Artificial Neural Network: MLP

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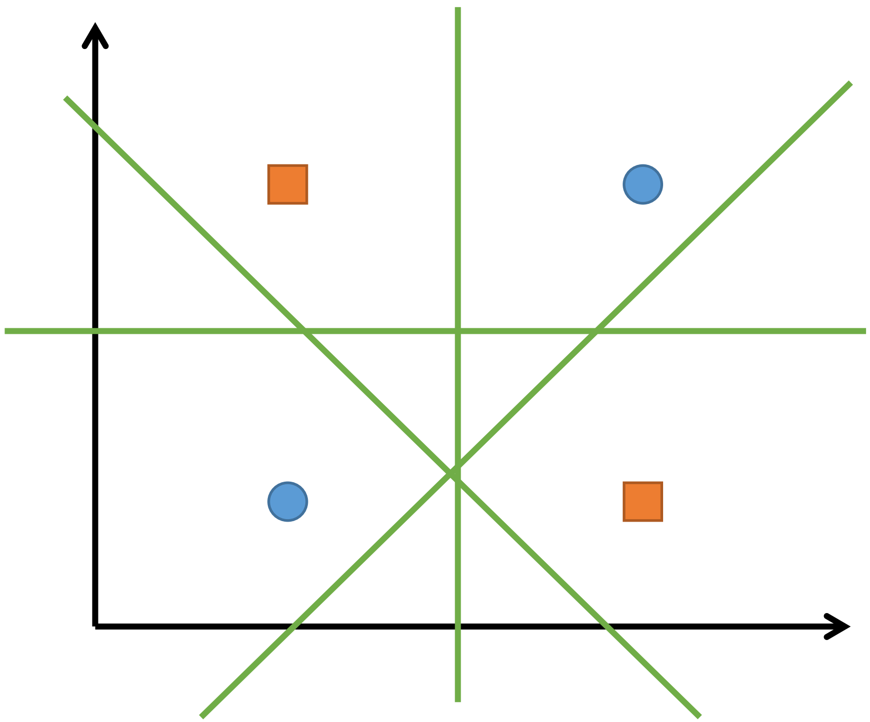
AGENDA

Perceptron: Limitation

- 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***

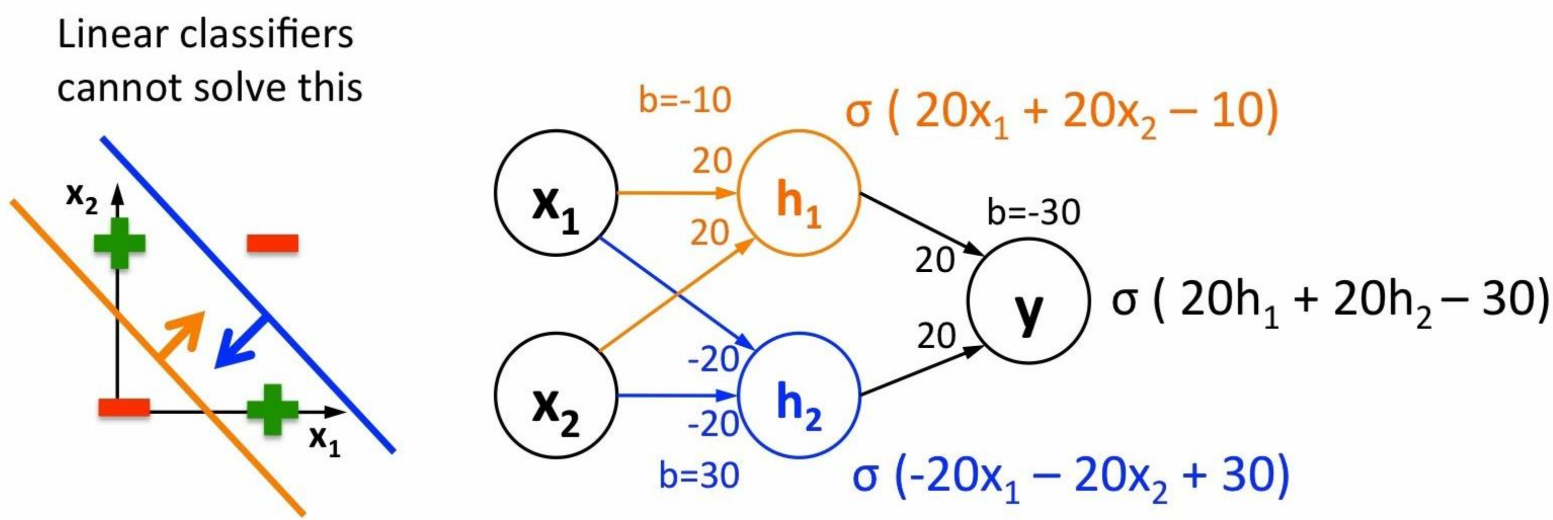
Perceptron: Limitation

- 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!



