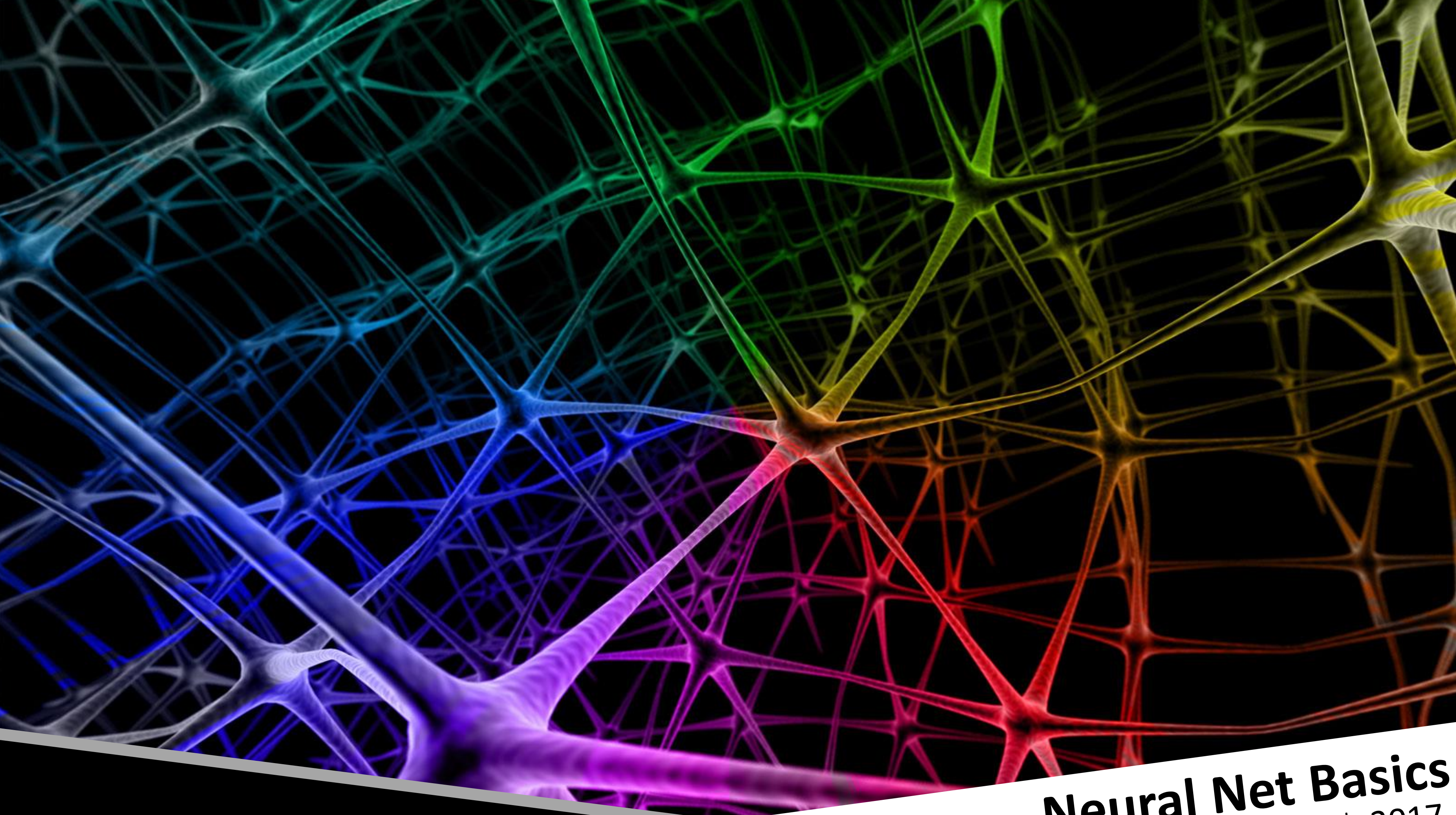


Neural Net Basics

Sep 18th & 21st, 2017

ADL x MLDS

Yun-Nung (Vivian) Chen

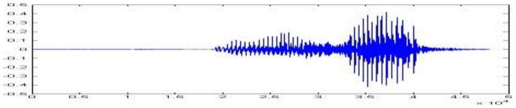
HTTP://ADL.MIULAB.TW
HTTP://MLDS.MIULAB.TW

國立臺灣大學
National Taiwan University

Slides credited from Prof. Hung-Yi Lee

Learning ≈ Looking for a Function

Speech Recognition

$f($  $)=$ "你好"

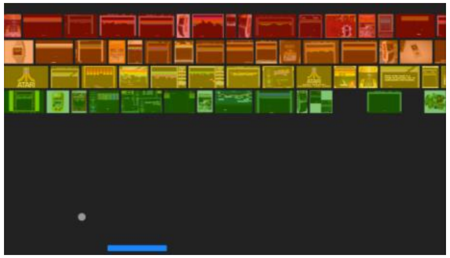
Handwritten Recognition

$f($  $)=$ "2"

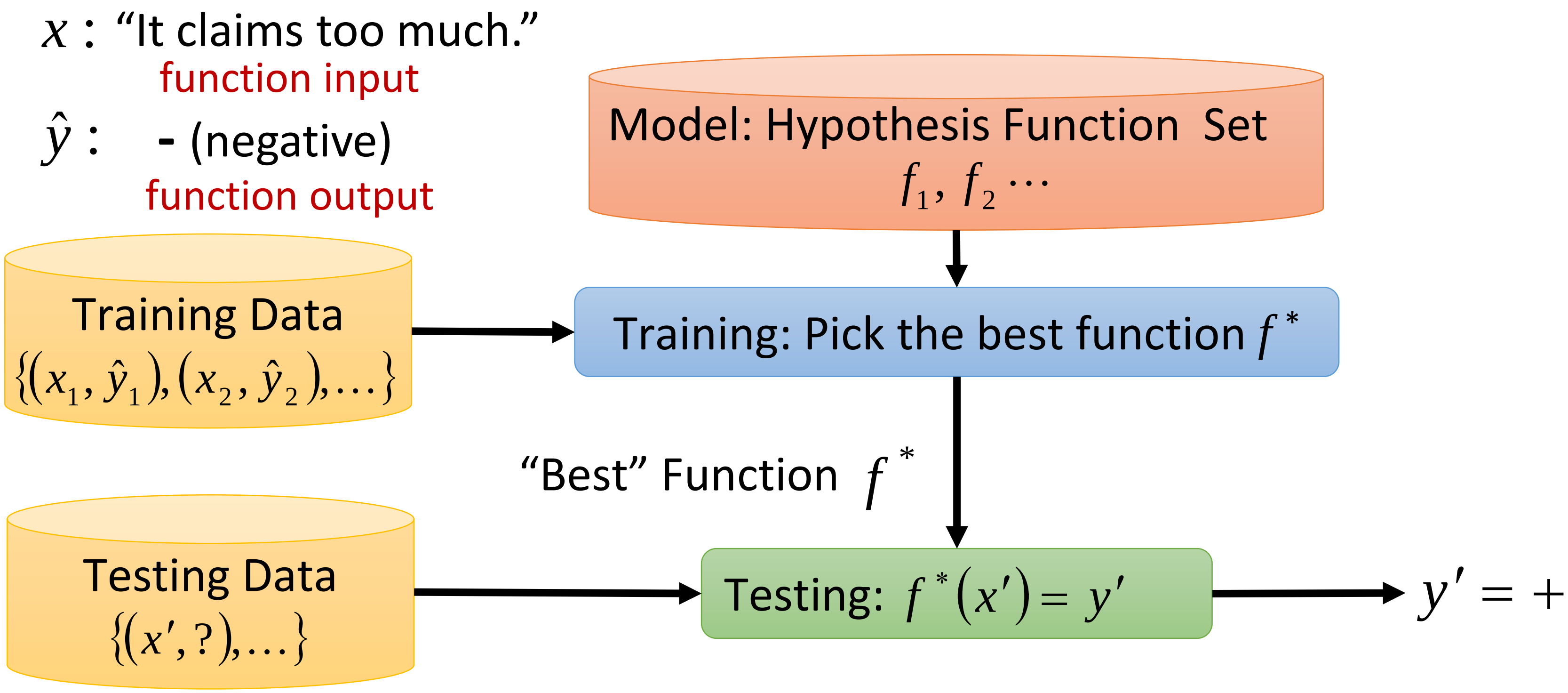
Weather forecast

$f($  Thursday $)=$ "  Saturday"

Play video games

$f($  $)=$ "move left"

Machine Learning Framework



x : "It claims too much."

function input

$\hat{y}$: - (negative)

function output

Model: Hypothesis Function Set

$f_1, f_2 \cdots$

Training Data

$\{(x_1, \hat{y}_1), (x_2, \hat{y}_2), \ldots\}$

Training: Pick the best function f^*

"Best" Function f^*

Testing Data

$\{(x', ?), \ldots\}$

Testing: $f^*(x') = y'$

$y' = +$

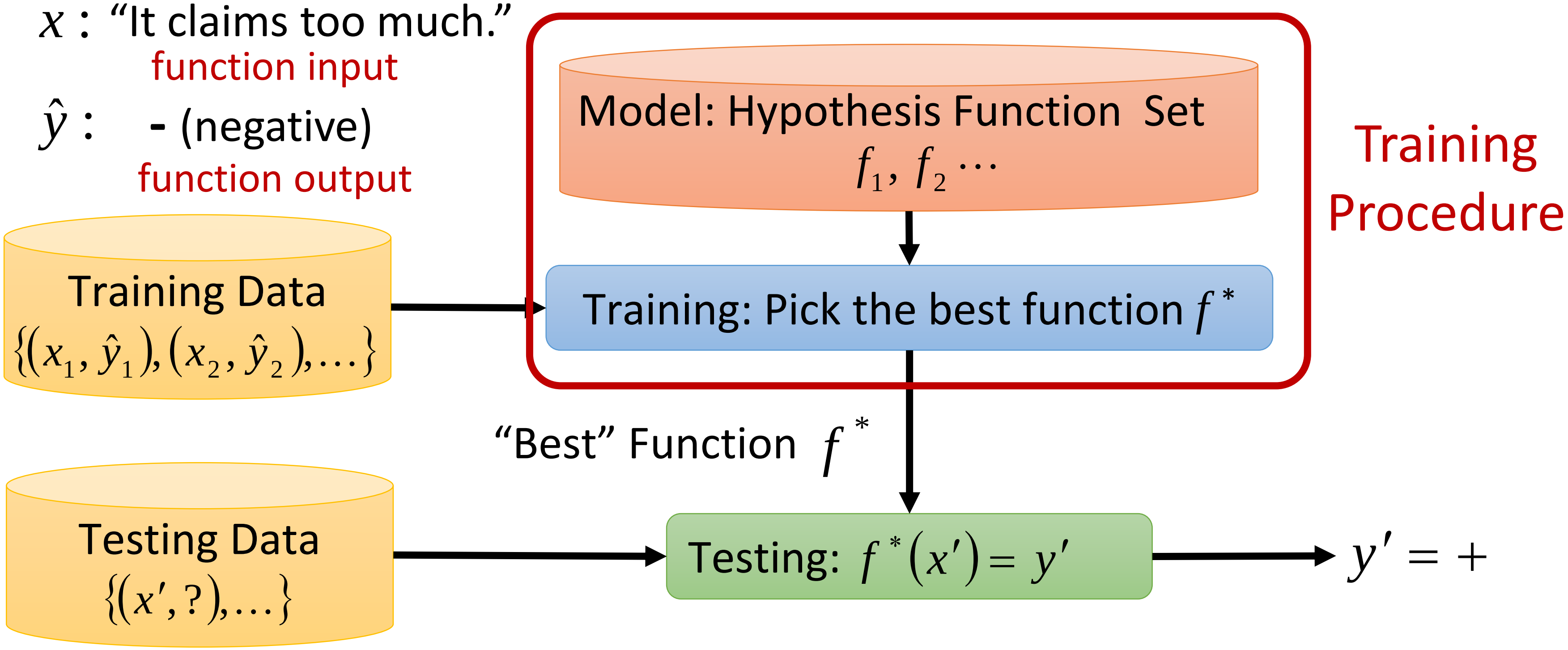
Training is to pick the best function given the observed data

Testing is to predict the label using the learned function

**Training &
Resources**

How to Train a Model?

Machine Learning Framework



x : "It claims too much."

function input

$\hat{y}$: - (negative)

function output

Training Data

$\{(x_1, \hat{y}_1), (x_2, \hat{y}_2), \dots\}$

Model: Hypothesis Function Set

$f_1, f_2 \cdots$

Training: Pick the best function f^*

Training Procedure

"Best" Function f^*

Testing Data

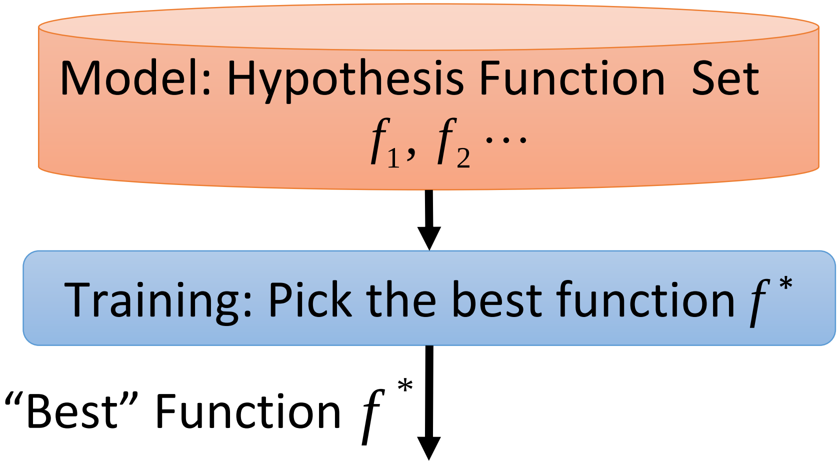
$\{(x', ?), \dots\}$

Testing: $f^*(x') = y'$

$y' = +$

Training is to pick the best function given the observed data
Testing is to predict the label using the learned function

Training Procedure



Model: Hypothesis Function Set

$f_1, f_2 \cdots$

Training: Pick the best function f^*

"Best" Function f^*

Q1. What is the model? (function hypothesis set)

Q2. What does a "good" function mean?

Q3. How do we pick the "best" function?

Training Procedure Outline

① Model Architecture

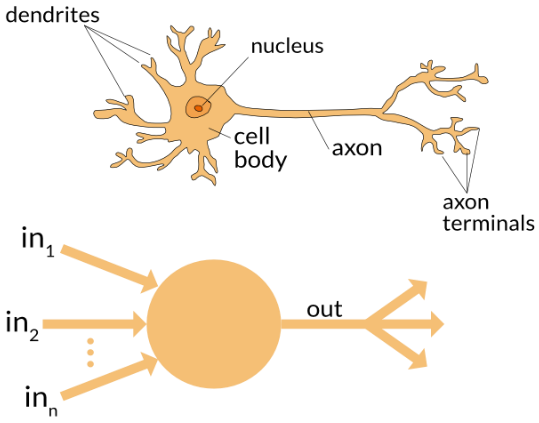
- ✓ A Single Layer of Neurons (Perceptron)
- ✓ Limitation of Perceptron
- ✓ Neural Network Model (Multi-Layer Perceptron)

② Loss Function Design

- ✓ Function = Model Parameters
- ✓ Model Parameter Measurement

③ Optimization

- ✓ Gradient Descent
- ✓ Stochastic Gradient Descent (SGD)
- ✓ Mini-Batch SGD
- ✓ Practical Tips



What is the Model?

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- ✓ Practical Tips

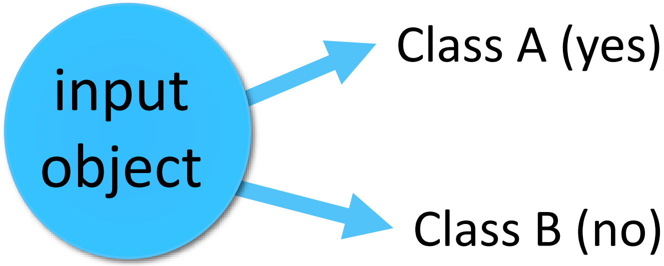
Classification Task

Sentiment Analysis

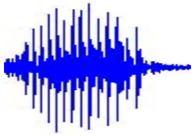
“這規格有誠意!” → +

“太爛了吧~” → -

Binary Classification



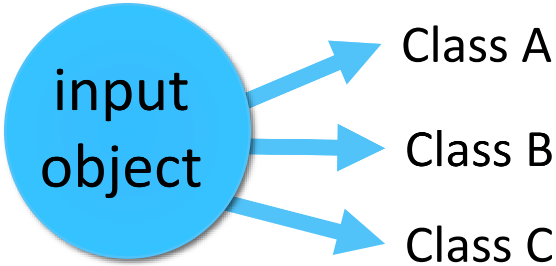
Speech Phoneme Recognition


→ /h/

Handwritten Recognition


→ 2

Multi-class Classification



Some cases are not easy to be formulated as classification problems

Target Function

Classification Task

$$f(x) = y \quad \Longrightarrow \quad f : R^N \to R^M$$

- x: input object to be classified → a N-dim vector
- y: class/label → a M-dim vector

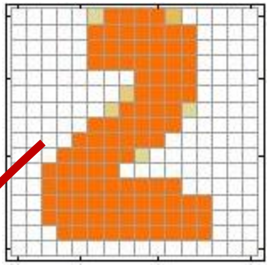
Assume both x and y can be represented as fixed-size vectors

Vector Representation Example

Handwriting Digit Classification

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

***x*: image**



16 x 16

Each pixel corresponds to an element in the vector

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

1: for ink

0: otherwise

16 x 16 = 256 dimensions

***y*: class/label**

10 dimensions for digit recognition

$$\begin{array}{cccc} \text{“1”} & & \text{“2”} & \\ \downarrow & & \downarrow & \\ \begin{bmatrix}1\\0\\0\\\vdots\end{bmatrix} & \begin{array}{c}\text{“1”}\\\text{“2”}\\\text{“3”}\\ \\ \end{array} & \begin{bmatrix}0\\1\\0\\\vdots\end{bmatrix} & \begin{array}{l}\text{“1”} \rightarrow \text{“1” or not}\\\text{“2”} \rightarrow \text{“2” or not}\\\text{“3”} \rightarrow \text{“3” or not}\\ \\ \end{array} \end{array}$$

Vector Representation Example

Sentiment Analysis

x: word

“love”

Each element in the vector corresponds to a word in the vocabulary

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

1: indicates the word

0: otherwise

dimensions = size of vocab

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

y: class/label

3 dimensions (positive, negative, neutral)

“+” “-”

$$\begin{bmatrix} 1 \\ 0 \\ 0 \\ \vdots \end{bmatrix} \begin{array}{c} \text{“+”} \\ \text{“-”} \\ \text{“?”} \\ \\ \end{array} \begin{bmatrix} 0 \\ 1 \\ 0 \\ \vdots \end{bmatrix}$$

“+” → “+” or not

“-” → “-” or not

“?” → “?” or not

Target Function

Classification Task

$$f(x) = y \quad \Longrightarrow \quad f : R^{N} \rightarrow R^{M}$$

◦ x: input object to be classified	→ a N-dim vector
◦ y: class/label	→ a M-dim vector

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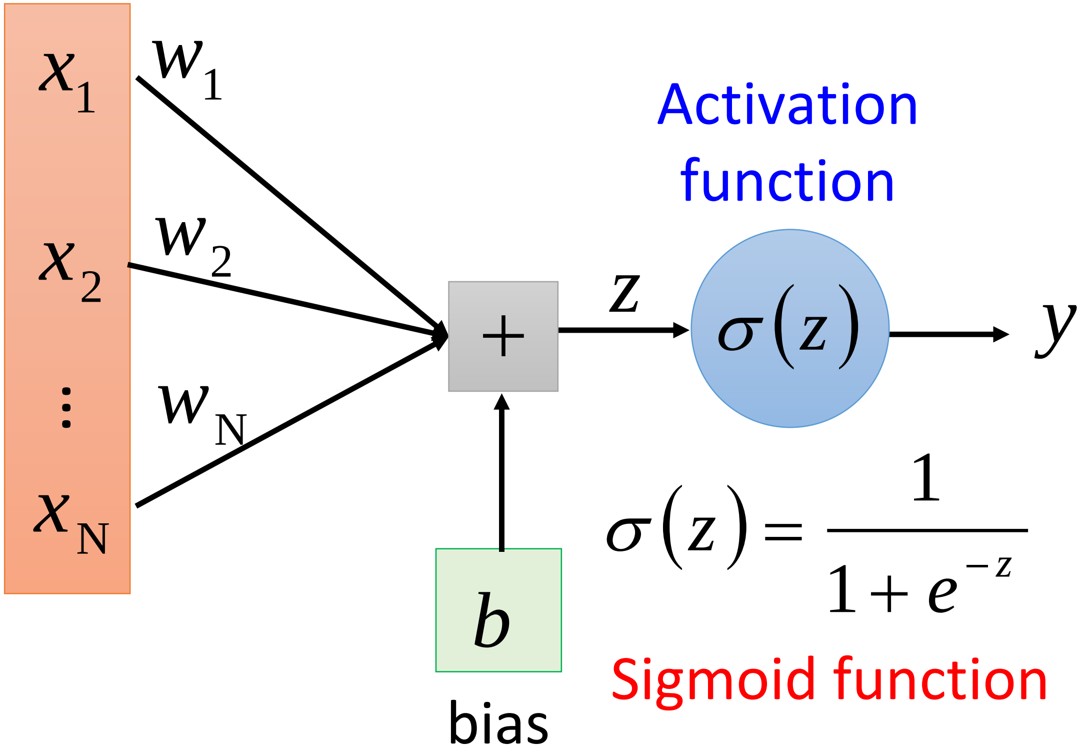
- ✓ Practical Tips

