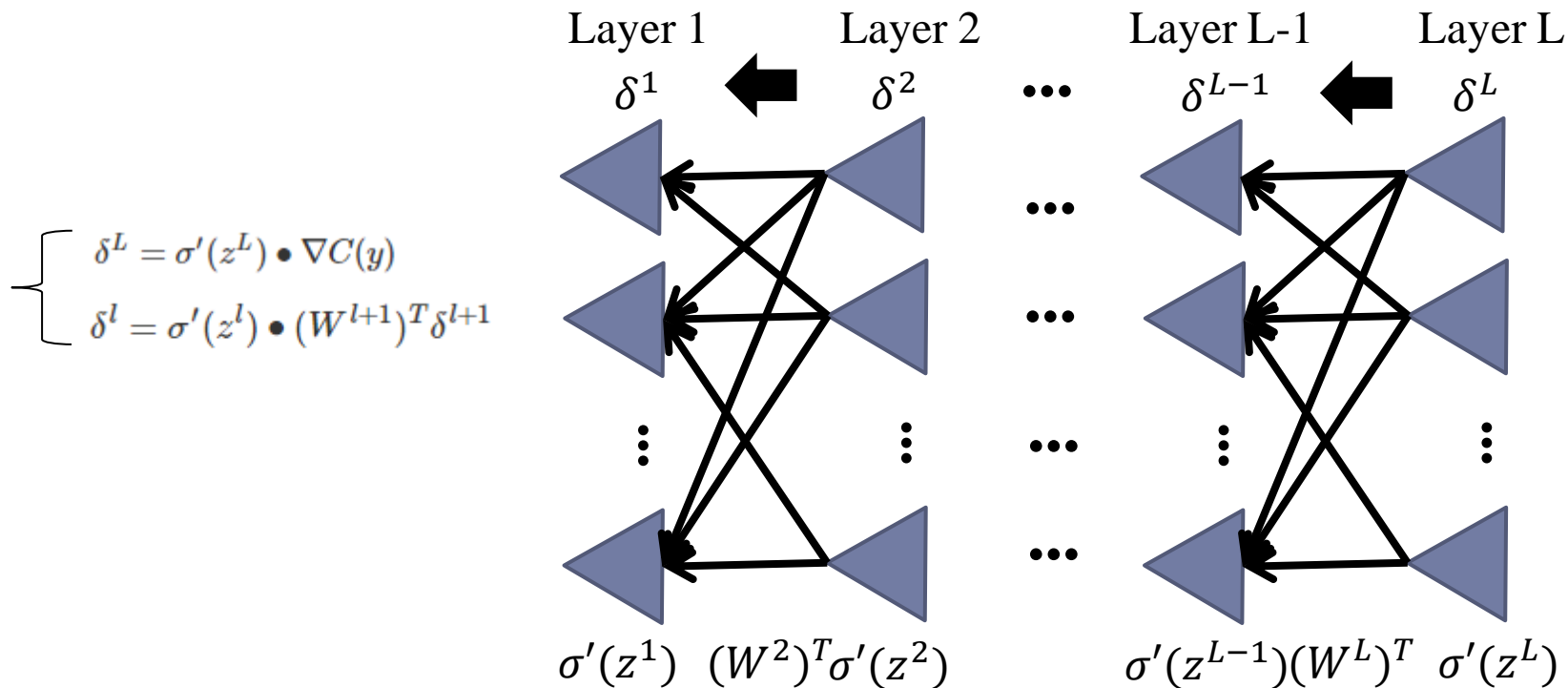
$$\delta^l = \sigma'(z^l) \bullet (W^{l+1})^T \delta^{l+1}$$

Backpropagation


$$\begin{cases} \delta^L = \sigma'(z^L) \bullet \nabla C(y) \\ \delta^l = \sigma'(z^l) \bullet (W^{l+1})^T \delta^{l+1} \end{cases}$$