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

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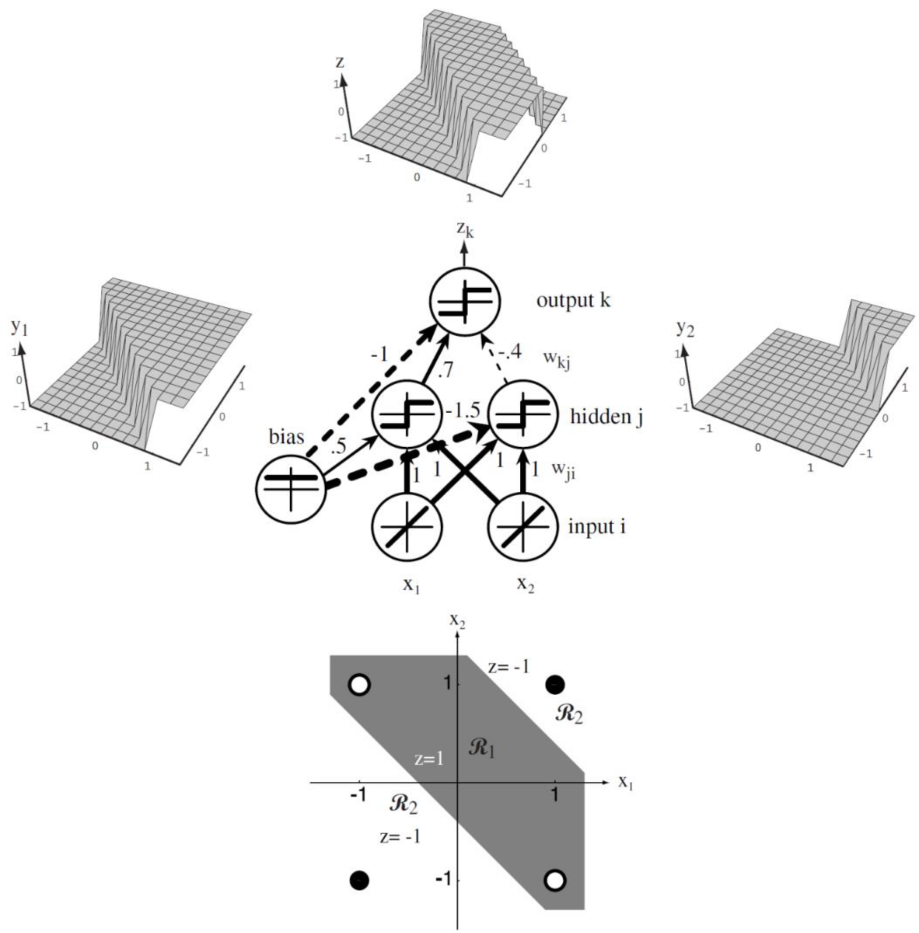
Multi-Layer Perceptron (MLP)

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

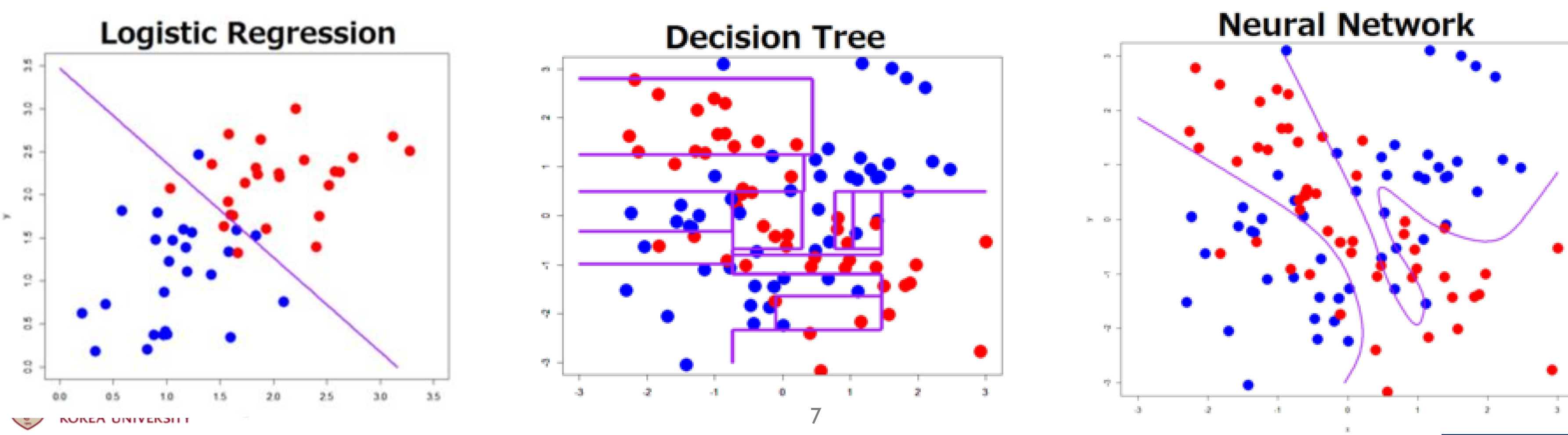


Multi-Layer Perceptron (MLP)

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

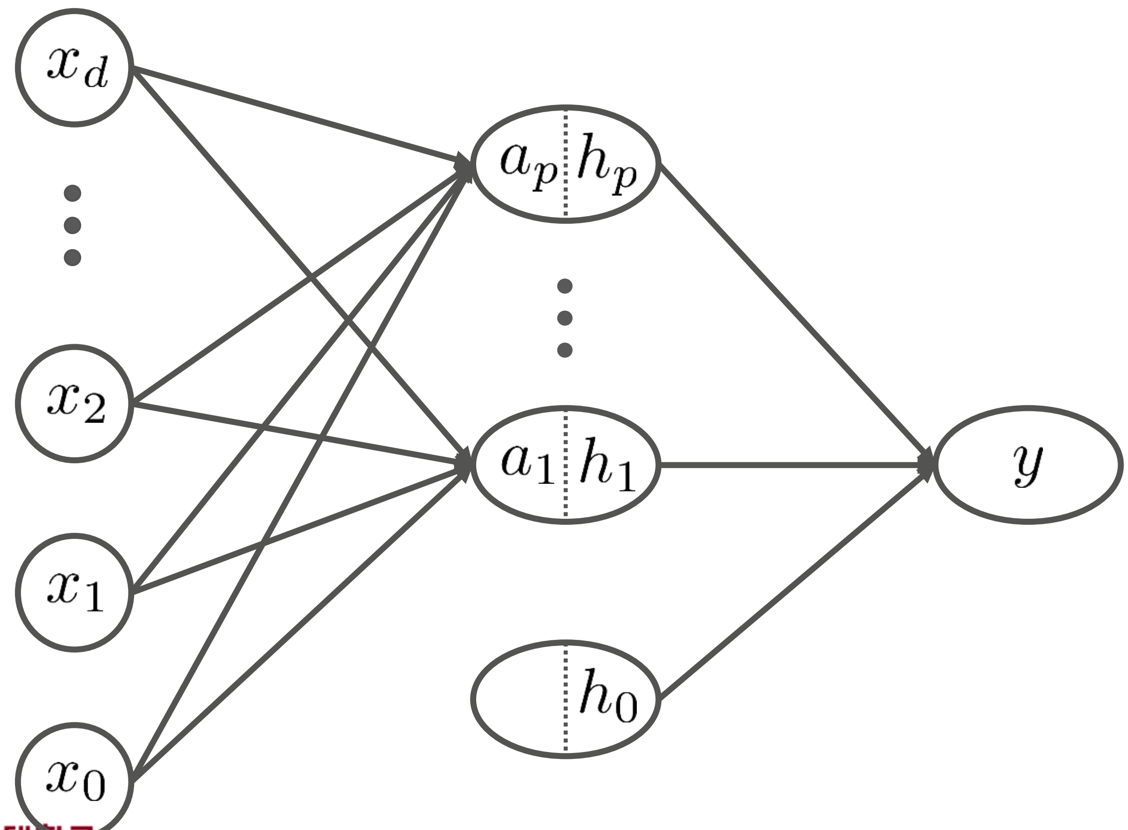
	Logstic Regression	Decision Tree	MLP
No. of lines	1	No restriction	User defined (No of hidden layers and hidden nodes)
Direction of lines	No restriction	Vertical to an axis	No restriction