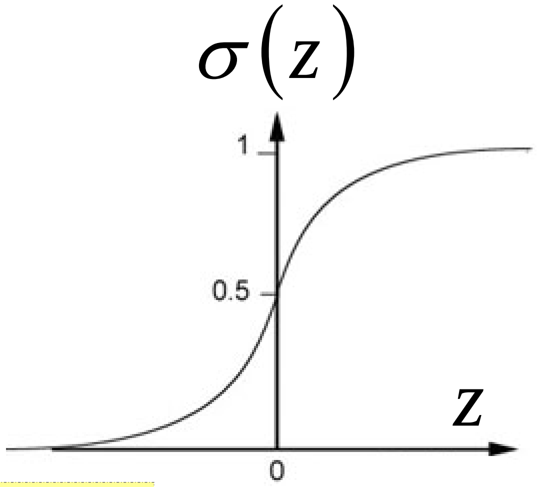
A Single Neuron



Activation function

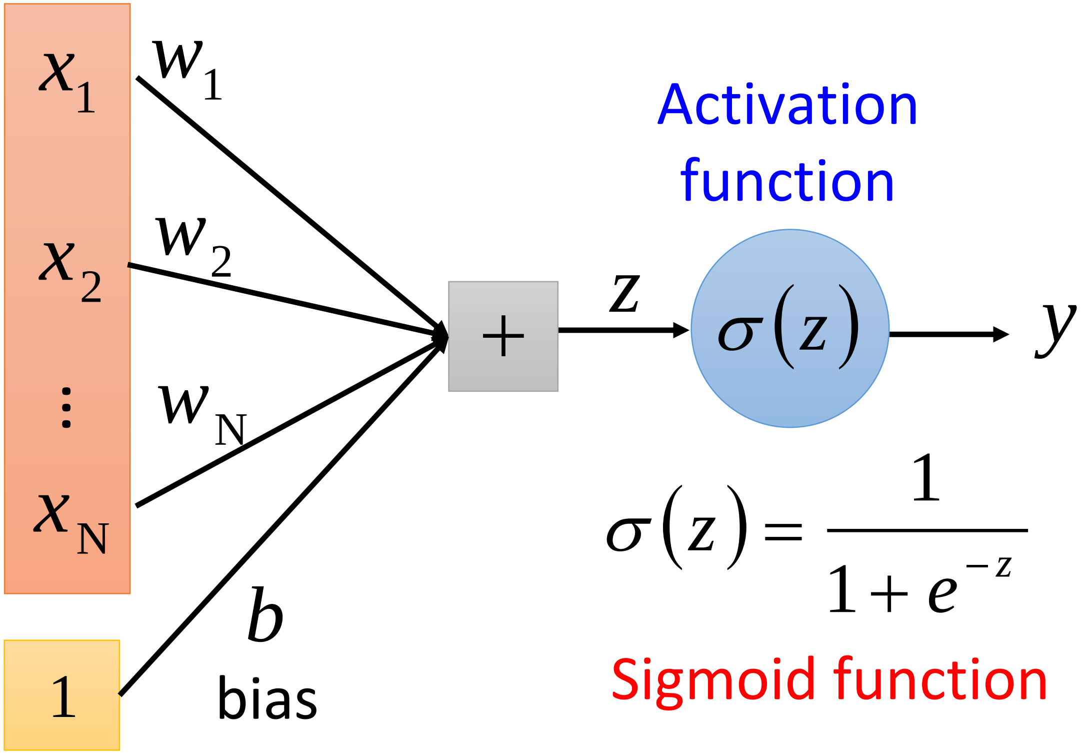
$$\sigma(z) = \frac{1}{1+e^{-z}}$$

Sigmoid function



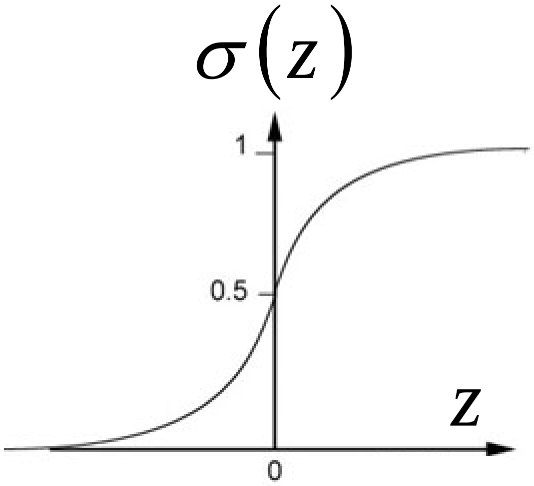
Each neuron is a very simple function

A Single Neuron



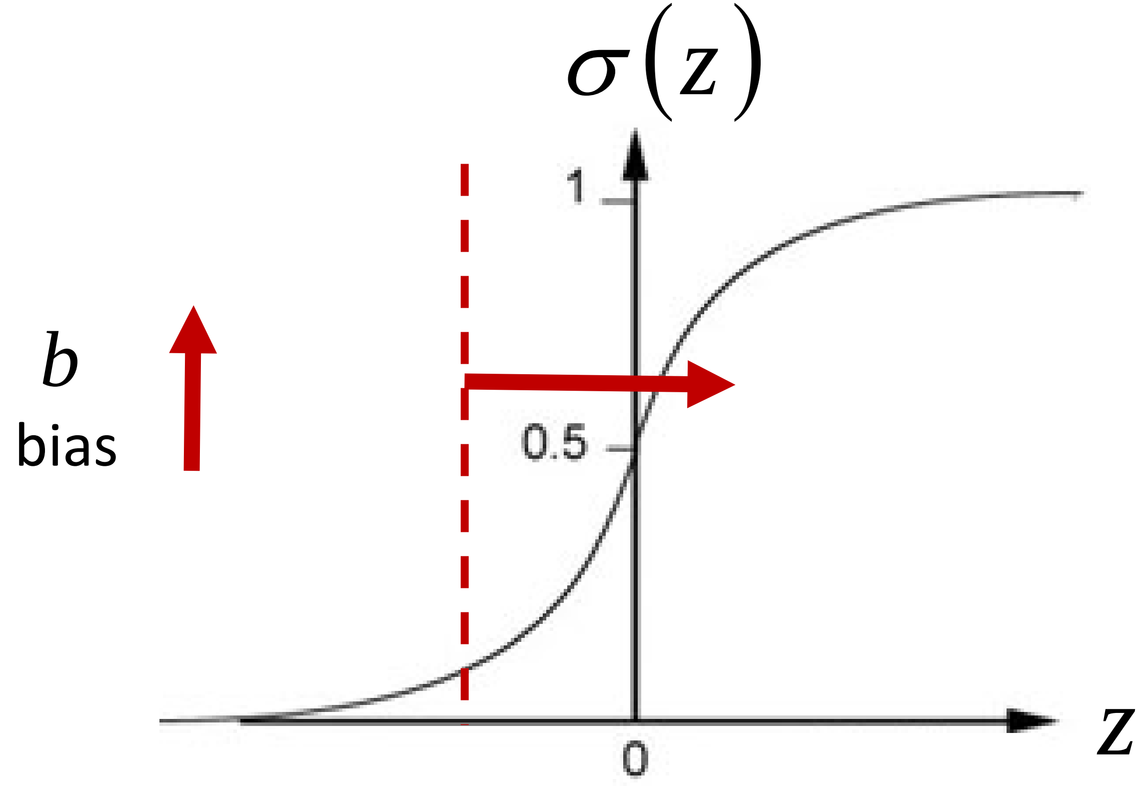
$$\sigma(z) = \frac{1}{1+e^{-z}}$$

Sigmoid function



The bias term is an “always on” feature

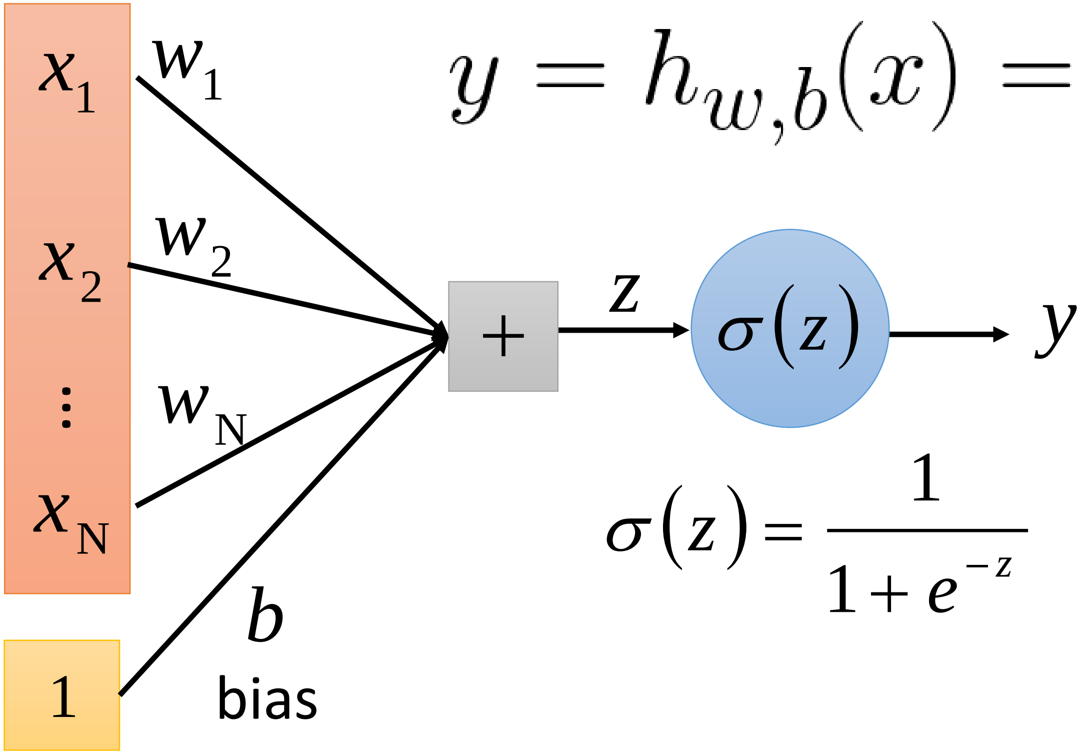
Why Bias?



The bias term gives a class prior

Model Parameters of A Single Neuron

$$y = h_{w,b}(x) = \sigma(w^T x + b)$$

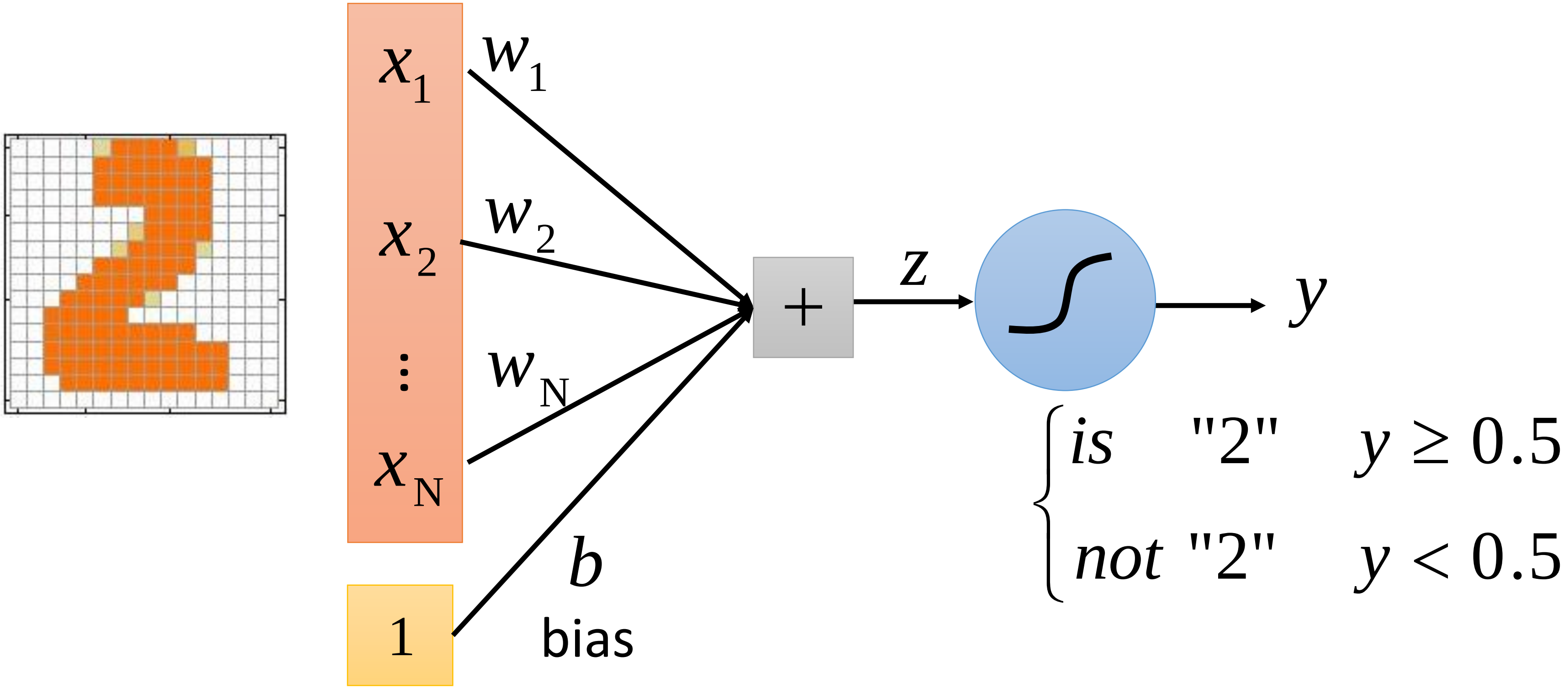


$$\sigma(z) = \frac{1}{1+e^{-z}}$$

w, b are the parameters of this neuron

A Single Neuron

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

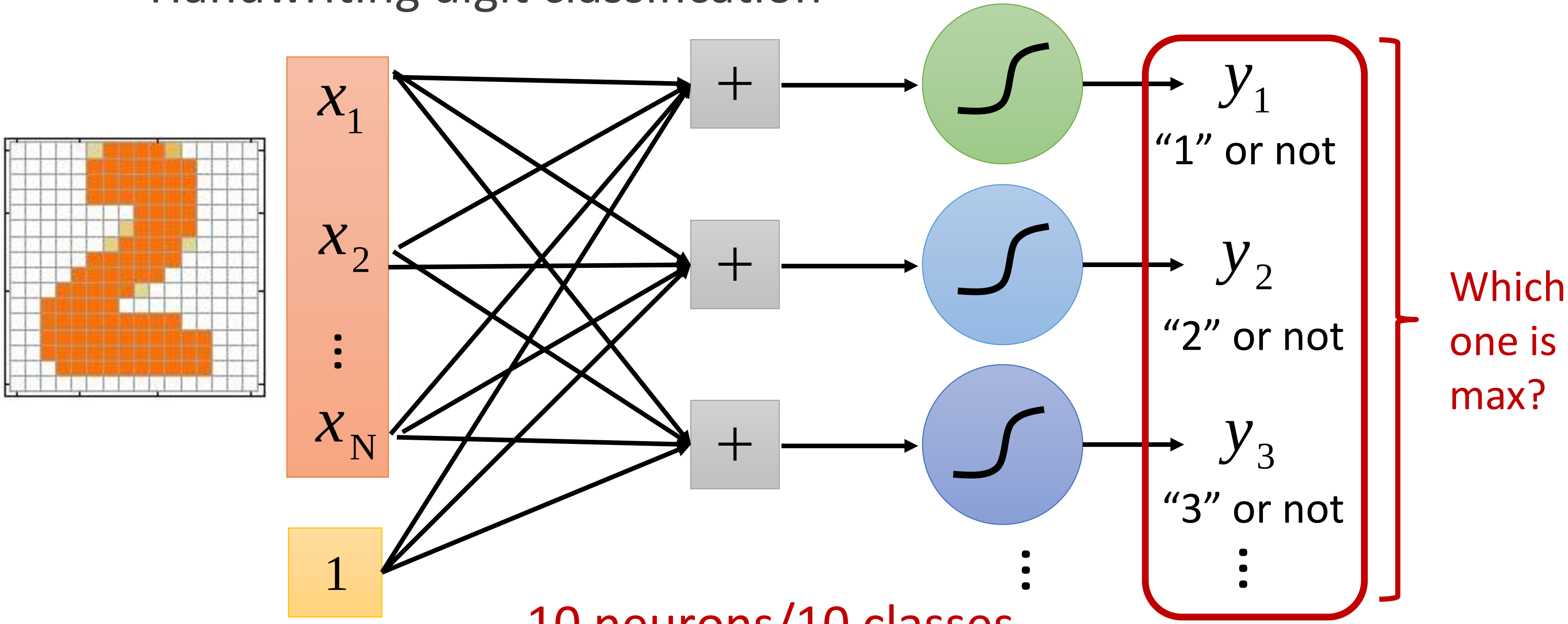


$$\begin{cases} is \quad "2" & y \geq 0.5 \\ not \; "2" & y < 0.5 \end{cases}$$

A single neuron can only handle binary classification

A Layer of Neurons $f : R^N \to R^M$

Handwriting digit classification



10 neurons/10 classes

A layer of neurons can handle multiple possible output, and the result depends on the max one

Training Procedure Outline

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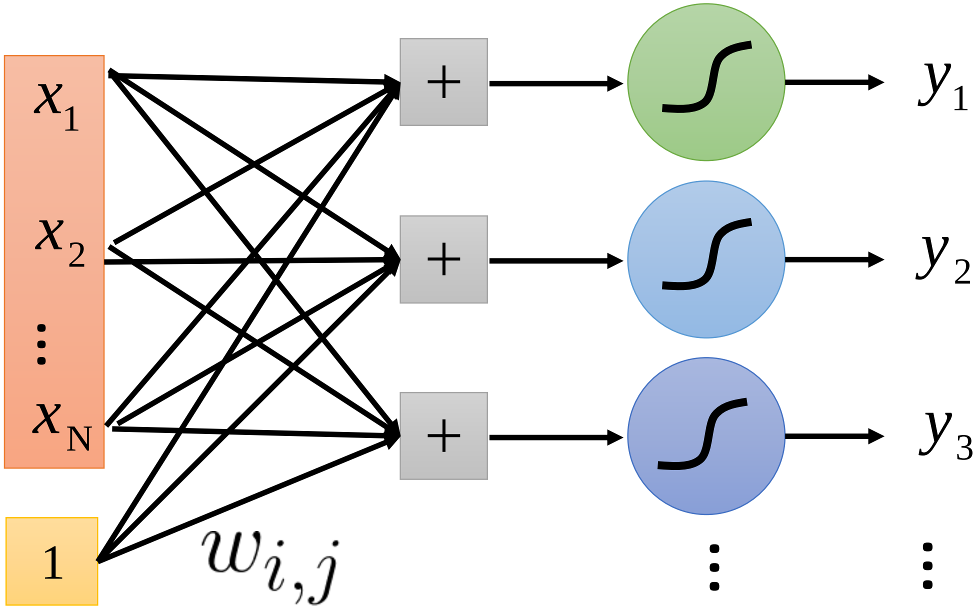
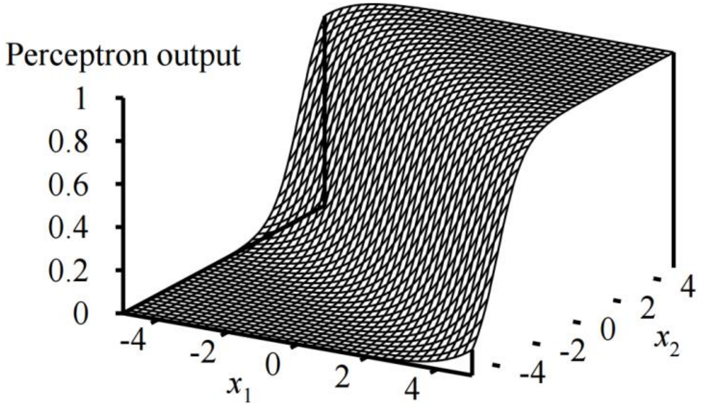
A Layer of Neurons – Perceptron

Output units all operate separately – no shared weights

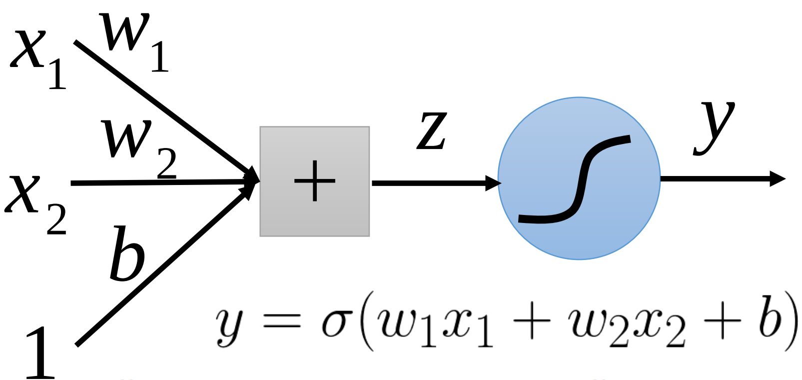




Adjusting weights moves the location, orientation, and steepness of cliff

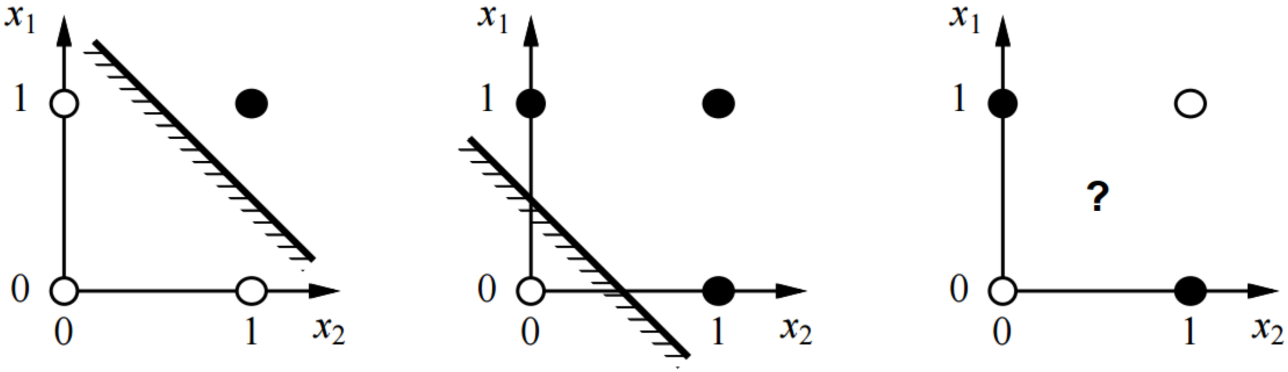
http://aima.eecs.berkeley.edu/slides-pdf/chapter20b.pdf

Expression of Perceptron



$$y = \sigma(w_1 x_1 + w_2 x_2 + b)$$

$$\begin{cases} \text{yes} & y \geq \theta \ \text{(threshold)} \\ \text{no} & y < \theta \end{cases}$$



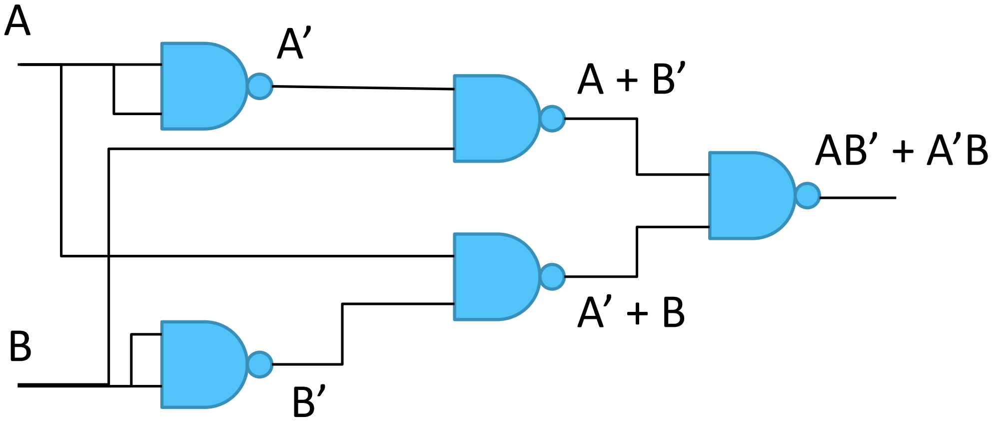
(a) x_1 **and** x_2 (b) x_1 **or** x_2 (c) x_1 **xor** x_2

A perceptron can represent AND, OR, NOT, etc., but not XOR → linear separator

http://aima.eecs.berkeley.edu/slides-pdf/chapter20b.pdf

How to Implement XOR?