Backpropagation



Backpropagation

$$\frac{\partial C}{\partial w_{ij}^l} = \frac{\partial C}{\partial z_i^l} * \frac{\partial z_i^l}{\partial w_{ij}^l}$$


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

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

\vdots

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

\vdots

if $l = 1$ (input layer \rightarrow layer 1)

$$z_i^1 = \sum_j w_{ij}^1 x_j^r + b_i^1 \quad \frac{\partial z_i^1}{\partial w_{ij}^1} = x_j$$

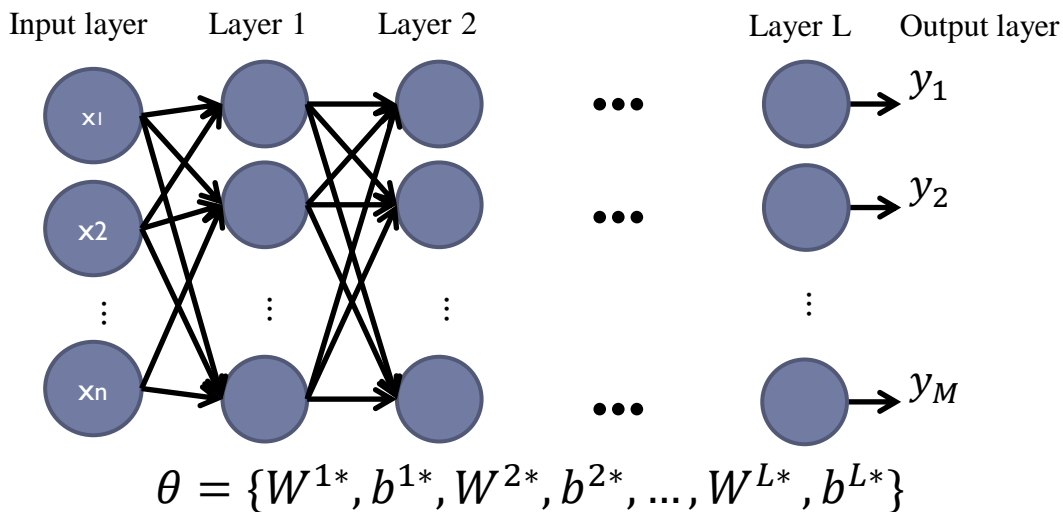
if $l > 1$ (layer $l - 1 \rightarrow$ layer 1)

$$z_i^l = \sum_j w_{ij}^l a_j^{l-1} + b_i^l \quad \frac{\partial z_i^l}{\partial w_{ij}^l} = a_j^{l-1}$$

Predict/Validate Result

Predict/Validate Result

- ▶ “*” mean a better set of parameters we have found
- ▶ Use test data to find model accuracy (supervised learning)
 - ▶ # correct predict / # total data