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



Multi-Layer Perceptron (MLP)

- 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



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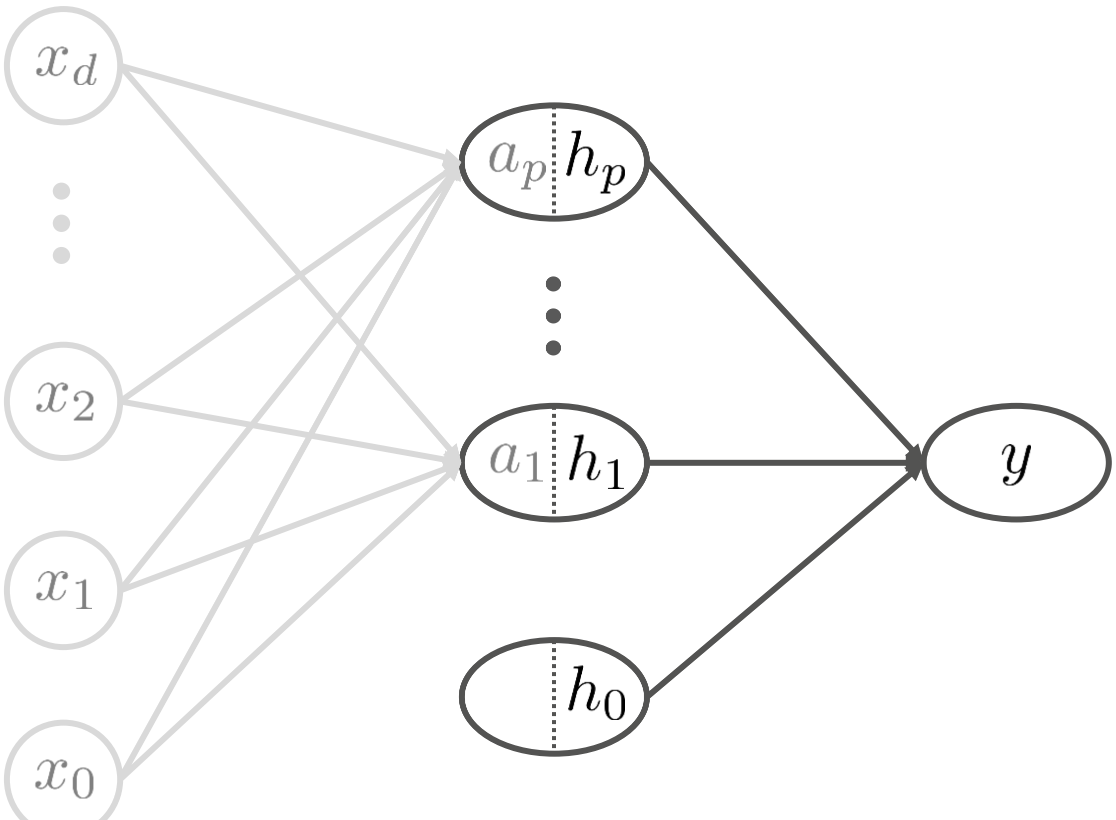

$$y = \sum_{i=0}^{p} w_p^{(2)} h_p$$

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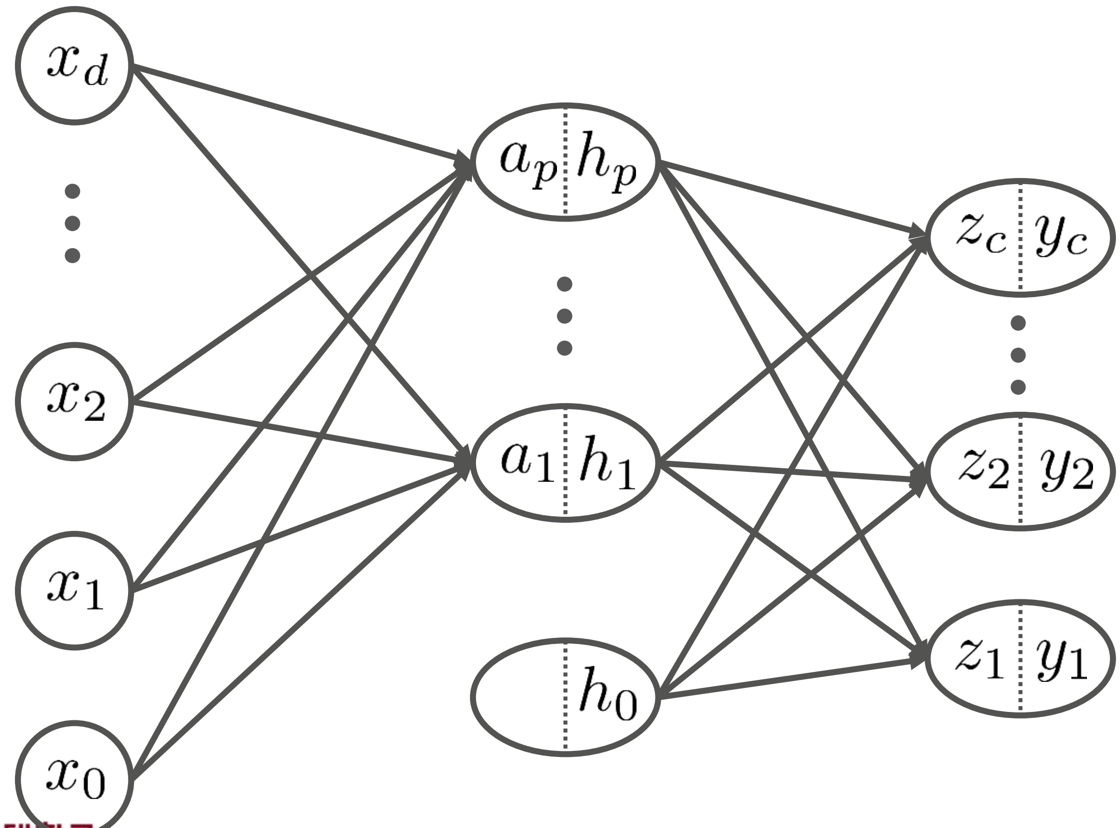