Input		Output
A	B	
0	0	0
0	1	1
1	0	1
1	1	0



A xor B = AB’ + A’B

Multiple operations can produce more complicate output

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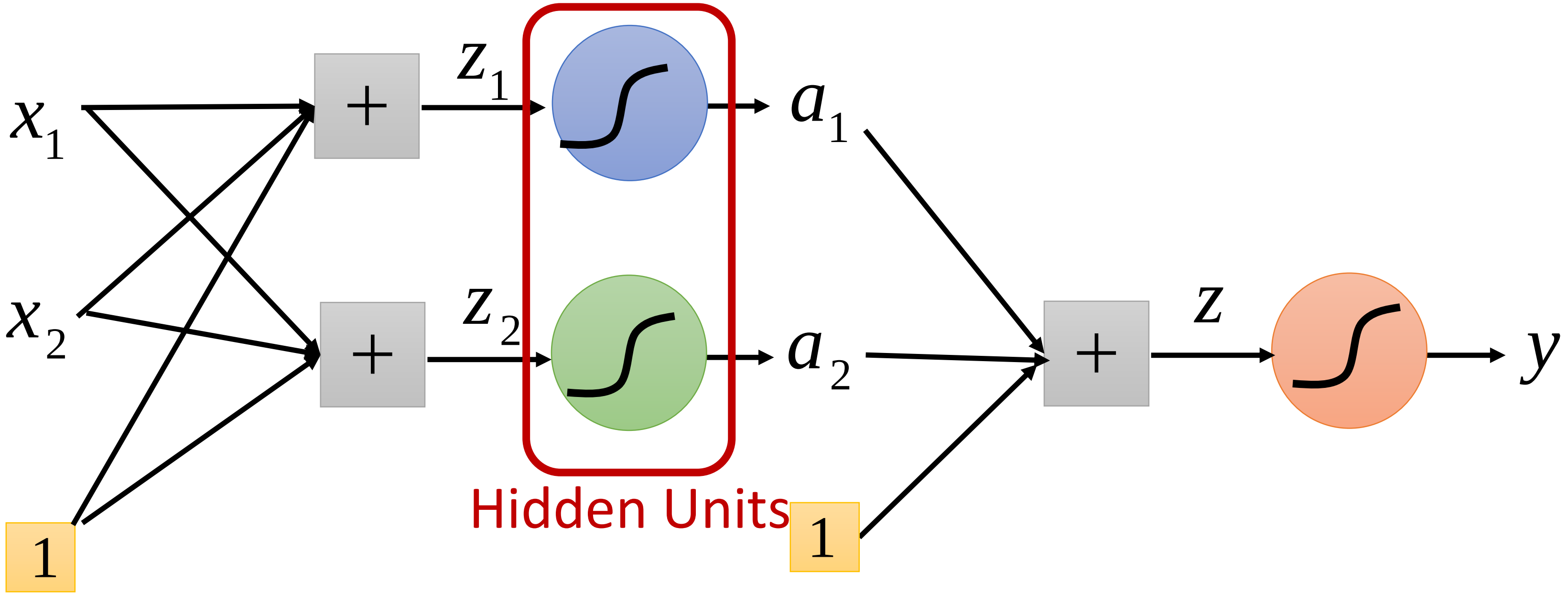
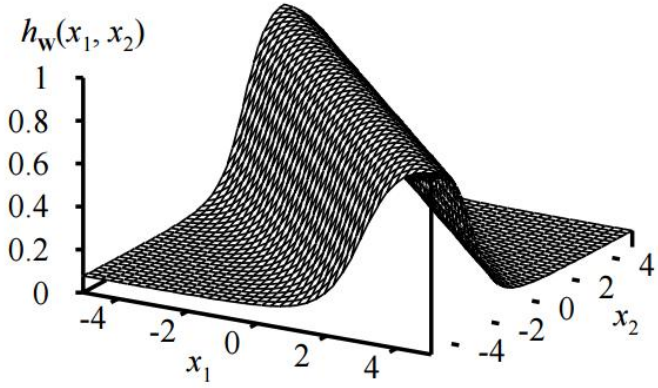
Neural Networks – Multi-Layer Perceptron



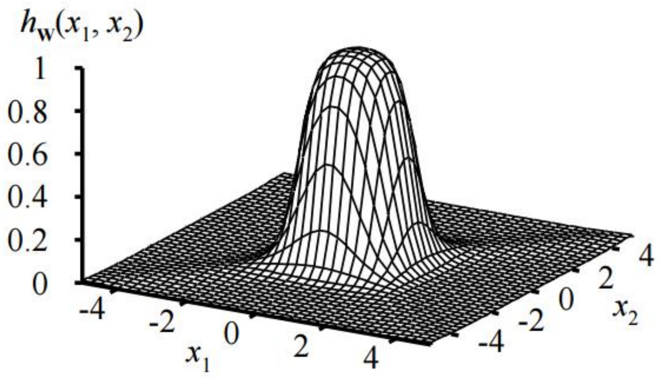
Expression of Multi-Layer Perceptron

Continuous function w/ 2 layers



Combine two opposite-facing threshold functions to make a ridge

Continuous function w/ 3 layers



Combine two perpendicular ridges to make a bump

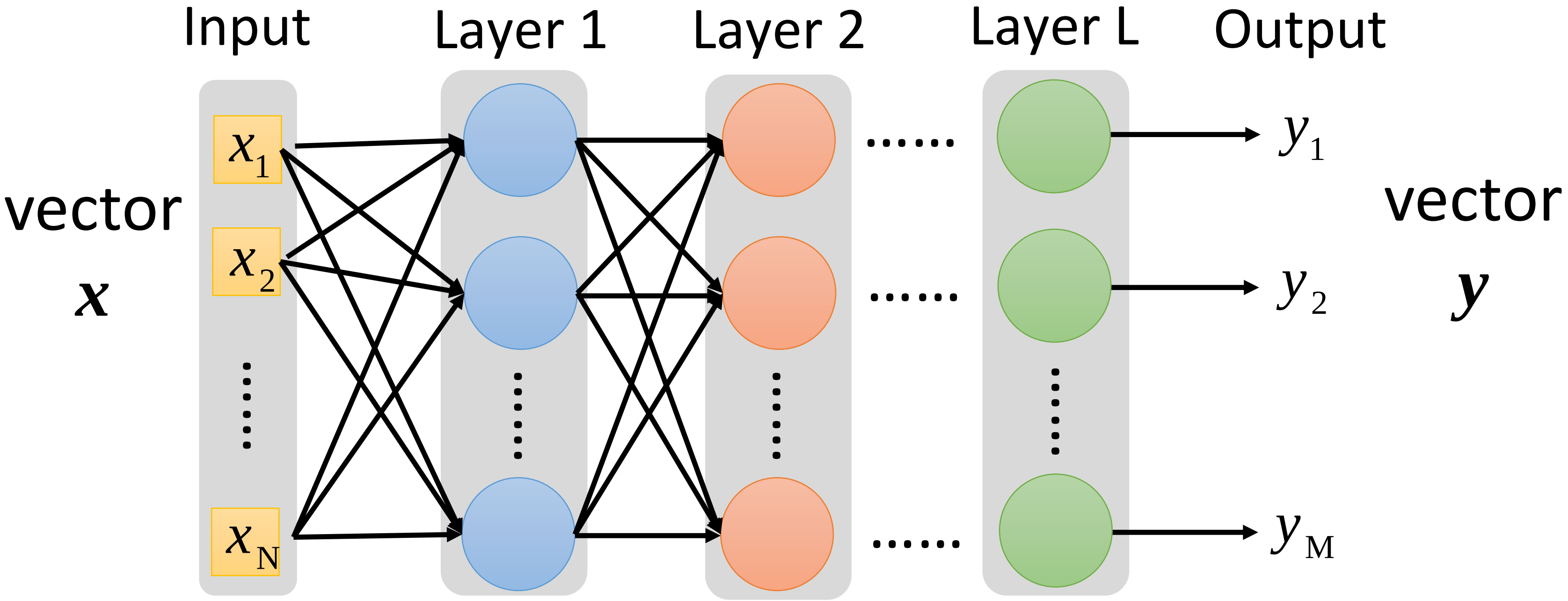
→ Add bumps of various sizes and locations to fit any surface

multiple layers enhance the model expression
→ the model can approximate more complex functions

http://aima.eecs.berkeley.edu/slides-pdf/chapter20b.pdf

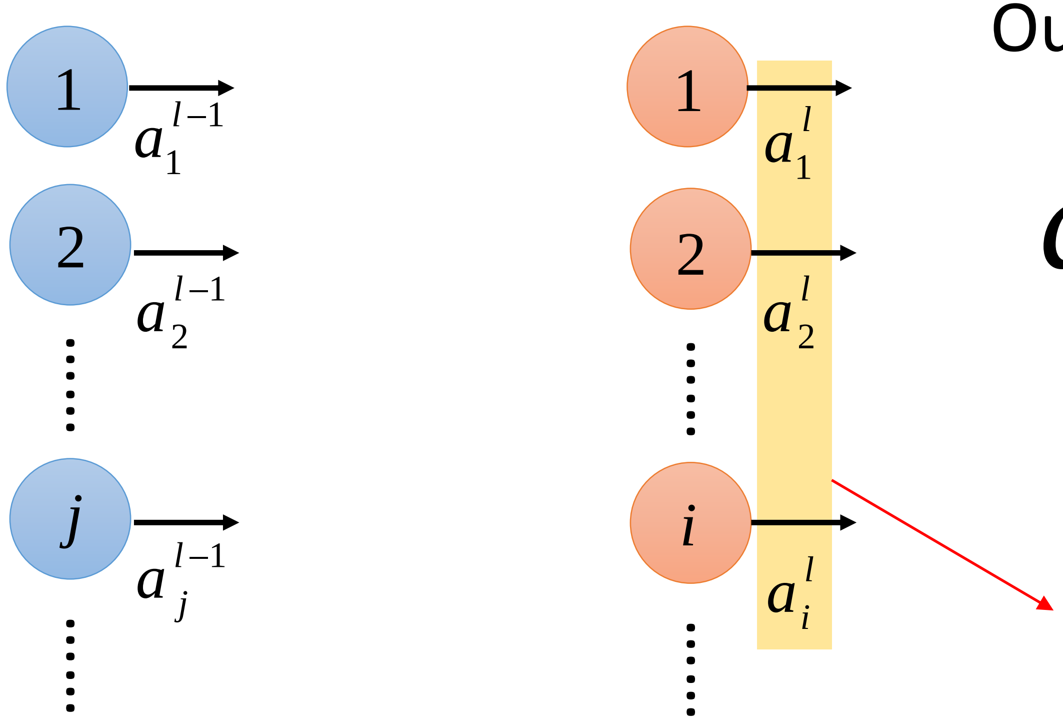
Deep Neural Networks (DNN) $f: R^N \to R^M$

Fully connected feedforward network



Deep NN: multiple hidden layers

Notation Definition



Output of a neuron:

a_i^l → layer l

a_i^l → neuron i

$$a^l = \begin{bmatrix} \vdots \\ a_i^l \\ \vdots \end{bmatrix}$$

Layer $l-1$

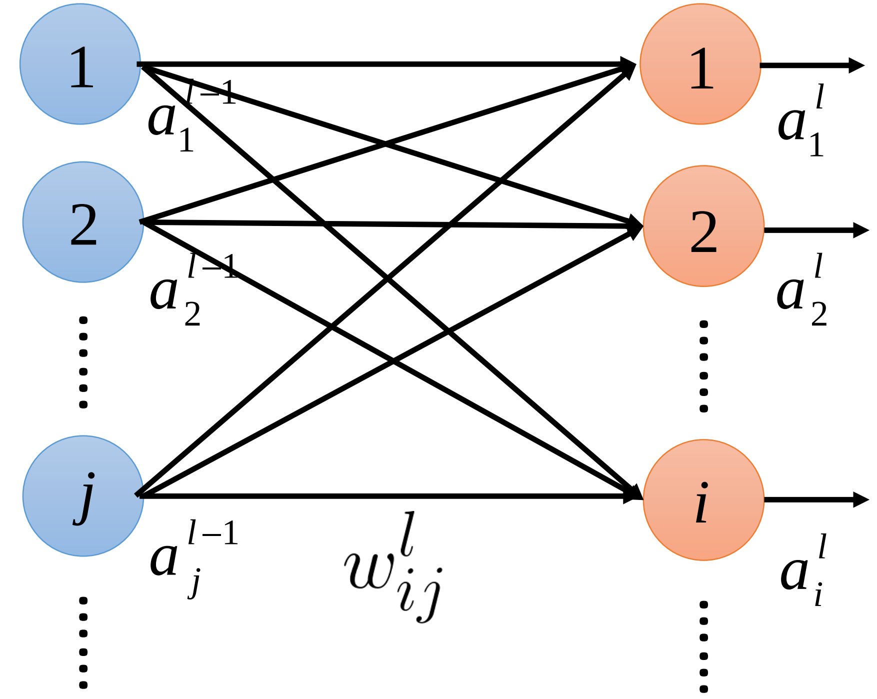
N_{l-1} nodes

Layer l

N_l nodes

output of one layer → a vector

Notation Definition



Layer $l-1$

N_{l-1} nodes

Layer l

N_l nodes

$$w_{ij}^{l}$$

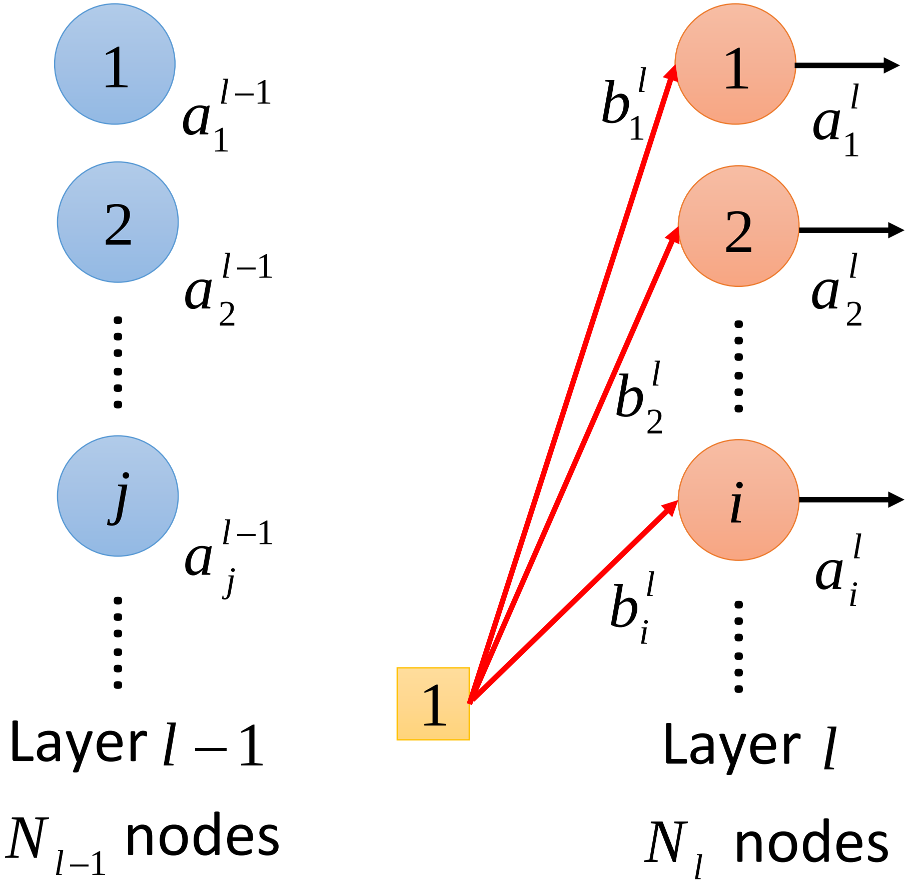
layer $l-1$
to layer l

from neuron *j* (layer *l-1*)
to neuron *i* (layer *l*)

$$\begin{array}{ccc} & \xleftrightarrow{\quad N_{l-1} \quad} & \\ W^l = & \begin{bmatrix} w_{11}^{l} & w_{12}^{l} & \cdots \\ w_{21}^{l} & w_{22}^{l} & \\ \vdots & & \ddots \end{bmatrix} & \updownarrow N_l \end{array}$$

