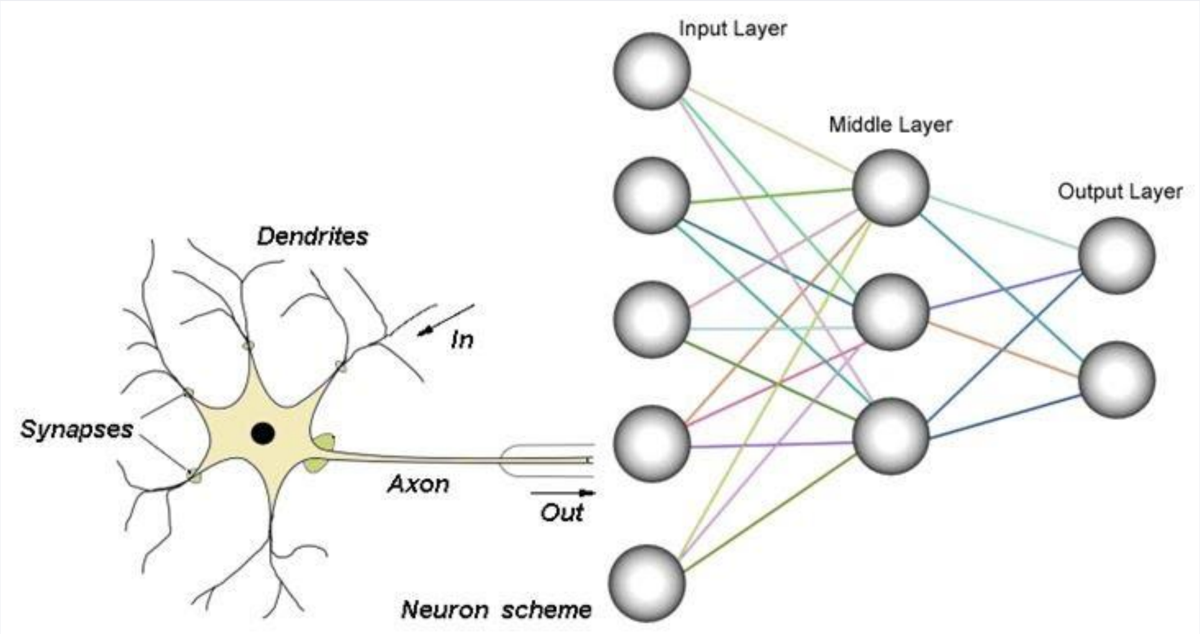

Lecture 11: Artificial Neural Networks

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School of Industrial Management Engineering
Korea University

AGENDA

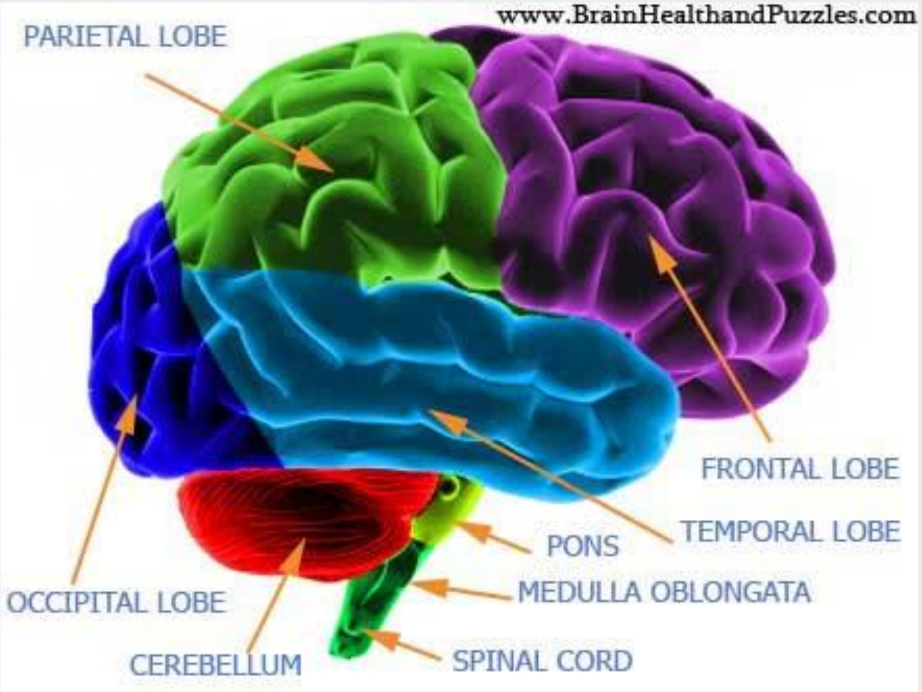
01 Artificial Neural Networks: Perceptron

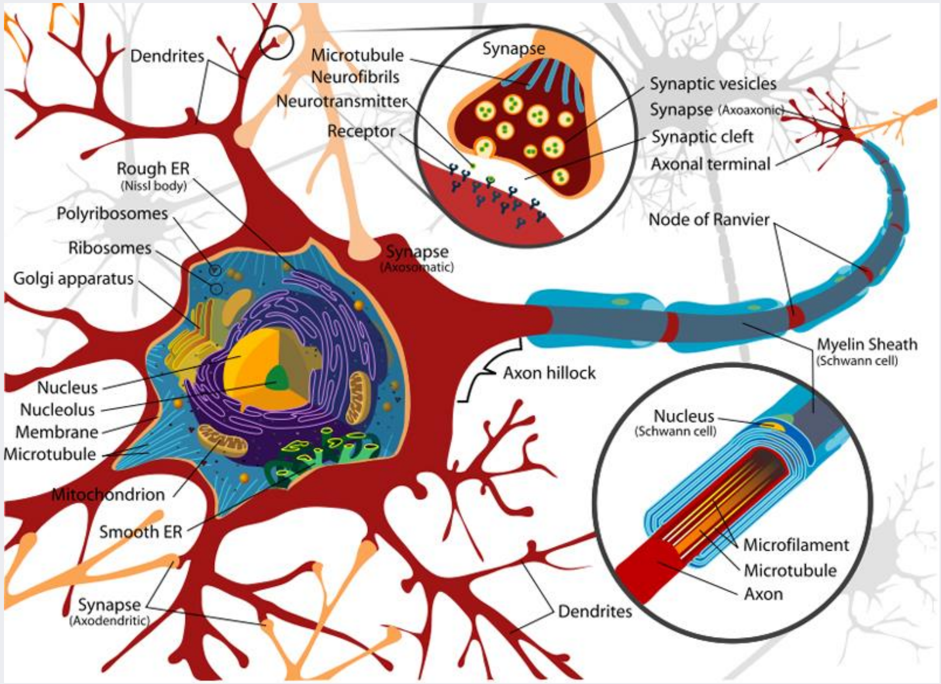
02 Multi-layer Perceptron (MLP)

03 R Exercise

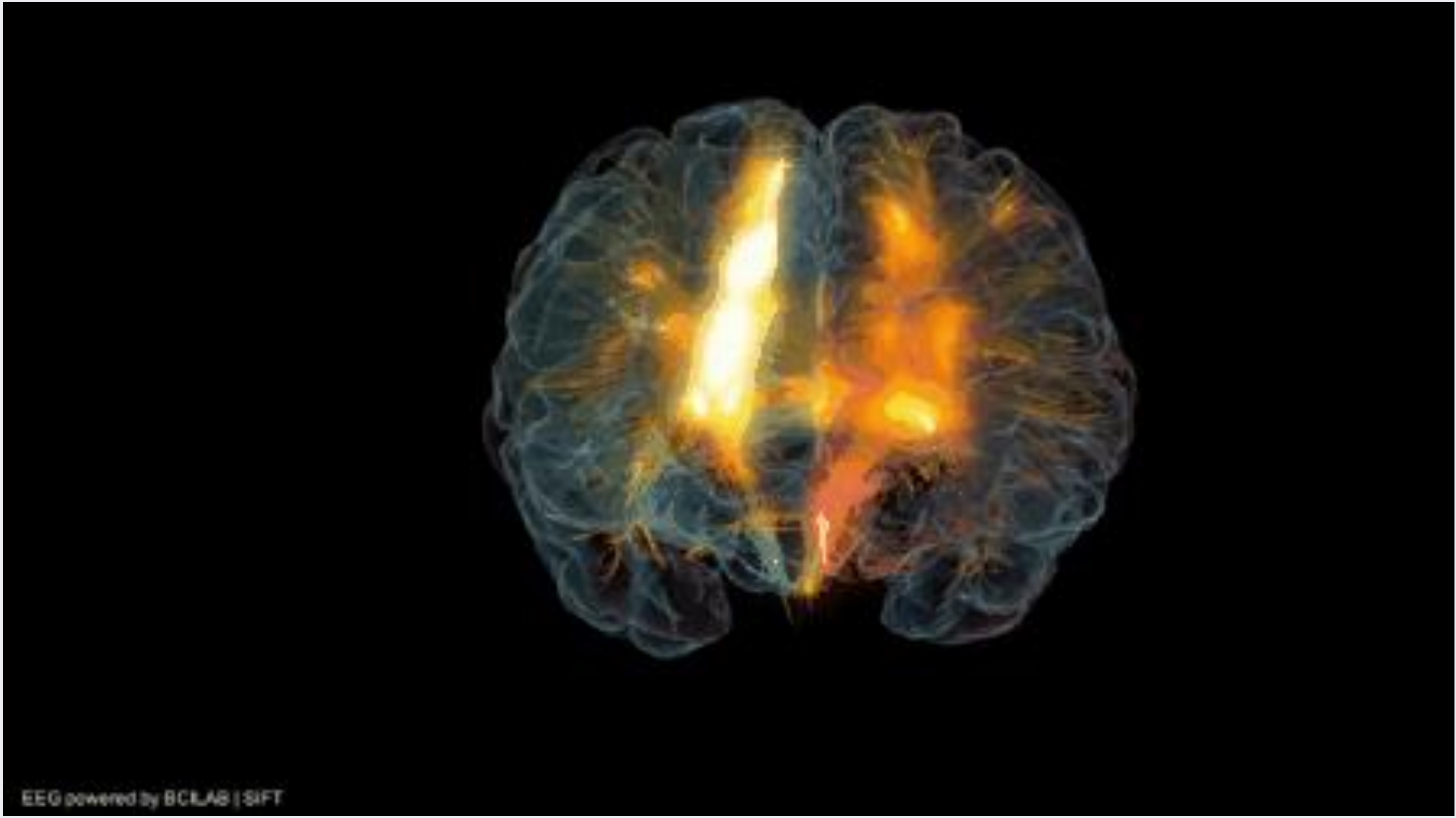
Brain Structure

- How our brain works…
  - ✓ Neurons transmit and analyze communication within the brain and other parts of the nervous system
  - ✓ A message within the brain is converted to electronic signs





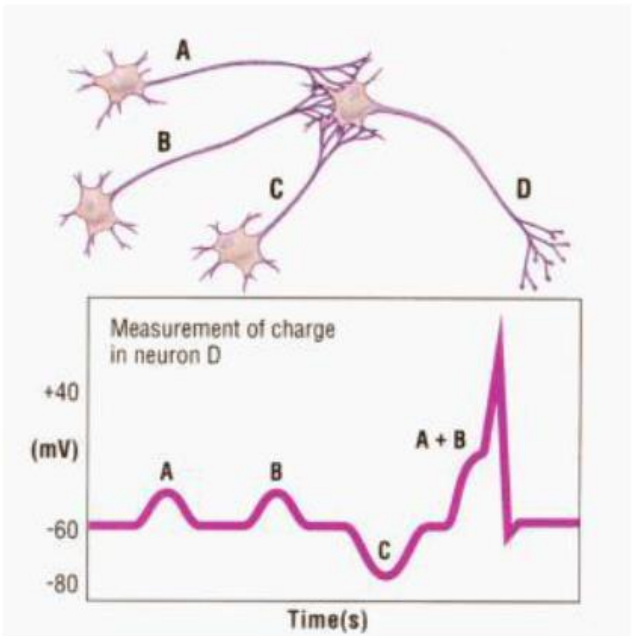
Neuron Firing Off in Real-Time

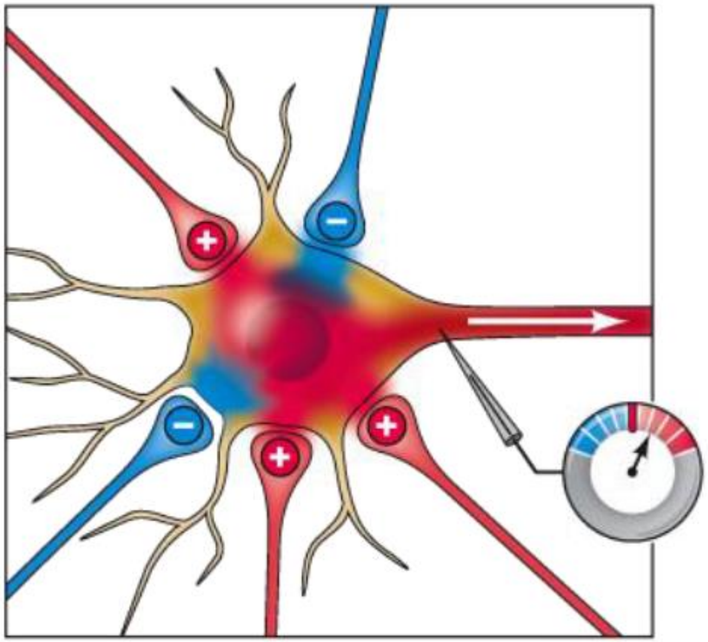


http://www.dailymail.co.uk/sciencetech/article-2581184/The-dynamic-mind-Stunning-3D-glass-brain-shows-neurons-firing-real-time.html

The Way Our Brain Works

- The way neurons work





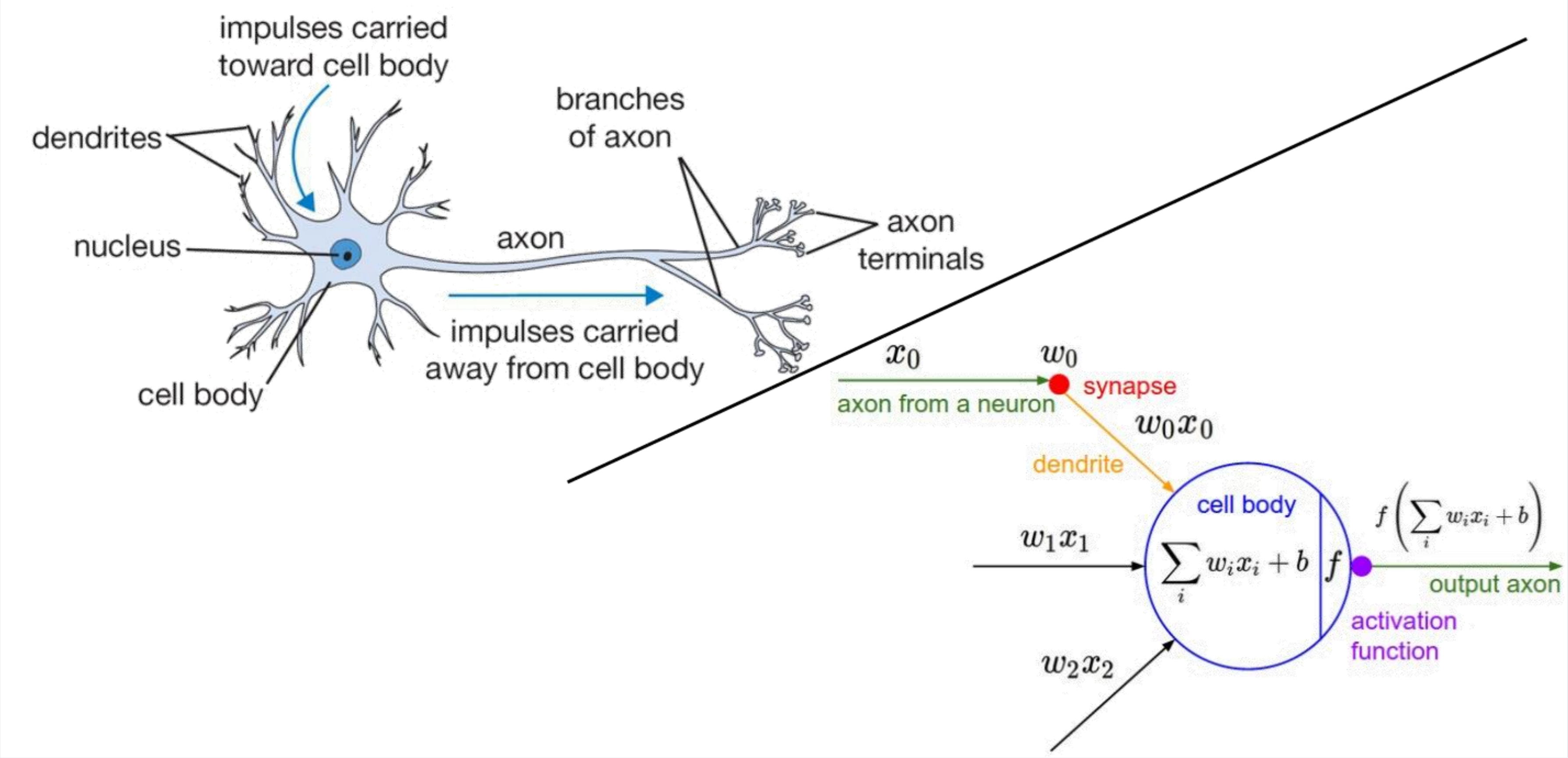
Neurons receive signals

✓ Combine those signals – **sum** the stimulus

✓ Fire if the stimulus exceed the **threshold**

Perceptron

- Imitate a single neuron

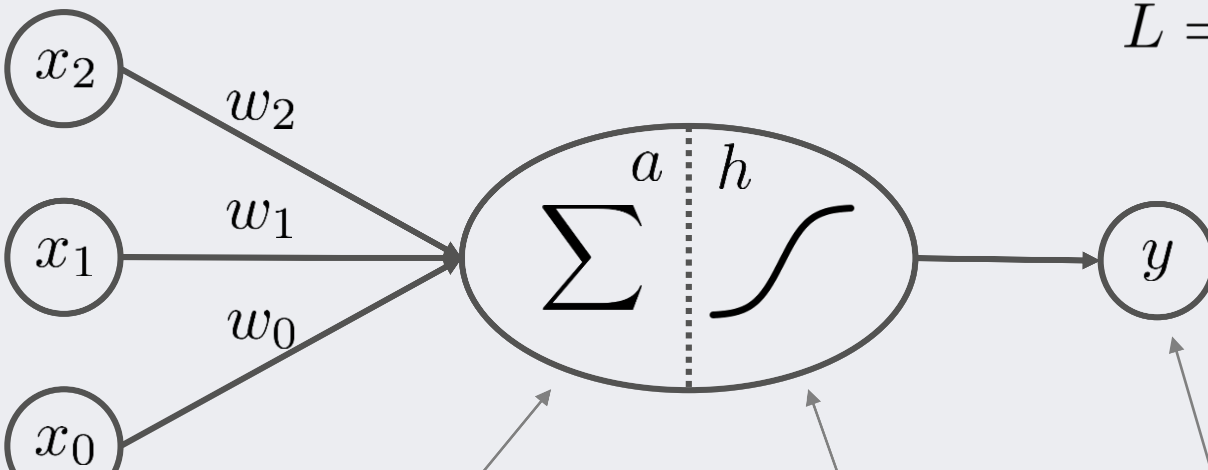


Perceptron

- Perceptron
  - ✓ An organism with only 1 neuron

원하는 값(t)과
예측값(y)의 차이를
손실함수로 정의

$$L = \frac{1}{2}(t-y)^2$$



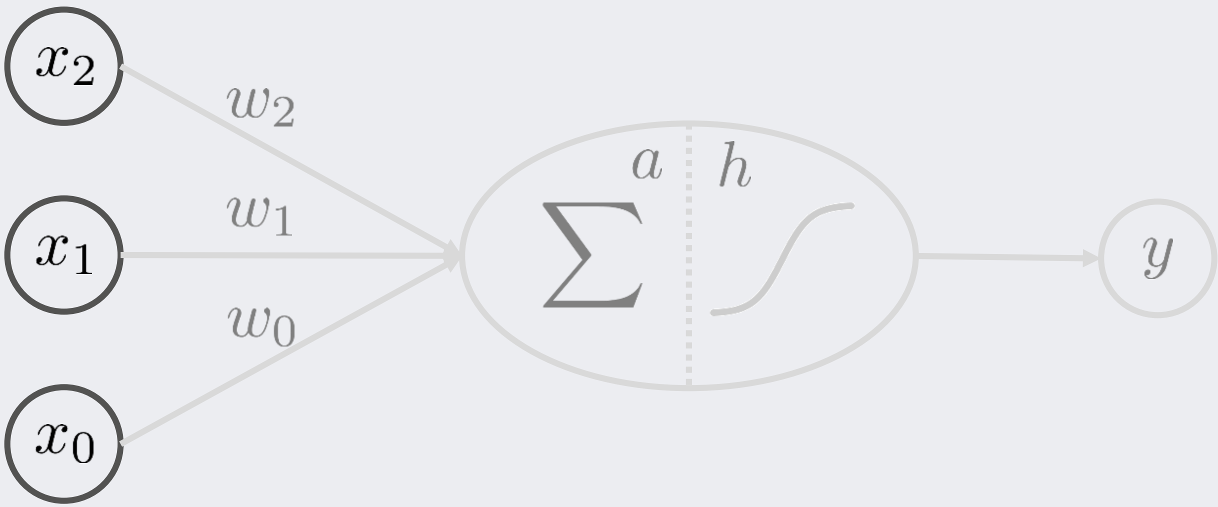
$$a = \sum_{i=0}^{2} w_i x_i \qquad h = \frac{1}{1+exp(-a)} \qquad y = h$$

여러 변수들의 정보를
나름대로 취합해서

얼마만큼 다음 단계로
전달할지 결정한다
(활성화)

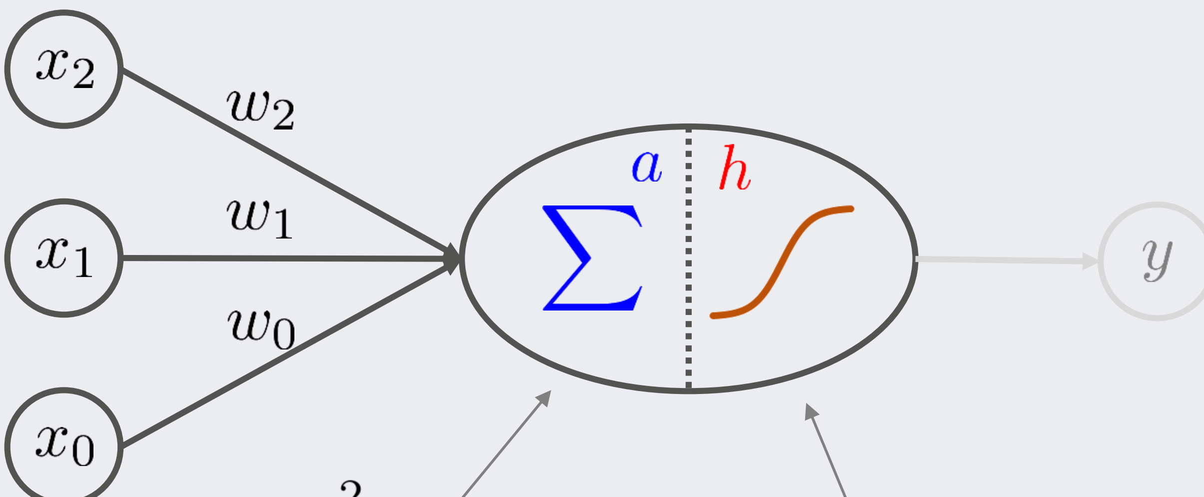
Perceptron

- Input node
  - ✓ Input (predictor, explanatory) variables



Perceptron

- Hidden node
  - ✓ Take the weighted sum of input values and perform a non-linear activation



$$a = \sum_{i=0}^{2} w_i x_i \qquad h = \frac{1}{1 + exp(-a)}$$

여러 변수들의 정보를
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얼마만큼 다음 단계로
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(활성화)