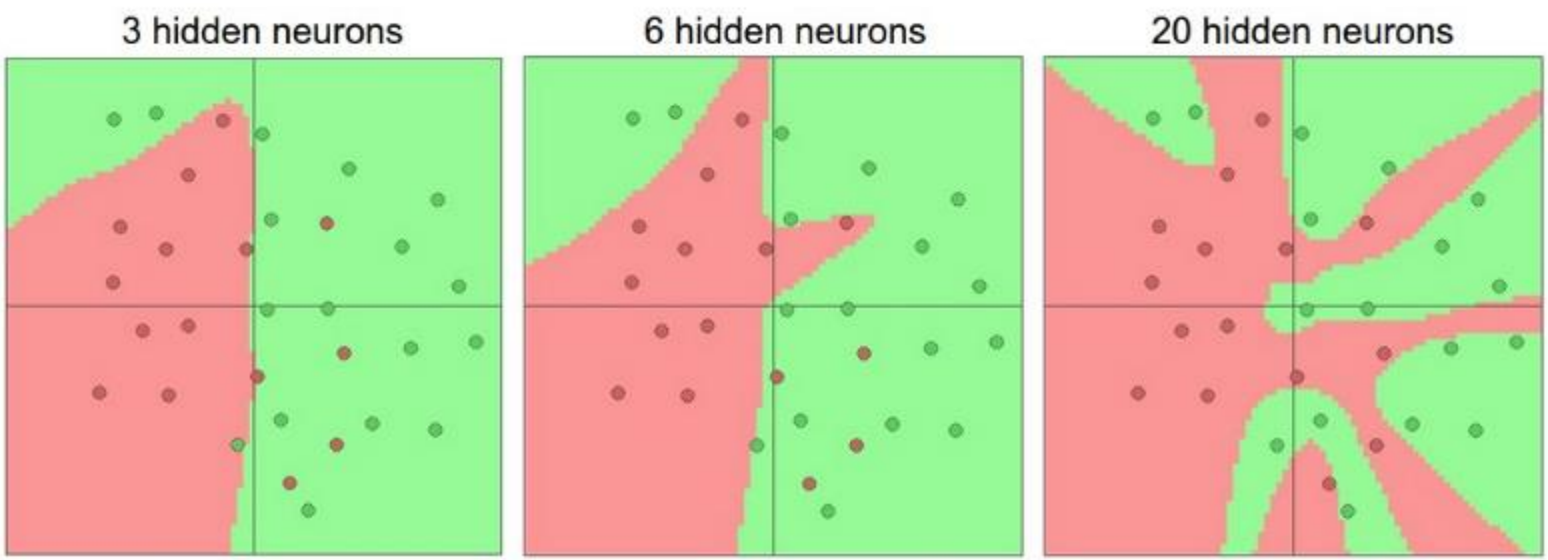
$$z_j = \sum_{i=0}^{p} w_{jp}^{(2)} h_p$$

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

각 출력 노드의 출력값을 해당 범주에
속하는 확률로 해석할 수 있음

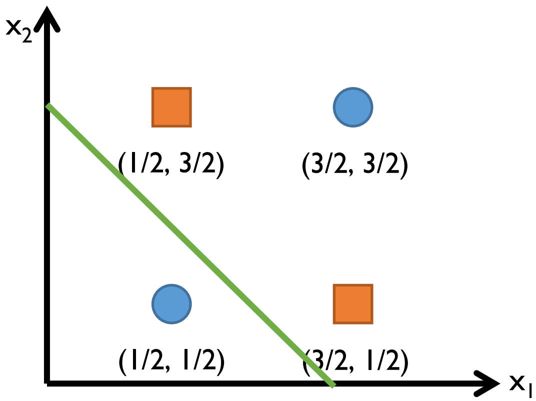
Multi-Layer Perceptron (MLP)

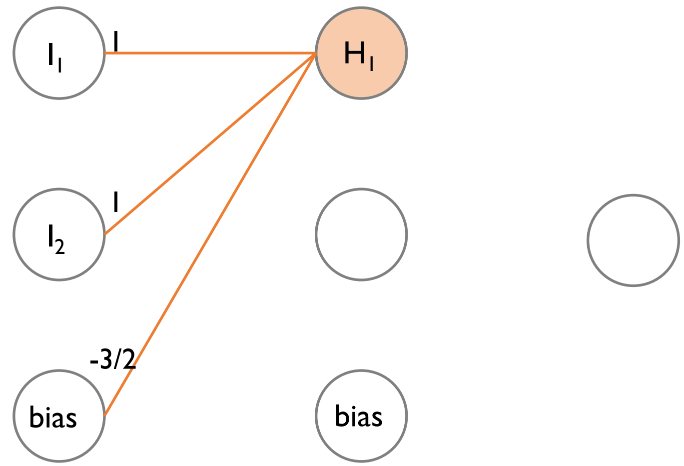
- The role of hidden nodes
  - ✓ Determines the complexity of ANN
  - ✓ If we use more number of hidden nodes, we can find a more sophisticated decision boundary (classification) or an arbitrary shape of function (regression)



Multi-Layer Perceptron (MLP)