weights between two layers
→ a matrix

Notation Definition

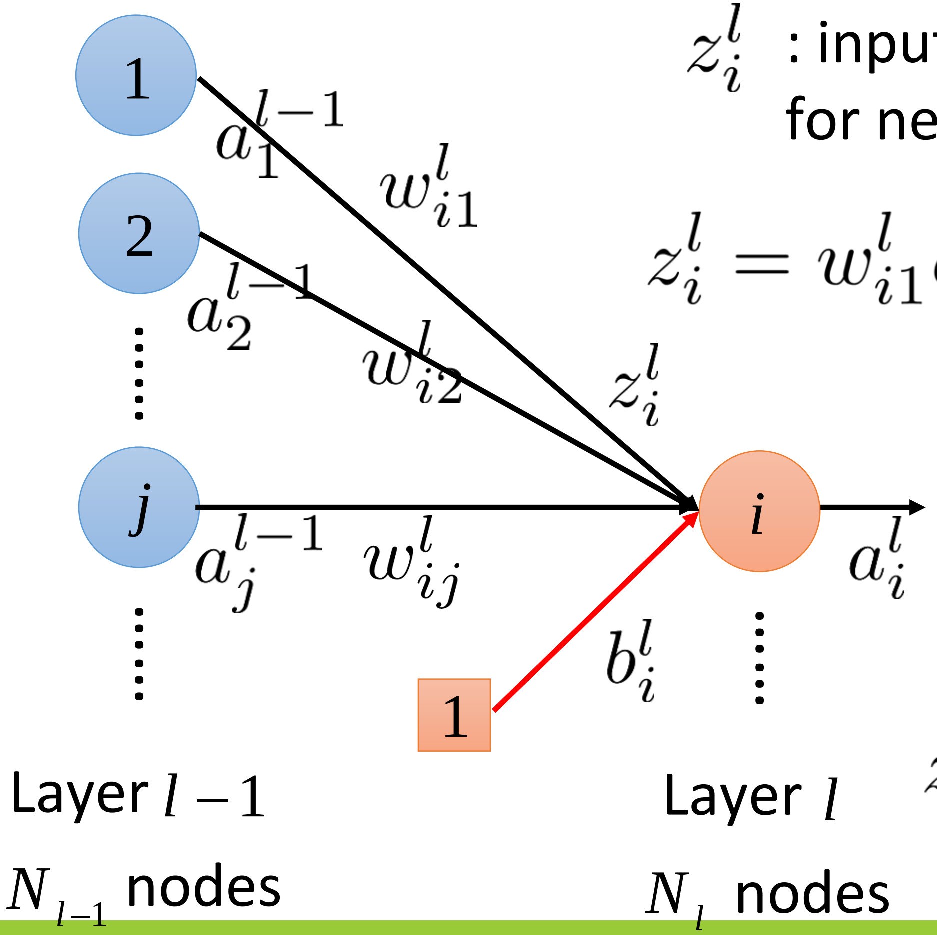


b_i^l : bias for neuron i at layer l

$$b^l = \begin{bmatrix} \vdots \\ b_i^l \\ \vdots \end{bmatrix}$$

bias of all neurons at each layer
→ a vector

Notation Definition



z_i^l : input of the activation function for neuron *i* at layer *l*

$$z_i^l = w_{i1}^l a_1^{l-1} + w_{i2}^l a_2^{l-1} + \ldots + b_i^l$$

$$z_i^l = \sum_{j=1}^{N_{l-1}} w_{ij}^l a_j^{l-1} + b_i^l$$

$$z^l = \begin{bmatrix} \vdots \\ z_i^l \\ \vdots \end{bmatrix}$$

activation function input at each layer → a vector

Notation Summary

a_i^l : output of a neuron

a^l : output vector of a layer

z_i^l : input of activation function

z^l : input vector of activation function for a layer

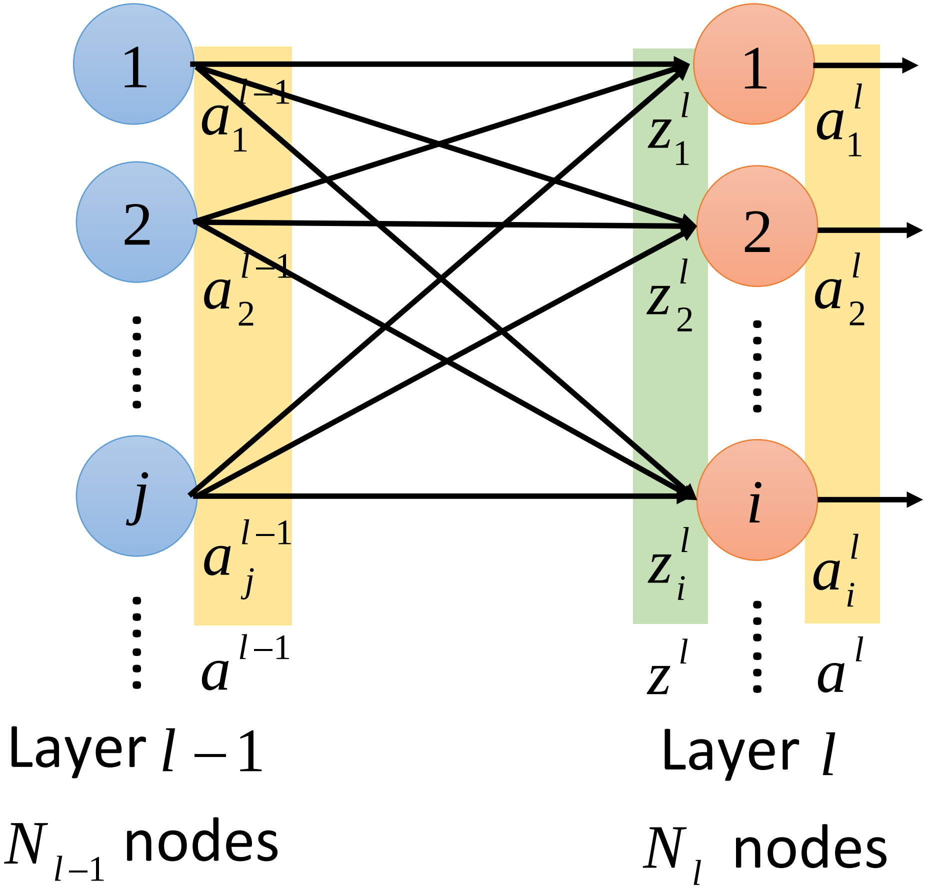
w_{ij}^l : a weight

W^l : a weight matrix

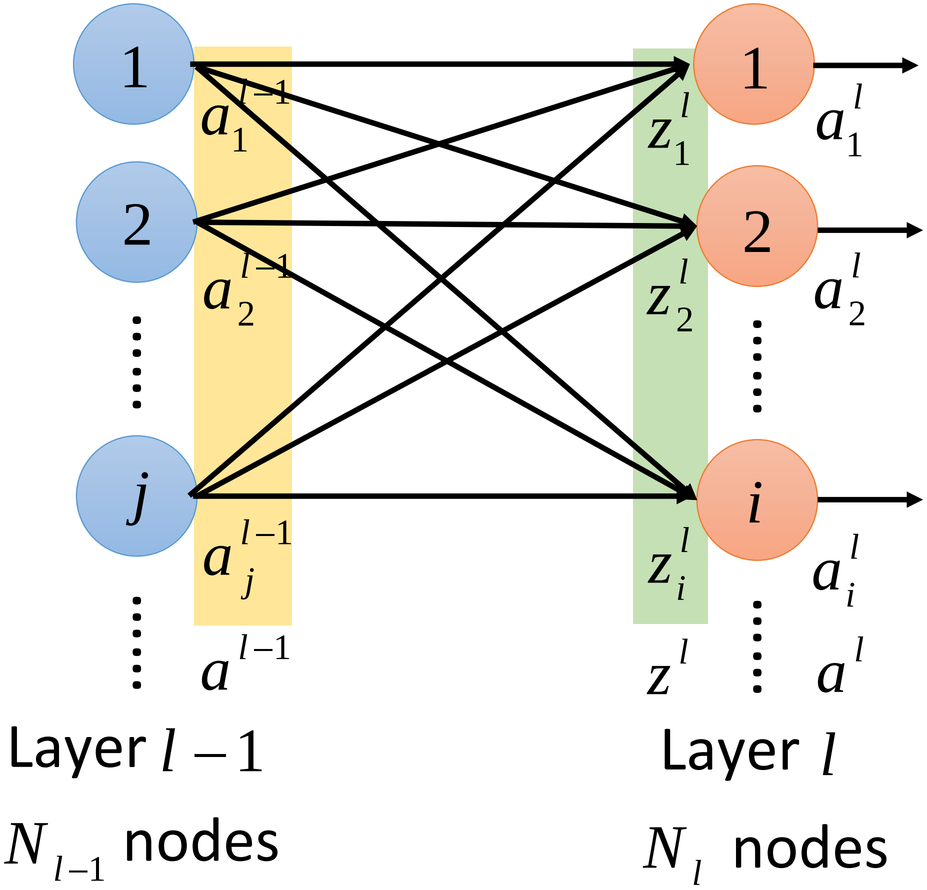
b_i^l : a bias

b^l : a bias vector

Layer Output Relation



Layer Output Relation – from *a* to *z*



$$z_1^l = w_{11}^1 a_1^{l-1} + w_{12}^1 a_2^{l-1} + \cdots + b_1^l$$

$$\vdots$$

$$z_i^l = w_{i1}^1 a_1^{l-1} + w_{i2}^1 a_2^{l-1} + \cdots + b_i^l$$

$$\vdots$$

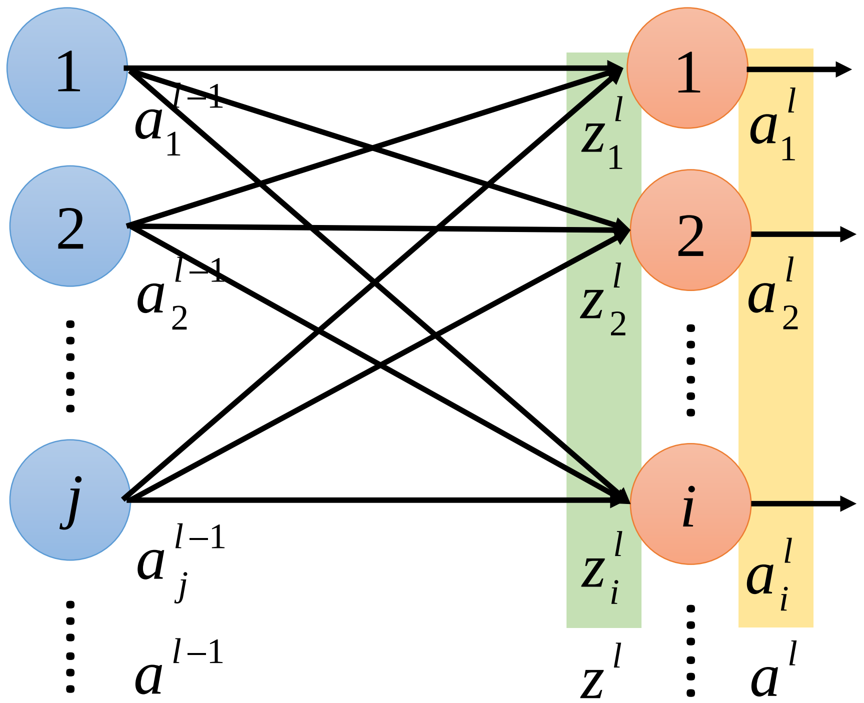
$$\Downarrow$$

$$\begin{bmatrix} z_1^l \\ \vdots \\ z_i^l \\ \vdots \end{bmatrix} = \begin{bmatrix} w_{11}^l & w_{12}^l & \cdots \\ w_{21}^l & w_{22}^l & \\ \vdots & & \ddots \end{bmatrix} \begin{bmatrix} a_1^{l-1} \\ \vdots \\ a_i^{l-1} \\ \vdots \end{bmatrix} + \begin{bmatrix} b_1^l \\ \vdots \\ b_i^l \\ \vdots \end{bmatrix}$$

$$\Downarrow$$

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

Layer Output Relation – from z to a



Layer $l-1$

N_{l-1} nodes

Layer l

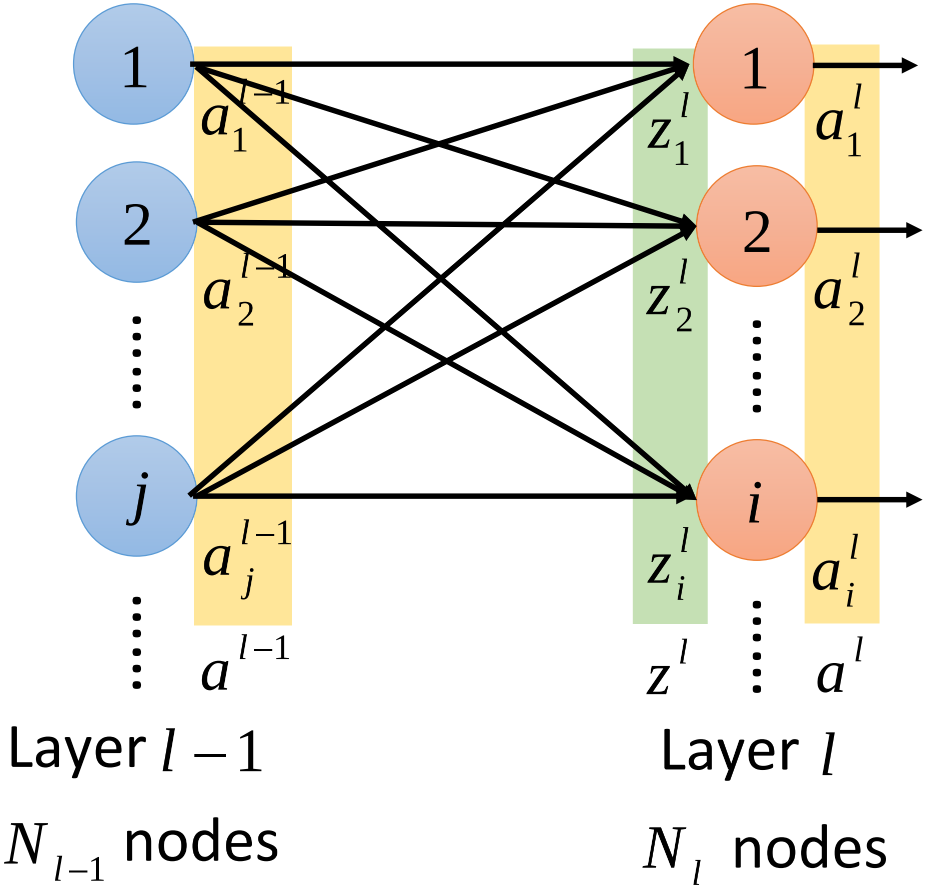
N_l nodes

$$a_i^l = \sigma\left(z_i^l\right)$$

$$\begin{bmatrix} a_1^l \\ a_2^l \\ \vdots \\ a_i^l \\ \vdots \end{bmatrix} = \begin{bmatrix} \sigma\left(z_1^l\right) \\ \sigma\left(z_2^l\right) \\ \vdots \\ \sigma\left(z_i^l\right) \\ \vdots \end{bmatrix}$$

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

Layer Output Relation



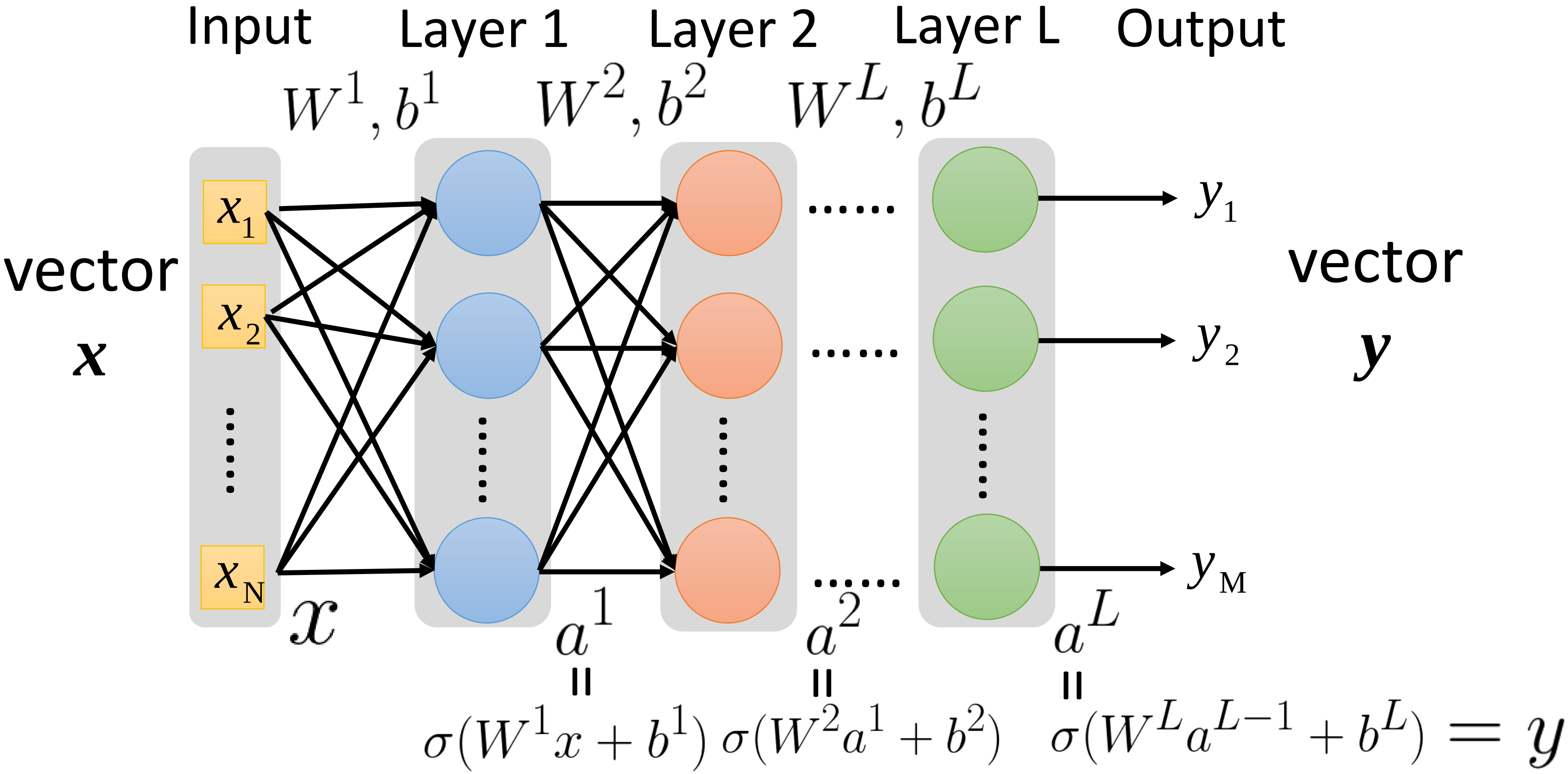
$$z^l = W^l a^{l-1} + b^l$$

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

$$a^l = \sigma(W^l a^{l-1} + b^l)$$

Neural Network Formulation $f : R^N \to R^M$

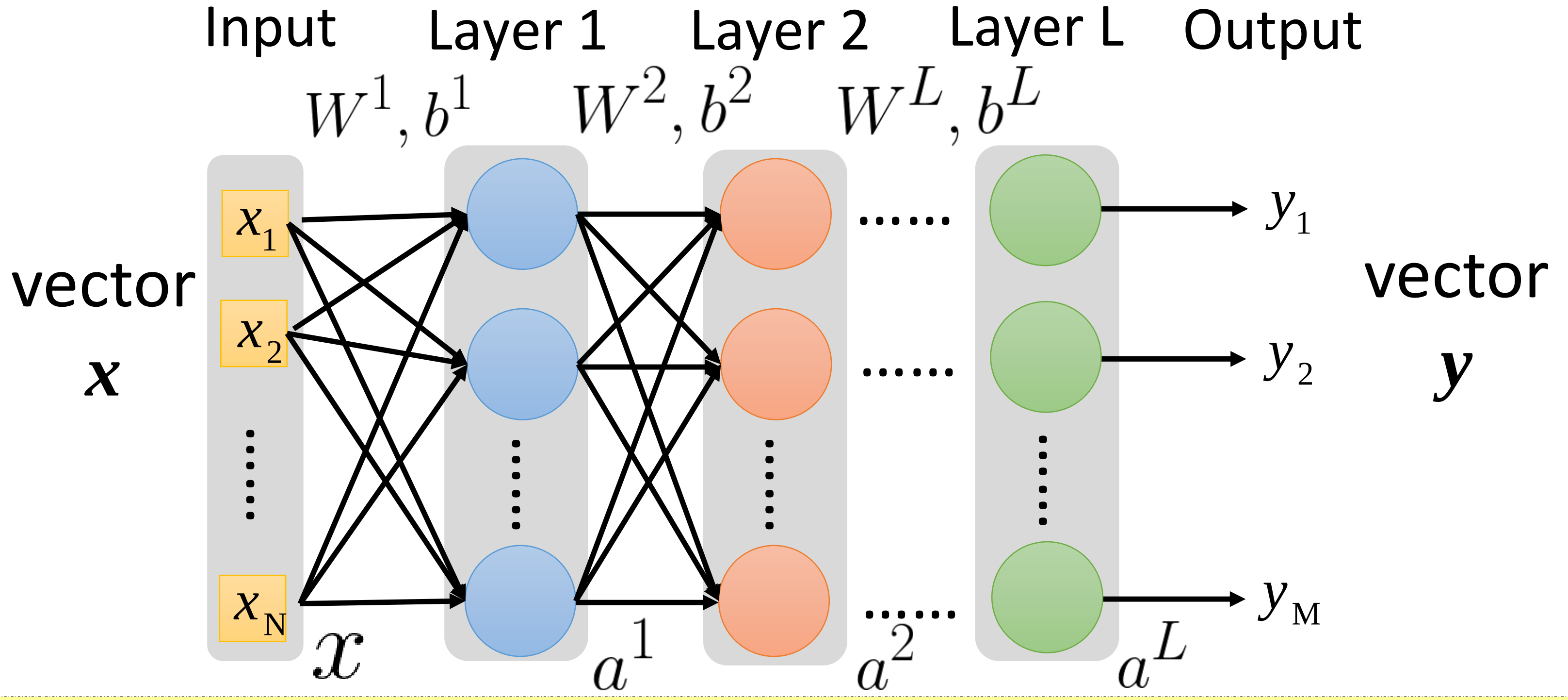
Fully connected feedforward network



$$a^1 = \sigma(W^1 x + b^1) \quad a^2 = \sigma(W^2 a^1 + b^2) \quad a^L = \sigma(W^L a^{L-1} + b^L) = y$$

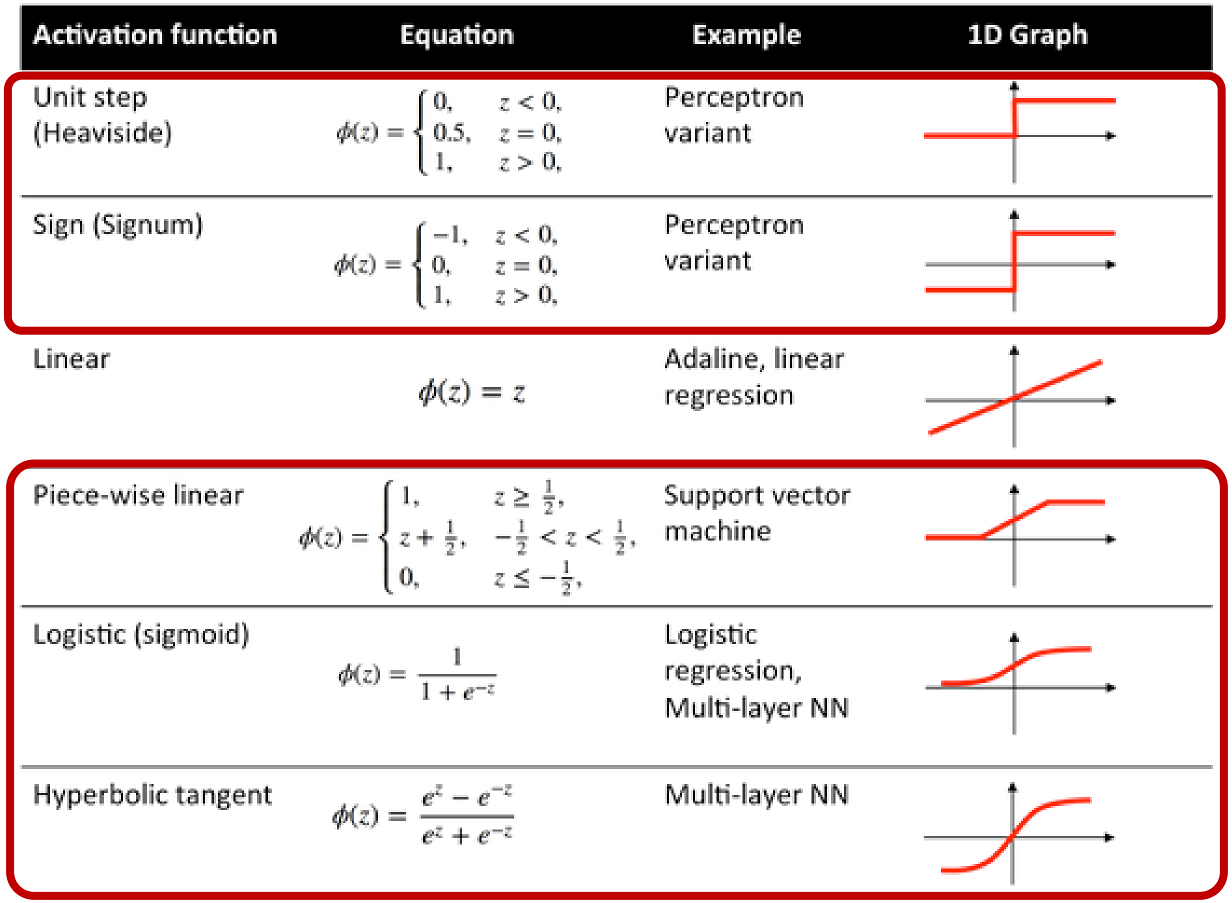
Neural Network Formulation $f: R^N \rightarrow R^M$