Overfitting



Training error is going lower but testing error is not

Overfitting

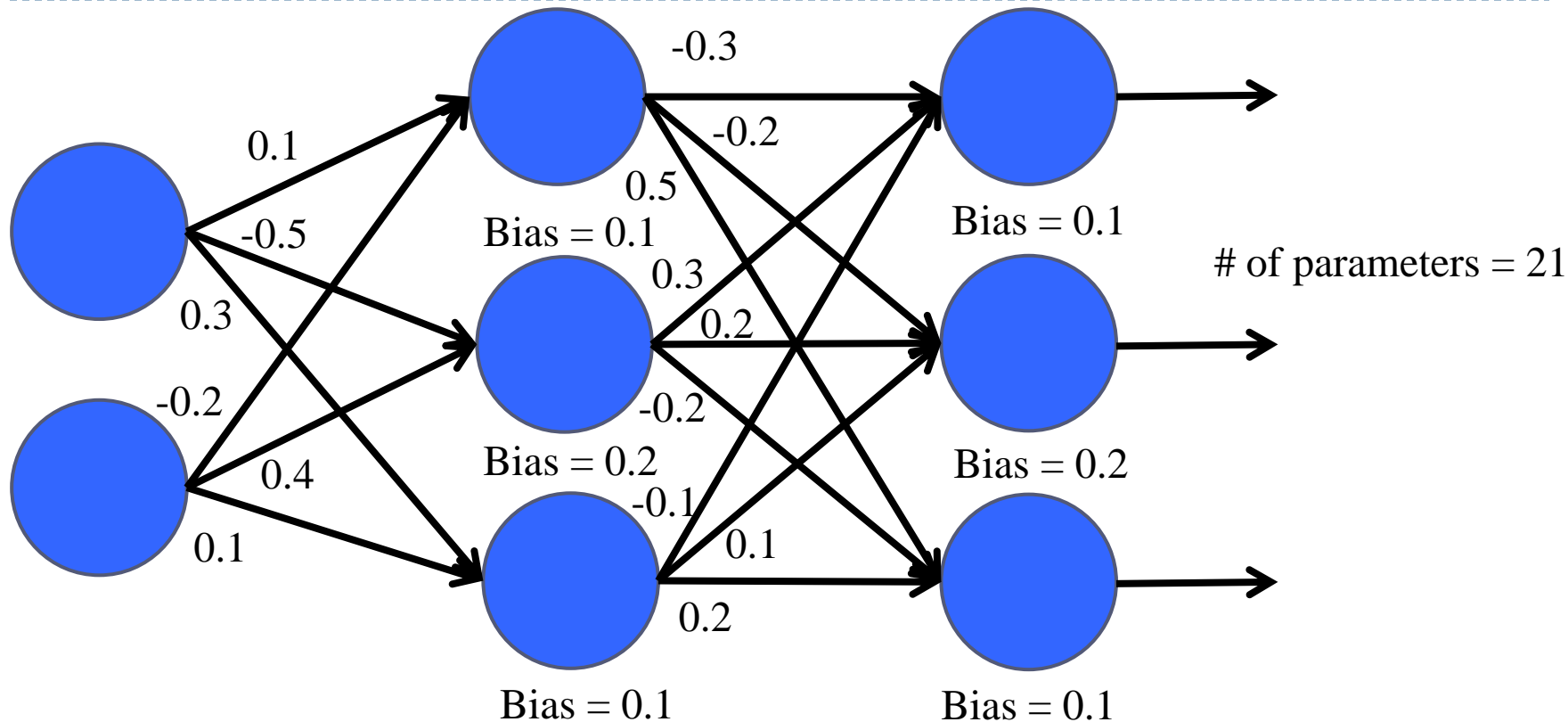
- ▶ **Prevent overfitting**
 - ▶ Use more data
 - ▶ Stronger regularization
 - ▶ Data augmentation
 - ▶ Reduce complexity of model