Perceptron

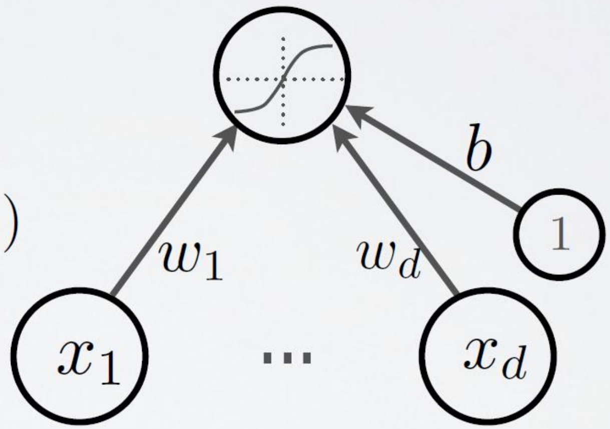
- Role of activation
  - ✓ Determine how much information from the previous layer is forward to the next layer

- Neuron pre-activation (or input activation):

$$a(\mathbf{x}) = b + \sum_i w_i x_i = b + \mathbf{w}^\top \mathbf{x}$$

- Neuron (output) activation

$$h(\mathbf{x}) = g(a(\mathbf{x})) = g(b + \sum_i w_i x_i)$$



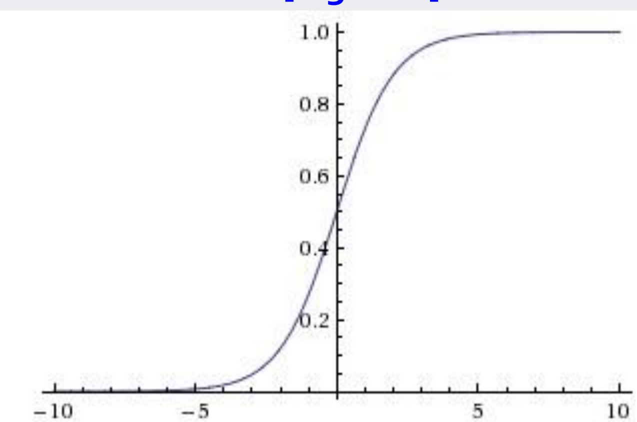
- $\mathbf{w}$ are the connection weights
- b is the neuron bias
- $g(\cdot)$ is called the activation function

http://info.usherbrooke.ca/hlarochelle/cours/ift725_A2013/contenu.html

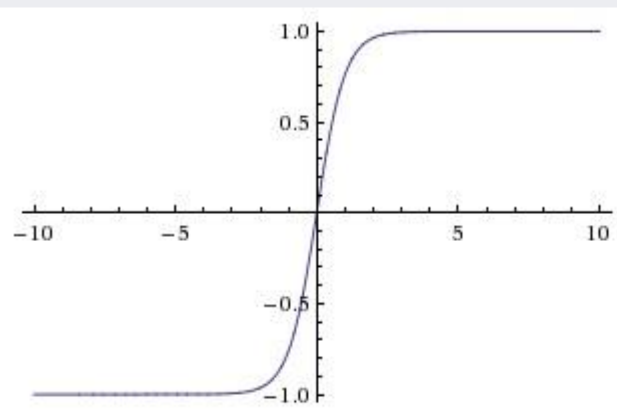
Perceptron

- Representative activation functions
  - ✓ Sigmoid: the most commonly used activation, [0, 1] range, learning speed is relatively slow
  - ✓ Tanh: Similar to sigmoid but [-1, 1] range, learning speed is relatively fast
  - ✓ ReLU (Rectified linear unit): very fast learning speed, easy to compute (without exponential function)

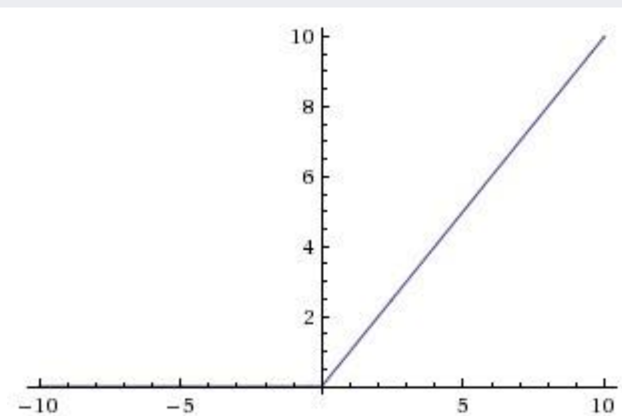
[Sigmoid]



[Tanh]



[ReLU]



$$g(a) = \mathrm{sigm}(a) = \frac{1}{1+\exp(-a)}$$

$$g(a) = \tanh(a) = \frac{\exp(a)-\exp(-a)}{\exp(a)+\exp(-a)} = \frac{\exp(2a)-1}{\exp(2a)+1}$$

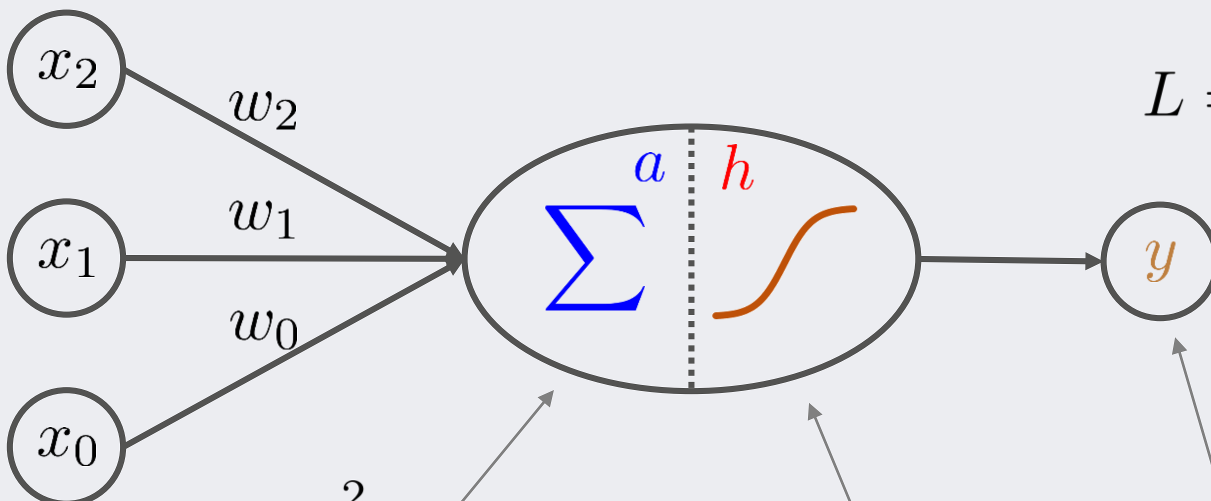
$$g(a) = \mathrm{reclin}(a) = \max(0, a)$$

Perceptron

- Output node
  - ✓ Take the value from the hidden node (Perceptron has only one hidden node)
  - ✓ It takes a weighted sum of hidden nodes in a multi-layer perceptron

원하는 값(t)과 예측값(y)의
차이를 손실함수로 정의

$$L = \frac{1}{2}(t - y)^2$$



$$a = \sum_{i=0}^{2} w_i x_i \qquad h = \frac{1}{1 + exp(-a)} \qquad y = h$$

여러 변수들의 정보를
나름대로 취합해서

얼마만큼 다음 단계로
전달할지 결정한다
(활성화)

Perceptron

- Purpose of perceptron
  - ✓ Find the weight w that can best match the input (x) and the target (t)
- How do we know that the relationship is accurately found?
  - ✓ Use a loss function (how the output y is close to the target t)
    - Regression: squared loss is commonly used

$$L = \frac{1}{2}(t-y)^2$$

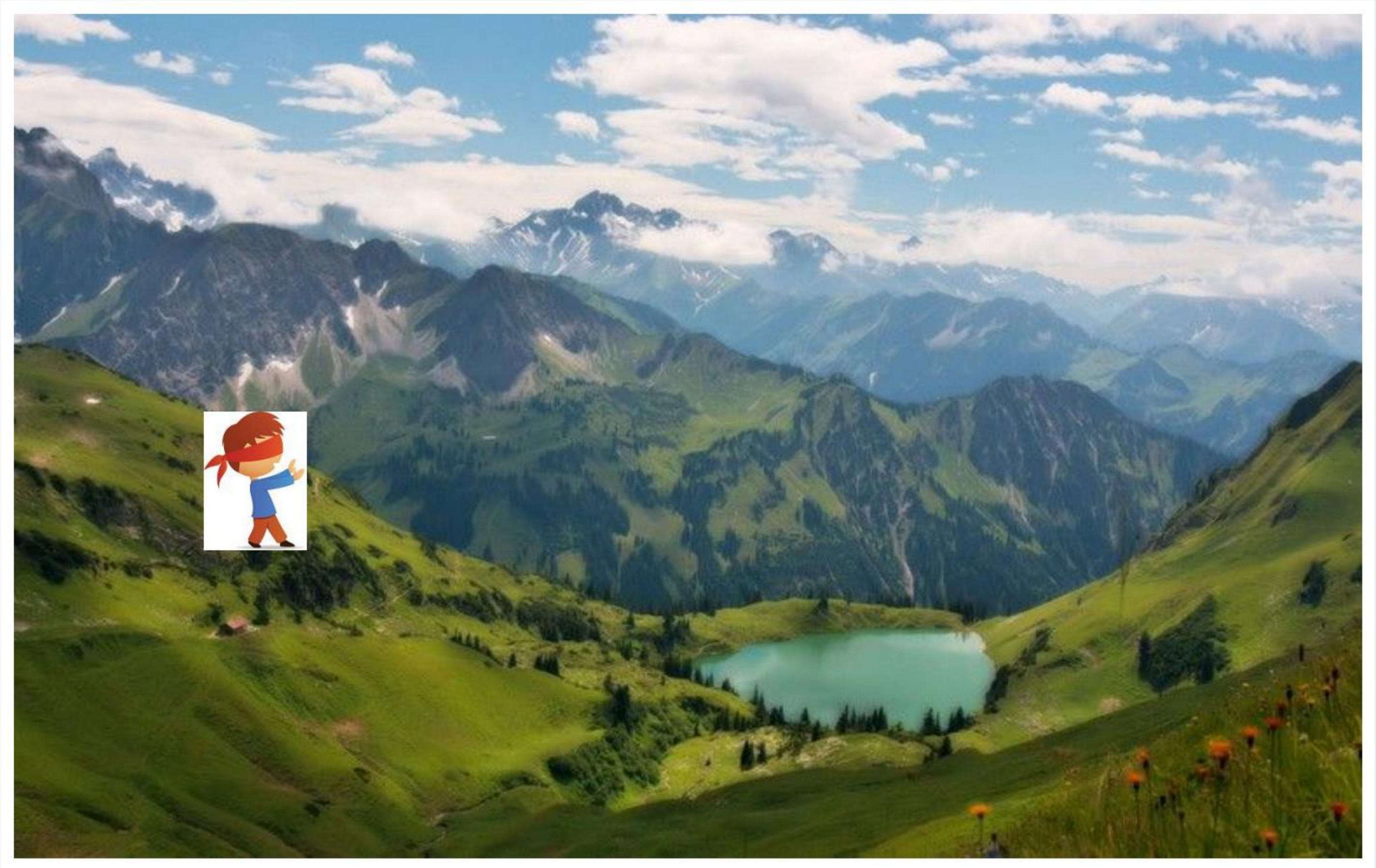
    - Classification: cross-entropy is usually used (only binary classification is possible with perceptron)

$$L = \sum_{i=1}^{2} t_i \log p_i$$

  - ✓ Cost function
    - Computes how inaccurate the current model is (the average of loss function values is commonly used)

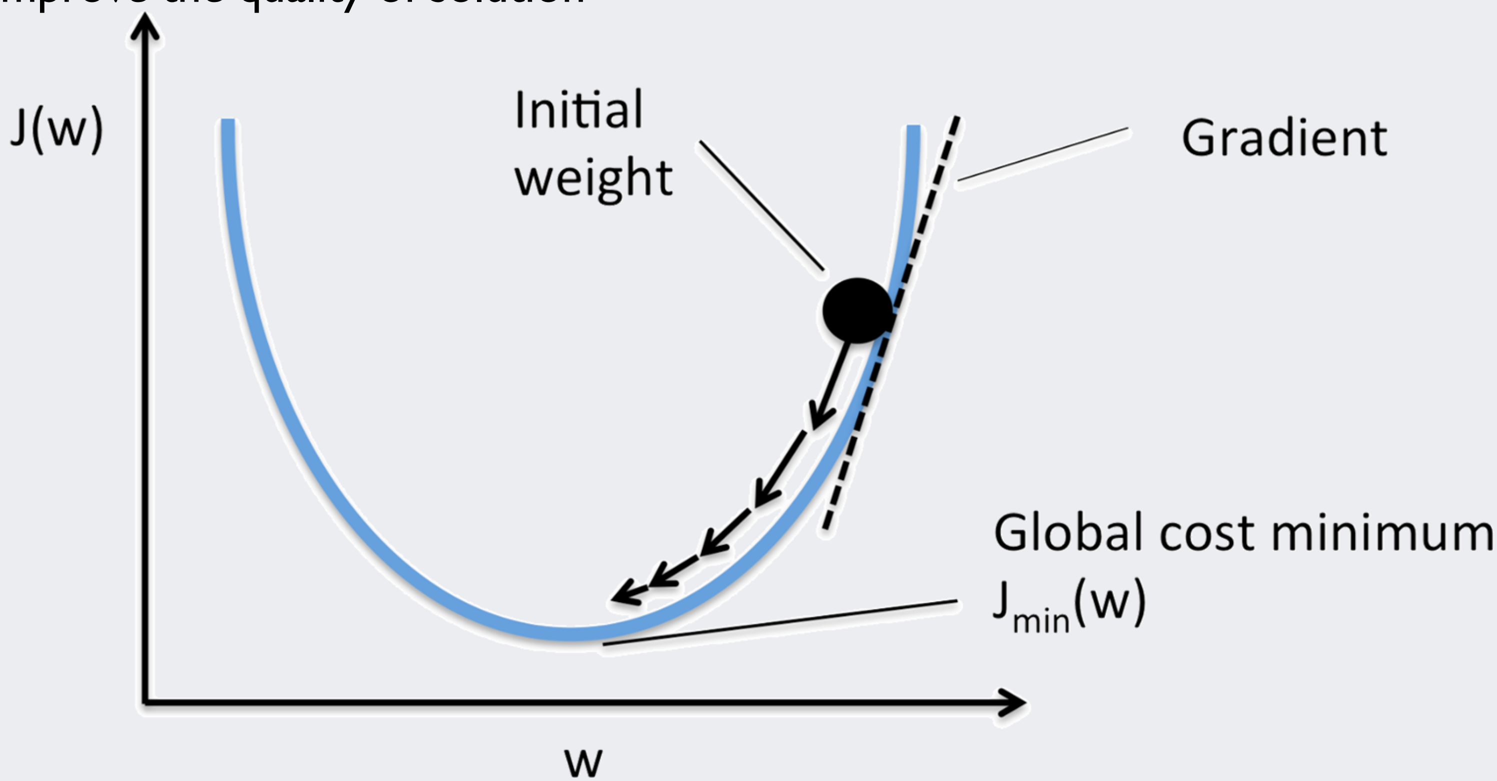
Learning: Gradient Descent

- Gradient Descent



Learning: Gradient Descent

- Gradient Descent Algorithm
  - ✓ Blue line: the objective function to be minimized
  - ✓ Black circle: the current solution
  - ✓ Direction of the arrows: the direction that the current solution should move to improve the quality of solution



Learning: Gradient Descent

- Take the first derivative of the cost function w.r.t the current weight w
  - ✓ Is the gradient 0?
    - Yes: Current weights are the optimum! → end of learning
    - No: Current weights can be improved → learn more
  - ✓ How can we improve the current weights if the gradient is not 0?
    - Move the current weight toward to the opposite direction of the gradient
  - ✓ How much should the weights be moved?
    - Not sure
    - Move them a little and compute the gradient again
    - It will converge

Learning: Gradient Descent

- Theoretical Background

  ✓ Taylor expansion

$$f(x+\Delta x) = f(x) + \frac{f'(x)}{1!}\Delta x + \frac{f''(x)}{2!}\Delta x^2 + \cdots$$

  ✓ If the first derivative is not zero, we can decrease the function value by moving x toward the opposite direction of its first derivative

$$x_{new} = x_{old} - \eta f'(x), \quad where \;\; 0 < \eta < 1$$

  ✓ Then the function value of the new x is always smaller than that of the old x

$$f(x_{new}) = f(x_{old} - \eta f'(x)) \cong f(x_{old}) - \eta |f'(x)|^2 < f(x_{old})$$

https://www.youtube.com/watch?v=3d6DsjIBzJ4&t=322s

Learning: Gradient Descent

- Use chain rule

$$\frac{\partial L}{\partial y} = y - t \qquad \frac{\partial y}{\partial h} = 1$$

$$\frac{\partial h}{\partial a} = \frac{exp(-a)}{(1 + exp(-a))^2} = \frac{1}{1 + exp(-a)} \cdot \frac{exp(-a)}{1 + exp(-a)} = h(1 - h)$$

$$\frac{\partial a}{\partial w_i} = x_i$$

- Gradients for w and x

$$\frac{L}{\partial w_i} = \frac{L}{\partial y} \cdot \frac{\partial y}{\partial h} \cdot \frac{\partial h}{\partial a} \cdot \frac{\partial a}{\partial w_i} = (y - t) \cdot 1 \cdot h(1 - h) \cdot x_i$$

Learning: Gradient Descent

- Weight update by Gradient Descent

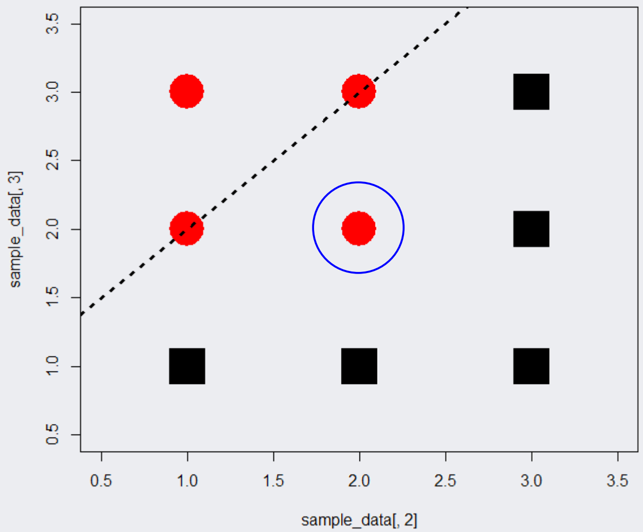
$$w_i^{new} = w_i^{old} - \alpha \times (y - t) \cdot 1 \cdot h(1 - h) \cdot x_i$$

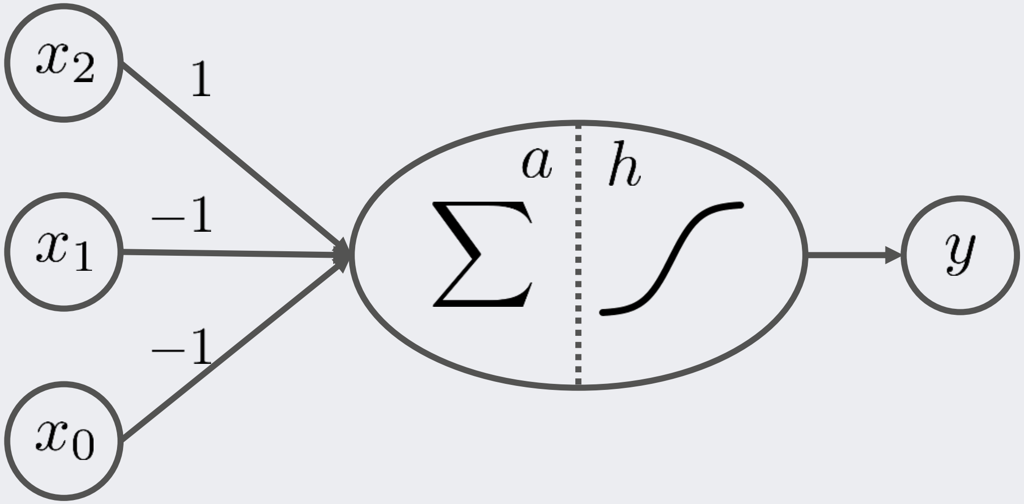
현재의 출력값(y)과 정답(t)이
차이가 많이 날 수록
가중치를 많이 업데이트 하라

대상 가중치와 연결된 입력
변수의 값이 클 수록
가중치를 많이 업데이트 하라

Training Perceptron: Example 1 (alpha = 1)

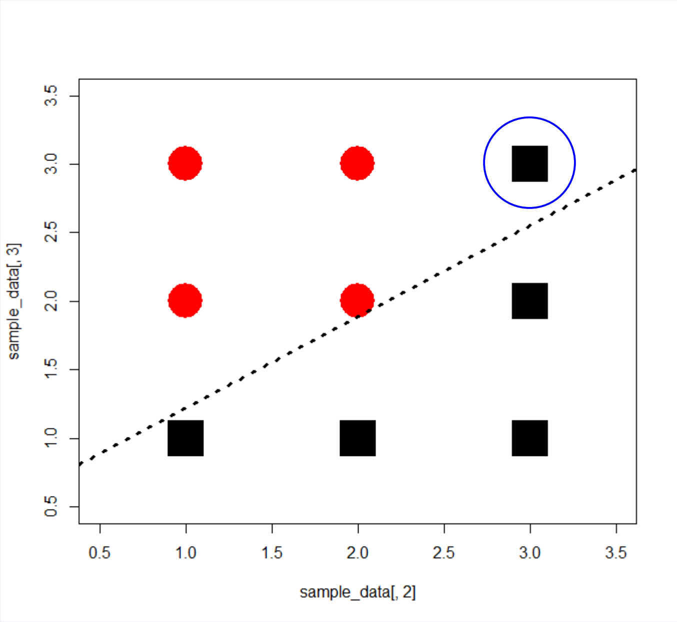
- Initialize and select the first training example (x_1=2, x_2=2, t=1)