Fully connected feedforward network



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

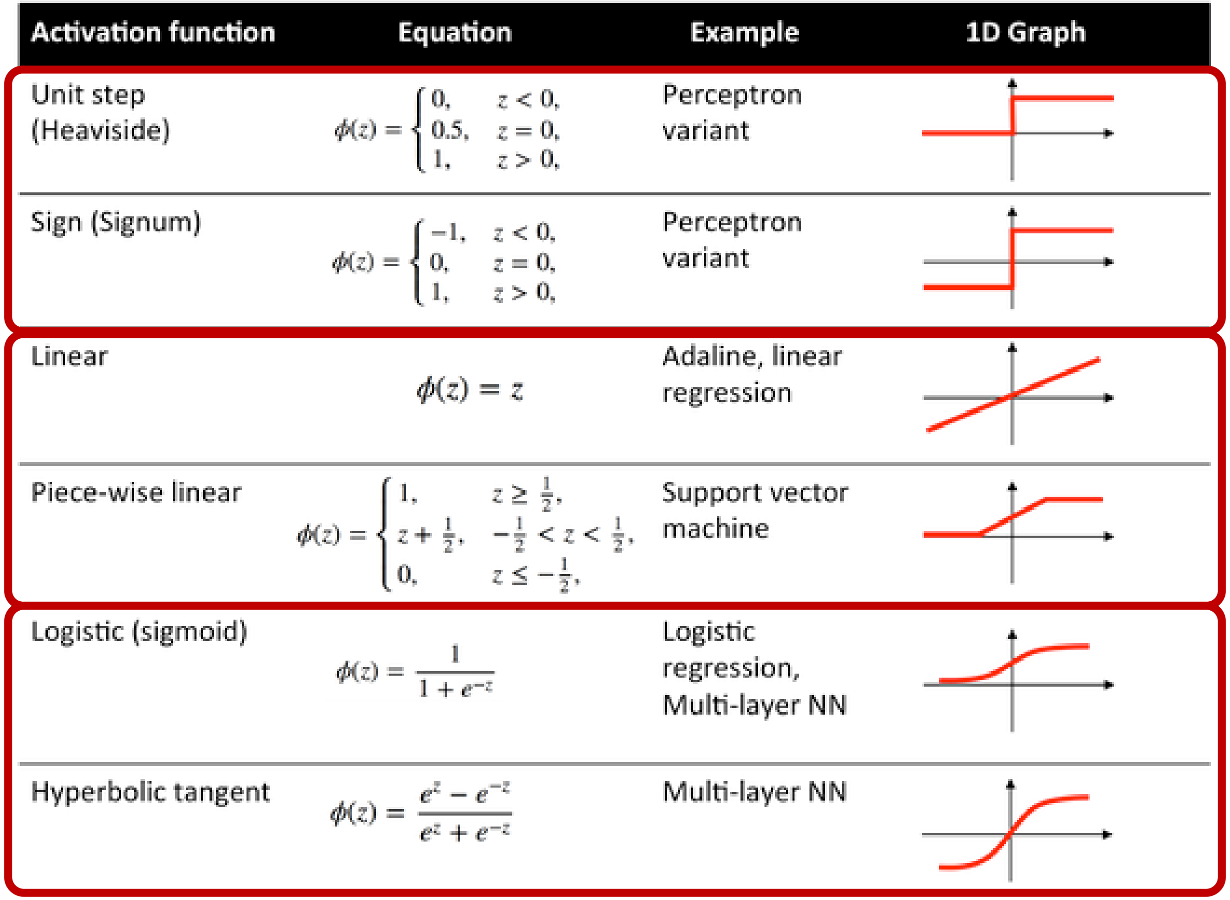
Activation Function $\sigma(\cdot)$



Activation function	Equation	Example	1D Graph
Unit step (Heaviside)	$\phi(z) = \begin{cases} 0, & z < 0, \\ 0.5, & z = 0, \\ 1, & z > 0, \end{cases}$	Perceptron variant	
Sign (Signum)	$\phi(z) = \begin{cases} -1, & z < 0, \\ 0, & z = 0, \\ 1, & z > 0, \end{cases}$	Perceptron variant	
Linear	$\phi(z) = z$	Adaline, linear regression	
Piece-wise linear	$\phi(z) = \begin{cases} 1, & z \geq \frac{1}{2}, \\ z + \frac{1}{2}, & -\frac{1}{2} < z < \frac{1}{2}, \\ 0, & z \leq -\frac{1}{2}, \end{cases}$	Support vector machine	
Logistic (sigmoid)	$\phi(z) = \frac{1}{1 + e^{-z}}$	Logistic regression, Multi-layer NN	
Hyperbolic tangent	$\phi(z) = \frac{e^z - e^{-z}}{e^z + e^{-z}}$	Multi-layer NN	

bounded function

Activation Function $\sigma(\cdot)$



Activation function	Equation	Example	1D Graph
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Hyperbolic tangent	$\phi(z) = \frac{e^z - e^{-z}}{e^z + e^{-z}}$	Multi-layer NN	

boolean

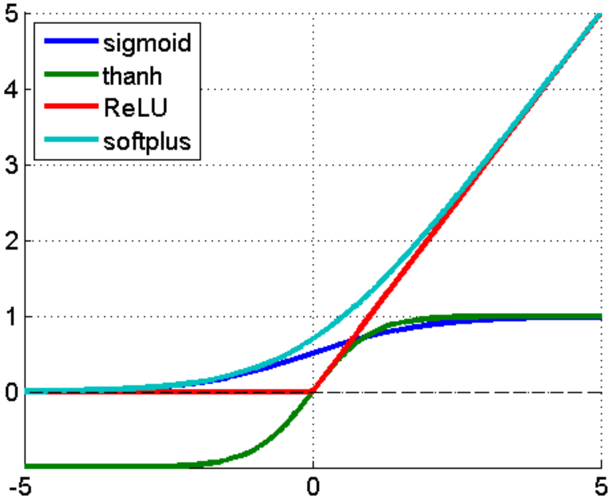
linear

non-linear

Non-Linear Activation Function

Sigmoid

$$\mathrm{sigmoid}(x) = \frac{1}{1 + e^{-x}}$$



Tanh

$$\tanh(x) = \frac{\sinh(x)}{\cosh(x)} = \frac{e^x - e^{-x}}{e^x + e^{-x}}$$

Rectified Linear Unit (ReLU)

$$\mathrm{ReLU}(x) = \max(x, 0)$$

Non-linear functions are frequently used in neural net

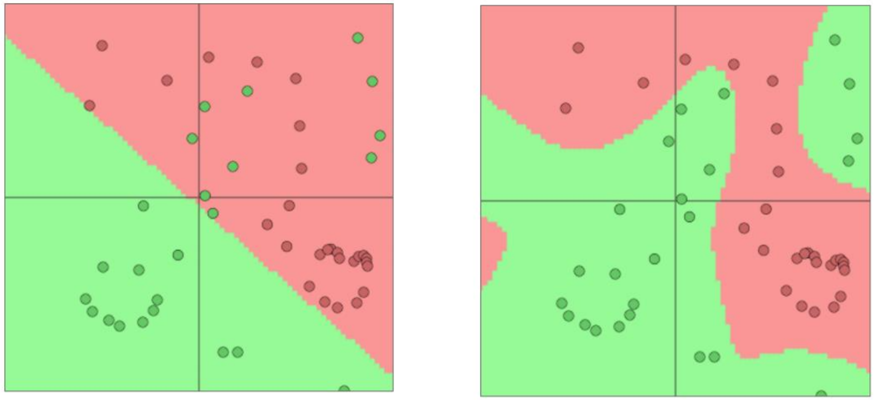
Why Non-Linearity?

Function approximation

- ***Without non-linearity***, deep neural networks work the same as linear transform

$$W_1(W_2 \cdot x) = (W_1 W_2)x = Wx$$

- ***With non-linearity***, networks with more layers can approximate more complex function



What does the “Good” Function mean?

Training Procedure Outline

① Model Architecture

- ✓ A Single Layer of Neurons (Perceptron)
- ✓ Limitation of Perceptron
- ✓ Neural Network Model (Multi-Layer Perceptron)

② Loss Function Design

- ✓ Function = Model Parameters
- ✓ Model Parameter Measurement

③ Optimization

- ✓ Gradient Descent
- ✓ Stochastic Gradient Descent (SGD)
- ✓ Mini-Batch SGD
- ✓ Practical Tips

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Function = Model Parameters

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

function set

different parameters W and b → different functions

Formal definition

$$f(x; \boxed{\theta})$$

model parameter set

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

pick a function f = pick a set of model parameters θ

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Model Parameter Measurement

Define a function to measure the quality of a parameter set θ

- Evaluating by a loss/cost/error function $C(\theta)$ → how bad θ is
- Best model parameter set

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

- Evaluating by an objective/reward function $O(\theta)$ → how good θ is
- Best model parameter set

$$\theta^* = \arg\max_{\theta} O(\theta)$$

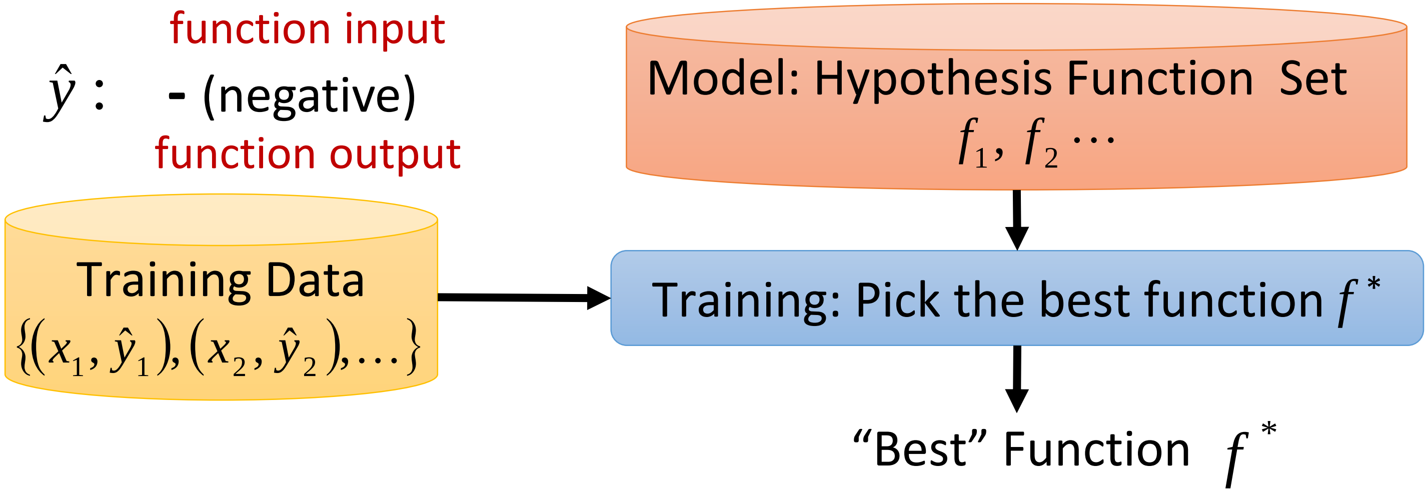
Loss Function Example

x : "It claims too much."

function input

$\hat{y}$: **-** (negative)

function output



Model: Hypothesis Function Set

$f_1, f_2 \cdots$

Training Data

$\{(x_1, \hat{y}_1), (x_2, \hat{y}_2), \ldots\}$

Training: Pick the best function f^*

"Best" Function f^*

A "Good" function: $f(x;\theta) \sim \hat{y} \Rightarrow \|\hat{y} - f(x;\theta)\| \approx 0$

Define an example loss function: $C(\theta) = \sum_k \|\hat{y}_k - f(x_k;\theta)\|$

sum over the error of all training samples

Frequent Loss Function

Square loss

$$C(\theta) = (1 - \hat{y} f(x;\theta))^2$$

Hinge loss

$$C(\theta) = \max(0, 1 - \hat{y} f(x;\theta))$$

Logistic loss

$$C(\theta) = -\hat{y} \log(f(x;\theta))$$

Cross entropy loss

$$C(\theta) = -\sum \hat{y} \log(f(x;\theta))$$

Others: large margin, etc.

https://en.wikipedia.org/wiki/Loss_functions_for_classification

How can we Pick the “Best” Function?

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Problem Statement

Given a loss function and several model parameter sets

- Loss function: $C(\theta)$
- Model parameter sets: $\{\theta_1, \theta_2, \cdots\}$

Find a model parameter set that minimizes $C(\theta)$

How to solve this optimization problem?

1) Brute force – enumerate all possible θ

2) Calculus – $\frac{\partial C(\theta)}{\partial \theta} = 0$

Issue: whole space of $C(\theta)$ is unknown

Training Procedure Outline

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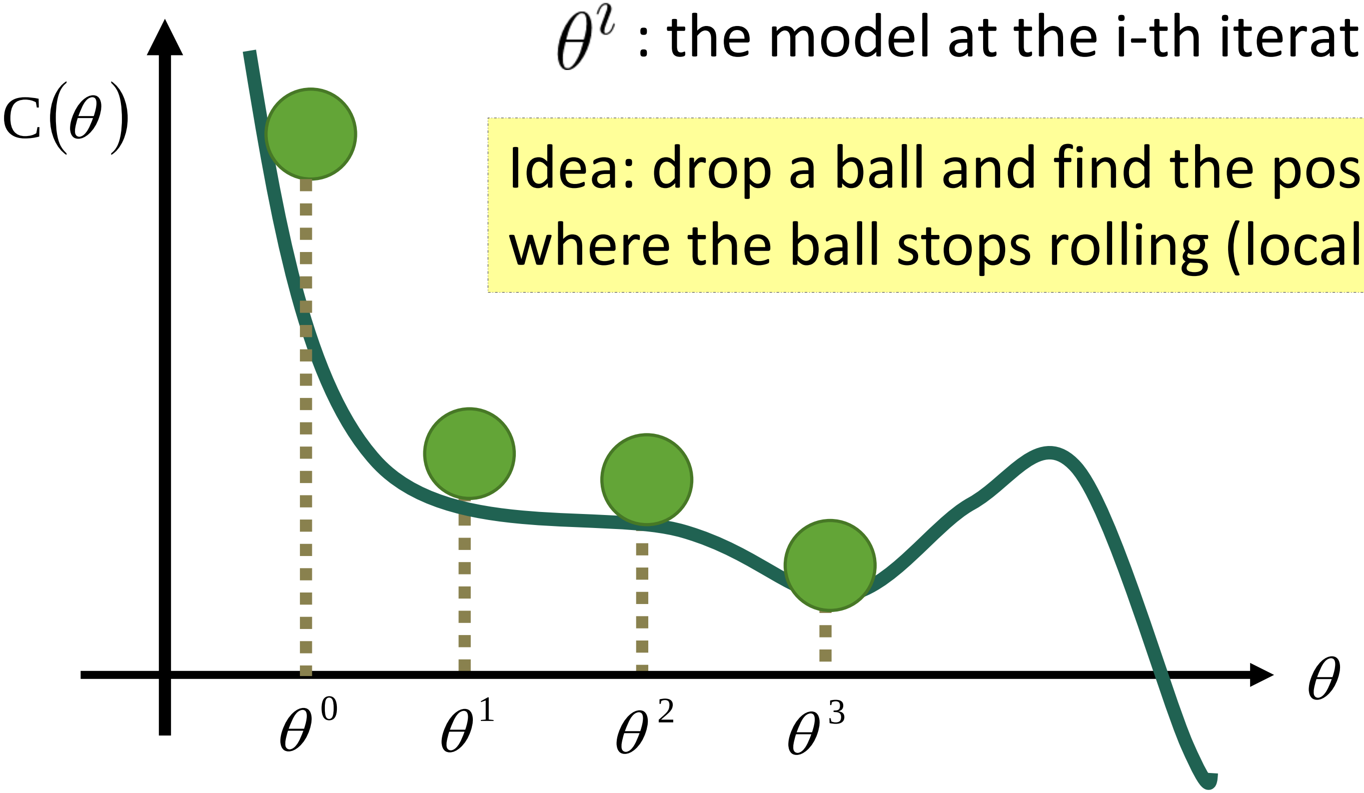
Gradient Descent for Optimization

Assume that θ has only one variable

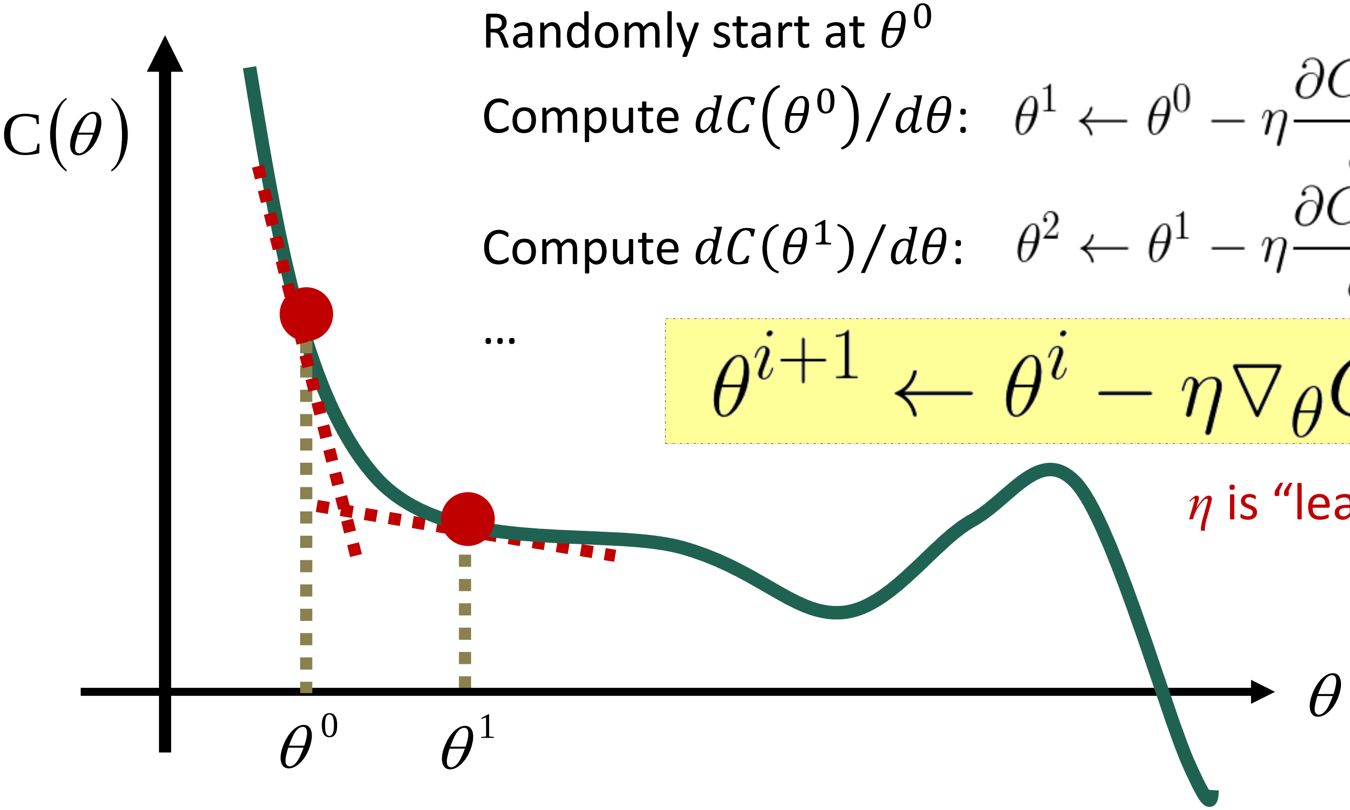
θ^i : the model at the i-th iteration

Idea: drop a ball and find the position where the ball stops rolling (local minima)



Gradient Descent for Optimization

Assume that θ has only one variable



Randomly start at θ^0

Compute $dC(\theta^0)/d\theta$: $\theta^1 \leftarrow \theta^0 - \eta \frac{\partial C(\theta^0)}{\partial \theta}$

Compute $dC(\theta^1)/d\theta$: $\theta^2 \leftarrow \theta^1 - \eta \frac{\partial C(\theta^1)}{\partial \theta}$

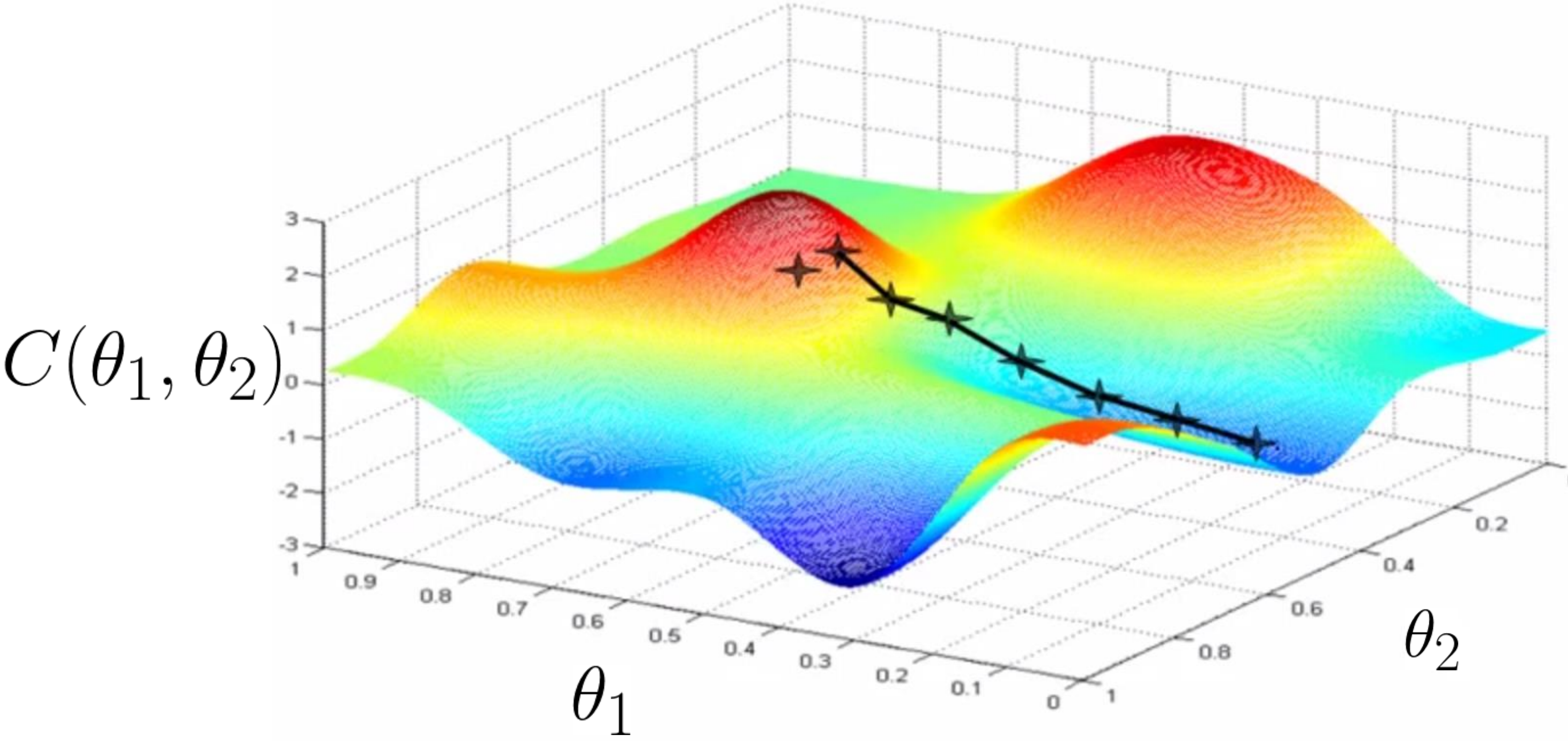
…

$$\theta^{i+1} \leftarrow \theta^i - \eta \nabla_\theta C(\theta^i)$$

η is “learning rate”