- XOR problem revisited





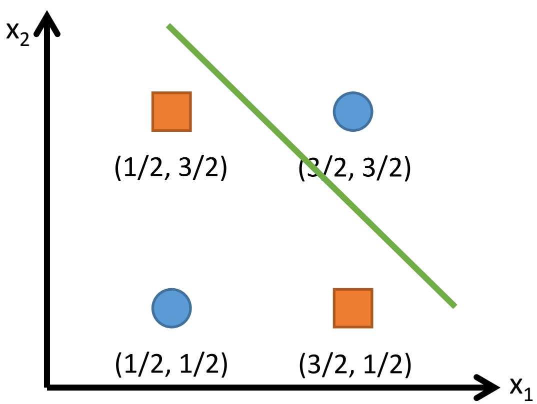
$$a_1 = x_1 + x_2 - \frac{3}{2}$$

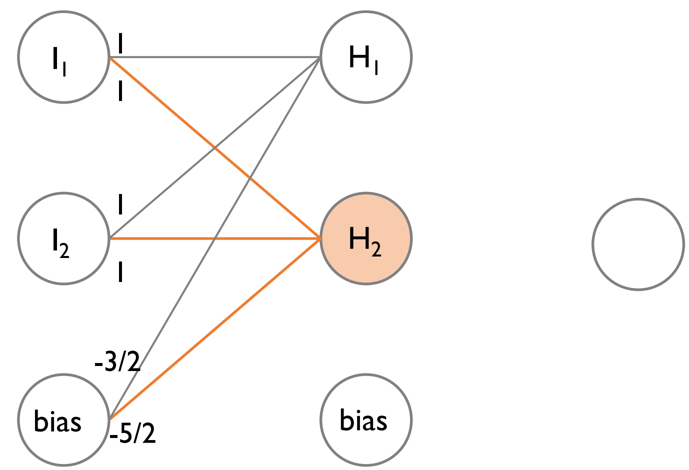
$$h_1 = g(a_1) = \begin{cases} 1 & \text{if} \quad a_1 \geq 0 \\ -1 & \text{if} \quad a_1 < 0 \end{cases}$$

x_1	x_2	a_1	h_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

Multi-Layer Perceptron (MLP)

- XOR problem revisited (cont')





$$a_2 = x_1 + x_2 - \frac{5}{2}$$

$$h_2 = g(a_2) = \begin{cases} 1 & \text{if} \quad a_2 \geq 0 \\ -1 & \text{if} \quad a_2 < 0 \end{cases}$$

x_1	x_2	a_2	h_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

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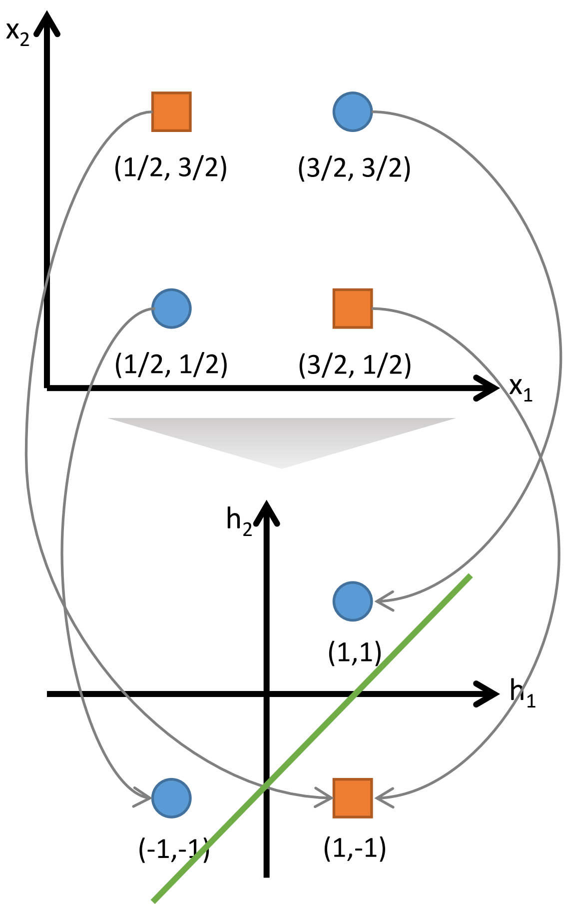
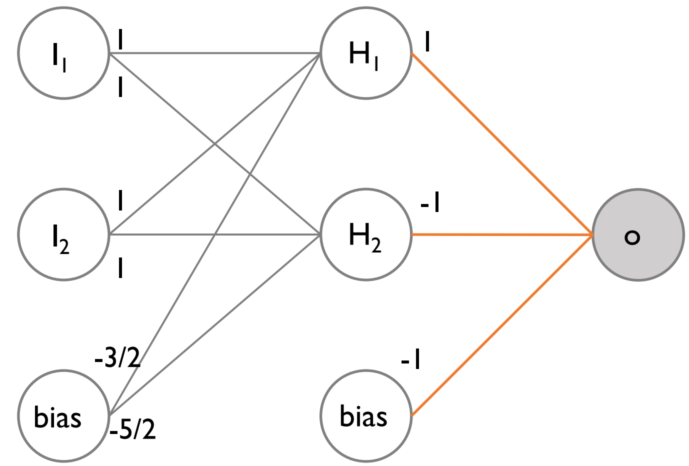
Multi-Layer Perceptron (MLP)

- XOR problem revisited (cont')





x_1	x_2	a_1	h_1	a_2	h_2	o	y
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

$$o = h_1 + h_2 - 1 \qquad y = g(o) = \begin{cases} 1 & \text{if} \quad o \geq 0 \\ -1 & \text{if} \quad o < 0 \end{cases}$$

Multi-Layer Perceptron (MLP)

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

$$a_j = \sum_{i=0}^{d} w_{ji}^{(1)} x_i, \quad h_j = g(a_j) = \frac{1}{1 + \exp(-a_j)}$$