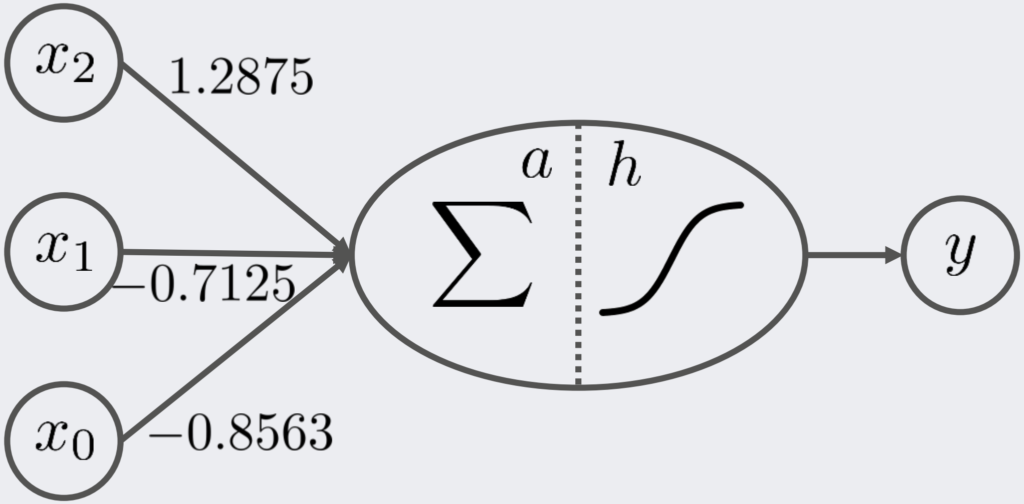




Training Perceptron: Example 1 (alpha = 1)

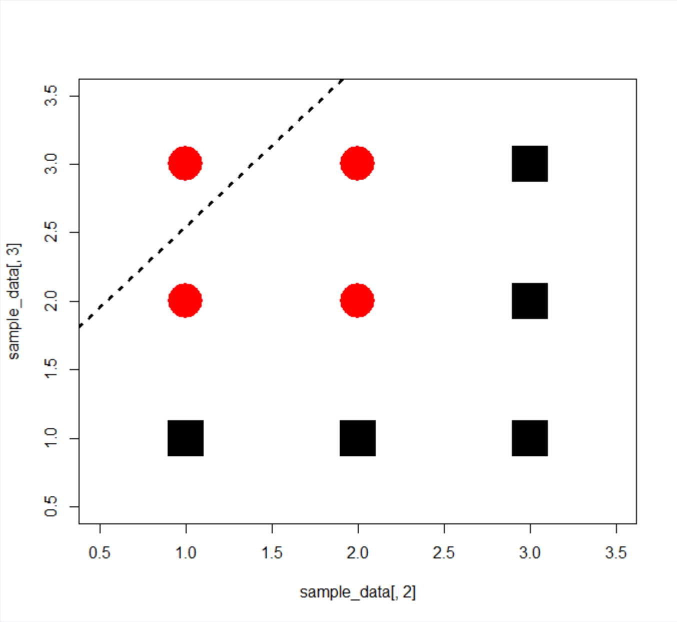
- Training result and selection of the second training example (x_1=3, x_2=3, t=0)

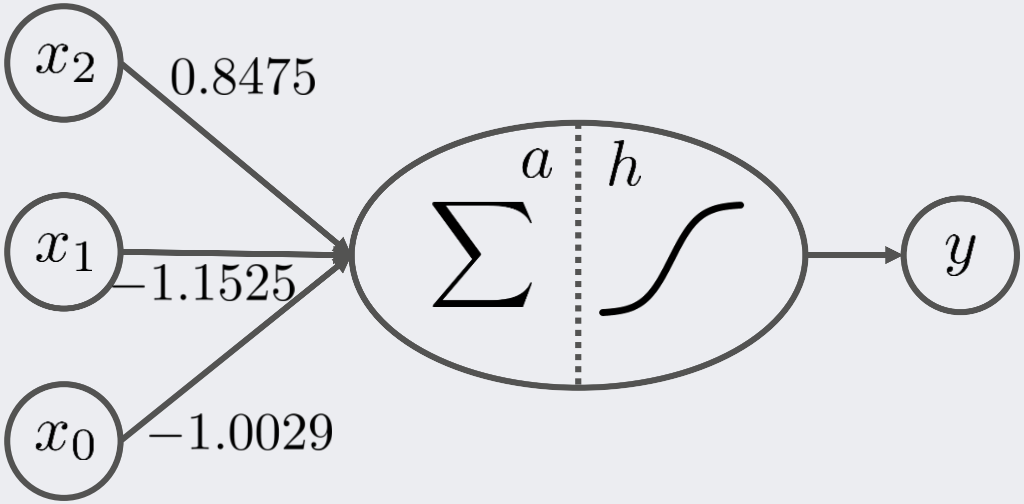




Training Perceptron: Example 1 (alpha = 1)

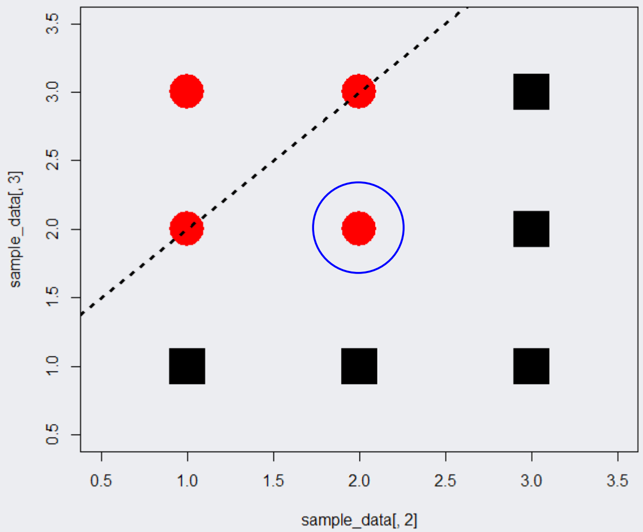
- Training result

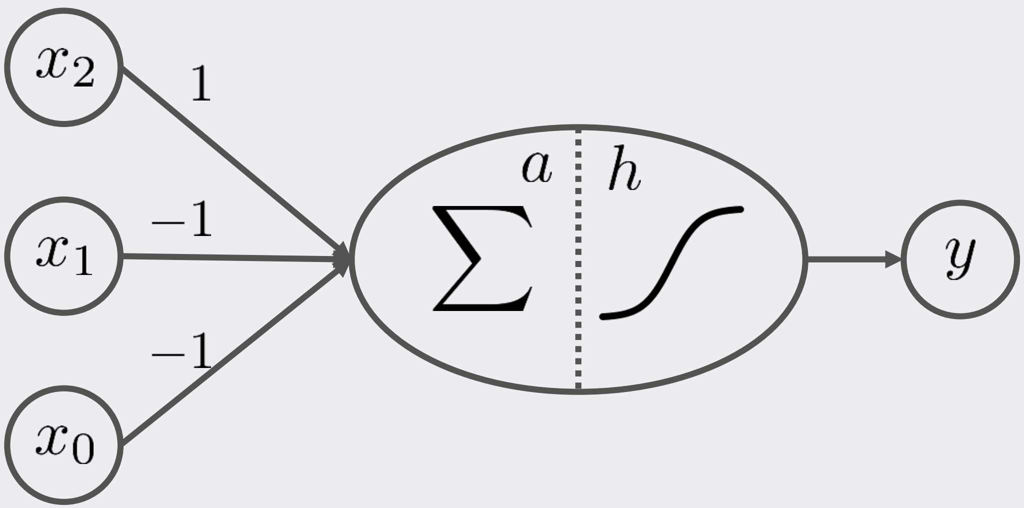




Training Perceptron: Example 1 (alpha = 0.5)

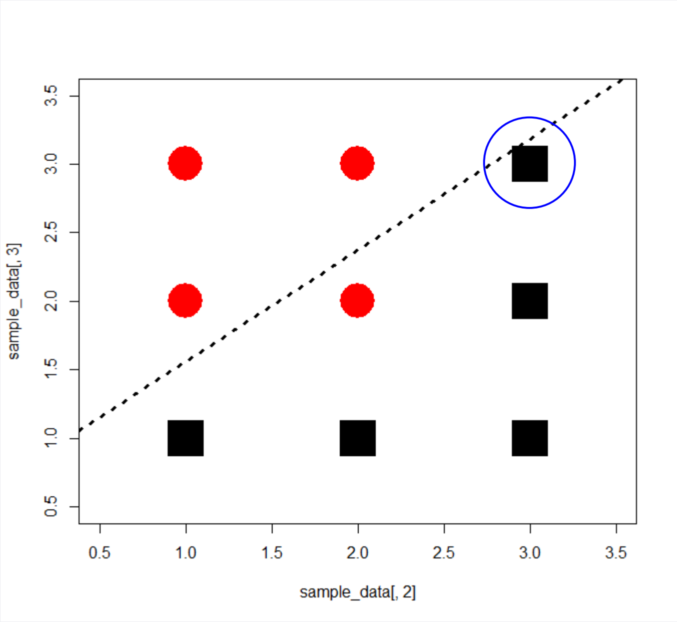
- Initialize and select the first training example (x_1=2, x_2=2, t=1)

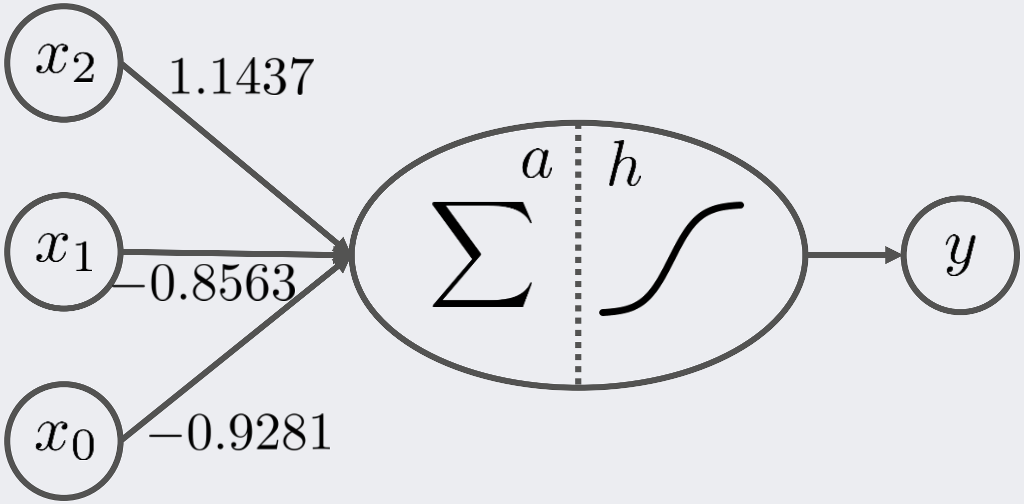




Training Perceptron: Example 1 (alpha = 0.5)

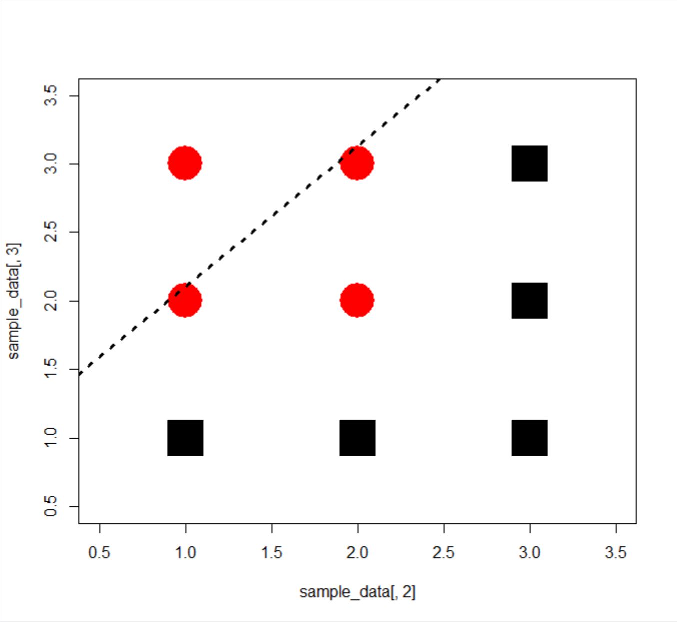
- Training result and selection of the second training example (x_1=3, x_2=3, t=0)

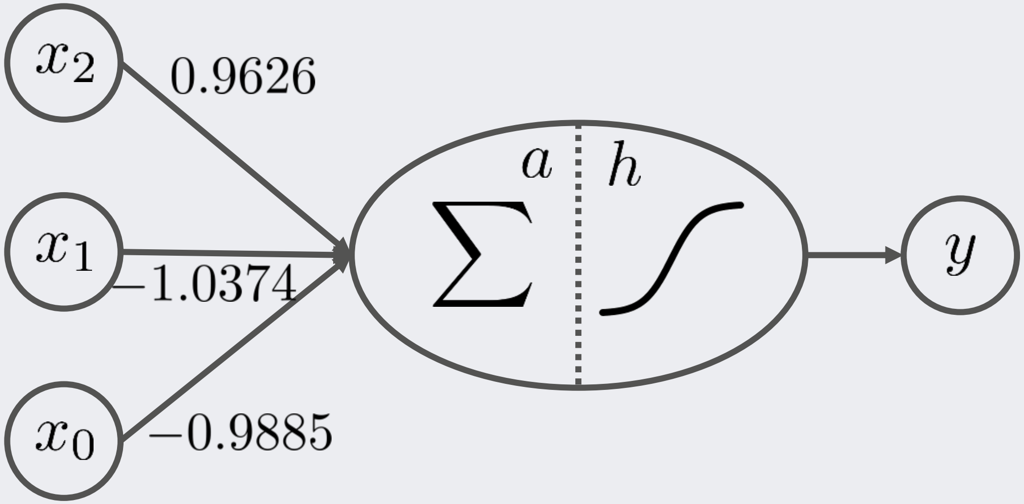




Training Perceptron: Example 1 (alpha = 0.5)

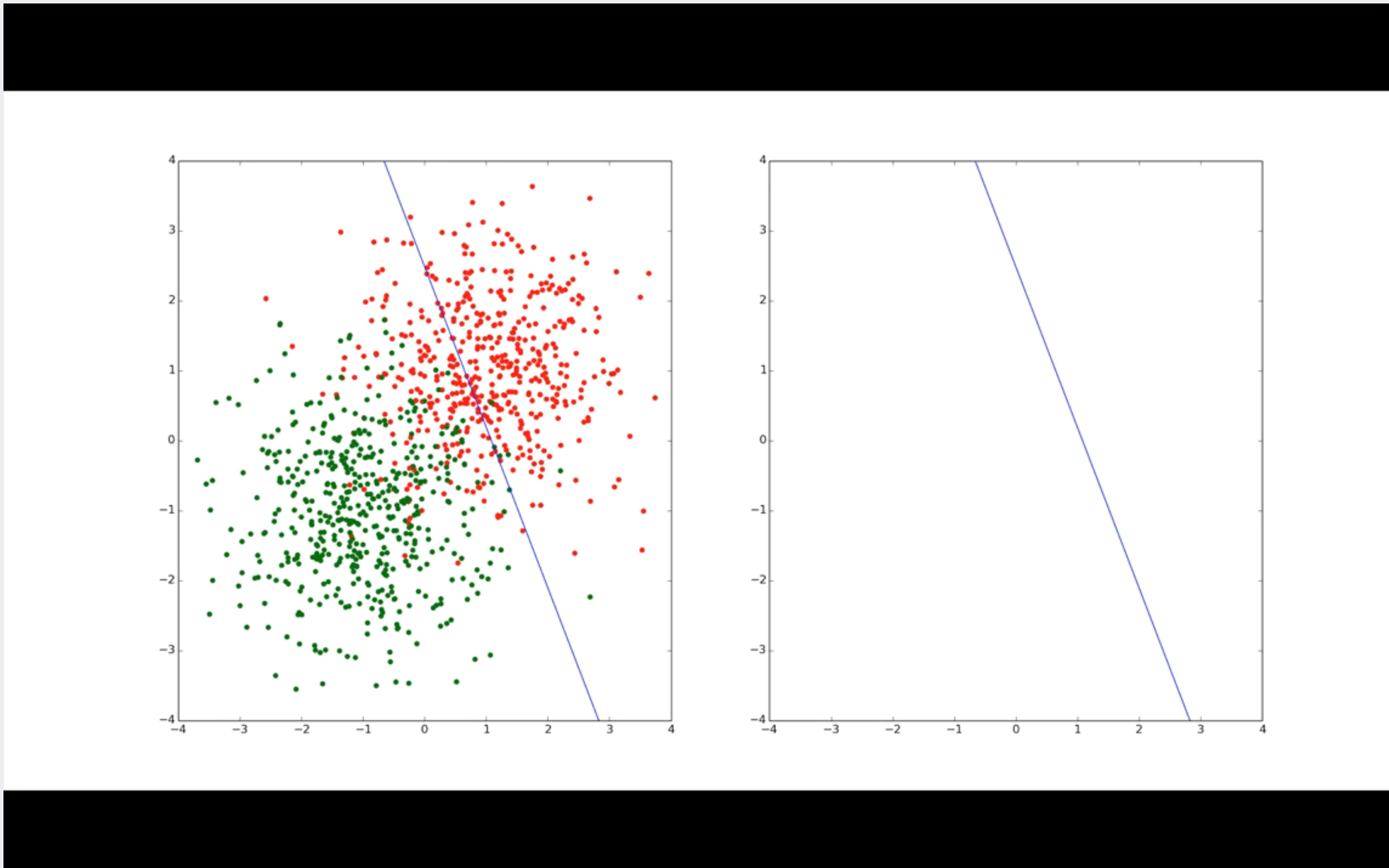
- Training result





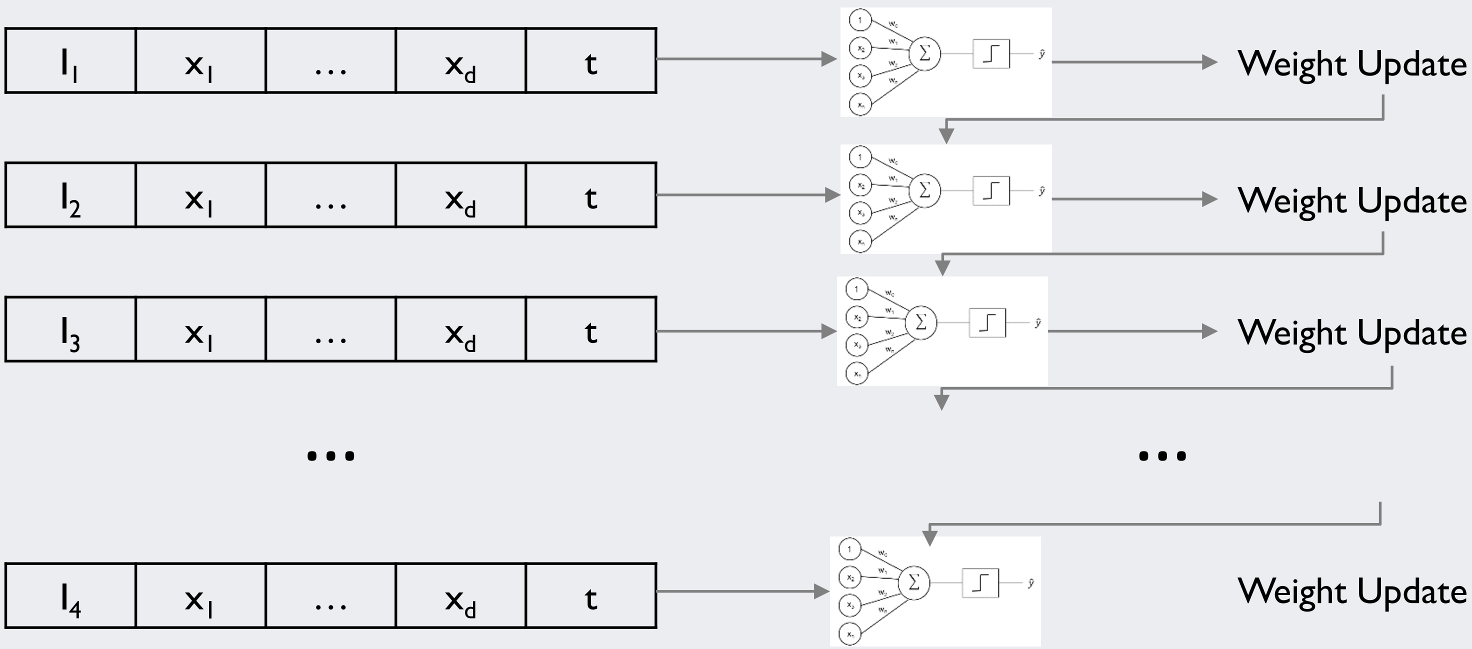
Perceptron

- Training Perceptron



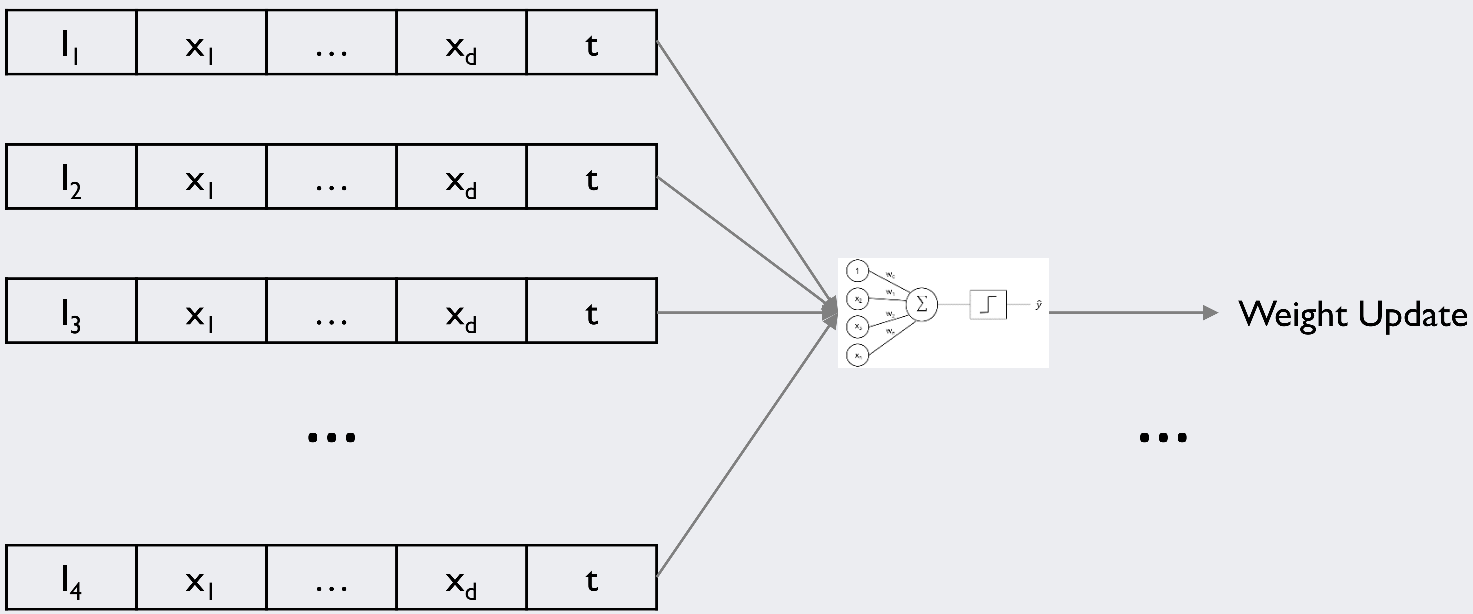
Issues on Gradient Descent

- Issue 1: How frequently should the weights be updated?
  - ✓ Stochastic Gradient Descent (SGD)
    - Compute the loss function for an individual training example and update the gradients