Quick Recap in this Lecture

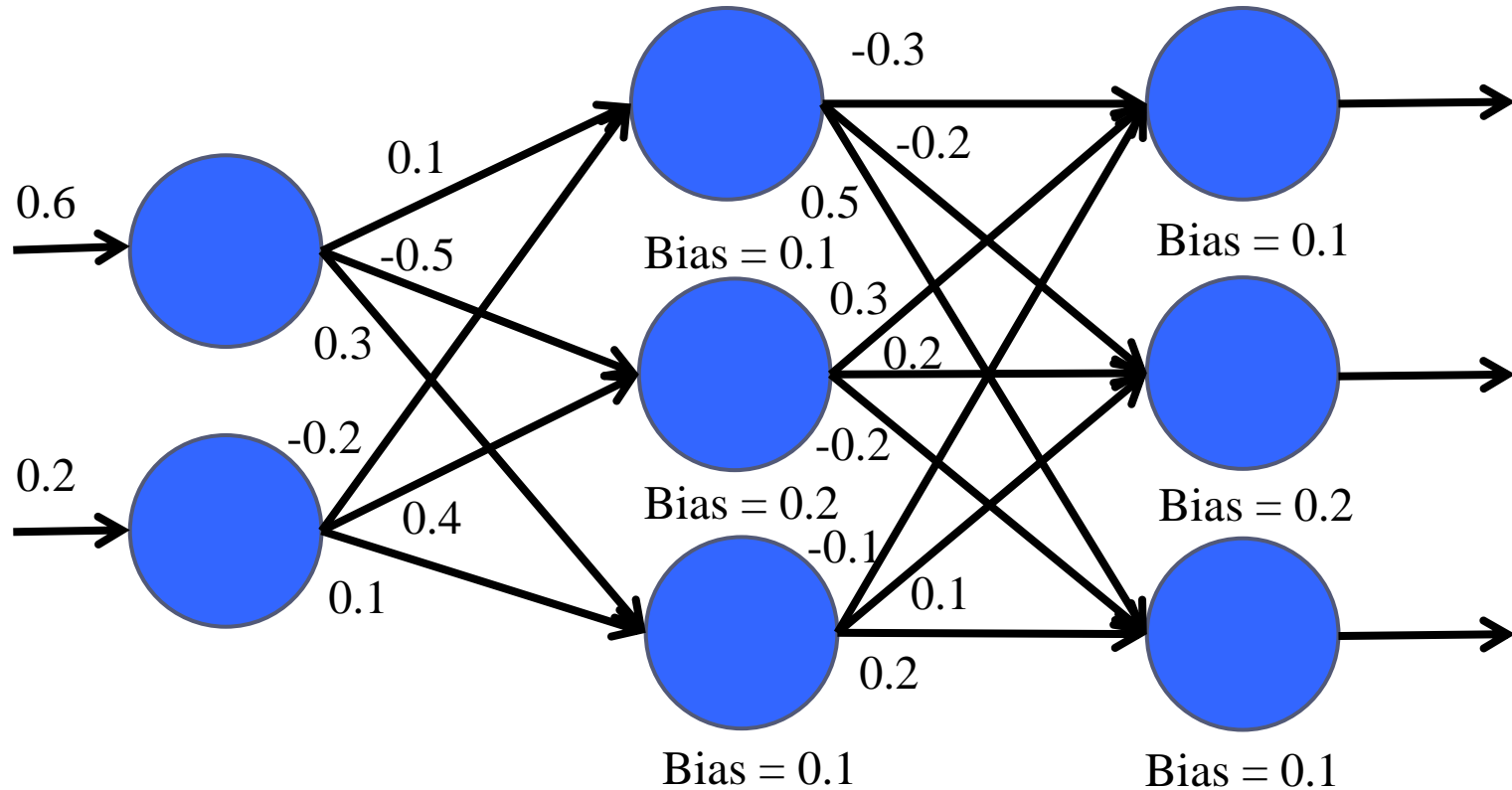
1. Build DNN model
2. Define loss (mean square/cross entropy with softmax)
3. Optimization (backpropagation)
4. Validate result