Gradient Descent for Optimization

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



Gradient Descent for Optimization

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

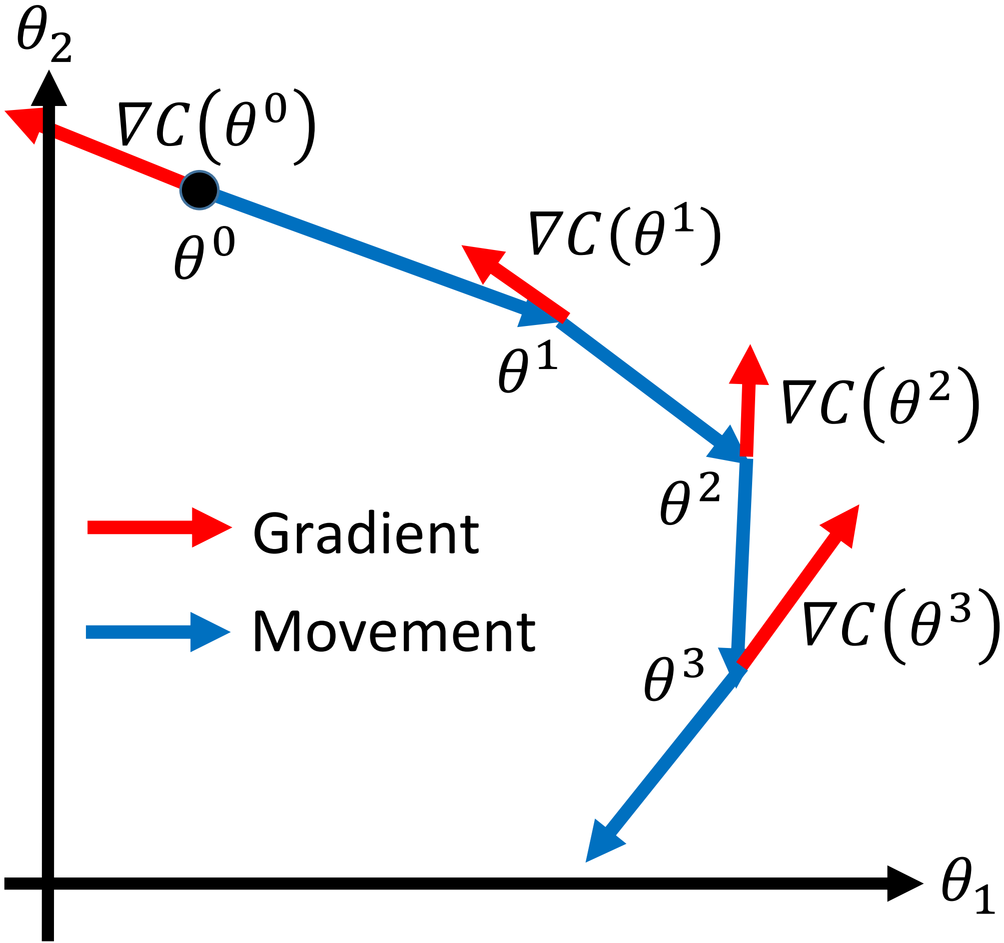
- Randomly start at θ^0: $\theta^0 = \begin{bmatrix} \theta_1^0 \\ \theta_2^0 \end{bmatrix}$
- Compute the gradients of $C(\theta)$ at θ^0: $\nabla_\theta C(\theta^0) = \begin{bmatrix} \frac{\partial C(\theta_1^0)}{\partial \theta_1} \\ \frac{\partial C(\theta_2^0)}{\partial \theta_2} \end{bmatrix}$
- Update parameters:

$$\begin{bmatrix} \theta_1^1 \\ \theta_2^1 \end{bmatrix} = \begin{bmatrix} \theta_1^0 \\ \theta_2^0 \end{bmatrix} - \eta \begin{bmatrix} \frac{\partial C(\theta_1^0)}{\partial \theta_1} \\ \frac{\partial C(\theta_2^0)}{\partial \theta_2} \end{bmatrix}$$

$$\theta^{i+1} \leftarrow \theta^i - \eta \nabla_\theta C(\theta^i)$$

- Compute the gradients of $C(\theta)$ at θ^1: $\nabla_\theta C(\theta^1) = \begin{bmatrix} \frac{\partial C(\theta_1^1)}{\partial \theta_1} \\ \frac{\partial C(\theta_2^1)}{\partial \theta_2} \end{bmatrix}$

Gradient Descent for Optimization

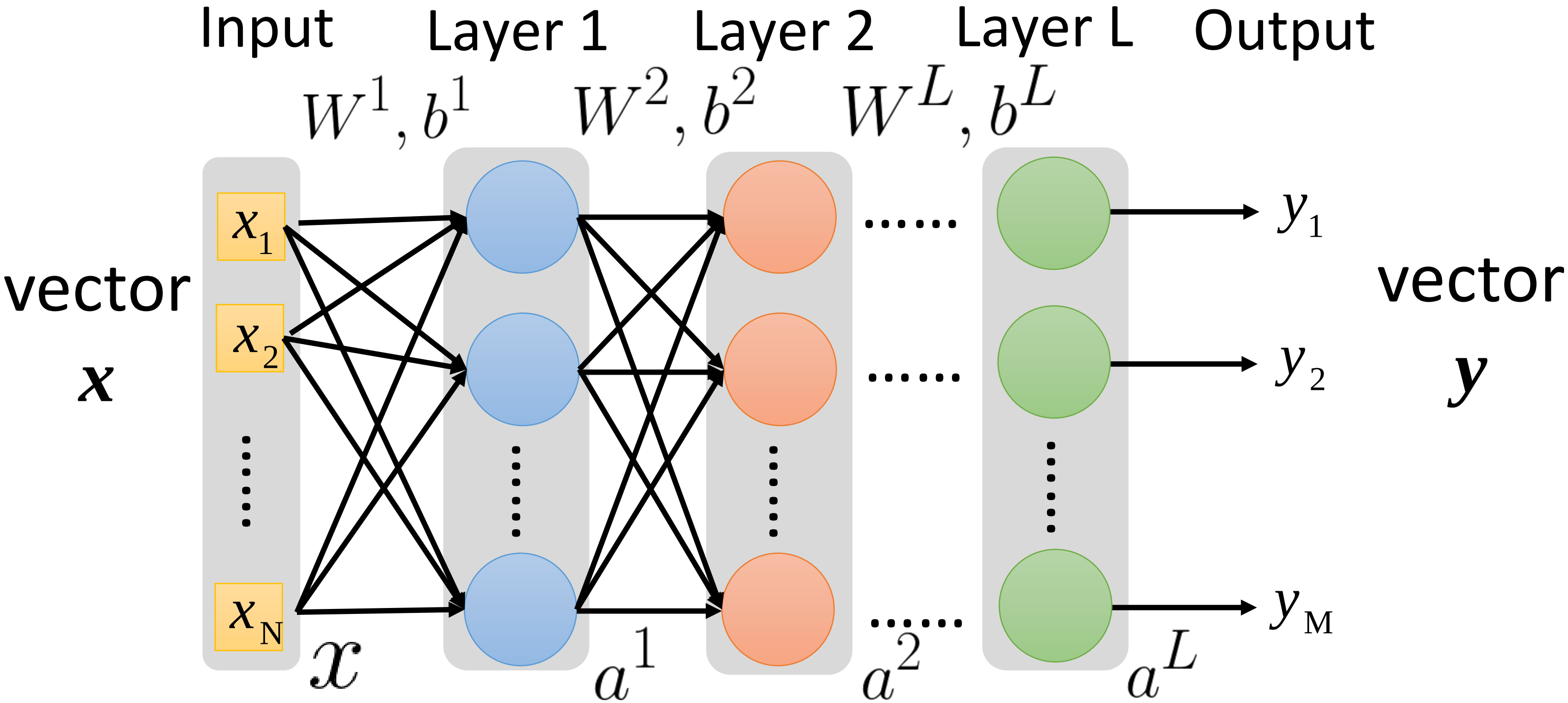


Algorithm

```
Initialization: start at $\theta^0$
while($\theta^{(i+1)} \neq \theta^i$)
{
    compute gradient at $\theta^i$
    update parameters
      $\theta^{i+1} \leftarrow \theta^i - \eta \nabla_\theta C(\theta^i)$
}
```

Revisit Neural Network Formulation

Fully connected feedforward network



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

Gradient Descent for Neural Network

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

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

$$W^l = \begin{bmatrix} w_{11}^l & w_{12}^l & \cdots \\ w_{21}^l & w_{22}^l & \\ \vdots & & \ddots \end{bmatrix} \quad b^l = \begin{bmatrix} \vdots \\ b_i^l \\ \vdots \end{bmatrix}$$

$$\nabla C(\theta) = \begin{bmatrix} \vdots \\ \frac{\partial C(\theta)}{\partial w_{ij}^l} \\ \vdots \\ \frac{\partial C(\theta)}{\partial b_i^l} \end{bmatrix}$$

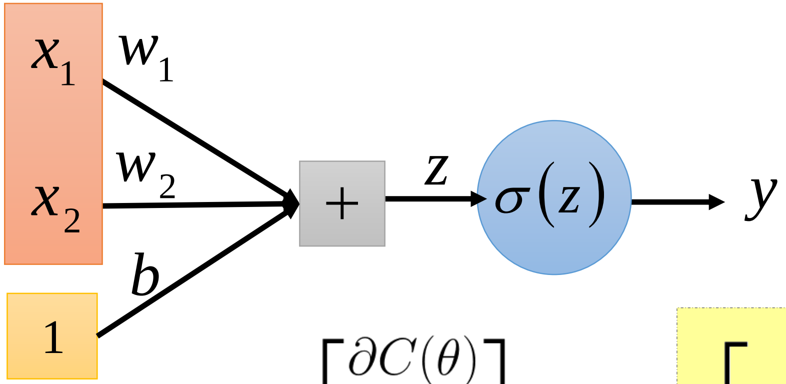
```
Algorithm
Initialization: start at $\theta^0$
while($\theta^{(i+1)} \neq \theta^i$)
{
    compute gradient at $\theta^i$
    update parameters
    $\theta^{i+1} \leftarrow \theta^i - \eta\nabla_\theta C(\theta^i)$
}
```

Gradient Descent for Optimization

Simple Case

$$y = f(x;\theta) = \sigma(Wx + b)$$

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



$$\nabla_\theta C(\theta) = \begin{bmatrix} \frac{\partial C(\theta)}{\partial w_1} \\ \frac{\partial C(\theta)}{\partial w_2} \\ \frac{\partial C(\theta)}{\partial b} \end{bmatrix}$$

```
Algorithm
Initialization: start at $\theta^0$
while($\theta^{(i+1)} \neq \theta^i$)
{
    compute gradient at $\theta^i$
    update parameters
    $\theta^{i+1} \leftarrow \theta^i - \eta \nabla_\theta C(\theta^i)$
}
```

$$\begin{bmatrix} w_1^{i+1} \\ w_2^{i+1} \\ b^{i+1} \end{bmatrix} \leftarrow \begin{bmatrix} w_1^i \\ w_2^i \\ b^i \end{bmatrix} - \eta \begin{bmatrix} \frac{\partial C(\theta)}{\partial w_1} \\ \frac{\partial C(\theta)}{\partial w_2} \\ \frac{\partial C(\theta)}{\partial b} \end{bmatrix}$$

Gradient Descent for Optimization

Simple Case – Three Parameters & Square Error Loss

Update three parameters for t-th iteration

$$w_1^{(t+1)} = w_1^{(t)} - \eta \frac{\partial C(\theta^{(t)})}{\partial w_1}$$

$$w_2^{(t+1)} = w_2^{(t)} - \eta \frac{\partial C(\theta^{(t)})}{\partial w_2}$$

$$b^{(t+1)} = b^{(t)} - \eta \frac{\partial C(\theta^{(t)})}{\partial b}$$

$$\begin{bmatrix} w_1^{i+1} \\ w_2^{i+1} \\ b^{i+1} \end{bmatrix} \leftarrow \begin{bmatrix} w_1^{i} \\ w_2^{i} \\ b^{i} \end{bmatrix} - \eta \begin{bmatrix} \frac{\partial C(\theta)}{\partial w_1} \\ \frac{\partial C(\theta)}{\partial w_2} \\ \frac{\partial C(\theta)}{\partial b} \end{bmatrix}$$

Square error loss

$$C(\theta) = \sum_{\forall x} \|\hat{y} - f(x;\theta)\| = (\hat{y} - f(x;\theta))^2$$

Gradient Descent for Optimization

Simple Case – Square Error Loss

Square Error Loss

$$\frac{\partial C(\theta)}{\partial w_1} = \frac{\partial}{\partial w_1}(f(x;\theta) - \hat{y})^2$$

$$= 2(f(x;\theta) - \hat{y})\frac{\partial}{\partial w_1}f(x;\theta)$$

$$= 2(\sigma(Wx+b) - \hat{y})\boxed{\frac{\partial}{\partial w_1}\sigma(Wx+b)}$$

$$f(x;\theta) = \sigma(Wx+b)$$

Gradient Descent for Optimization

Simple Case – Square Error Loss

$$\frac{\partial \sigma(Wx+b)}{\partial w_1} = \frac{\partial \sigma(Wx+b)}{\partial (Wx+b)} \frac{\partial (Wx+b)}{\partial w_1}$$

$$\frac{\partial g}{\partial x} = \frac{\partial g}{\partial f} \frac{\partial f}{\partial x}$$ chain rule $$\frac{\partial g(z)}{\partial z} = [1 - g(z)]g(z)$$ sigmoid func $g(z) = \frac{1}{1+e^{-x}}$

$$= [1 - \sigma(Wx+b)]\sigma(Wx+b) \boxed{\frac{\partial (Wx+b)}{\partial w_1}}$$

$$\frac{\partial (Wx+b)}{\partial w_1} = \frac{\partial (w_1 x_1 + w_2 x_2 + b)}{\partial w_1} = x_1$$

$$\frac{\partial \sigma(Wx+b)}{\partial w_1} = [1 - \sigma(Wx+b)]\sigma(Wx+b)x_1$$

Gradient Descent for Optimization

Simple Case – Square Error Loss

Square Error Loss

$$\frac{\partial C(\theta)}{\partial w_1} = \frac{\partial}{\partial w_1}(f(x;\theta) - \hat{y})^2$$

$$= 2(f(x;\theta) - \hat{y})\frac{\partial}{\partial w_1}f(x;\theta)$$

$$f(x;\theta) = \sigma(Wx + b)$$

$$= 2(\sigma(Wx + b) - \hat{y})\boxed{\frac{\partial}{\partial w_1}\sigma(Wx + b)}$$

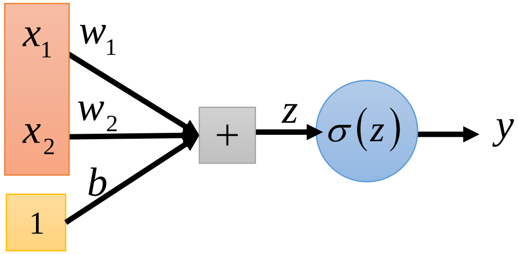
$$\frac{\partial \sigma(Wx + b)}{\partial w_1} = [1 - \sigma(Wx + b)]\sigma(Wx + b)x_1$$

$$\frac{\partial C(\theta)}{\partial w_1} = 2(\sigma(Wx + b) - \hat{y})[1 - \sigma(Wx + b)]\sigma(Wx + b)x_1$$

Gradient Descent for Optimization

Simple Case – Three Parameters & Square Error Loss

Update three parameters for t-th iteration



$$w_1^{(t+1)} = w_1^{(t)} - \eta \frac{\partial C(\theta^{(t)})}{\partial w_1}$$

$$\frac{\partial C(\theta)}{\partial w_1} = 2(\sigma(Wx+b) - \hat{y})[1 - \sigma(Wx+b)]\sigma(Wx+b)x_1$$

$$w_2^{(t+1)} = w_2^{(t)} - \eta \frac{\partial C(\theta^{(t)})}{\partial w_2}$$

$$\frac{\partial C(\theta)}{\partial w_2} = 2(\sigma(Wx+b) - \hat{y})[1 - \sigma(Wx+b)]\sigma(Wx+b)x_2$$

$$b^{(t+1)} = b^{(t)} - \eta \frac{\partial C(\theta^{(t)})}{\partial b}$$

$$\frac{\partial C(\theta)}{\partial b} = 2(\sigma(Wx+b) - \hat{y})[1 - \sigma(Wx+b)]\sigma(Wx+b)$$

Optimization Algorithm

```
Algorithm
Initialization: set the parameters $\theta, b$ at random
while(stopping criteria not met)
{
    for training sample $\{x, \hat{y}\}$, compute gradient and update parameters
        $\theta^{i+1} \leftarrow \theta^{i} - \eta \nabla_{\theta} C(\theta^{i})$
}
```

$$w_1^{(t+1)} = w_1^{(t)} - \eta \frac{\partial C(\theta^{(t)})}{\partial w_1} \quad \frac{\partial C(\theta)}{\partial w_1} = 2(\sigma(Wx+b) - \hat{y})[1 - \sigma(Wx+b)]\sigma(Wx+b)x_1$$

$$w_2^{(t+1)} = w_2^{(t)} - \eta \frac{\partial C(\theta^{(t)})}{\partial w_2} \quad \frac{\partial C(\theta)}{\partial w_2} = 2(\sigma(Wx+b) - \hat{y})[1 - \sigma(Wx+b)]\sigma(Wx+b)x_2$$

$$b^{(t+1)} = b^{(t)} - \eta \frac{\partial C(\theta^{(t)})}{\partial b} \quad \frac{\partial C(\theta)}{\partial b} = 2(\sigma(Wx+b) - \hat{y})[1 - \sigma(Wx+b)]\sigma(Wx+b)$$

Gradient Descent for Neural Network

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

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

$$W^l = \begin{bmatrix} w^l_{11} & w^l_{12} & \cdots \\ w^l_{21} & w^l_{22} & \\ \vdots & & \ddots \end{bmatrix} \quad b^l = \begin{bmatrix} \vdots \\ b^l_i \\ \vdots \end{bmatrix}$$

$$\nabla C(\theta) = \begin{bmatrix} \vdots \\ \frac{\partial C(\theta)}{\partial w^l_{ij}} \\ \vdots \\ \frac{\partial C(\theta)}{\partial b^l_i} \end{bmatrix}$$

```
Algorithm
Initialization: start at $\theta^0$
while($\theta^{(i+1)} \neq \theta^i$)
{
    compute gradient at $\theta^i$
    update parameters
     $\theta^{i+1} \leftarrow \theta^i - \eta\nabla_\theta C(\theta^i)$
}
```

Computing the gradient includes millions of parameters.
To compute it efficiently, we use **backpropagation**.