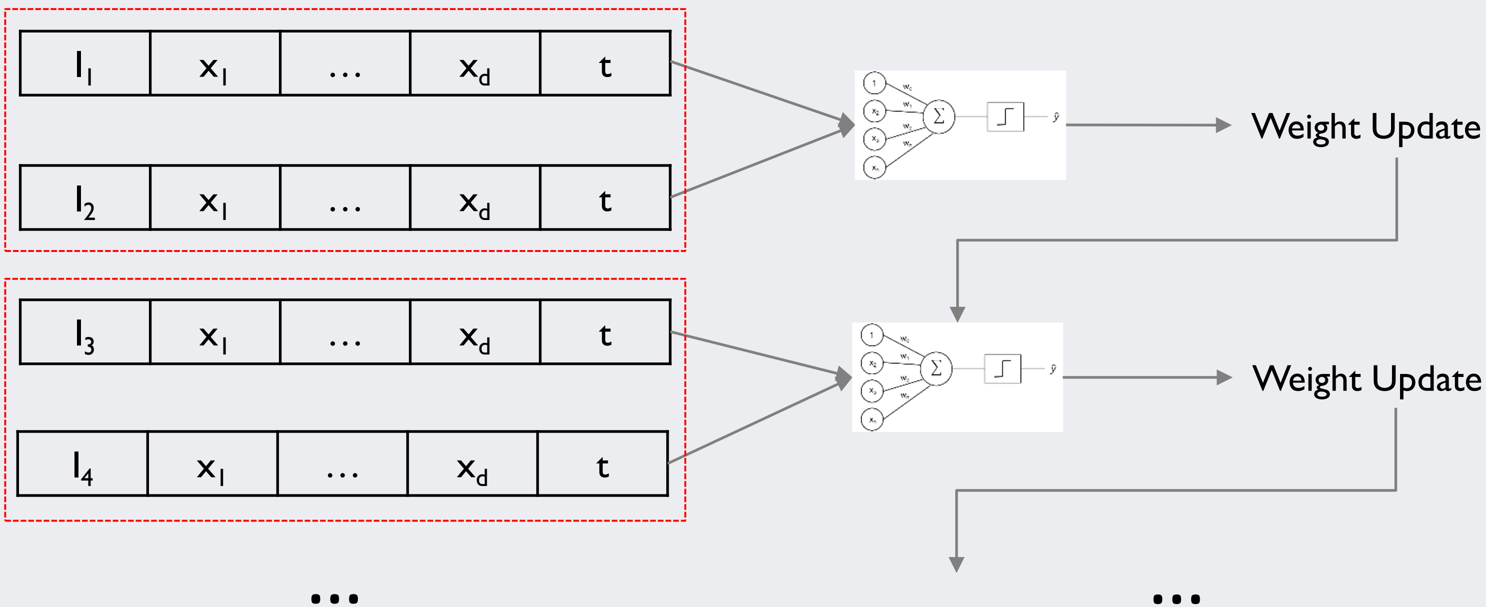
Issues on Gradient Descent

- Issue 1: How frequently should the weights be updated?
  - ✓ Batch Gradient Descent (BGD)
    - Fix the network weights, compute the cost function using all training examples, compute the gradient, and update the weights



Issues on Gradient Descent

- Issue 1: How frequently should the weights be updated?
  - ✓ Mini-Batch Gradient Descent
    - A strategy between SGD and BGD
    - Construct a mini-batch with n examples from N training examples and compute the gradient using the n examples (when the mini-batch size is set to 2)



Issues on Gradient Descent

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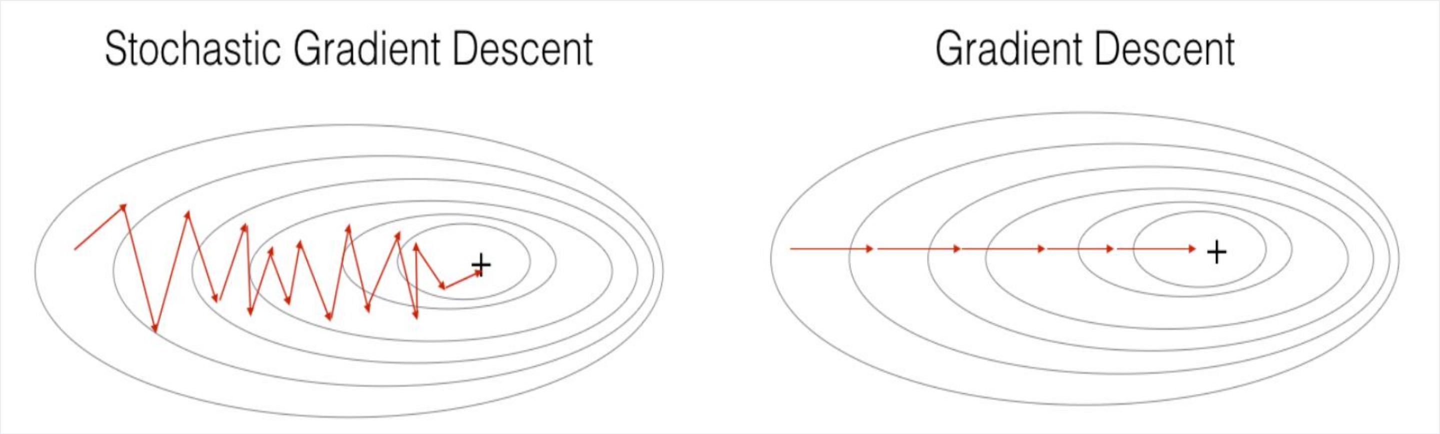
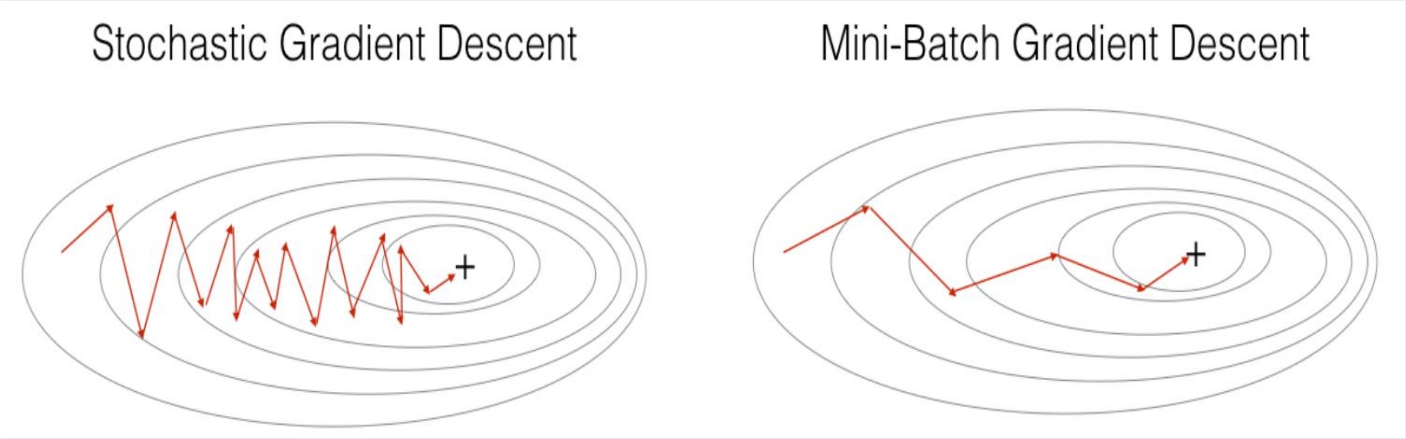
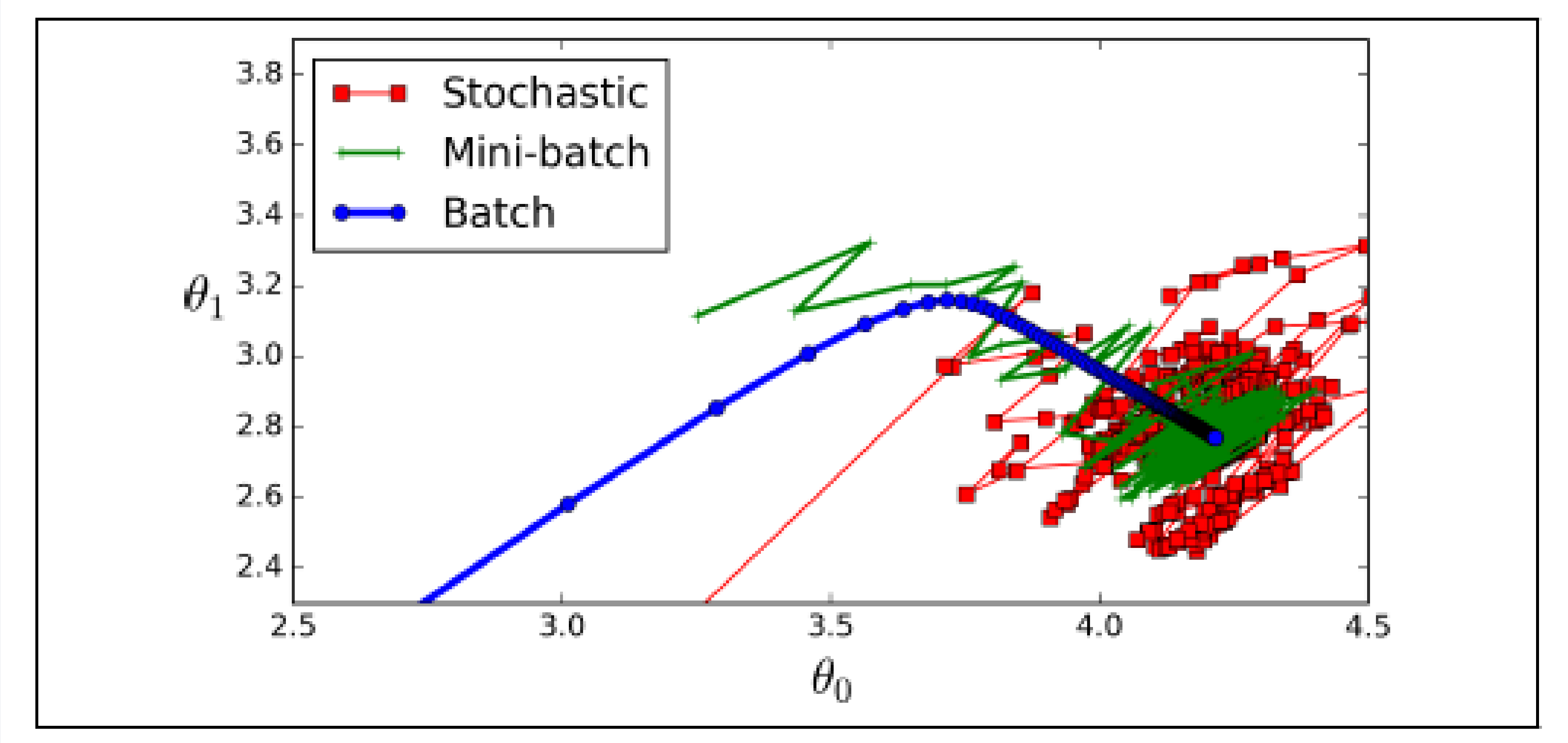




http://pengcheng.tech/2017/09/28/gradient-descent-momentum-and-adam/

Issues on Gradient Descent

- Issue 1: How frequently should the weights be updated?

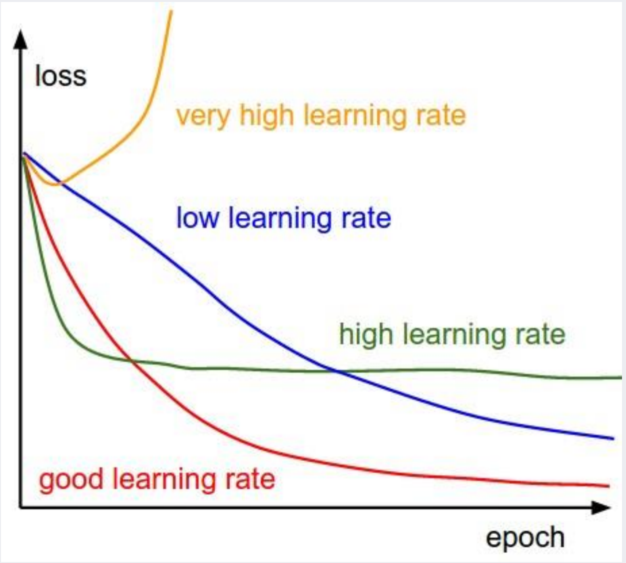


Issues on Gradient Descent

- Issue 2: How much should the weights be updated?
  - ✓ A problem of deciding learning rate

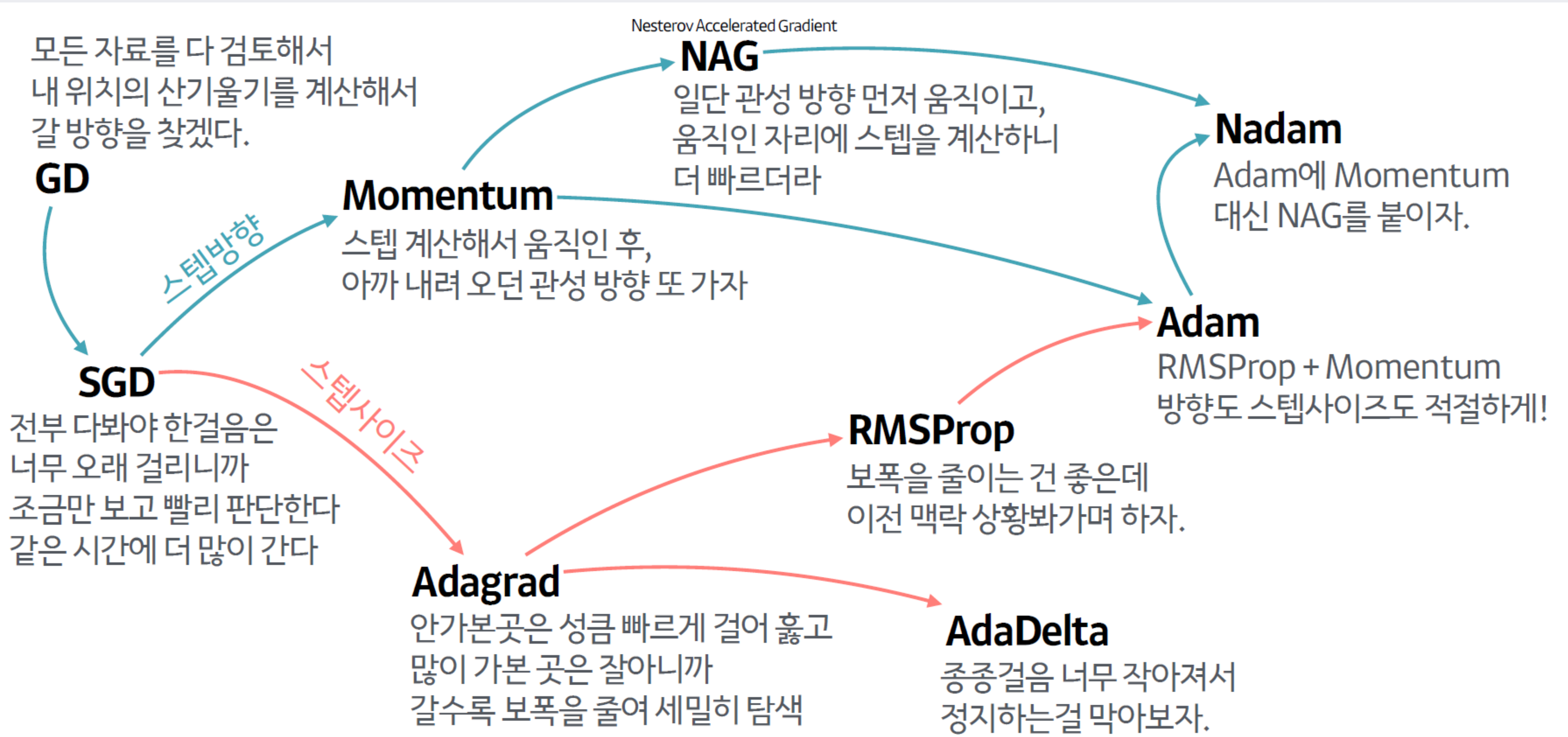
$$w_{new} = w_{old} - \alpha f'(w)$$

    - If the learning rate is too large, the network will not converge
    - If the learning rate is too small, it takes too long time to converge
  - ✓ An appropriate (?) learning rate is required



Issues on Gradient Descent

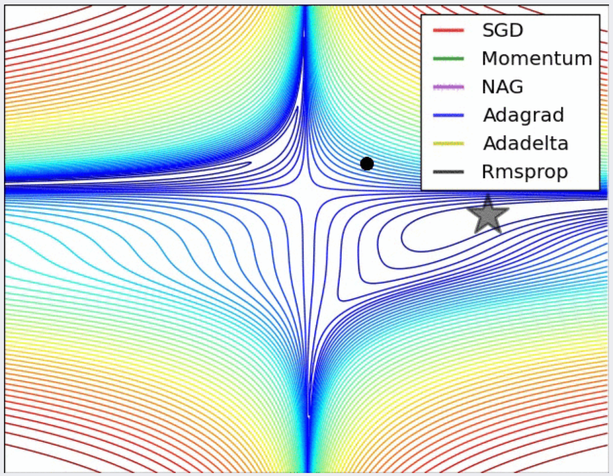
- Issue 2: How much should the weights be updated?



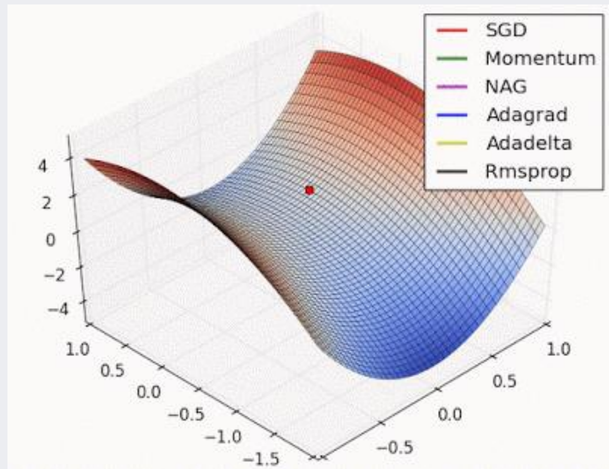
하용호. 자습해도 모르겠던 딥러닝, 머리속에 인스톨 시켜드립니다. (https://www.slideshare.net/yongho/ss-79607172)

Issues on Gradient Descent

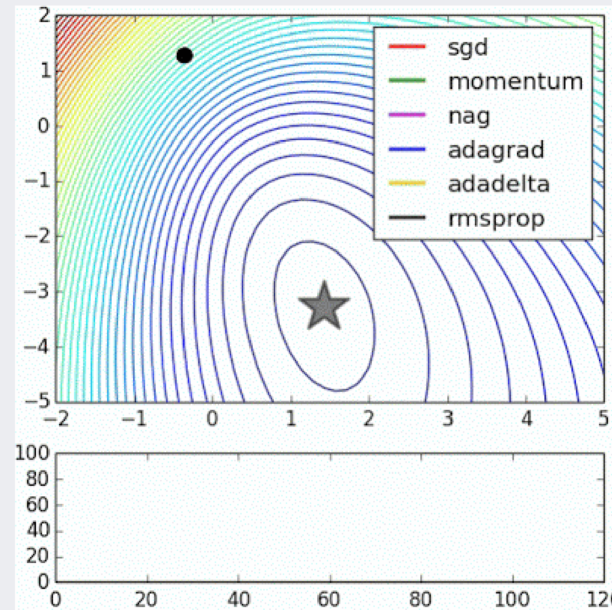
- Issue 2: How much should the weights be updated?