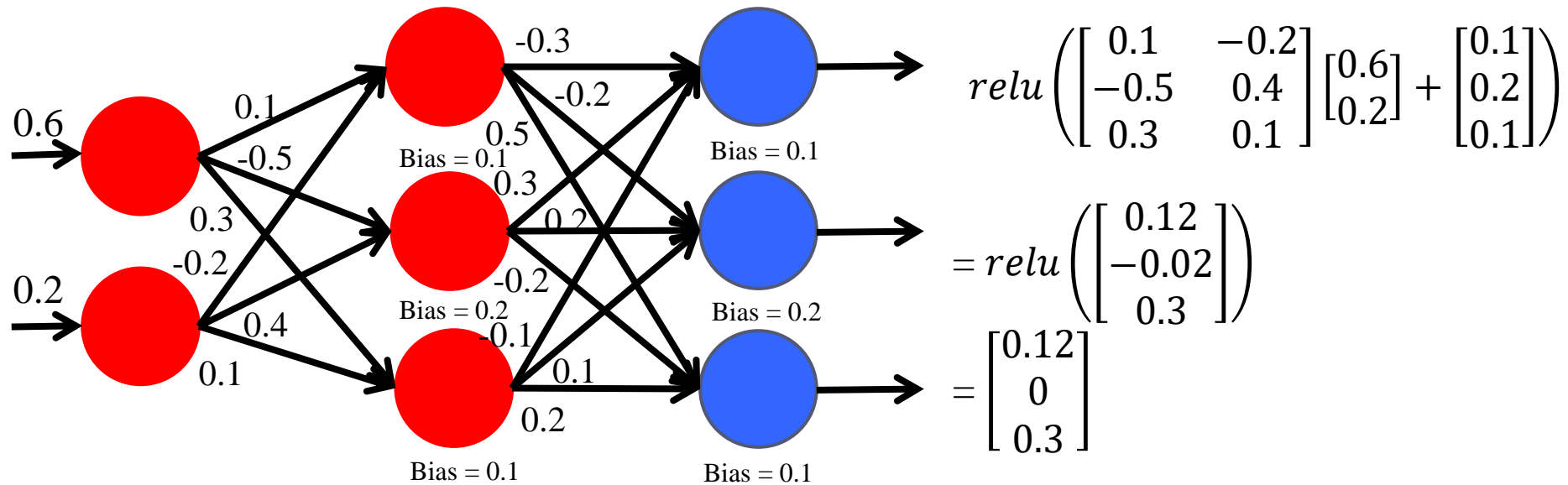
Example-initialization



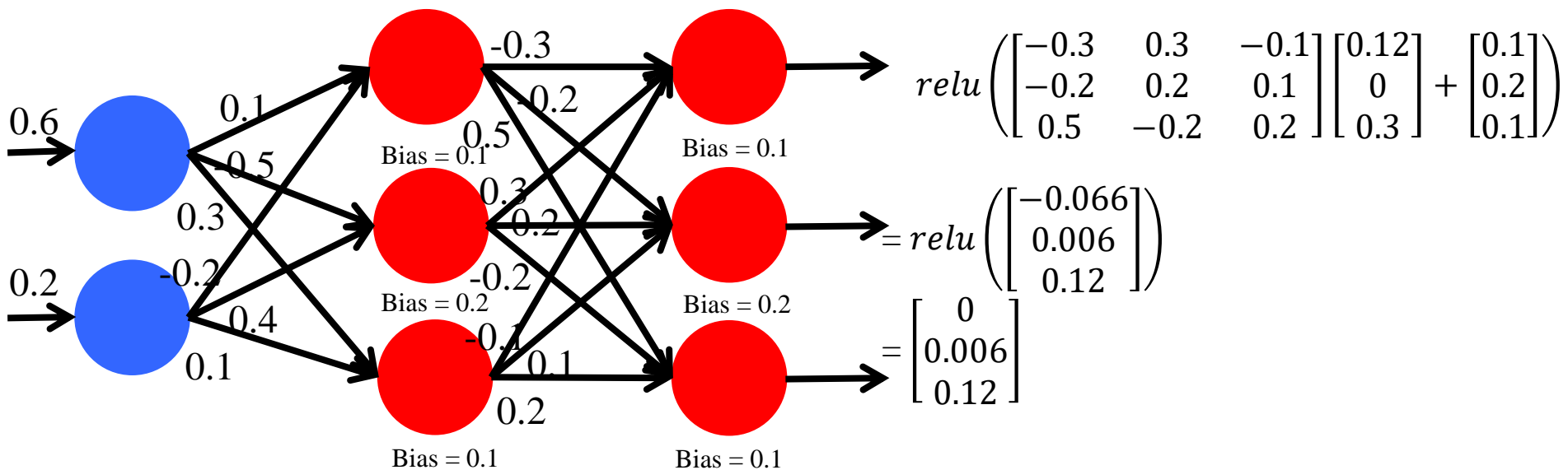
Example-feed data



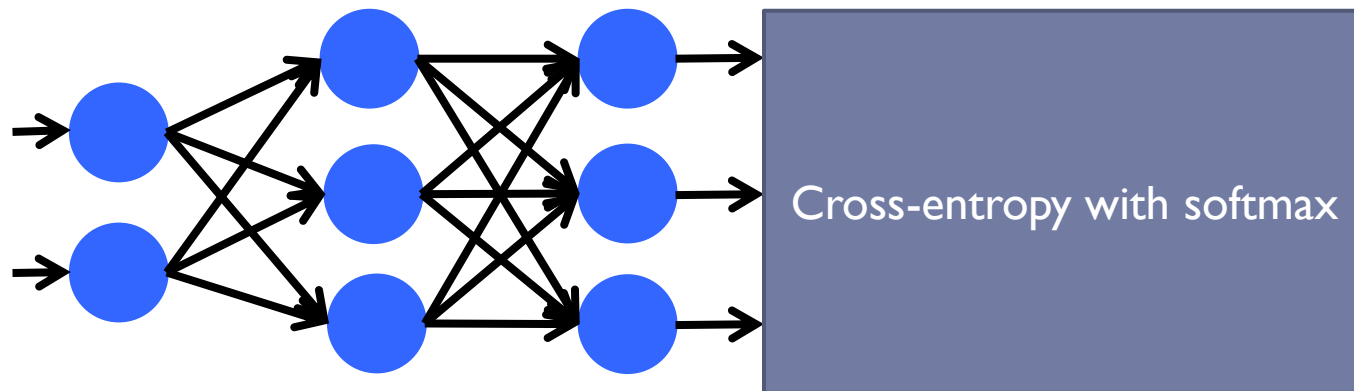
Example-forward pass



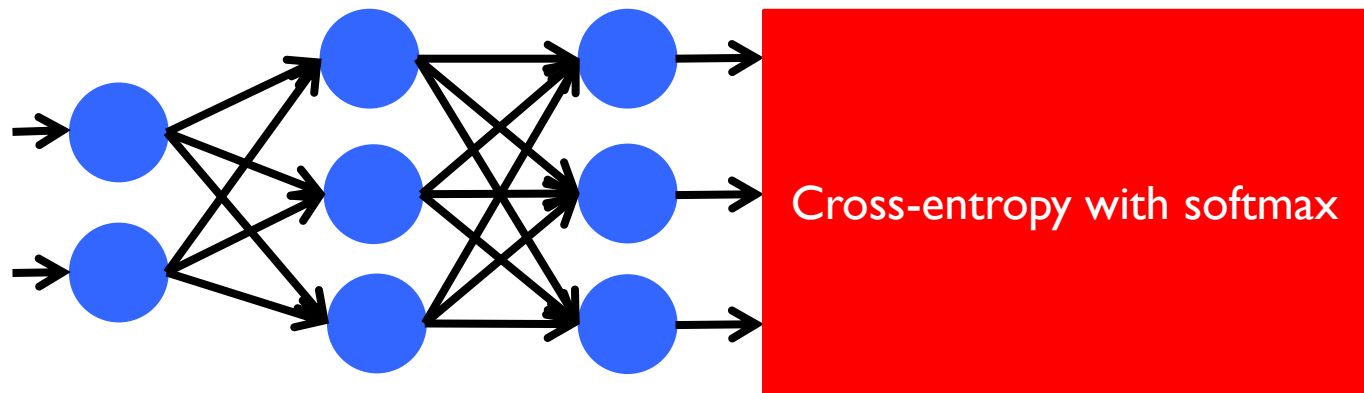
Example-forward pass