Gradient Descent Issue

$$\theta^{i+1} = \theta^i - \eta \nabla C(\theta^i)$$

Training Data

$\{(x_1, \hat{y}_1), (x_2, \hat{y}_2), \ldots\}$

$$C(\theta) = \frac{1}{K}\sum_k \|f(x_k;\theta) - \hat{y}_k\| = \frac{1}{K}\sum_k C_k(\theta)$$

$$\nabla C(\theta^i) = \frac{1}{K}\sum_k \nabla C_k(\theta^i)$$

After seeing all training samples, the model can be updated → slow

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Stochastic Gradient Descent (SGD)

Gradient Descent

$$\theta^{i+1} = \theta^i - \eta \nabla C(\theta^i) \quad \nabla C(\theta^i) = \boxed{\frac{1}{K}\sum_k \nabla C_k(\theta^i)}$$

Stochastic Gradient Descent (SGD)

- Pick a training sample x_k

$$\theta^{i+1} = \theta^i - \eta \nabla C_k(\theta^i)$$

- If all training samples have same probability to be picked

$$E[\nabla C_k(\theta^i)] = \boxed{\frac{1}{K}\sum_k \nabla C_k(\theta^i)}$$

Training Data

$\{(x_1, \hat{y}_1), (x_2, \hat{y}_2), \ldots\}$

The model can be updated after seeing one training sample → faster

Epoch Definition

When running SGD, the model starts θ^0

Training Data

$\{(x_1, \hat{y}_1), (x_2, \hat{y}_2), \ldots\}$

pick x_1 $\quad \theta^1 = \theta^0 - \eta \nabla C_1(\theta^0)$

pick x_2 $\quad \theta^2 = \theta^1 - \eta \nabla C_2(\theta^1)$

$\vdots \qquad \vdots$

pick x_k $\quad \theta^k = \theta^{k-1} - \eta \nabla C_k(\theta^{k-1})$

$\vdots \qquad \vdots$

pick x_K $\quad \theta^K = \theta^{K-1} - \eta \nabla C_K(\theta^{K-1})$

see all training samples once

→ one epoch

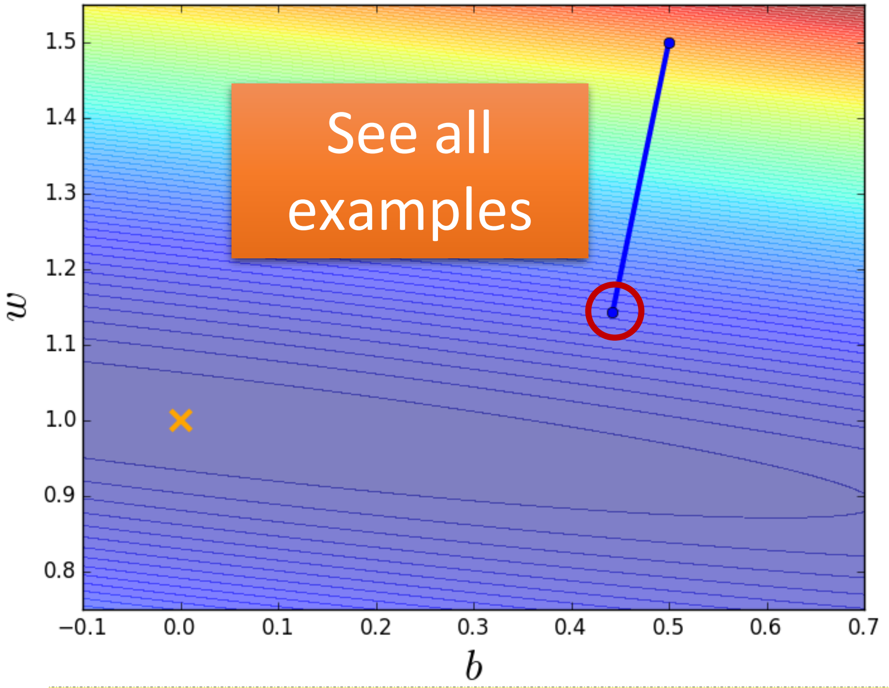
---

pick x_1 $\quad \theta^{K+1} = \theta^K - \eta \nabla C_1(\theta^K)$

Gradient Descent v.s. SGD

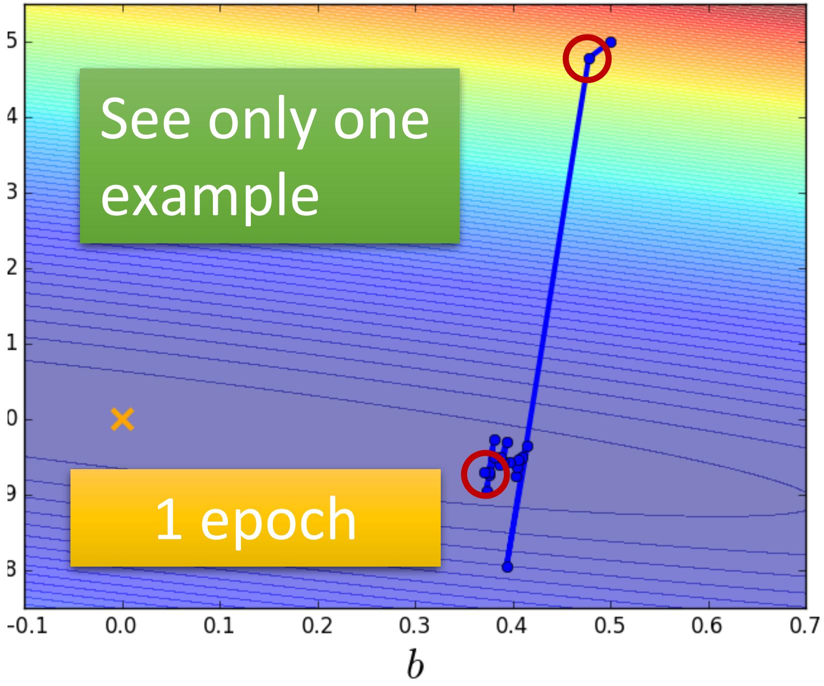
Gradient Descent

Update after seeing all examples



Stochastic Gradient Descent

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



SGD approaches to the target point faster than gradient descent

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Mini-Batch SGD

Batch Gradient Descent

$$\theta^{i+1} = \theta^i - \eta \frac{1}{K} \sum_k \nabla C_k(\theta^i)$$

Use all K samples in each iteration

Stochastic Gradient Descent (SGD)

- Pick a training sample x_k

$$\theta^{i+1} = \theta^i - \eta \nabla C_k(\theta^i)$$

Use *1* samples in each iteration

Mini-Batch SGD

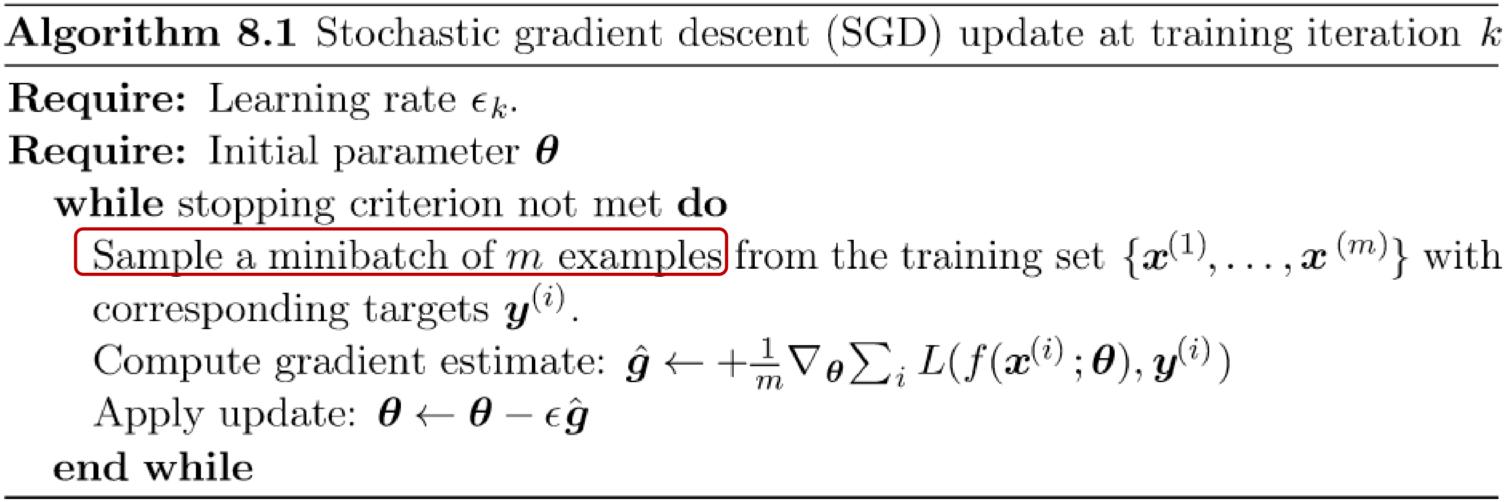
- Pick a set of B training samples as a batch b

B is "batch size"

$$\theta^{i+1} = \theta^i - \eta \frac{1}{B} \sum_{x_k \in b} \nabla C_k(\theta^i)$$

Use all B samples in each iteration

Mini-Batch SGD

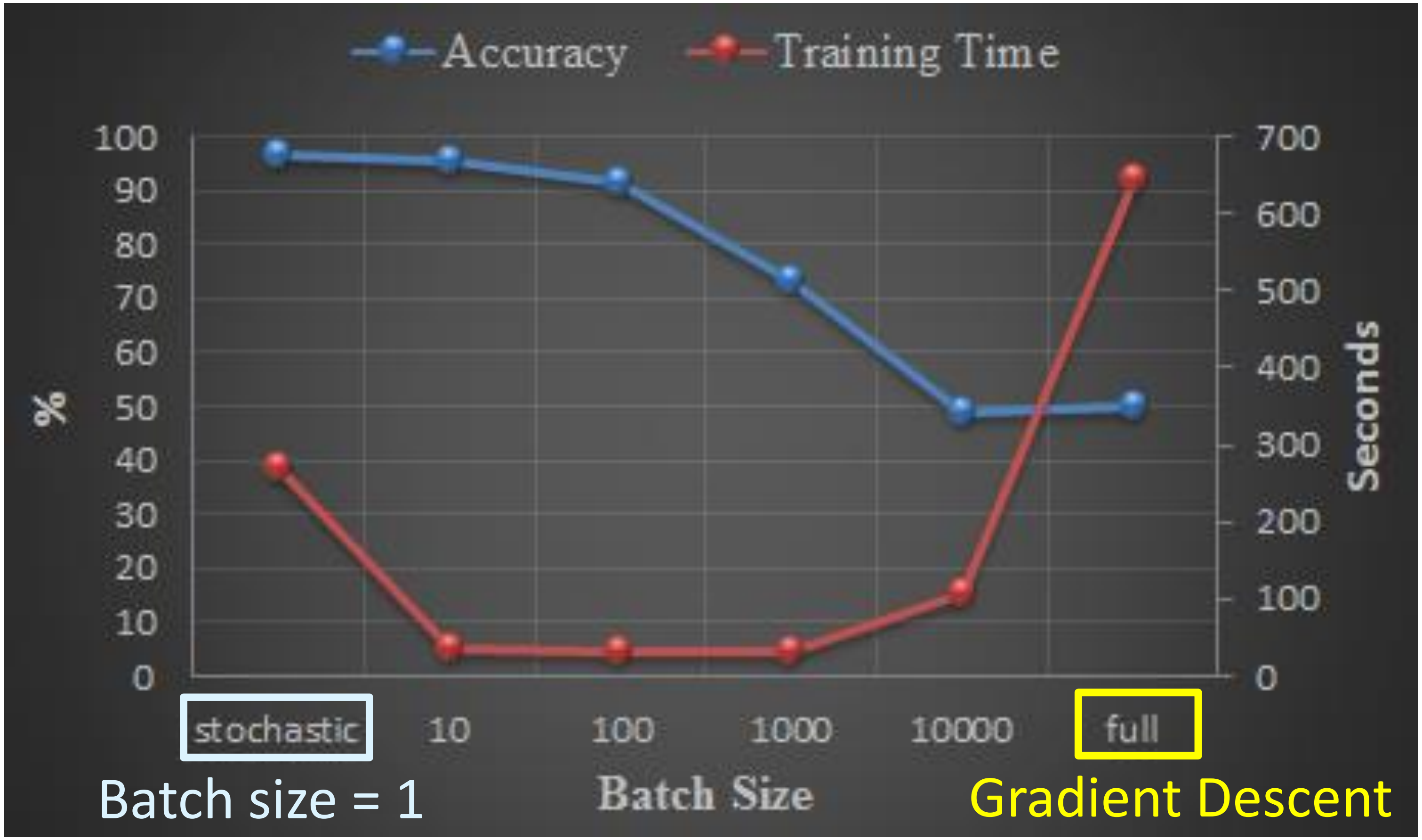


Algorithm 8.1 Stochastic gradient descent (SGD) update at training iteration k

```
Require: Learning rate $\epsilon_k$.
Require: Initial parameter $\boldsymbol{\theta}$
  while stopping criterion not met do
    Sample a minibatch of $m$ examples from the training set $\{\boldsymbol{x}^{(1)}, \dots, \boldsymbol{x}^{(m)}\}$ with corresponding targets $\boldsymbol{y}^{(i)}$.
    Compute gradient estimate: $\hat{\boldsymbol{g}} \leftarrow +\frac{1}{m}\nabla_{\boldsymbol{\theta}}\sum_i L(f(\boldsymbol{x}^{(i)};\boldsymbol{\theta}), \boldsymbol{y}^{(i)})$
    Apply update: $\boldsymbol{\theta} \leftarrow \boldsymbol{\theta} - \epsilon\hat{\boldsymbol{g}}$
  end while
```

Batch v.s. Mini-Batch

Handwritting Digit Classification

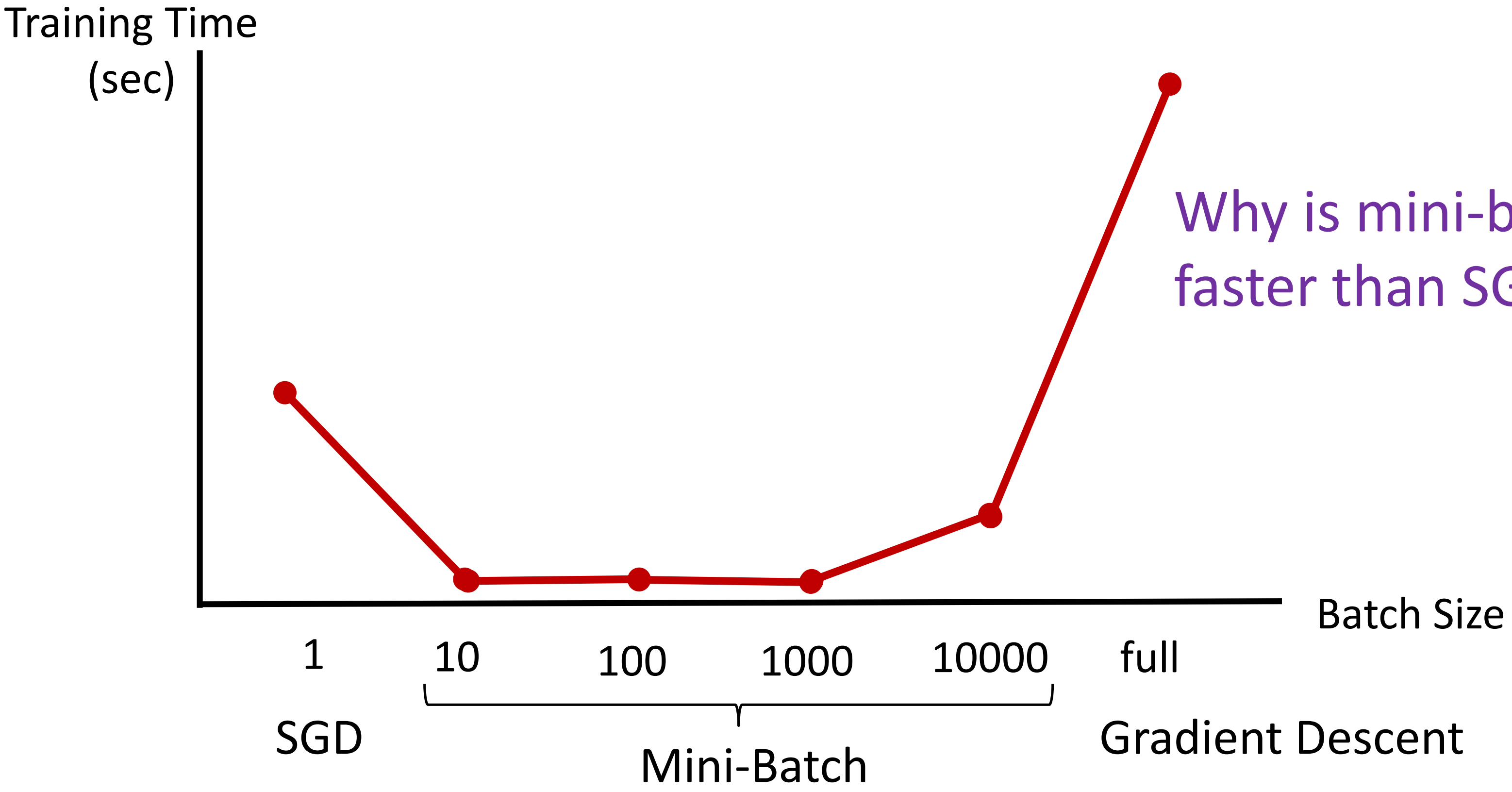


Batch size = 1

Gradient Descent

Gradient Descent v.s. SGD v.s. Mini-Batch

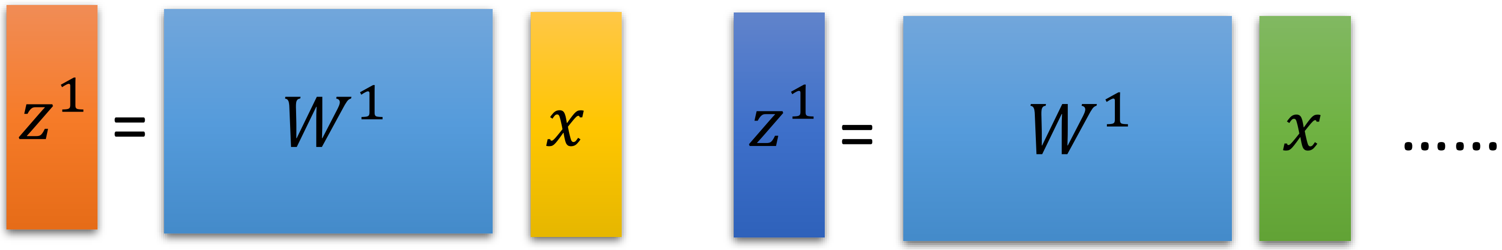
Training speed: mini-batch > SGD > Gradient Descent



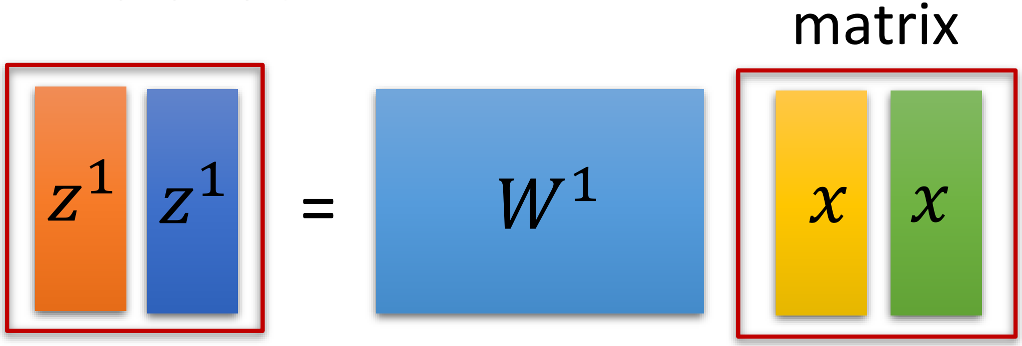
Why is mini-batch faster than SGD?

SGD v.s. Mini-Batch

Stochastic Gradient Descent (SGD)

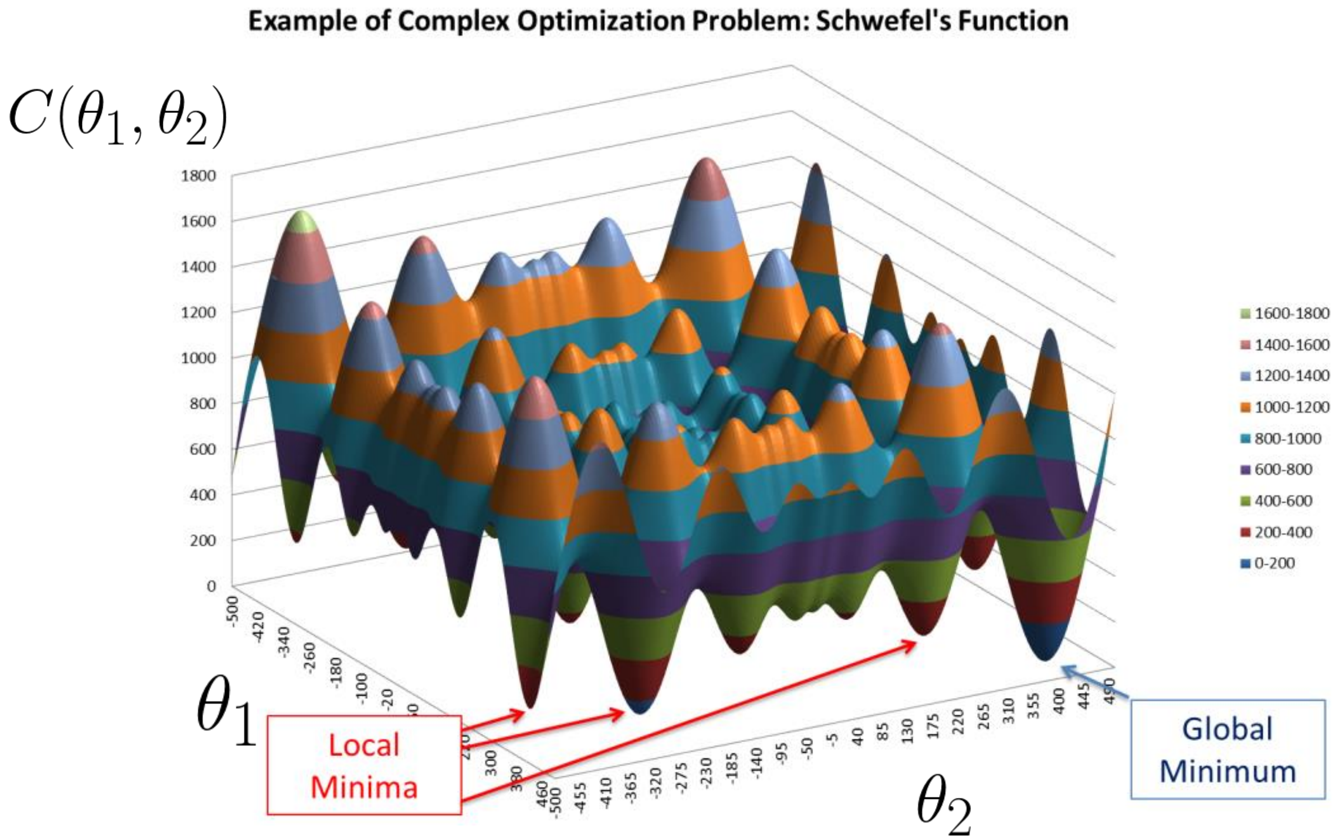


Mini-Batch SGD



Modern computers run matrix-matrix multiplication faster than matrix-vector multiplication

Big Issue: Local Optima



Neural networks has <u>no guarantee</u> for obtaining global optimal solution

Training Procedure Outline

① Model Architecture

- ✓ A Single Layer of Neurons (Perceptron)
- ✓ Limitation of Perceptron
- ✓ Neural Network Model (Multi-Layer Perceptron)