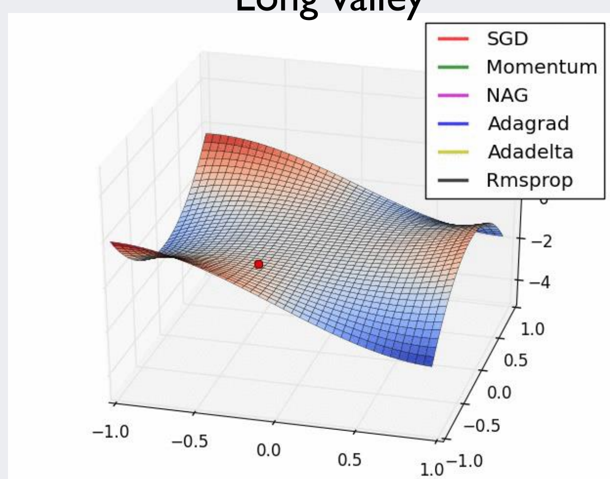
Beale's function



Long valley



Noisy moons



Saddle point

http://www.denizyuret.com/2015/03/alec-radfords-animations-for.html

AGENDA

01 Artificial Neural Networks: Perceptron

02 Multi-layer Perceptron (MLP)

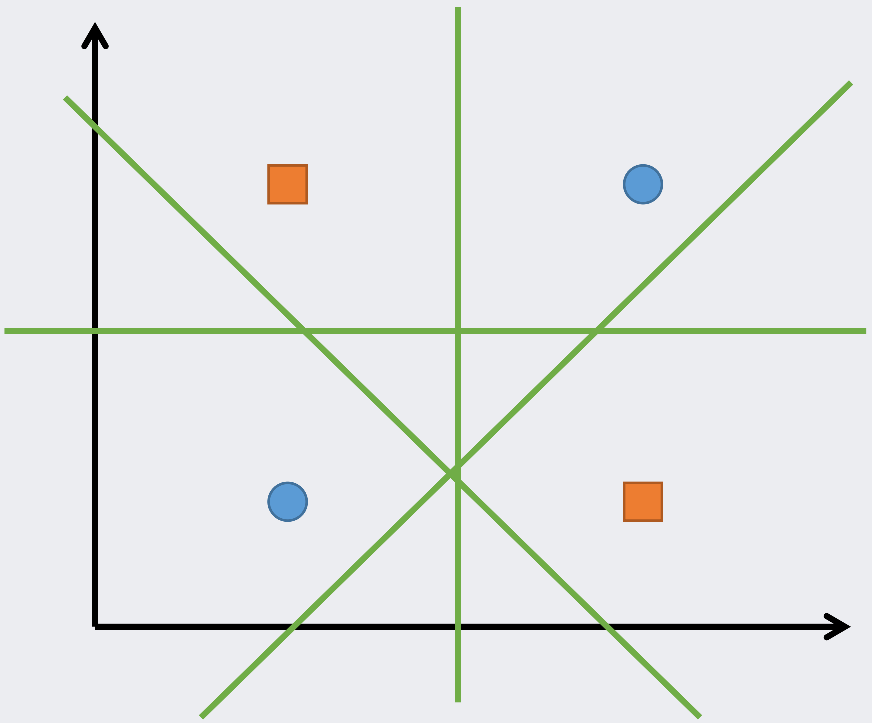
03 R Exercise

Limitation of Perceptron

- The Limitation of Linear Models
  - ✓ **Classification:**
    - Linear (Fisher) discriminant analysis, logistic regression, etc.
    - Can only produce a linear class boundary
  - ✓ **Regression:**
    - Multiple linear regression
    - Can only capture the linear relationship between the predictors and the outcome
  - ✓ Cannot results in good prediction performance ***when the classification boundary or the predictor/outcome relationship is not linear***

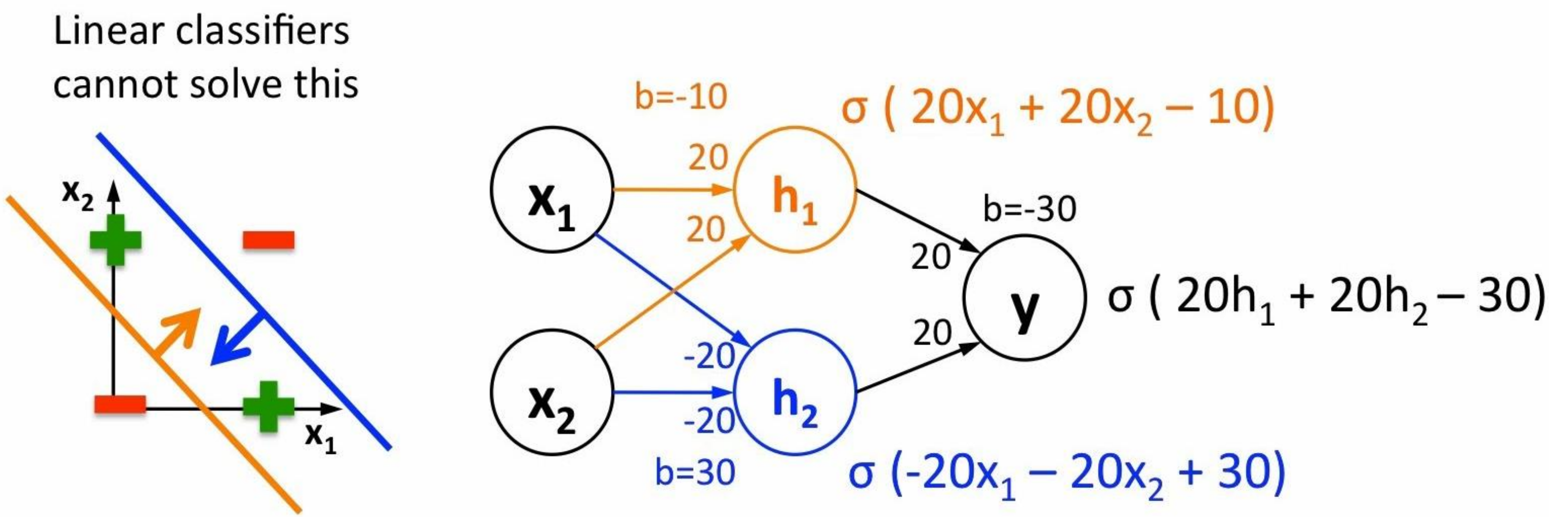
Limitation of Perceptron

- The Limitation of Linear Models
  - ✓ Draw a straight line that perfectly separates the circles and crosses (XOR)



Multi-Layer Perceptron (MLP)

- Combine multiple perceptrons!
  - ✓ If we cannot solve a complex problem directly, then it is better to decompose it into some small and simple problems that can be solved!



$\sigma(20*0 + 20*0 - 10) \approx 0$ $\quad$ $\sigma(-20*0 - 20*0 + 30) \approx 1$ $\quad$ $\sigma(20*0 + 20*1 - 30) \approx 0$

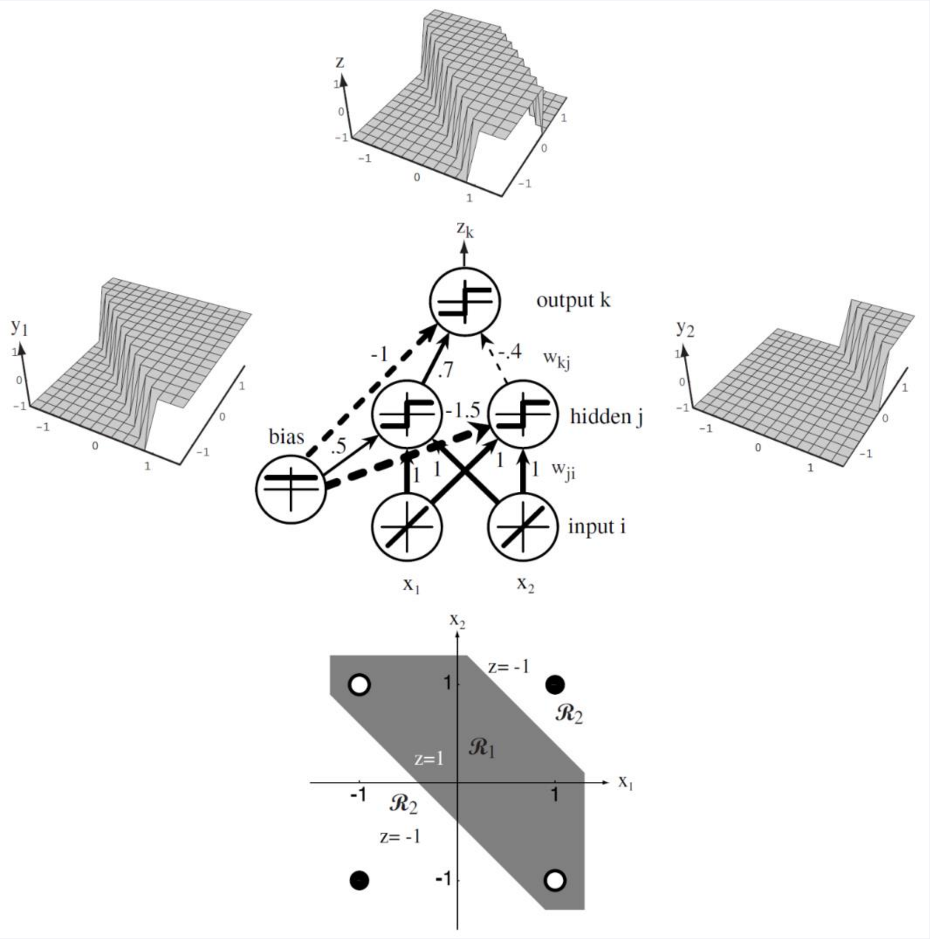
$\sigma(20*1 + 20*1 - 10) \approx 1$ $\quad$ $\sigma(-20*1 - 20*1 + 30) \approx 0$ $\quad$ $\sigma(20*1 + 20*0 - 30) \approx 0$

$\sigma(20*0 + 20*1 - 10) \approx 1$ $\quad$ $\sigma(-20*0 - 20*1 + 30) \approx 1$ $\quad$ $\sigma(20*1 + 20*1 - 30) \approx 1$

$\sigma(20*1 + 20*0 - 10) \approx 1$ $\quad$ $\sigma(-20*1 - 20*0 + 30) \approx 1$ $\quad$ $\sigma(20*1 + 20*1 - 30) \approx 1$

Multi-Layer Perceptron (MLP)

- Non-linear model
  - ✓ Can find an arbitrary shape of class boundary or regression functions

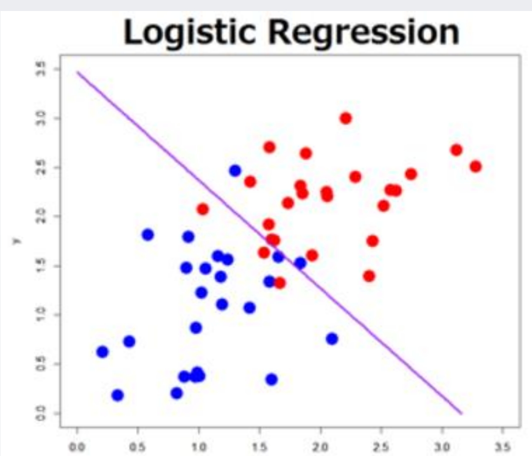


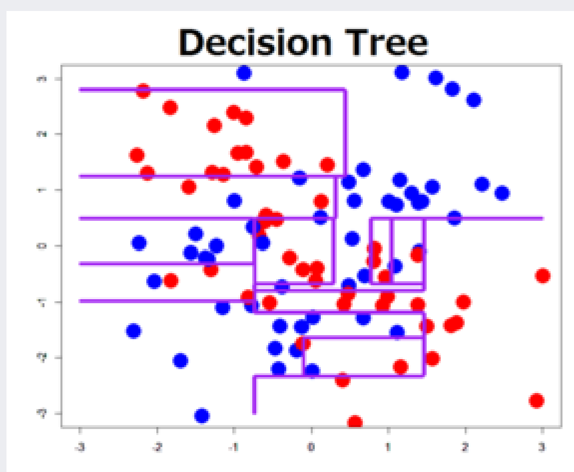
Multi-Layer Perceptron (MLP)

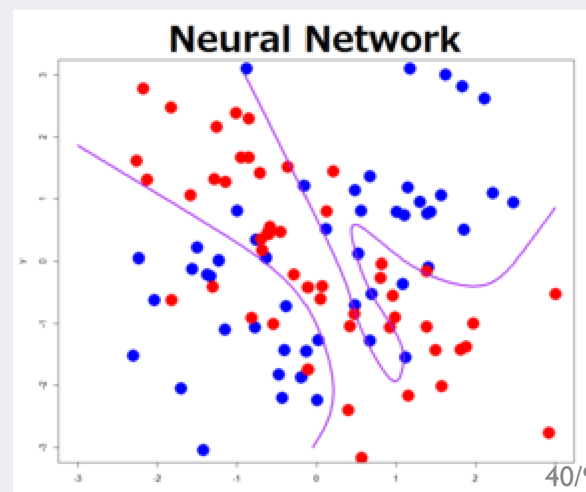
- Decision boundary of MLP
  - ✓ Assume that the class decision boundary can be regarded as a combination of piecewise linear boundaries

	Logstic Regression	Decision Tree	MLP
No. of lines	1	No restriction	User defined (No of hidden layers and hidden nodes)
Direction of lines	No restriction	Vertical to an axis	No restriction

  - ▪ MLP has the highest degree of freedom to defined the decision boundary

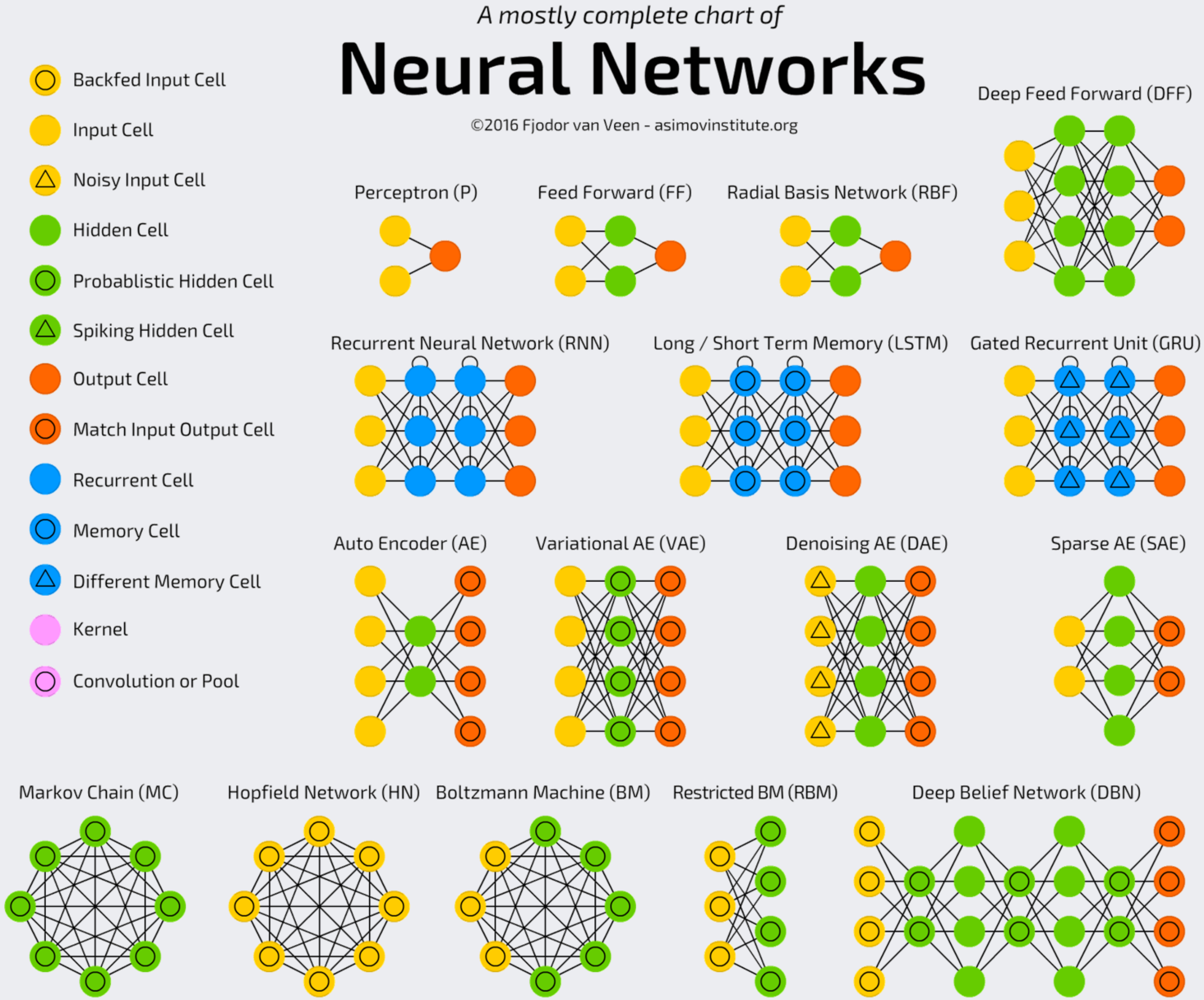






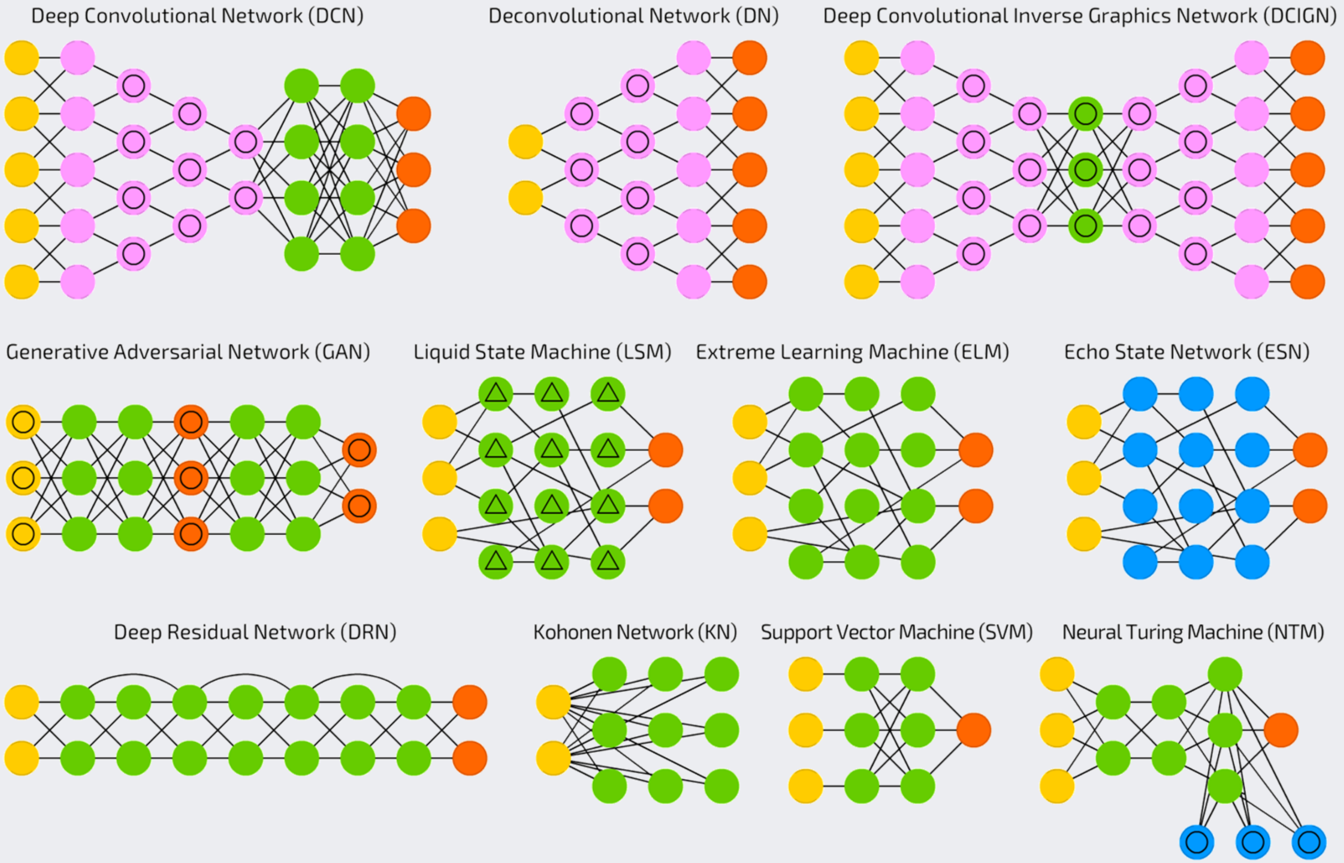
Multi-Layer Perceptron (MLP)

- Various Structure of Artificial Neural Networks



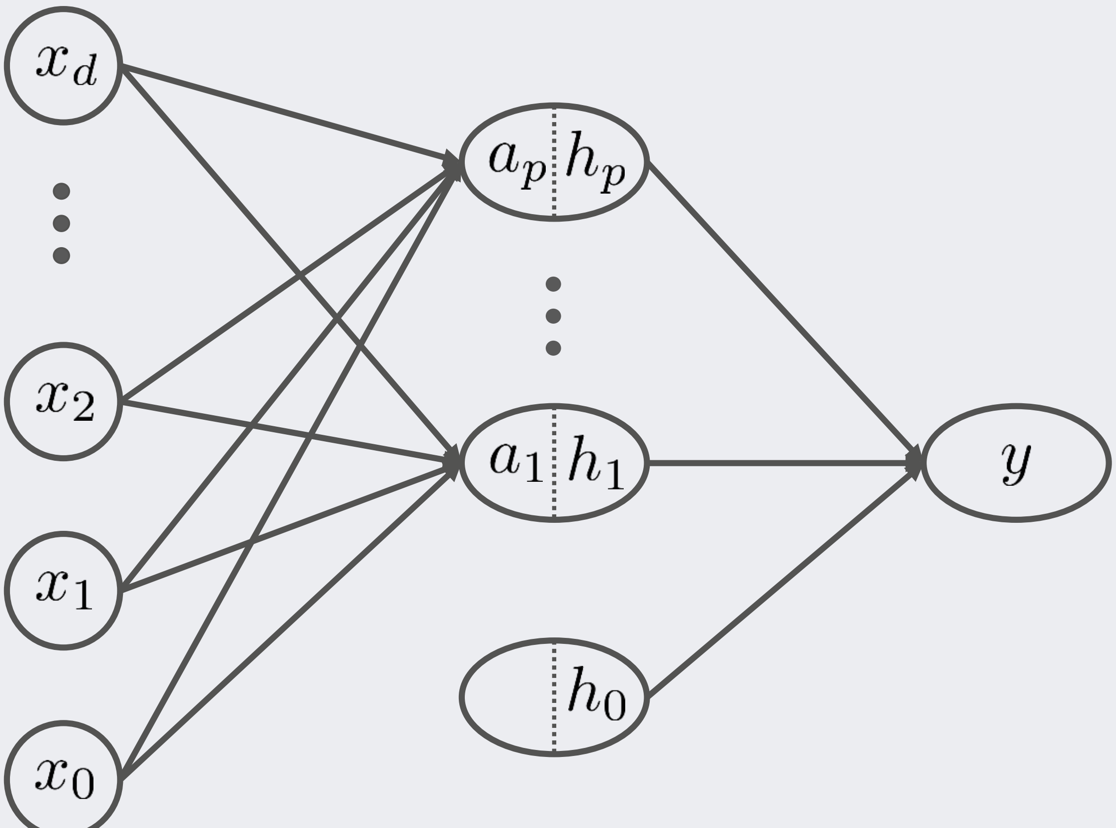
Multi-Layer Perceptron (MLP)

- Various Structure of Artificial Neural Networks



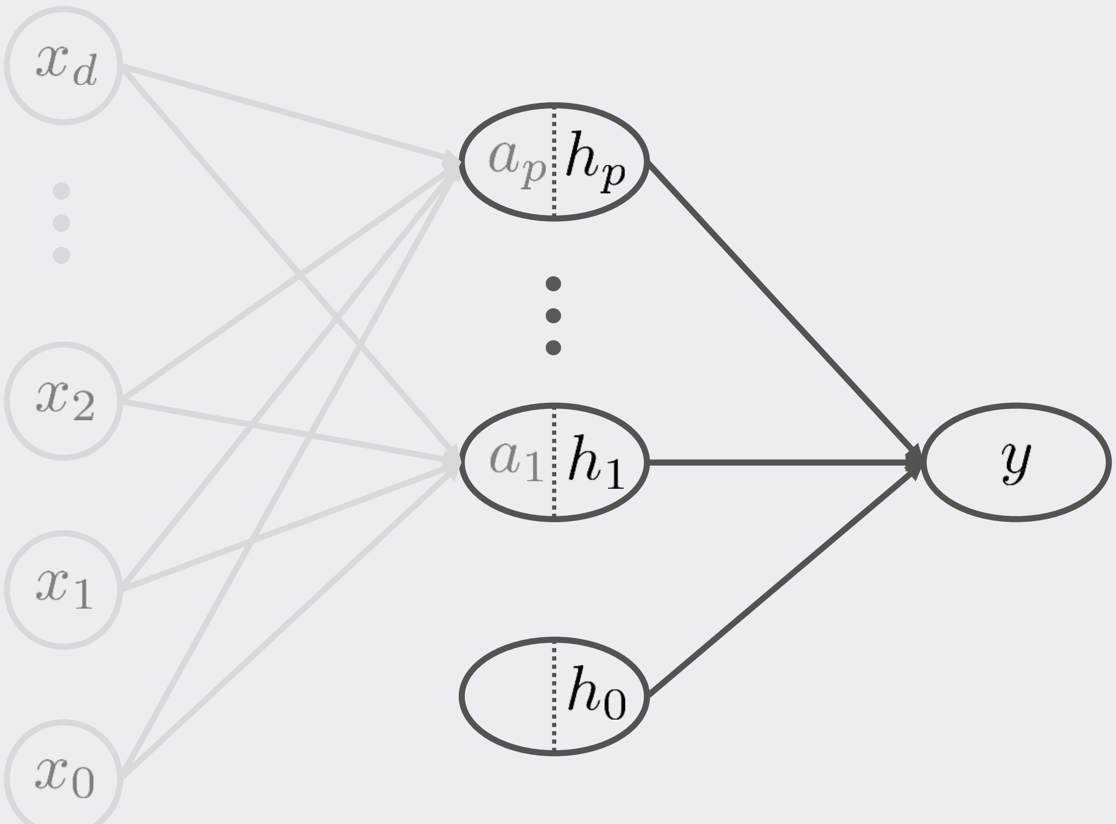
MLP with One Hidden Layer

- Basic Structure: Feed-forward Neural Network with One Hidden Layer
  - ✓ Each hidden node can be considered as an independent perceptron
  - ✓ The output node is a combination of all perceptrons