Example-forward pass



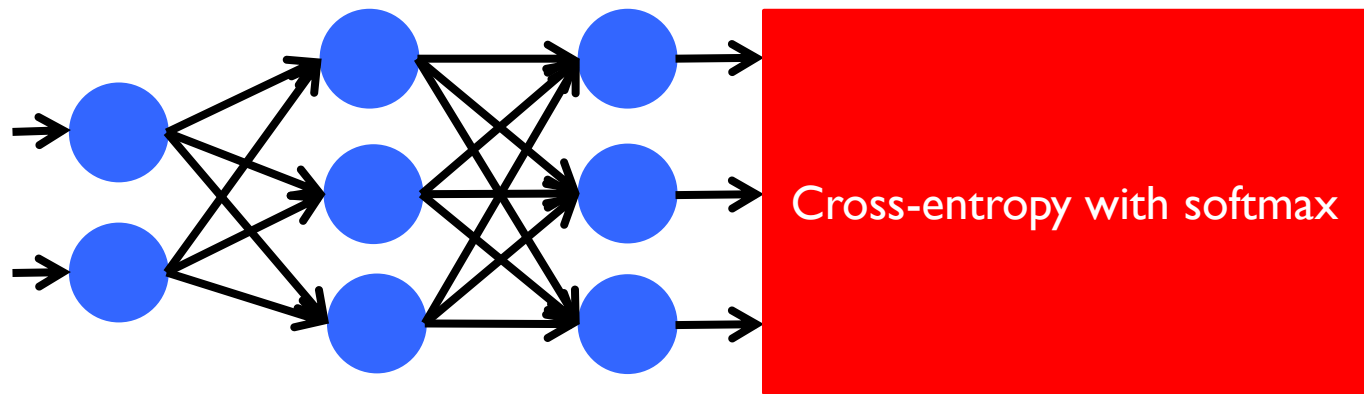
Example-forward pass



$$\text{Softmax}\left(\begin{bmatrix} 0 \\ 0.006 \\ 0.12 \end{bmatrix}\right) = \begin{bmatrix} 0.319 \\ 0.321 \\ 0.36 \end{bmatrix}$$

$$\sigma(\mathbf{z})_j = \frac{e^{z_j}}{\sum_{k=1}^K e^{z_k}} \quad \text{for } j = 1, \dots, K.$$

Example-forward pass



What we expect
(label)

$$\begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix}$$

$$\begin{aligned} & - 0 * \ln(0.319) - 1 * \ln(0.321) - 0 * \ln(0.36) \\ & = 1.1363 \end{aligned}$$