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

$$y = \sum_{j=0}^{p} w_j^{(2)} h_j$$

  - ✓ The final outcome of the neural network:

$$y = \sum_{j=0}^{p} w_j^{(2)} \cdot g(\sum_{i=0}^{d} w_{ji}^{(1)} x_i)$$

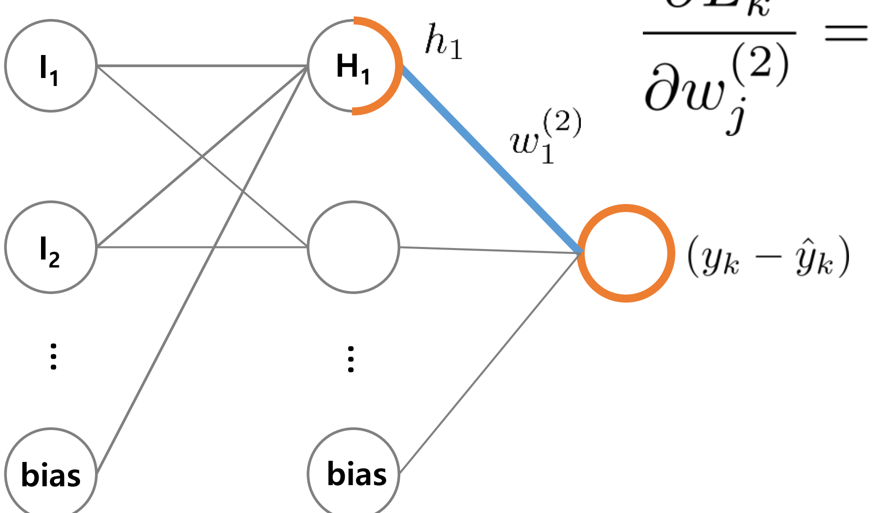
Multi-Layer Perceptron (MLP)

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

$$L_k = \frac{1}{2}(y_k - \hat{y}_k)^2 \quad , \quad y_k = \sum_{j=0}^{p} w_j^{(2)} \cdot g(\sum_{i=0}^{d} w_{ji}^{(1)} \mathbf{x}_{ki})$$

  - ✓ The weight $w_j^{(2)}$ which connects the jth hidden node and the output node will be updated by

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

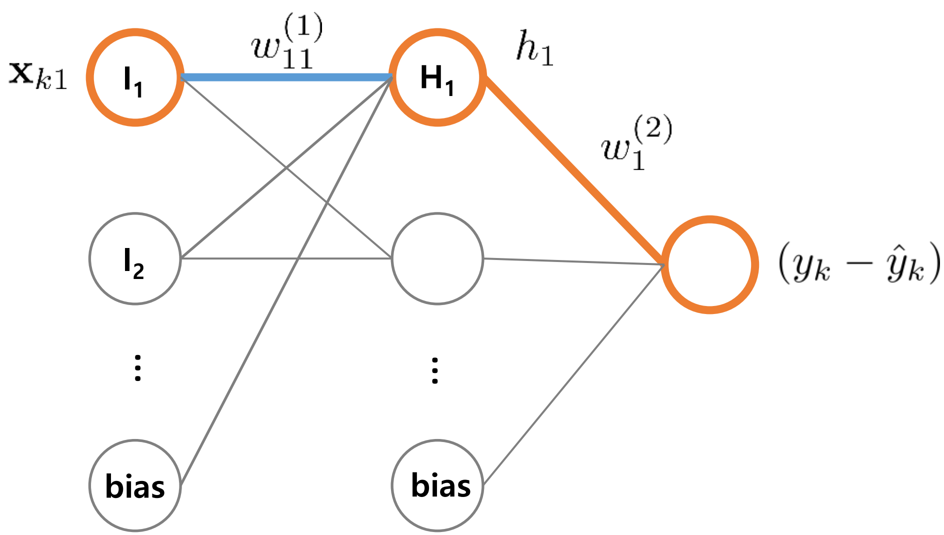


Multi-Layer Perceptron (MLP)

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

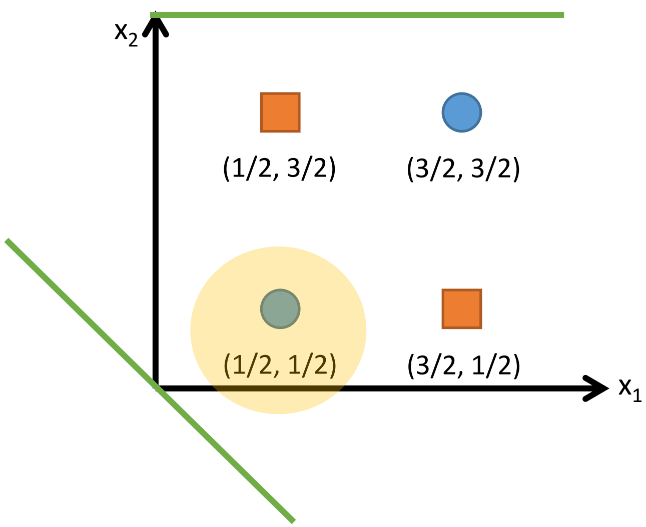
$$\frac{\partial L_k}{\partial w_{ji}^{(1)}} = \frac{\partial L_k}{\partial y_k} \cdot \frac{\partial y_k}{\partial w_j^{(2)}} \cdot \frac{\partial h_j}{\partial a_j} \cdot \frac{\partial a_j}{\partial w_{ji}^{(1)}}$$

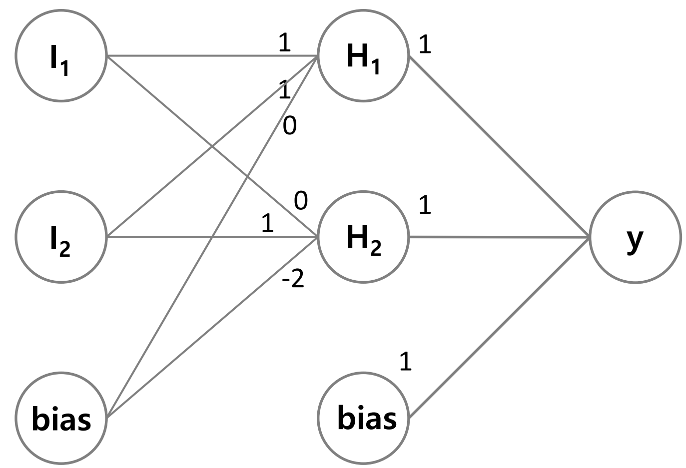
$$= (y_k - \hat{y}_k) \cdot w_j^{(2)} \cdot a_j \cdot (1 - a_j) \cdot \mathbf{x}_{ki}$$