MLP with One Hidden Layer

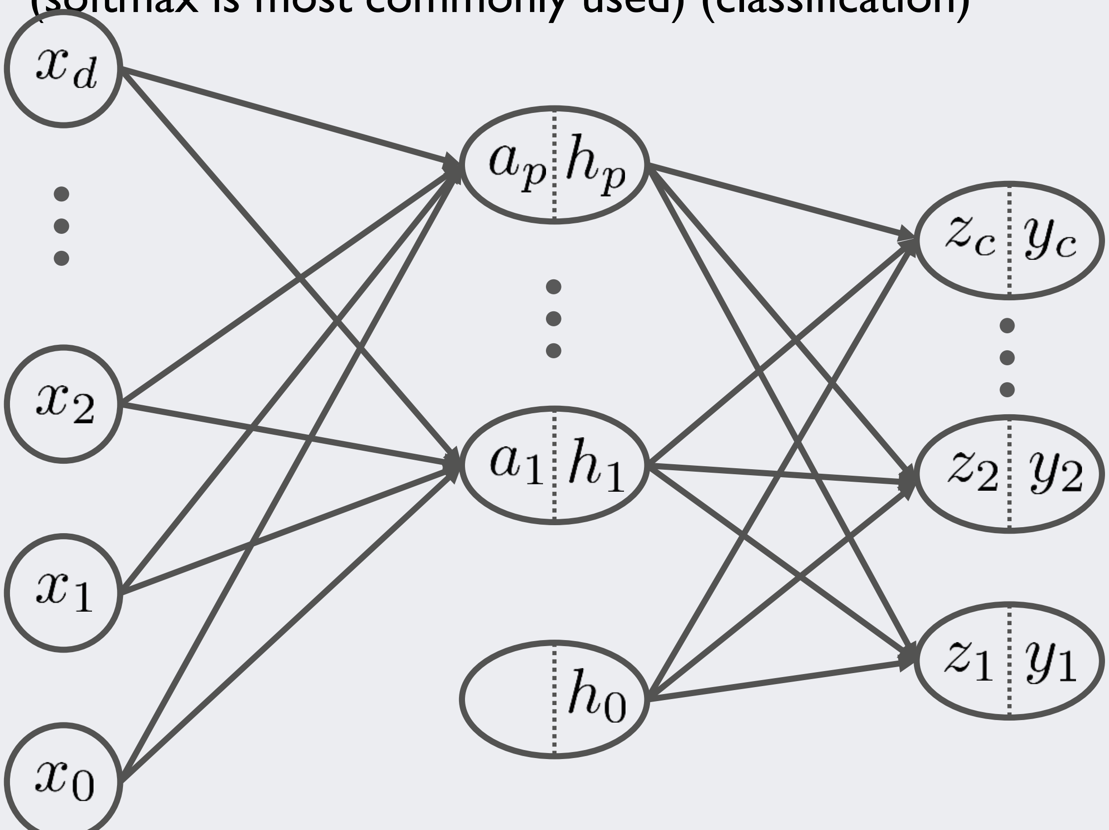
- Basic Structure: Feed-forward Neural Network with One Hidden Layer
  - ✓ Each hidden node can be considered as an independent perceptron
  - ✓ The output node is a linear combination of all perceptrons (regression)



$$y = \sum_{i=0}^{p} w_p^{(2)} h_p$$

MLP with One Hidden Layer

- Basic Structure: Feed-forward Neural Network with One Hidden Layer
  - ✓ Each hidden node can be considered as an independent perceptron
  - ✓ The output node is a combination of all perceptrons with a non-linear transformation (softmax is most commonly used) (classification)



MLP with One Hidden Layer

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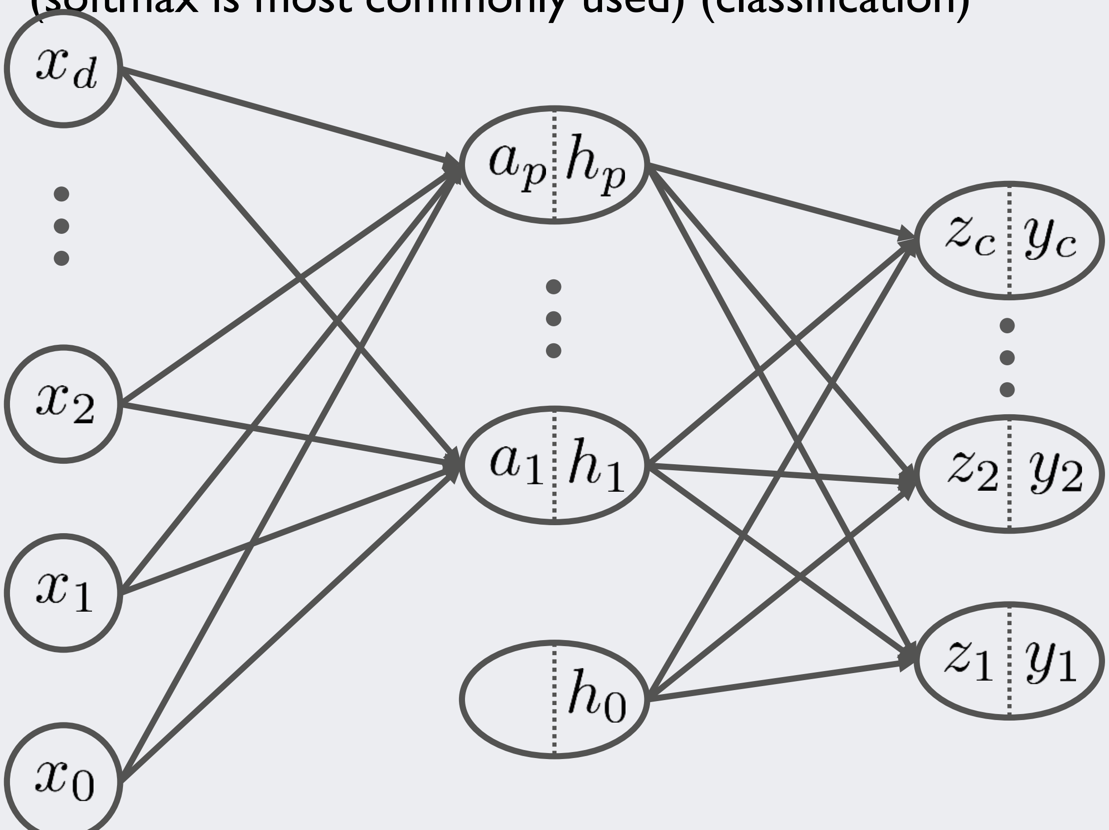


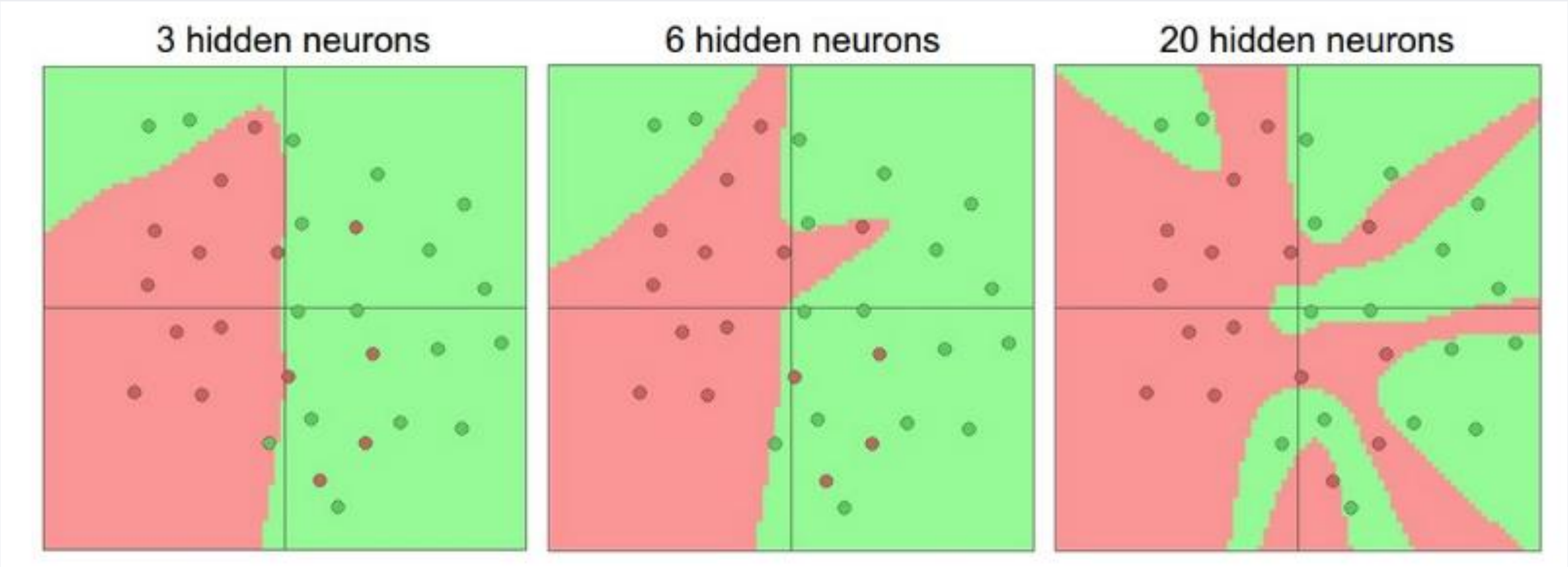
$$z_j = \sum_{i=0}^{p} w_{jp}^{(2)} h_p$$

$$y_j = \frac{e^{z_j}}{\sum_{k=1}^{c} e^{z_k}}$$

각 출력 노드의 출력값을 해당 범주에 속하는 확률로 해석할 수 있음

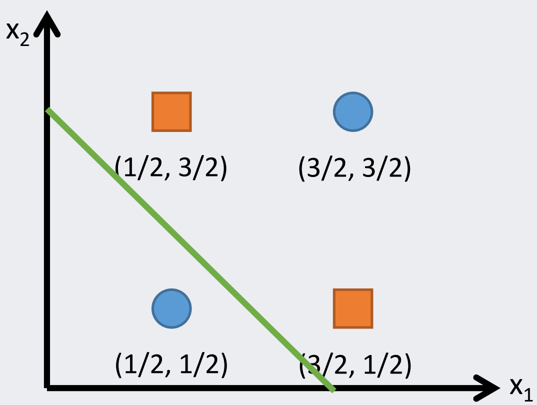
MLP: Hidden Nodes

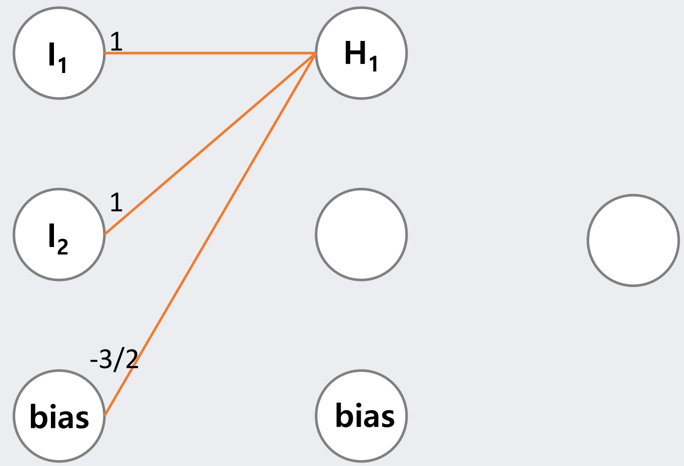
- The role of hidden nodes
  - ✓ Determines the complexity of ANN
  - ✓ If we use more number of hidden nodes, we can find a more sophisticated decision boundary (classification) or an arbitrary shape of function (regression)



MLP: How it works?

- XOR problem revisited





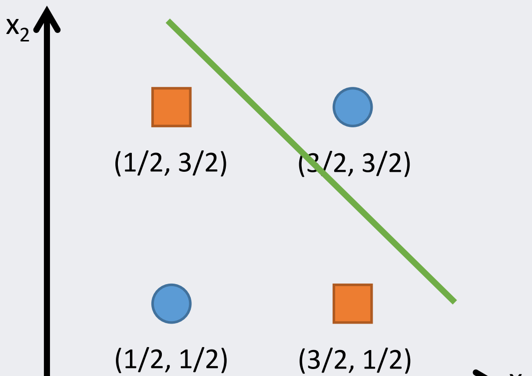
$$h_1 = x_1 + x_2 - \frac{3}{2}$$

$$z_1 = g(h_1) = \begin{cases} 1 & if \;\; h_1 \geq 0 \\ -1 & if \;\; h_1 < 0 \end{cases}$$

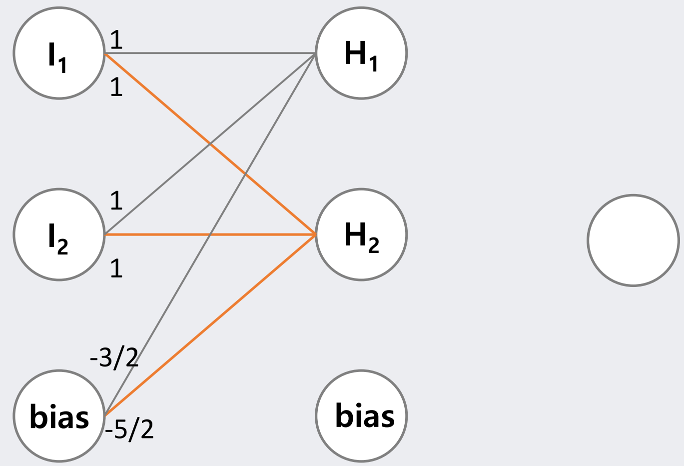
x_1	x_2	h_1	z_1
1/2	1/2	-1/2	-1
3/2	1/2	1/2	1
1/2	3/2	1/2	1
3/2	3/2	3/2	1

MLP: How it works?

- XOR problem revisited (cont')



$$h_2 = x_1 + x_2 - \frac{5}{2}$$

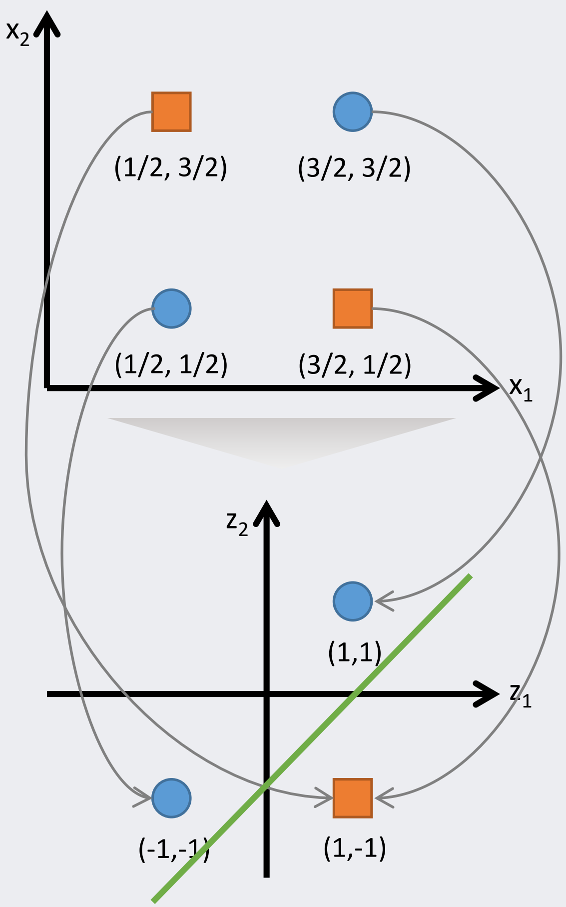


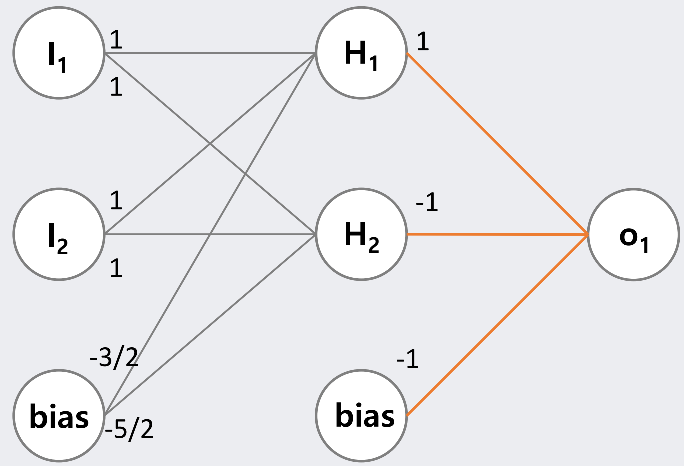
$$z_2 = g(h_2) = \begin{cases} 1 & if\ h_2 \geq 0 \\ -1 & if\ h_2 < 0 \end{cases}$$

x_1	x_2	h_2	z_2
1/2	1/2	-3/2	-1
3/2	1/2	-1/2	-1
1/2	3/2	-1/2	-1
3/2	3/2	1/2	1

MLP: How it works?

- XOR problem revisited (cont')





x_1	x_2	h_1	z_1	h_2	z_2	o_1	z
1/2	1/2	-1/2	-1	-3/2	-1	-1	-1
3/2	1/2	1/2	1	-1/2	-1	1	1
1/2	3/2	1/2	1	-1/2	-1	1	1
3/2	3/2	3/2	1	1/2	1	-1	-1

$$o_1 = z_1 - z_2 - 1$$

$$z = g(o_1) = \begin{cases} 1 & if \ o_1 \geq 0 \\ -1 & if \ o_1 < 0 \end{cases}$$

MLP: Formulation

- General formulation

  ✓ The output of the hidden node j (when the activation function is sigmoid):

$$h_j = \sum_{i=1}^{d+1} w_{ji}^{(1)} x_i, \quad z_j = g(h_j) = \frac{1}{1+\exp(-h_j)}$$

  ✓ The output of the output node (when the activation function is sigmoid):

$$o = \sum_{j=1}^{p+1} w_j^{(2)} g(h_j), \quad z = g(o) = \frac{1}{1+\exp(-o)}$$

  ✓ The final outcome of the neural network:

$$\hat{y} = g\left(\sum_{j=1}^{p+1} w_j^{(2)} g\left(\sum_{i=1}^{d+1} w_{ji}^{(1)} x_i\right)\right)$$

MLP: Training

- Gradient descent algorithm
  - ✓ Taylor expansion of a function

$$f(x+\Delta x) = f(x) + \frac{f'(x)}{1!}\Delta x + \frac{f''(x)}{2!}\Delta x^2 + \cdots$$

  - ✓ For the minimization problem, we can reduce the objective function value by moving the current solution to the opposite direction of the first derivative if it is not zero

$$x_{new} = x_{old} - \eta f'(x), \quad where \quad 0 < \eta < 1$$

  - ✓ The objective function value become lower compared to the previous solution

$$f(x_{new}) = f(x_{old} - \eta f'(x)) \cong f(x_{old}) - \eta |f'(x)|^2 < f(x_{old})$$

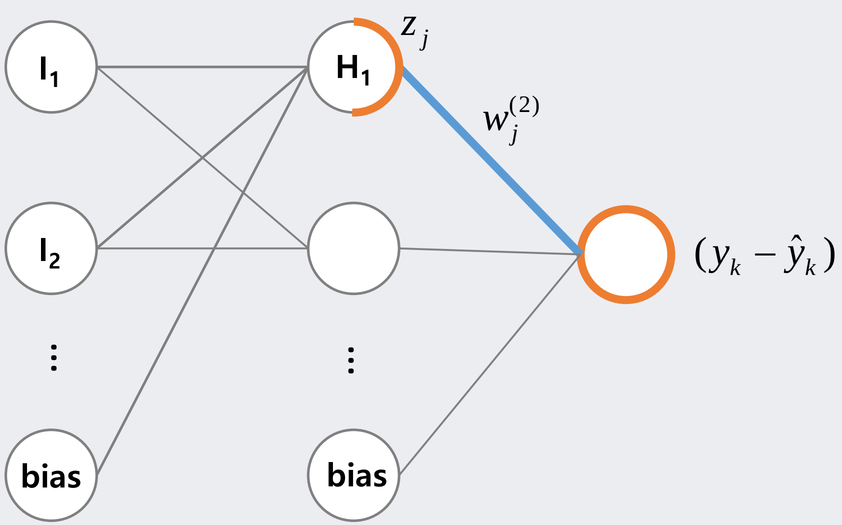
MLP: Training

- Error Back-Propagation
  - ✓ The error of k^th observation

$$Err_k = \frac{1}{2}(y_k - \hat{y}_k)^2, \quad \hat{y}_k = \sum_{j=1}^{p+1} w_j^{(2)} g\left(\sum_{i=1}^{d+1} w_{ji}^{(1)} x_i\right)$$

  - ✓ The weight $w_j^{(2)}$ which connects the j^{th} hidden node

$$\frac{\partial Err_k}{\partial w_j^{(2)}} = \frac{\partial Err_k}{\partial \hat{y}_k} \cdot \frac{\partial \hat{y}_k}{\partial w_j^{(2)}} = (y_k - \hat{y}_k) \cdot z_j$$

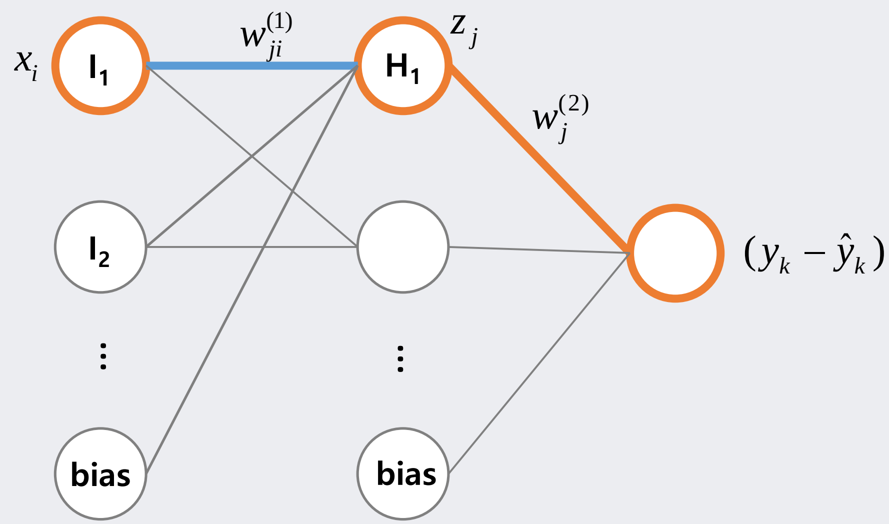


최종 결과물을 얻고	**Feed Forward and Prediction**
그 결과물과 우리가 원하는 결과물과의 차이점을 찾은 후	**Cost Function**
그 차이가 무엇으로 인해 생기는 지	**Differentiation (미분)**
역으로 내려가면서 추정하여	**Back Propagation**
새로운 Parameter 값을 배움	**Weight Update**