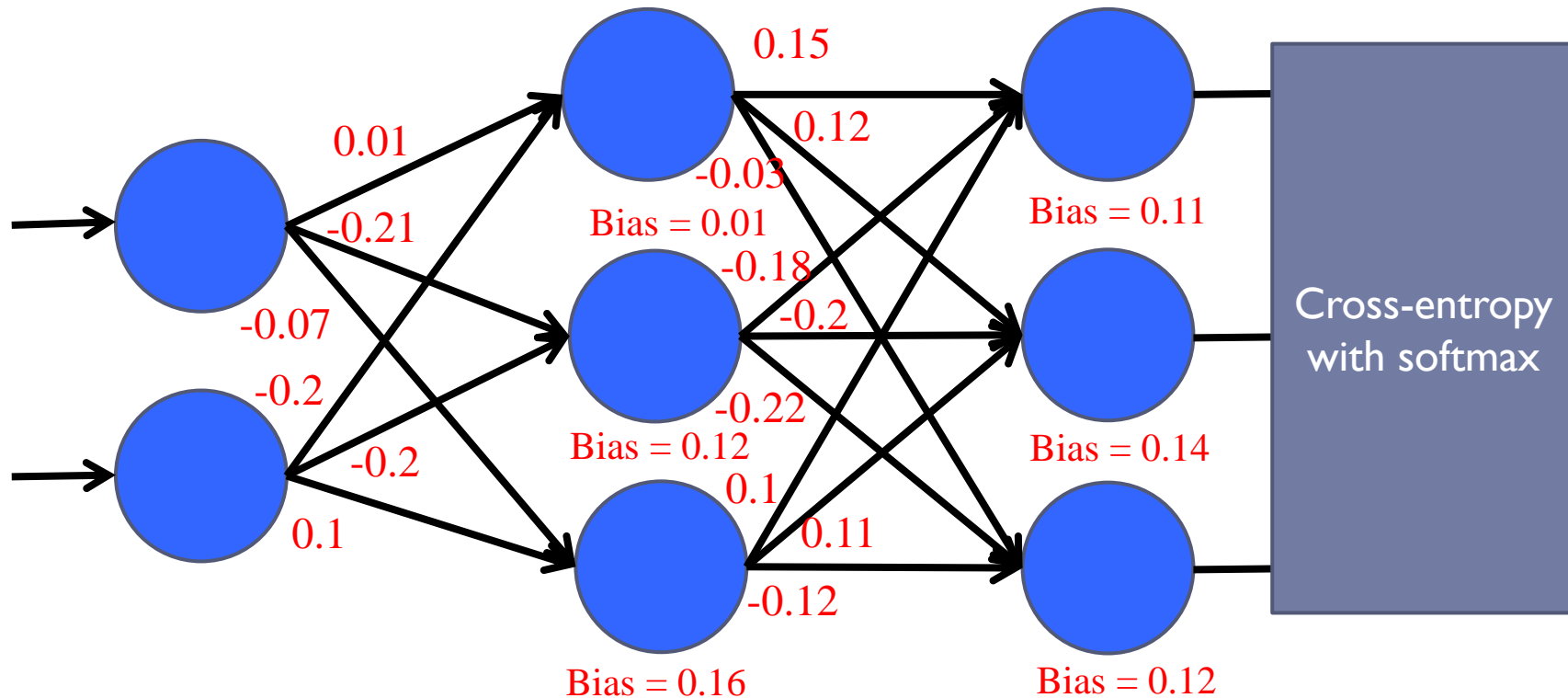
$$- \sum_{i=0}^{class \#} \hat{y}_i \ln(y_i)$$

This is large at the beginning. During training, this should decrease.

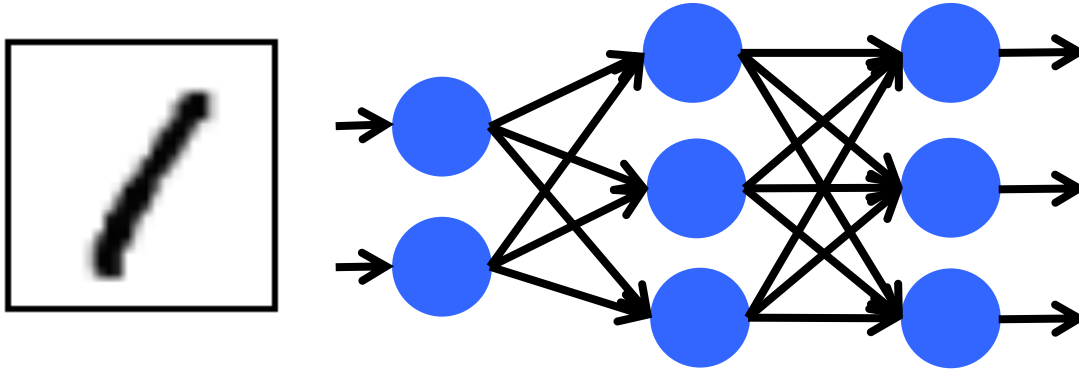
Example-optimization

Use optimizer to optimize
and wait.....

Example-after optimization

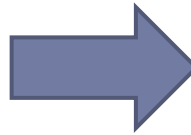


Example-predict



Feed you test data

You may get something like this

$$\begin{bmatrix} 0.1 \\ 0.5 \\ 0.4 \end{bmatrix}$$


Model predict this is class #2
(0.5 is greater than others)