MLP: Training

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





$$a_1 = \sum w_{1i}^{(1)} x_i = 1 \times 0.5 + 1 \times 0.5 + 0 \times 1 = 1$$

$$h_1 = \frac{1}{1 + \exp(1)} = 0.269$$

$$a_2 = \sum w_{2i}^{(1)} x_i = 0 \times 0.5 + 1 \times 0.5 + (-2) \times 1 = -1.5$$

$$h_2 = \frac{1}{1 + \exp(-1.5)} = 0.818$$

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

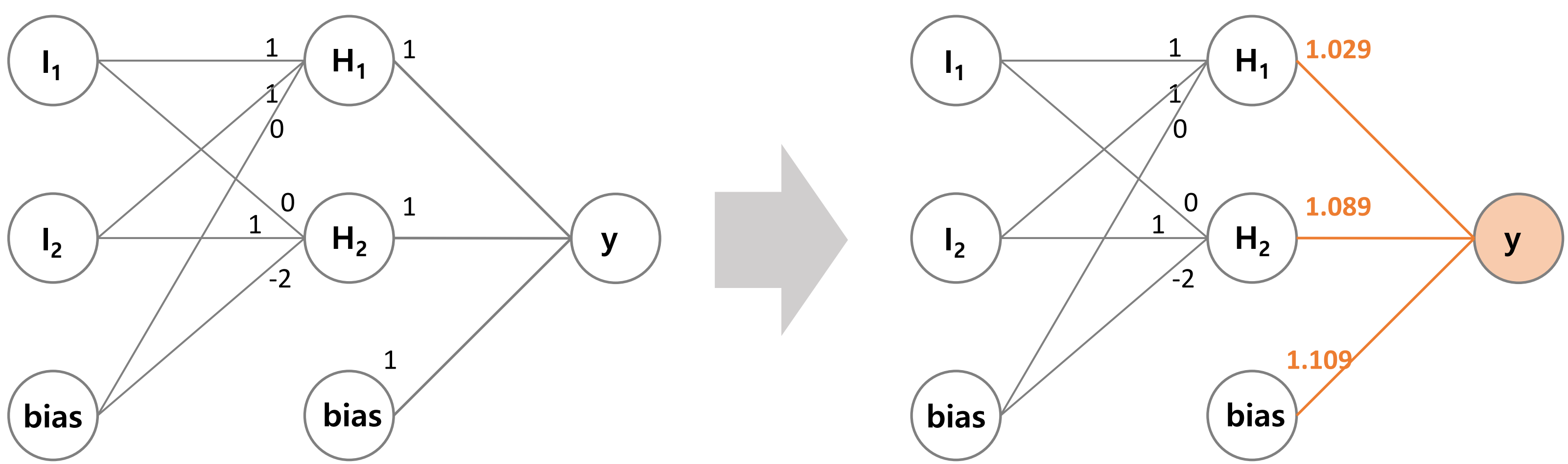
MLP: Training

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

$$w_1^{(2)}(new) = w_1^{(2)}(old) - \eta \times (y - \hat{y}) \times h_1 = 1 - 0.1 \times (1 - 2.087) \times 0.269 = 1.029$$

$$w_2^{(2)}(new) = w_2^{(2)}(old) - \eta \times (y - \hat{y}) \times h_2 = 1 - 0.1 \times (1 - 2.087) \times 0.818 = 1.089$$

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



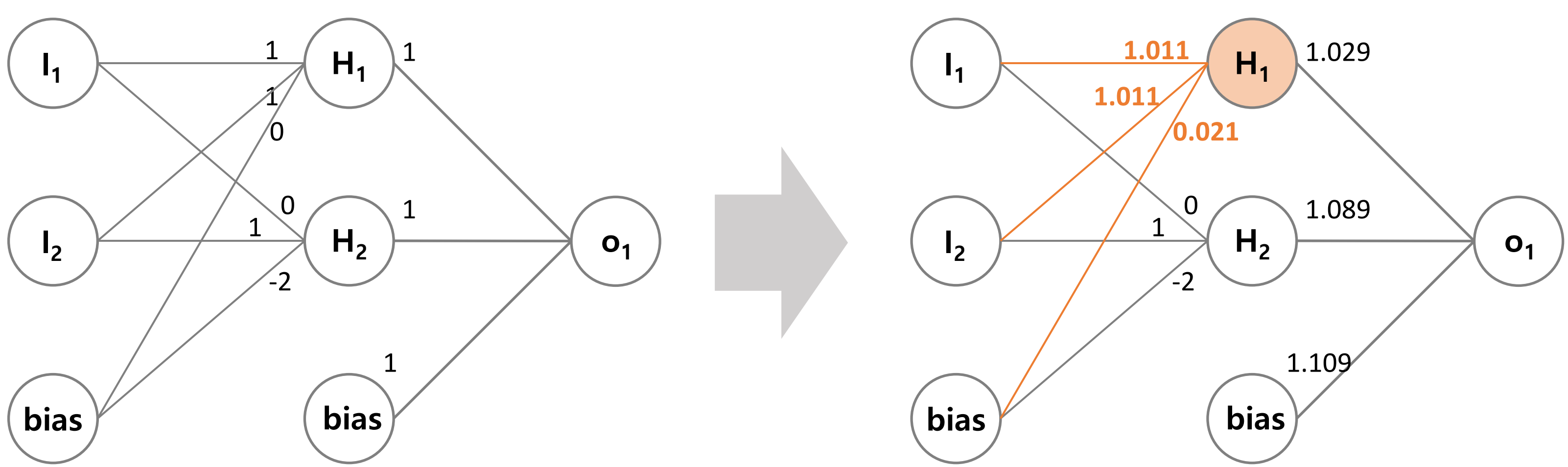
MLP: Training

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

$$w_{11}^{(1)}(new) = w_{11}^{(1)}(old) - \eta \times (y - \hat{y}) \times w_1^{(2)} \times h_1 \times (1 - h_1) \times x_1 = 1.011$$

$$w_{12}^{(1)}(new) = w_{12}^{(1)}(old) - \eta \times (y - \hat{y}) \times w_1^{(2)} \times h_1 \times (1 - h_1) \times x_2 = 1.011$$

$$w_{10}^{(1)}(new) = w_{10}^{(1)}(old) - \eta \times (y - \hat{y}) \times w_1^{(2)} \times h_1 \times (1 - h_1) \times b^{(1)} = 0.021$$