② Loss Function Design

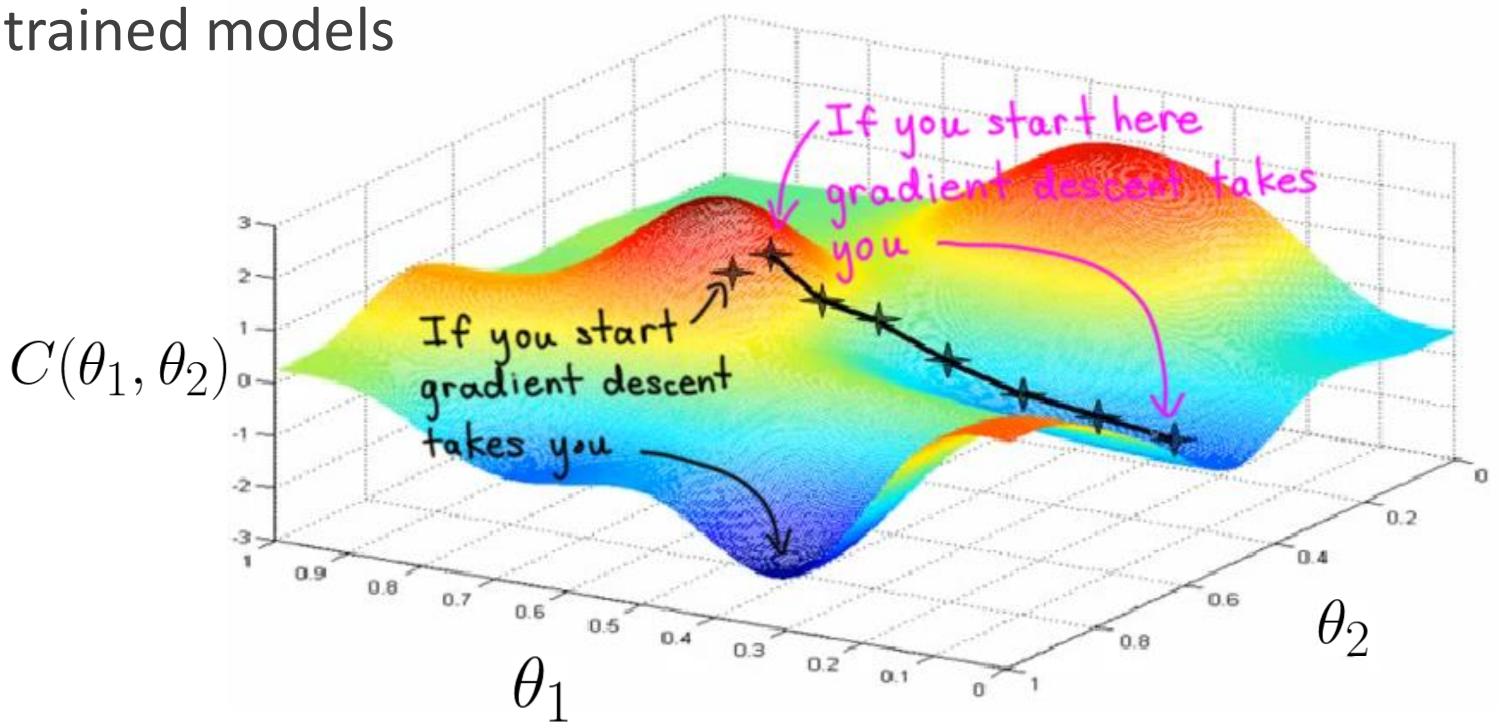
- ✓ Function = Model Parameters
- ✓ Model Parameter Measurement

③ Optimization

- ✓ Gradient Descent
- ✓ Stochastic Gradient Descent (SGD)
- ✓ Mini-Batch SGD
- ✓ Practical Tips

Initialization

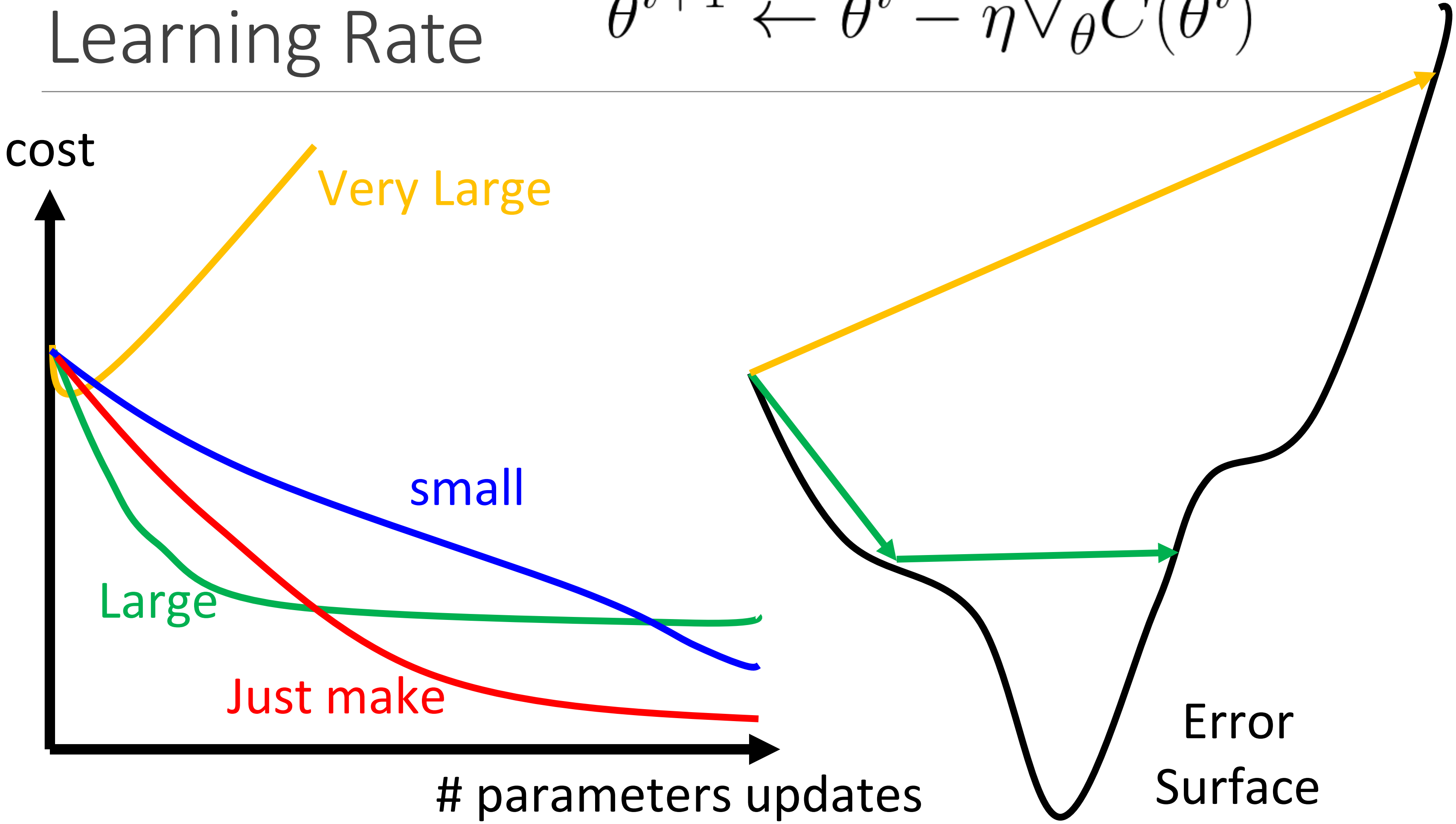
Different initialization parameters may result in different trained models



Do not initialize the parameters equally → set them randomly

Learning Rate

$$\theta^{i+1} \leftarrow \theta^{i} - \eta \nabla_{\theta} C(\theta^{i})$$



Learning rate should be set carefully

Tips for Mini-Batch Training

Shuffle training samples before every epoch

- the network might memorize the order you feed the samples

Use a fixed batch size for every epoch

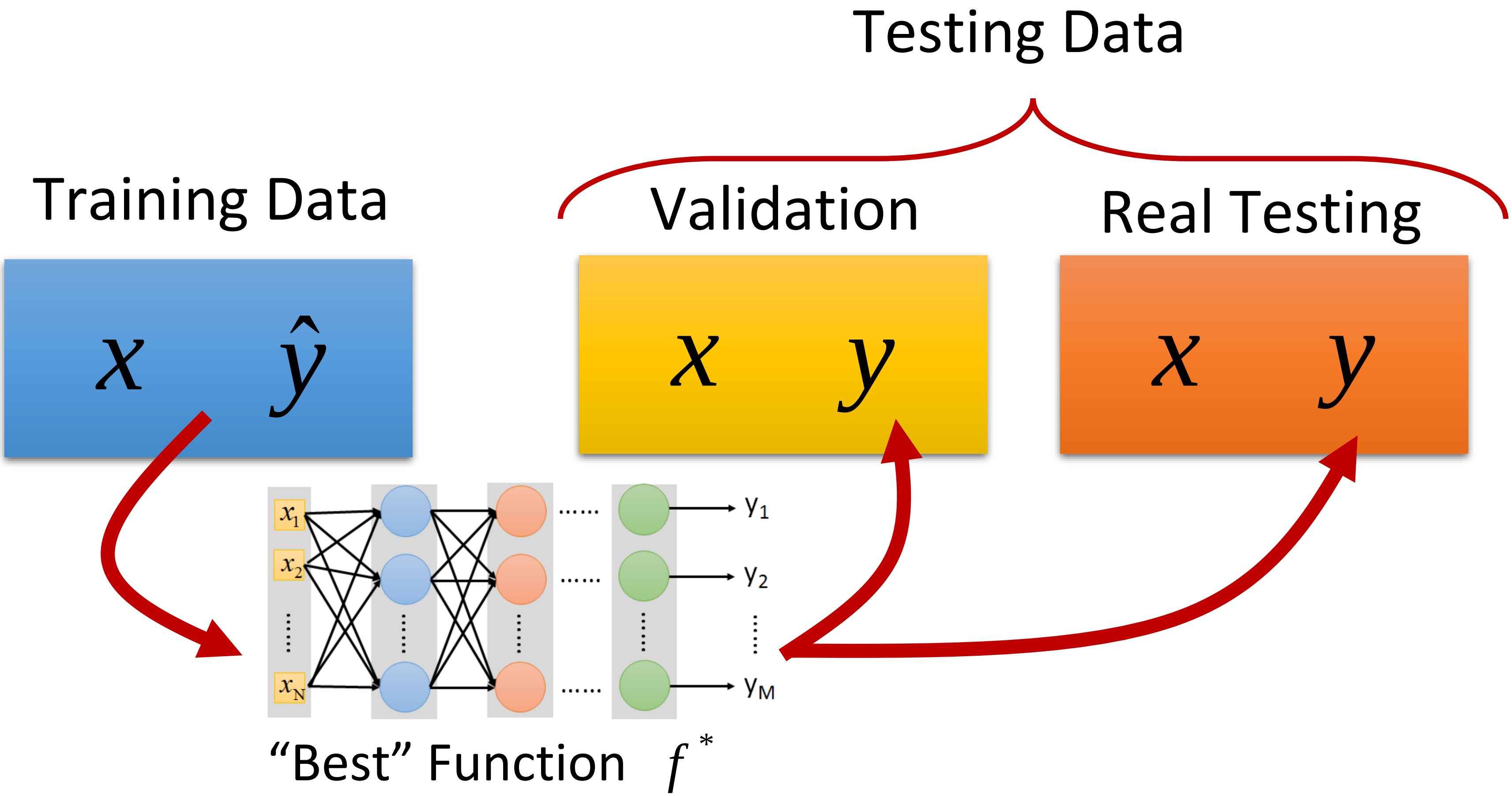
- enable to fast implement matrix multiplication for calculations

Adapt the learning rate to the batch size

- larger batch → smaller learning rate

http://stackoverflow.com/questions/13693966/neural-net-selecting-data-for-each-mini-batch

Learning Recipe



Testing Data

Training Data

Validation

Real Testing

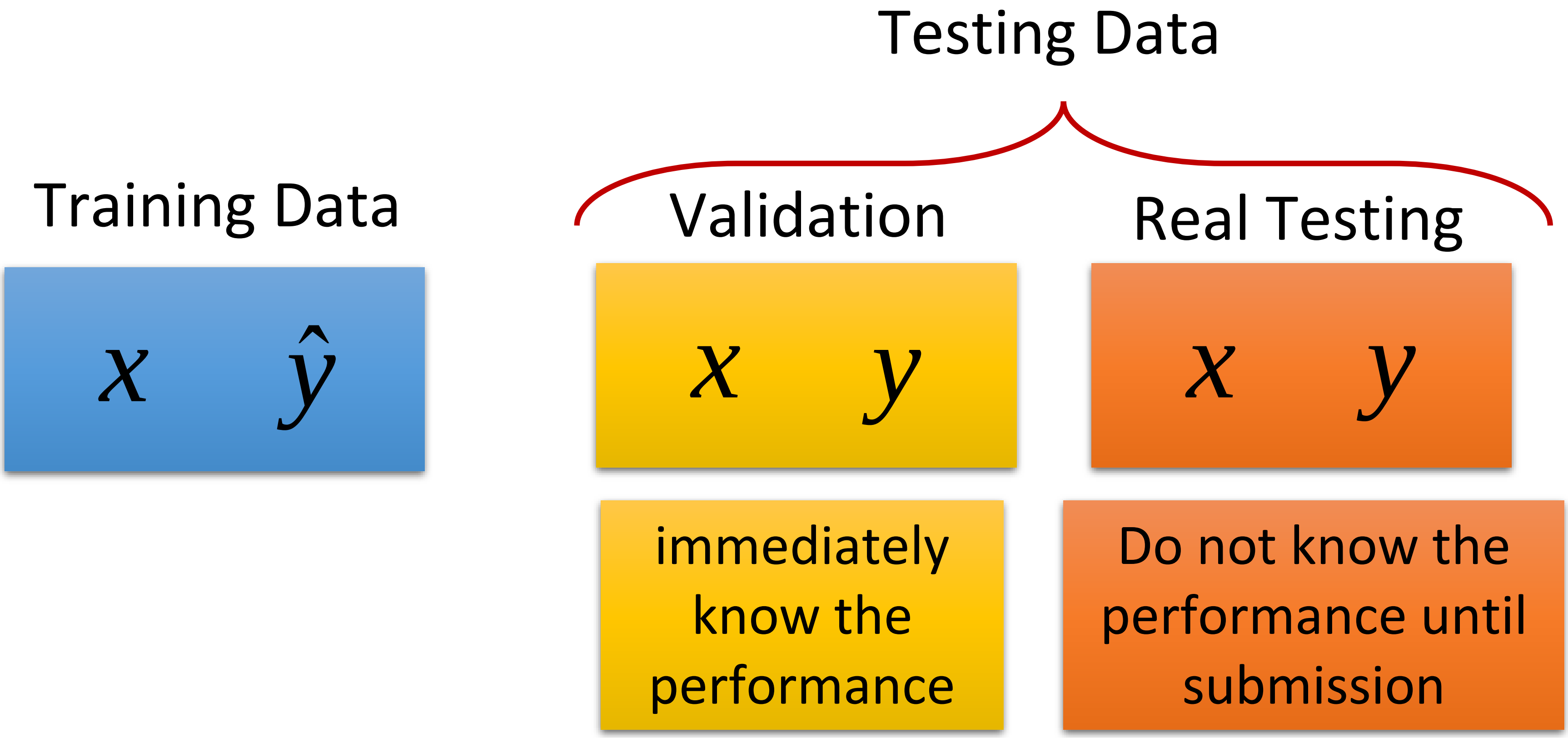
x $\hat{y}$

x y

x y

“Best” Function f^*

Learning Recipe



Testing Data

Training Data

x $\hat{y}$

Validation

x y

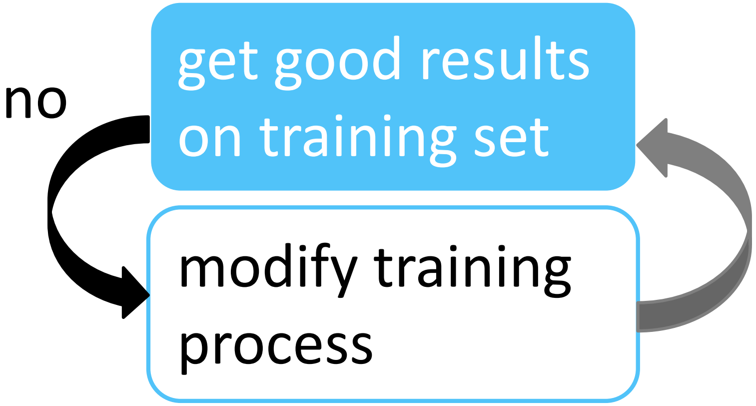
immediately know the performance

Real Testing

x y

Do not know the performance until submission

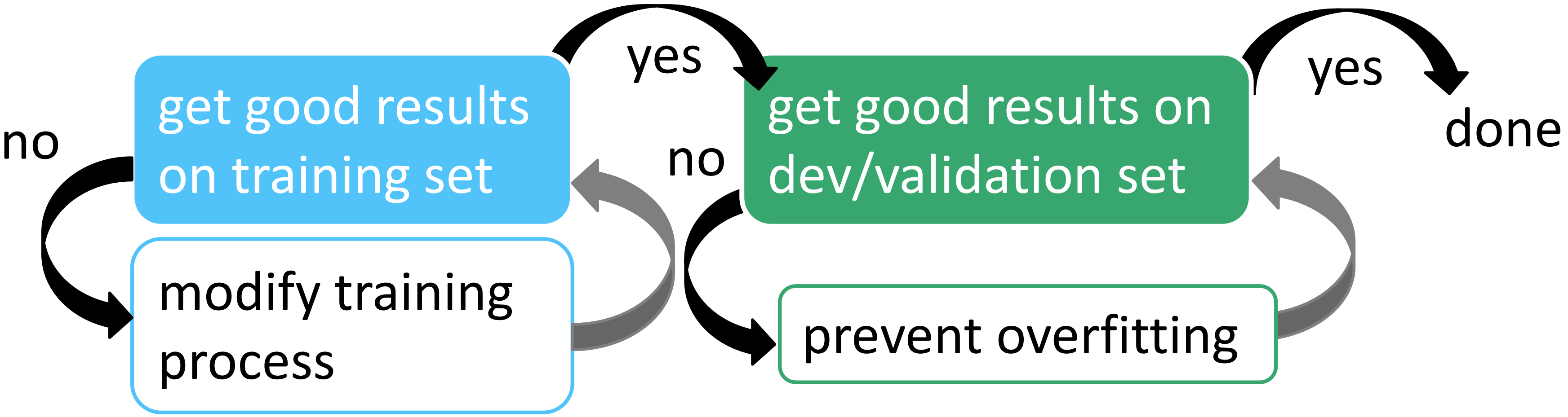
Learning Recipe



Possible reasons

- no good function exists: bad hypothesis function set
  → reconstruct the model architecture
- cannot find a good function: local optima
  → change the training strategy

Learning Recipe



get good results on training set

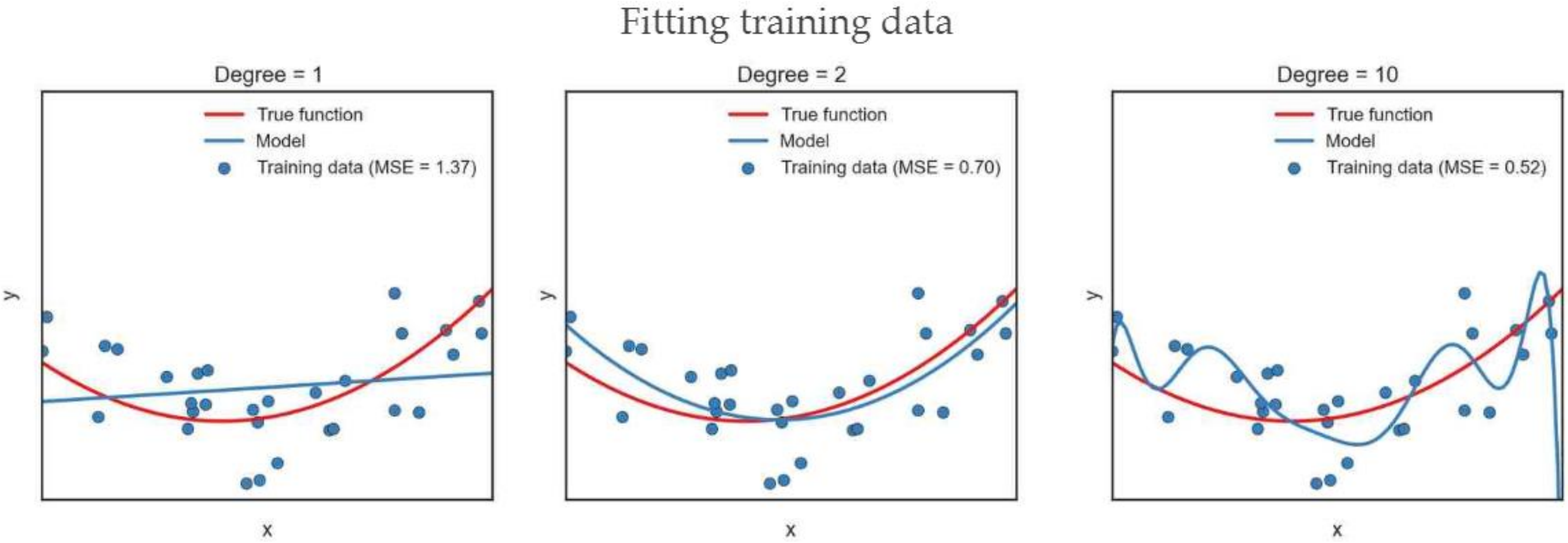
modify training process

get good results on dev/validation set

prevent overfitting

Better performance on training but worse performance on dev → overfitting

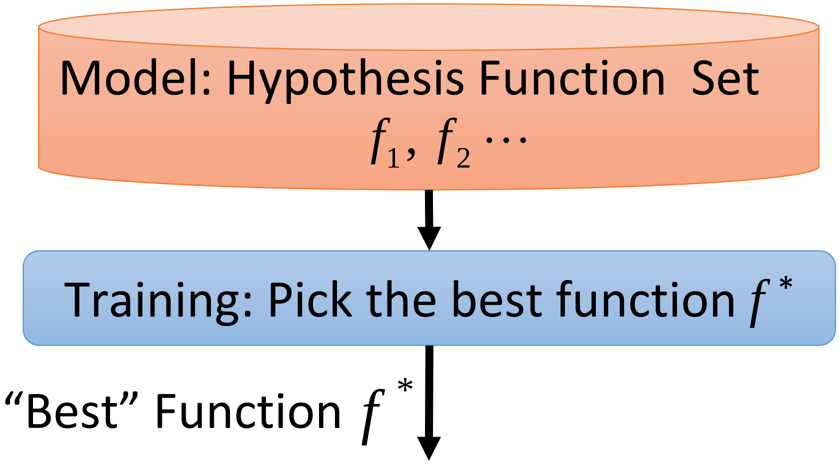
Overfitting



Possible solutions

- more training samples
- some tips: dropout, etc.

Concluding Remarks



Model: Hypothesis Function Set

$f_1, f_2 \cdots$

Training: Pick the best function f^*

"Best" Function f^*

Q1. What is the model?	**Model Architecture**
Q2. What does a "good" function mean?	**Loss Function Design**
Q3. How do we pick the "best" function?	**Optimization**