MLP: Training

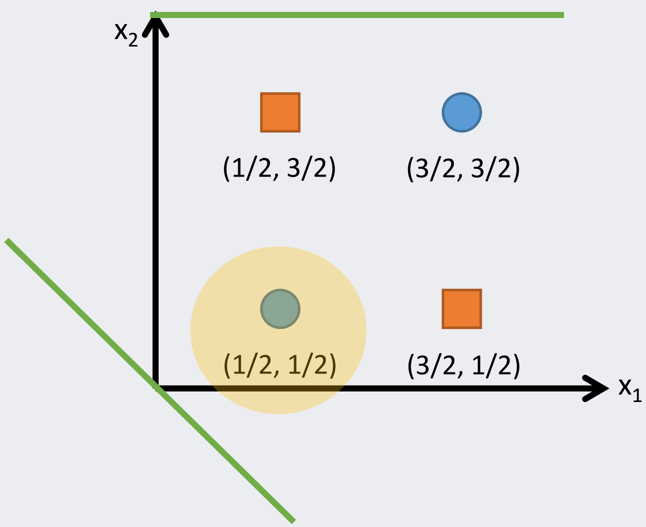
- Error Back-Propagation
  - ✓ The weight $w_{ji}^{(1)}$ which connects the i^{th} input node and j^{th} hidden node

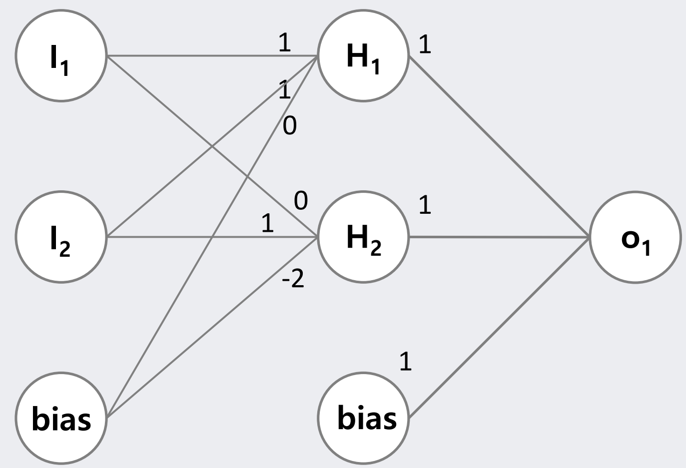
$$\frac{\partial Err_k}{\partial w_{ji}^{(1)}} = \frac{\partial Err_k}{\partial \hat{y}_k} \cdot \frac{\partial \hat{y}_k}{\partial z_j} \cdot \frac{\partial z_j}{\partial h_j} \cdot \frac{\partial h_j}{\partial w_{ji}^{(1)}} = (y_k - \hat{y}_k) \cdot w_j^{(2)} \cdot z_j \cdot (1 - z_j) \cdot x_i$$



MLP: Training

- Error Back-Propagation: Example
  - ✓ Initial weight: Random generation





$$h_1 = \sum w_{1i}^{(1)} x_i = 1 \times 0.5 + 1 \times 0.5 + 0 \times 1 = 1 \qquad z_1 = \frac{1}{1 + \exp(1)} = 0.269$$

$$h_2 = \sum w_{2i}^{(1)} x_i = 0 \times 0.5 + 1 \times 0.5 + (-2) \times 1 = -1.5 \qquad z_2 = \frac{1}{1 + \exp(-1.5)} = 0.818$$

$$\hat{y} = \sum w_j^{(2)} z_j = 1 \times 0.269 + 1 \times 0.818 + 1 \times 1 = 2.087$$

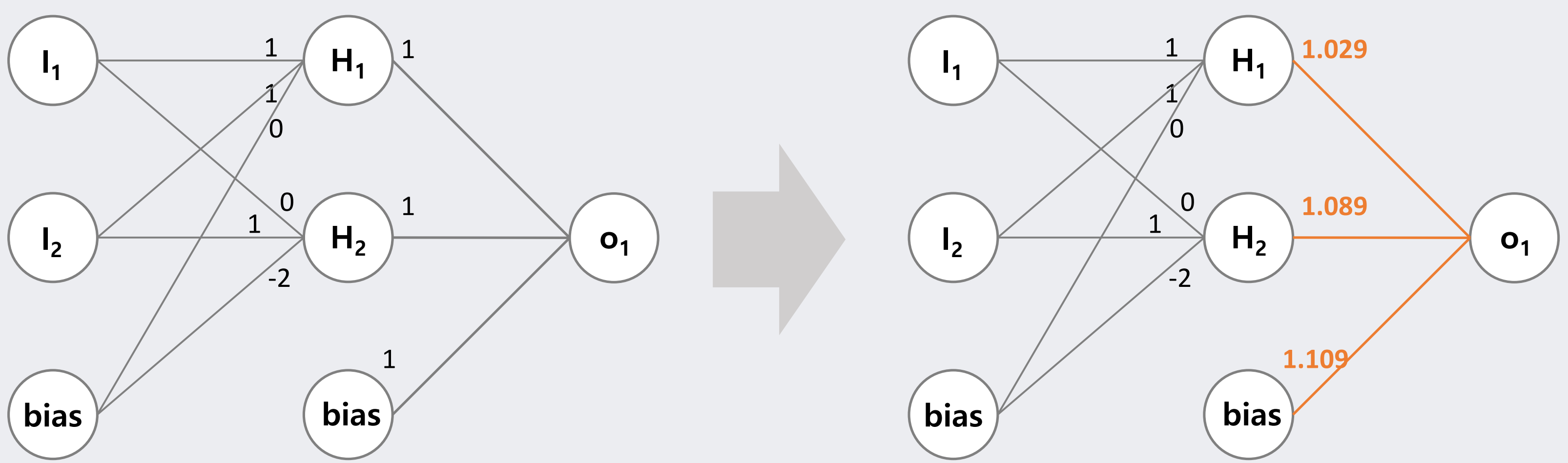
MLP: Training

- Error Back-Propagation: Example
  - ✓ Update the weights between the output and the hidden nodes

$$w_1^{(2)}(new) = w_1^{(2)}(old) - \eta \times (y - \hat{y}) \times z_1 = 1 - 0.1 \times (1 - 2.087) \times 0.269 = 1.029$$

$$w_2^{(2)}(new) = w_2^{(2)}(old) - \eta \times (y - \hat{y}) \times z_2 = 1 - 0.1 \times (1 - 2.087) \times 0.818 = 1.089$$

$$w_0^{(2)}(new) = w_0^{(2)}(old) - \eta \times (y - \hat{y}) \times b^{(2)} = 1 - 0.1 \times (1 - 2.087) \times 1 = 1.109$$



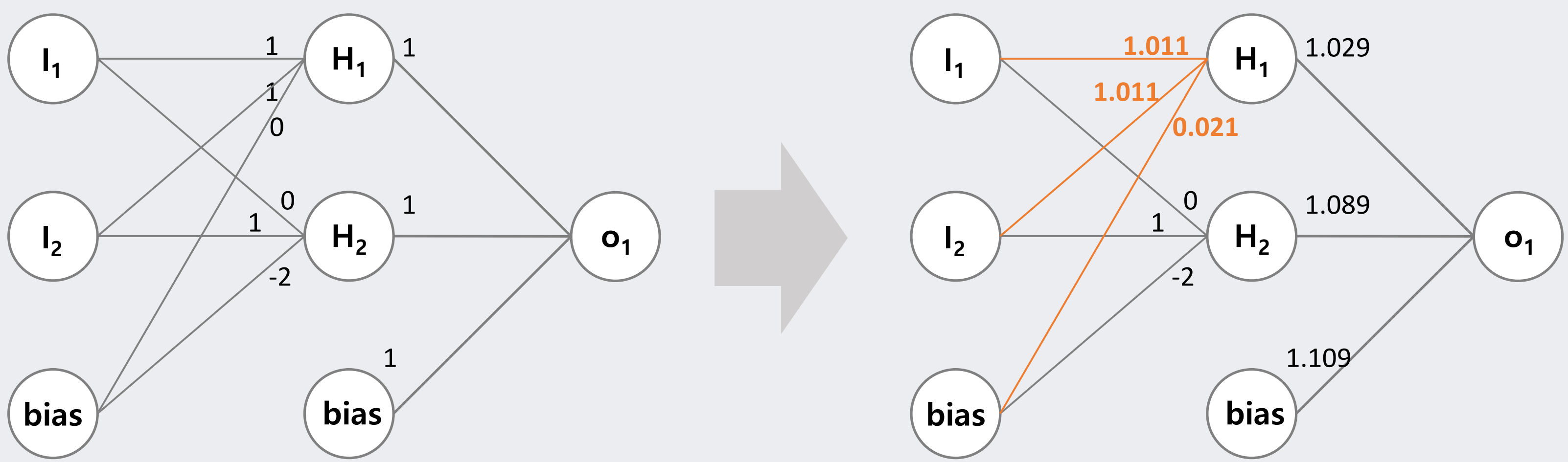
MLP: Training

- Error Back-Propagation: Example
  - ✓ Update the weights between the H_1 and the input nodes

$$w_{11}^{(1)}(new) = w_{11}^{(1)}(old) - \eta \times (y - \hat{y}) \times w_1^{(2)} \times z_1 \times (1 - z_1) \times x_1 = 1.011$$

$$w_{12}^{(1)}(new) = w_{12}^{(1)}(old) - \eta \times (y - \hat{y}) \times w_1^{(2)} \times z_1 \times (1 - z_1) \times x_2 = 1.011$$

$$w_{10}^{(1)}(new) = w_{10}^{(1)}(old) - \eta \times (y - \hat{y}) \times w_1^{(2)} \times z_1 \times (1 - z_1) \times b^{(1)} = 0.021$$



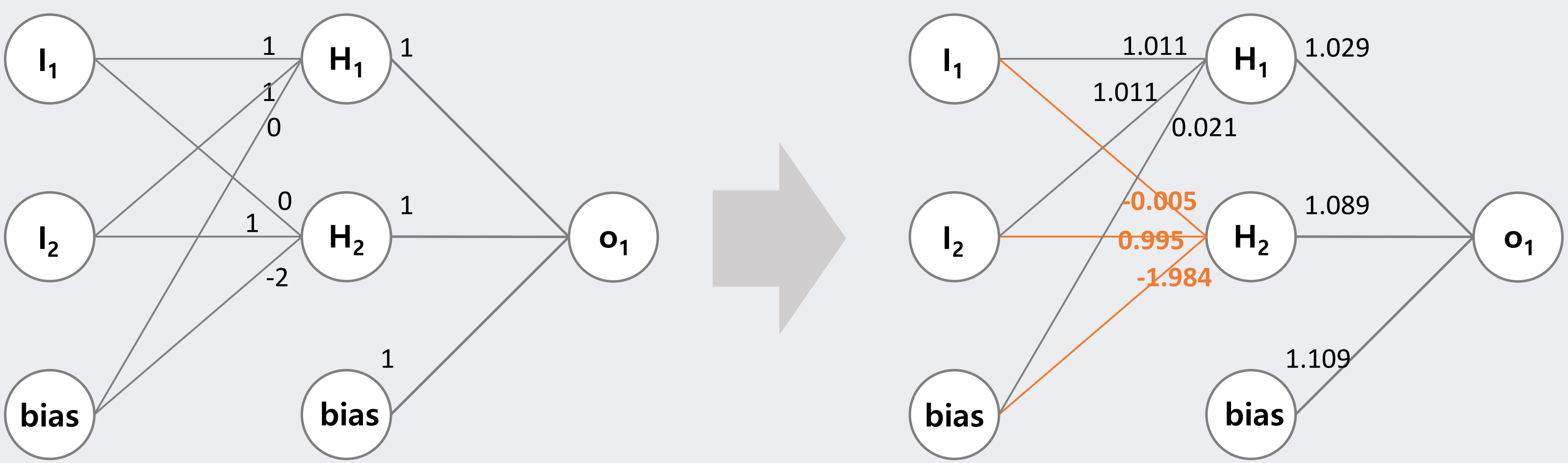
MLP: Training

- Error Back-Propagation: Example
  - ✓ Update the weights between the H_1 and the input nodes

$$w_{21}^{(1)}(new) = w_{21}^{(1)}(old) - \eta \times (y - \hat{y}) \times w_2^{(2)} \times z_2 \times (1 - z_2) \times x_1 = -0.005$$

$$w_{22}^{(1)}(new) = w_{22}^{(1)}(old) - \eta \times (y - \hat{y}) \times w_2^{(2)} \times z_2 \times (1 - z_2) \times x_2 = 0.995$$

$$w_{20}^{(1)}(new) = w_{20}^{(1)}(old) - \eta \times (y - \hat{y}) \times w_2^{(2)} \times z_2 \times (1 - z_2) \times b^{(1)} = -1.984$$



MLP: Training

- Goal
  - ✓ Find the weights that yield best predictions
- Features
  - ✓ The process described before is repeated for all records
  - ✓ At each record, compare the prediction to the actual target
  - ✓ Difference is the error for the output node
  - ✓ Error is propagated back and distributed to all the hidden nodes and used to update their weights

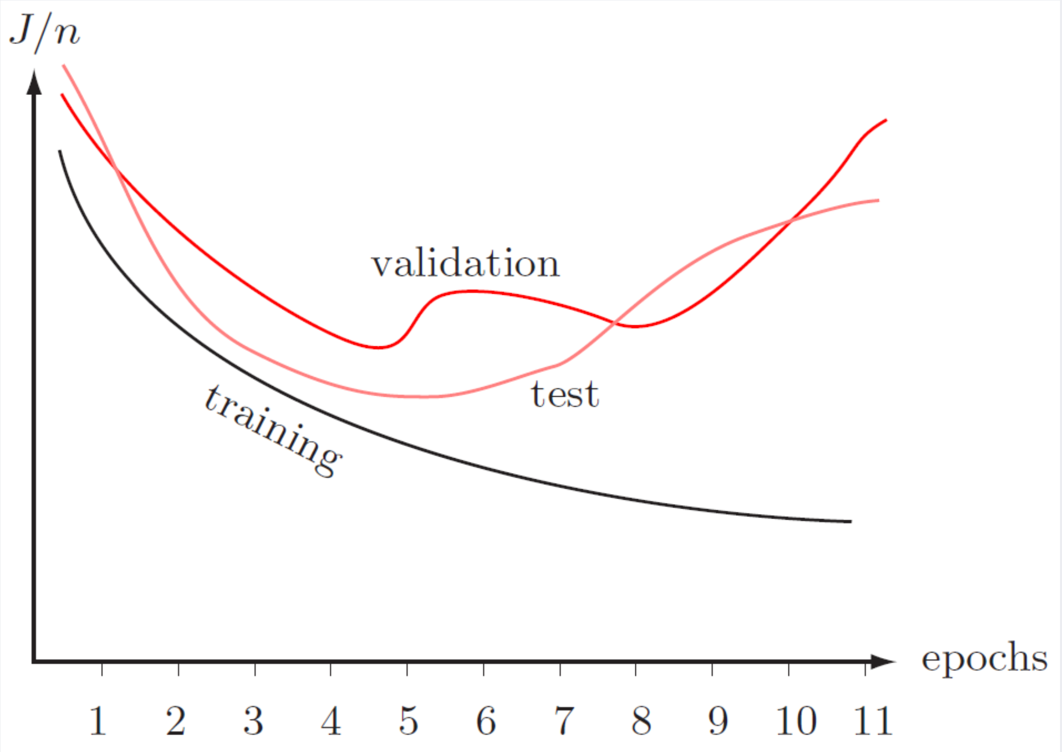
MLP: Training

- Why it works
  - ✓ Big errors lead to big changes in weights
  - ✓ Small errors leave weights relatively unchanged
  - ✓ Over thousand of updates, a given weight keeps changing until the error associated with it is negligible

- Common criteria to stop updating
  - ✓ When weights change very little from one epoch to the next
  - ✓ When the misclassification rate reaches a required threshold
  - ✓ When a limit on runs is reached

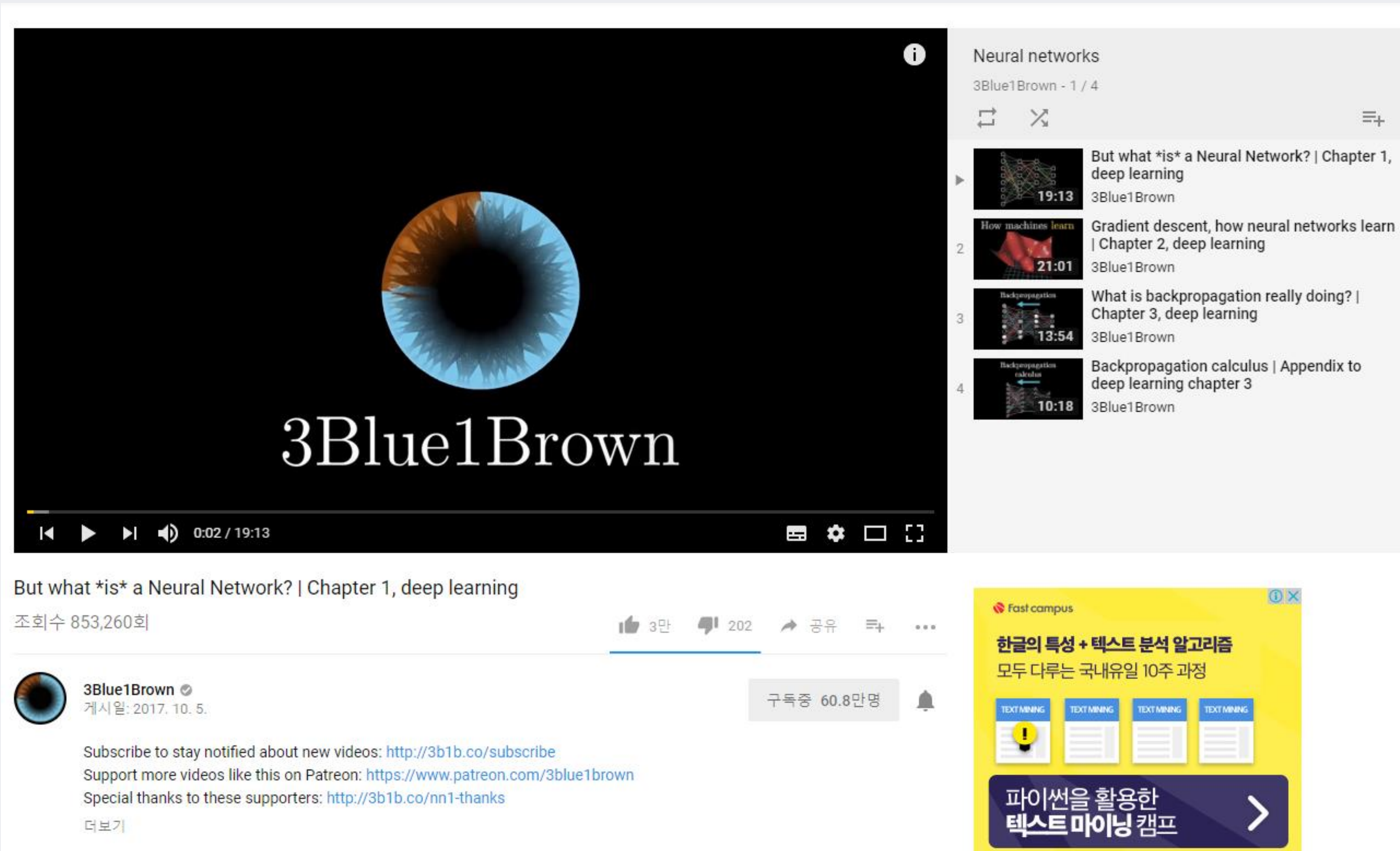
MLP: Training

- With sufficient iterations, neural networks can easily over-fit the data.
- To avoid over-fitting,
  - ✓ Track error in validation data
  - ✓ Limit iterations
  - ✓ Limit complexity of network
  - ✓ N. of hidden layers, nodes, etc.



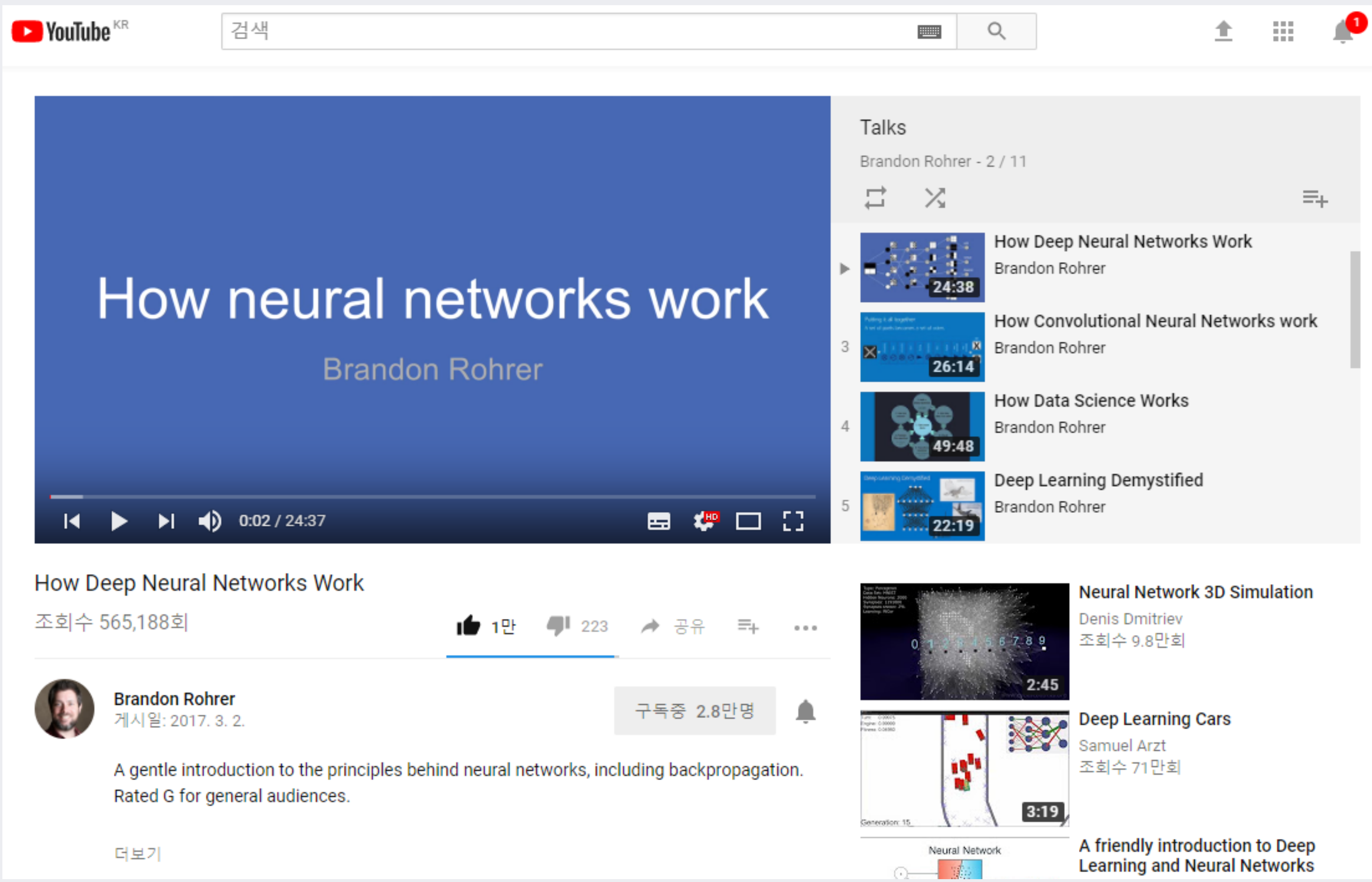
Recommended Video Lectures

- 유튜브 3Blue 1Brown Neural Network 강좌
  - ✓ https://www.youtube.com/channel/UCYO_jab_esuFRV4b17AJtAw



Recommended Video Lectures

- 유튜브 Brandon Rohrer 강좌
  - ✓ https://www.youtube.com/watch?v=ILsA4nyG7I0&list=PLVZqlMpoM6kbaeySxhdtgQPFEC5nV7Faa&index=2



AGENDA

01 Artificial Neural Networks: Perceptron

02 Multi-layer Perceptron (MLP)

03 R Exercise

R Exercise: Classification

- Dataset: Cardiotocography Data Set
  - ✓ https://archive.ics.uci.edu/ml/datasets/Cardiotocography

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Cardiotocography Data Set

Download: Data Folder, Data Set Description

Abstract: The dataset consists of measurements of fetal heart rate (FHR) and uterine contraction (UC) features on cardiotocograms classified by expert obstetricians.

Data Set Characteristics:	Multivariate	**Number of Instances:**	2126	**Area:**	Life
Attribute Characteristics:	Real	**Number of Attributes:**	23	**Date Donated**	2010-09-07
Associated Tasks:	Classification	**Missing Values?**	N/A	**Number of Web Hits:**	96768

Source:

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Bernardes, J., joaobern '@' med.up.pt, Faculty of Medicine, University of Porto, Portugal.
Ayres de Campos, D., sisporto '@' med.up.pt, Faculty of Medicine, University of Porto, Portugal.

Data Set Information:

2126 fetal cardiotocograms (CTGs) were automatically processed and the respective diagnostic features measured. The CTGs were also classified by three expert obstetricians and a consensus classification label assigned to each of them. Classification was both with respect to a morphologic pattern (A, B, C. ...) and to a fetal state (N, S, P). Therefore the dataset can be used either for 10-class or 3-class experiments.

R Exercise: Classification

- Dataset: Cardiotocography Data Set

Input variables

LB - FHR baseline (beats per minute)
AC - # of accelerations per second
FM - # of fetal movements per second
UC - # of uterine contractions per second
DL - # of light decelerations per second
DS - # of severe decelerations per second
DP - # of prolongued decelerations per second
ASTV - percentage of time with abnormal short term variability
MSTV - mean value of short term variability
ALTV - percentage of time with abnormal long term variability
MLTV - mean value of long term variability
Width - width of FHR histogram
Min - minimum of FHR histogram
Max - Maximum of FHR histogram
Nmax - # of histogram peaks
Nzeros - # of histogram zeros
Mode - histogram mode
Mean - histogram mean
Median - histogram median
Variance - histogram variance
Tendency - histogram tendency
CLASS - FHR pattern class code (1 to 10)
NSP - fetal state class code (N=normal; S=suspect; P=pathologic)

Target variable

R Exercise: Classification

- Performance evaluation function

```
# Part 1: Multi-class classification with ANN & Multinimial logistic regression
# Performance evaluation function for multi-class classification ----------
perf_eval_multi <- function(cm){
    # Simple Accuracy
    ACC = sum(diag(cm))/sum(cm)
    # Balanced Correction Rate
    BCR = 1
    for (i in 1:dim(cm)[1]){
        BCR = BCR*(cm[i,i]/sum(cm[i,]))
    }
    BCR = BCR^(1/dim(cm)[1])
    return(c(ACC, BCR))
}
```

✓ perf_eval_multi

- Argument: confusion matrix (cm)
- Outputs: simple accuracy (ACC), balanced correction rate (BCR)

R Exercise: Classification

- Install package

```
# Install nnet package and prepare it
install.packages("nnet")
library(nnet)
```

✓ "nnet" package

- Many packages provide neural network module
- "nnet" is one of the most widely used packages

R Exercise: Classification

- Data loading and preprocessing

```
# Multi-class classification (ctgs dataset)
ctgs_data <- read.csv("ctgs.csv")
n_instance <- dim(ctgs_data)[1]
n_var <- dim(ctgs_data)[2]

# Conduct normalization
ctgs_input <- ctgs_data[,-n_var]
ctgs_target <- ctgs_data[,n_var]
ctgs_input <- scale(ctgs_input, center = TRUE, scale = TRUE)
ctgs_target <- as.factor(ctgs_target)
ctgs_data_normalized <- data.frame(ctgs_input, Class = ctgs_target)
```

✓ Data loading

- read.csv( ) function, use header = TRUE option because the first row is the variable name
- Use dim( ) function to check the number of rows and columns in the dataset

✓ Data normalization

- Make the average and standard deviation of each variable to 0 and 1, respectively
- Covert the target variable type to "factor"

R Exercise: Classification

- Data loading and preprocessing

```
# Initialize performance matrix
perf_summary <- matrix(0, nrow = 2, ncol = 2)
colnames(perf_summary) <- c("ACC", "BCR")
rownames(perf_summary) <- c("Multi_Logit", "ANN")

# Split the data into the training/validation sets
set.seed(12345)
trn_idx <- sample(1:n_instance, round(0.8*n_instance))
ctgs_trn <- ctgs_data_normalized[trn_idx,]
ctgs_tst <- ctgs_data_normalized[-trn_idx,]
```

✓ Initialize the performance summary matrix

✓ Data partition

- set.seed( ): set the seed of random initialization
- Use 80% for training and 20% for test

R Exercise: Classification

- Training the Multinomial Logistic Regression

```
# Multinomial logistic regression -----------------------------------
# Train multinomial logistic regression
ml_logit <- multinom(Class ~ ., data = ctgs_trn)

# Check the coefficients
summary(ml_logit)
t(summary(ml_logit)$coefficients)
```

✓ Estimated regression coefficients

```
> t(summary(ml_logit)$coefficients)
                       2           3
(Intercept) -4.694977008 -11.58608545
LB          -1.136169974   2.94827810
AC          -3.747793932  -3.44072166
FM           0.469688181   1.07087196
UC          -0.907147801  -1.07874916
DL           0.028822895   0.15122342
DS          -0.433749154   0.23945220
DP           1.479317937   1.36253728
ASTV         1.376230801   3.46304432
MSTV        -0.269653587  -1.37476523
ALTV         0.413875887   1.48408278
```

```
MLTV        -0.056153529   0.68602348
Width       -0.007595327   0.13962712
Min          0.327512978   0.55153110
Max          0.523037010   1.21168222
Nmax         0.328949181  -0.92033096
Nzeros      -0.154133544   0.36098681
Mode        -1.041006093  -0.05063308
Mean         4.336477367  -1.34224223
Median      -0.604921319  -4.03591917
Variance     1.178814582   1.99001476
Tendency     0.117217134   0.16513548
```

R Exercise: Classification

- Classify the Test Examples using the Multinomial Logistic Regression

```
# Predict the class label
ml_logit_prey <- predict(ml_logit, newdata = ctgs_tst)
cfmatrix <- table(ctgs_tst$Class, ml_logit_prey)
cfmatrix

perf_summary[1,] <- perf_eval_multi(cfmatrix)
perf_summary
```

✓ Simple accuracy: 0.8941, Balanced correction rate: 0.7468

R Exercise: Classification

- Data transformation for MLR

```
# Artificial Neural Network -----------------------------------------------
# Train ANN
ann_trn_input <- ctgs_trn[,-n_var]
ann_trn_target <- class.ind(ctgs_trn[,n_var])
```

✓ For multi-class classification, the number of output nodes is the same as the number of classes

✓ Use class.ind( ) function to convert the target variable (factor type) to one-hot (1-of-C coding) vector

Class
1
2
3
1
2

C_1	C_2	C_3
1	0	0
0	1	0
0	0	1
1	0	0
0	1	0

R Exercise: Classification

- Search the best number of hidden nodes

```
# Find the best number of hidden nodes in terms of BCR
# Candidate hidden nodes
nH <- seq(from=5, to=30, by=5)
# 5-fold cross validation index
val_idx <- sample(c(1:5), dim(ann_trn_input)[1], replace = TRUE, prob = rep(0.2,5))
val_perf <- matrix(0, length(nH), 3)
```

  - ✓ The best number of hidden node depends on the dataset
  - ✓ Perform 5-fold cross validation
    - The range of hidden nodes: 5 ~ 30 (step by 5)
    - Initialize validation index
    - val_perf: store the performance for each number of hidden node

R Exercise: Classification

- Search the best number of hidden nodes

```
for (i in 1:length(nH)) {
    cat("Training ANN: the number of hidden nodes:", nH[i], "\n")
    eval_fold <- c()
    for (j in c(1:5)) {
        # Training with the data in (k-1) folds
        tmp_trn_input <- ann_trn_input[which(val_idx != j),]
        tmp_trn_target <- ann_trn_target[which(val_idx != j),]
        tmp_nnet <- nnet(tmp_trn_input, tmp_trn_target, size = nH[i],
                         decay = 5e-4, maxit = 500)
```

✓ Repeat the process for all candidate number of hidden node (i) and five folds (j)

  - If the val_idx is j, use the example for validation, otherwise use the example for training

✓ nnet( ): function for training the neural network

  - Arg 1: input (X) of training data
  - Arg 2: target (y) of training data
  - Arg 3: number of hidden nodes
  - Arg 4 & 5: weight decay threshold, maximum number of epochs

R Exercise: Classification

- Search the best number of hidden nodes

```
# Evaluate the model with the remaining 1 fold
tmp_val_input <- ann_trn_input[which(val_idx == j),]
tmp_val_target <- ann_trn_target[which(val_idx == j),]
eval_fold <- rbind(eval_fold, cbind(max.col(tmp_val_target),
         max.col(predict(tmp_nnet, tmp_val_input))))

# Confusion matrix
cfm <- table(eval_fold[,1], eval_fold[,2])
# nH
val_perf[i,1] <-nH[i]
# Record the validation performance
val_perf[i,2:3] <- t(perf_eval_multi(cfm))
```

✓ Combine the prediction results for 5 validation sets using rbind( ) and evaluate it together

R Exercise: Classification

- Search the best number of hidden nodes

```
ordered_val_perf <- val_perf[order(val_perf[,3], decreasing = TRUE),]
colnames(ordered_val_perf) <- c("nH", "ACC", "BCR")
ordered_val_perf
# Find the best number of hidden node
best_nH <- ordered_val_perf[1,1]
```

✓ Find the best hidden node in terms of BCR

  - Different results can be obtained for different trials

```
> ordered_val_perf
     nH       ACC       BCR
[1,] 30 0.9112287 0.8260219
[2,] 25 0.9118166 0.8226941
[3,] 20 0.9135802 0.8094907
[4,] 15 0.9012346 0.8008131
[5,] 10 0.8924162 0.7813366
[6,]  5 0.8847737 0.7753846
```

R Exercise: Classification

- Model training with the best number of hidden nodes

```
# Test the ANN
ann_tst_input = ctgs_tst[,-n_var]
ann_tst_target = class.ind(ctgs_tst[,n_var])
ctgs_nnet <- nnet(ann_trn_input, ann_trn_target, size = best_nH,
                  decay = 5e-4, maxit = 500)
```

✓ Use the best number of hidden nodes determined by the 5-fold cross validation to train the entire training dataset

R Exercise: Classification

- Evaluate the MLR and compare the results with the multinomial logistic regression

```
# Performance evaluation
prey <- predict(ctgs_nnet, ann_tst_input)
tst_cm <- table(max.col(ann_tst_target), max.col(prey))
tst_cm perf_summary[2,] <- perf_eval_multi(tst_cm)
perf_summary
```

```
> cfmatrix
   ml_logit_prey
      1   2   3
  1 318  14   0
  2  18  41   1
  3   4   8  21
```

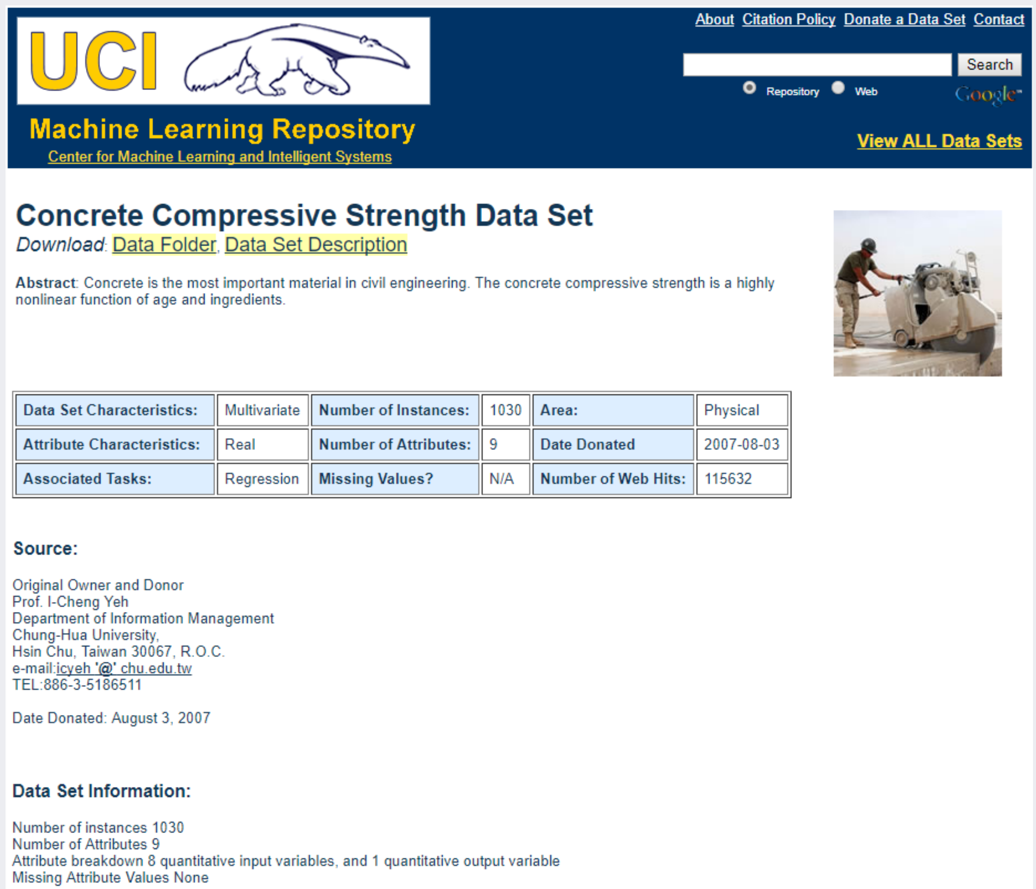
```
> tst_cm

      1   2   3
  1 321  11   0
  2  20  40   0
  3   4   5  24
```

```
> perf_summary
                  ACC       BCR
Multi_Logit 0.8941176 0.7468081
ANN         0.9058824 0.7768270
```

R Exercise: Regression

- Dataset: Concrete Compressive Strength Data Set
  - ✓ Predict the strength of concrete with different proportions of ingredients
  - ✓ https://archive.ics.uci.edu/ml/datasets/Concrete+Compressive+Strength



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Concrete Compressive Strength Data Set

Download: Data Folder, Data Set Description

Abstract: Concrete is the most important material in civil engineering. The concrete compressive strength is a highly nonlinear function of age and ingredients.

Data Set Characteristics:	Multivariate	Number of Instances:	1030	Area:	Physical
Attribute Characteristics:	Real	Number of Attributes:	9	Date Donated	2007-08-03
Associated Tasks:	Regression	Missing Values?	N/A	Number of Web Hits:	115632

Source:

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Date Donated: August 3, 2007

Data Set Information:

Number of instances 1030
Number of Attributes 9
Attribute breakdown 8 quantitative input variables, and 1 quantitative output variable
Missing Attribute Values None

R Exercise: Regression

- Dataset: Concrete Compressive Strength Data Set
  - ✓ Input and target variables

Cement (component 1) -- quantitative -- kg in a m3 mixture -- Input Variable
Blast Furnace Slag (component 2) -- quantitative -- kg in a m3 mixture -- Input Variable
Fly Ash (component 3) -- quantitative -- kg in a m3 mixture -- Input Variable
Water (component 4) -- quantitative -- kg in a m3 mixture -- Input Variable
Superplasticizer (component 5) -- quantitative -- kg in a m3 mixture -- Input Variable
Coarse Aggregate (component 6) -- quantitative -- kg in a m3 mixture -- Input Variable
Fine Aggregate (component 7) -- quantitative -- kg in a m3 mixture -- Input Variable
Age -- quantitative -- Day (1~365) -- Input Variable
Concrete compressive strength -- quantitative -- MPa -- Output Variable

R Exercise: Regression

- Compare MLR, k-NN, & ANN

  ✓ Performance evaluation function

```
# Part 2: Regression with MLR, k-NN, and ANN
# Performance evaluation function for regression --------------------------
perf_eval_reg <- function(tgt_y, pre_y){
    # RMSE
    rmse <- sqrt(mean((tgt_y - pre_y)^2))
    # MAE
    mae <- mean(abs(tgt_y - pre_y))
    # MAPE
    mape <- 100*mean(abs((tgt_y - pre_y)/tgt_y))
    return(c(rmse, mae, mape))
}
```

  ✓ Args: target value, predicted value

  ✓ Outputs: RMSE, MAE, MAPE

R Exercise: Regression

- Data loading and preprocessing

```
# Concrete strength data
concrete <- read.csv("concrete.csv", header = FALSE)
n_instance <- dim(concrete)[1]
n_var <- dim(concrete)[2]
RegX <- concrete[,-n_var]
RegY <- concrete[,n_var]
# Data Normalization
RegX <- scale(RegX, center = TRUE, scale = TRUE)
# Combine X and Y
RegData <- as.data.frame(cbind(RegX, RegY))
```

✓ Use read.csv( ) function

- Use header = FALSE option because the first row is not the name of variable

✓ Store the number of instances and variables

✓ Perform normalization for input variables

✓ Combine the normalized input variables and target variable for modeling

R Exercise: Regression

- Data loading and preprocessing

```
# Split the data into the training/test sets
set.seed(12345)
trn_idx <- sample(1:n_instance, round(0.7*n_instance))
trn_data <- RegData[trn_idx,]
tst_data <- RegData[-trn_idx,]
perf_summary_reg <- matrix(0,3,3)
rownames(perf_summary_reg) <- c("MLR", "k-NN", "ANN")
colnames(perf_summary_reg) <- c("RMSE", "MAE", "MAPE")
```

✓ Data partitioning: 70% for training 30% for test

✓ Initialize the performance summary table

  - Algorithms: MLR, k-NN, ANN
  - Metrics: RMSE, MAE, MAPE

R Exercise: Regression

- Training and Evaluating MLR

```
# Multiple linear regression
full_model <- lm(RegY ~ ., data = trn_data)
mlr_prey <- predict(full_model, newdata = tst_data)
perf_summary_reg[1,] <- perf_eval_reg(tst_data$RegY, mlr_prey)
perf_summary_reg
```

✓ Train the MLR with all variables

```
> perf_summary_reg
         RMSE      MAE     MAPE
MLR  10.44926 8.166065 30.85209
k-NN  0.00000 0.000000  0.00000
ANN   0.00000 0.000000  0.00000
```

R Exercise: Regression

- Training and Evaluating the k-NN

```
# Evaluate the k-NN with the test data
# k-Nearest Neighbor Learning (Regression) --------------------------------
install.packages("FNN", dependencies = TRUE)
library(FNN)

knn_reg <- knn.reg(trn_data[,-n_var], test = tst_data[,-n_var], trn_data$RegY, k=3)
knn_prey <- knn_reg$pred
perf_summary_reg[2,] <- perf_eval_reg(tst_data$RegY, knn_prey)
perf_summary_reg
```

✓ MAE is decreased by 1.7%p, MAPE is decreased by 7.5%p compared to MLR

```
> perf_summary_reg
          RMSE      MAE     MAPE
MLR  10.449259 8.166065 30.85209
k-NN  8.452958 6.462481 23.30499
ANN   0.000000 0.000000  0.00000
```

R Exercise: Regression

- Search the best number of hidden nodes

```
# Find the best number of hidden nodes in terms of BCR
# Candidate hidden nodes
nH <- seq(from=2, to=20, by=2)
# 5-fold cross validation index
val_idx <- sample(c(1:5), length(trn_idx), replace = TRUE, prob = rep(0.2,5))
val_perf <- matrix(0, length(nH), 4)
...
for (i in 1:length(nH)) {
    ...
    for (j in c(1:5)) {
        tmp_nnet <- nnet(RegY ~ ., data = tmp_trn_data, size = nH[i],
                                linout = TRUE, decay = 5e-4, maxit = 500)
...
```

✓ Perform the 5-fold cross validation by varying the number of hidden nodes from 2 to 20 with the step size of 2

✓ (Note) linout = TRUE option must be set to solve a regression problem

R Exercise: Regression

- Search the best number of hidden nodes

```
ordered_val_perf <- val_perf[order(val_perf[,3], decreasing = FALSE),]
colnames(ordered_val_perf) <- c("nH", "RMSE", "MAE", "MAPE")
ordered_val_perf

# Find the best number of hidden node
best_nH <- ordered_val_perf[1,1]
```

```
> ordered_val_perf
      nH     RMSE      MAE     MAPE
 [1,] 14 7.258657 5.028841 17.65126
 [2,] 20 6.933016 5.090388 17.76599
 [3,] 12 6.952557 5.093377 18.49242
 [4,] 16 6.975732 5.152586 18.37121
 [5,] 10 6.839858 5.161052 18.68690
 [6,]  8 7.298235 5.253384 18.67945
 [7,] 18 7.966798 5.494715 20.98212
 [8,]  4 7.290364 5.613038 19.26955
 [9,]  6 7.325283 5.643885 19.42178
[10,]  2 9.277461 6.734610 22.96352
```

R Exercise: Regression

- Training and Evaluating ANN

```
# Test the model and compare the performance
ann_prey <- predict(best_nnet, tst_data[,-n_var])
perf_summary_reg[3,] <- perf_eval_reg(tst_data$RegY, ann_prey)
perf_summary_reg
```

✓ ANN resulted in the lowest error rate among the three regression algorithms

```
> perf_summary_reg
           RMSE      MAE     MAPE
MLR   10.449259 8.166065 30.85209
k-NN   8.452958 6.462481 23.30499
ANN    7.056971 4.950896 16.08717
```


ANY
questions?