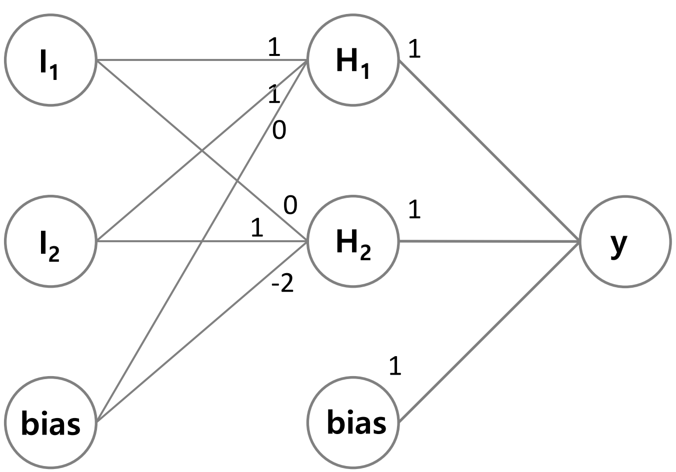
MLP: Training

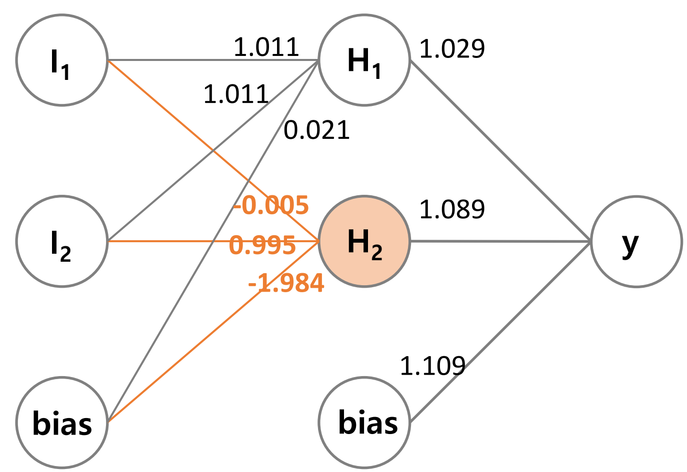
- Error Back-Propagation: Example
  - ✓ Update the weights between the H_1 and the input nodes

$$w_{21}^{(1)}(new) = w_{21}^{(1)}(old) - \eta \times (y - \hat{y}) \times w_2^{(2)} \times h_2 \times (1 - h_2) \times x_1 = -0.005$$

$$w_{22}^{(1)}(new) = w_{22}^{(1)}(old) - \eta \times (y - \hat{y}) \times w_2^{(2)} \times h_2 \times (1 - h_2) \times x_2 = 0.995$$

$$w_{20}^{(1)}(new) = w_{20}^{(1)}(old) - \eta \times (y - \hat{y}) \times w_2^{(2)} \times h_2 \times (1 - h_2) \times b^{(1)} = -1.984$$





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

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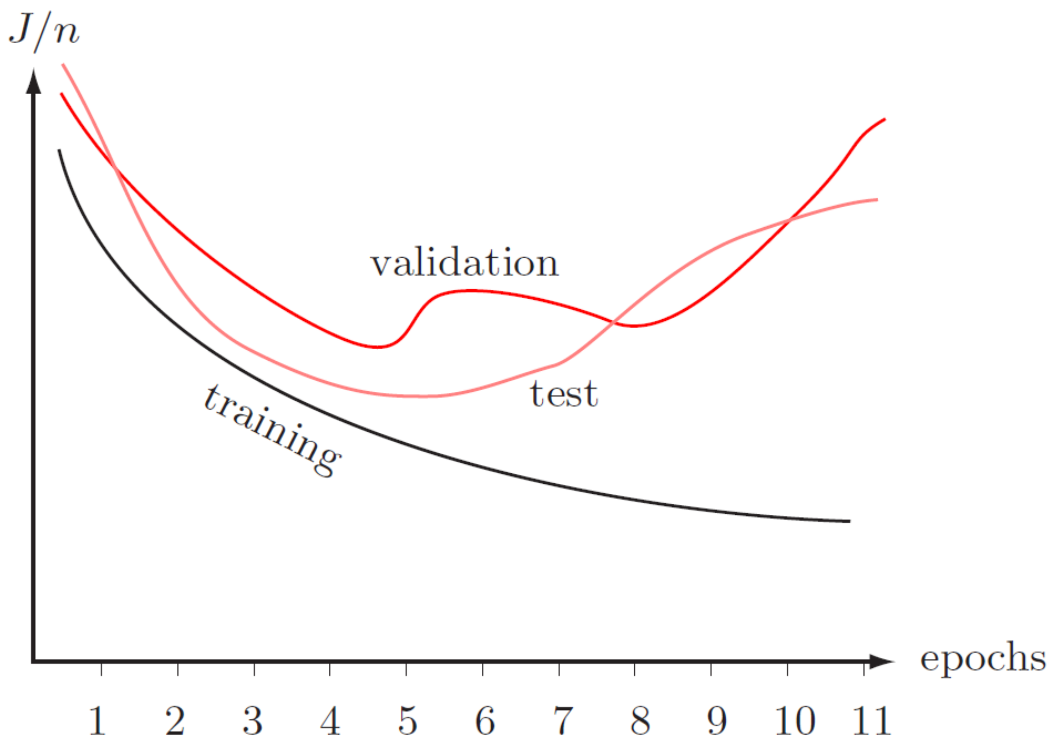
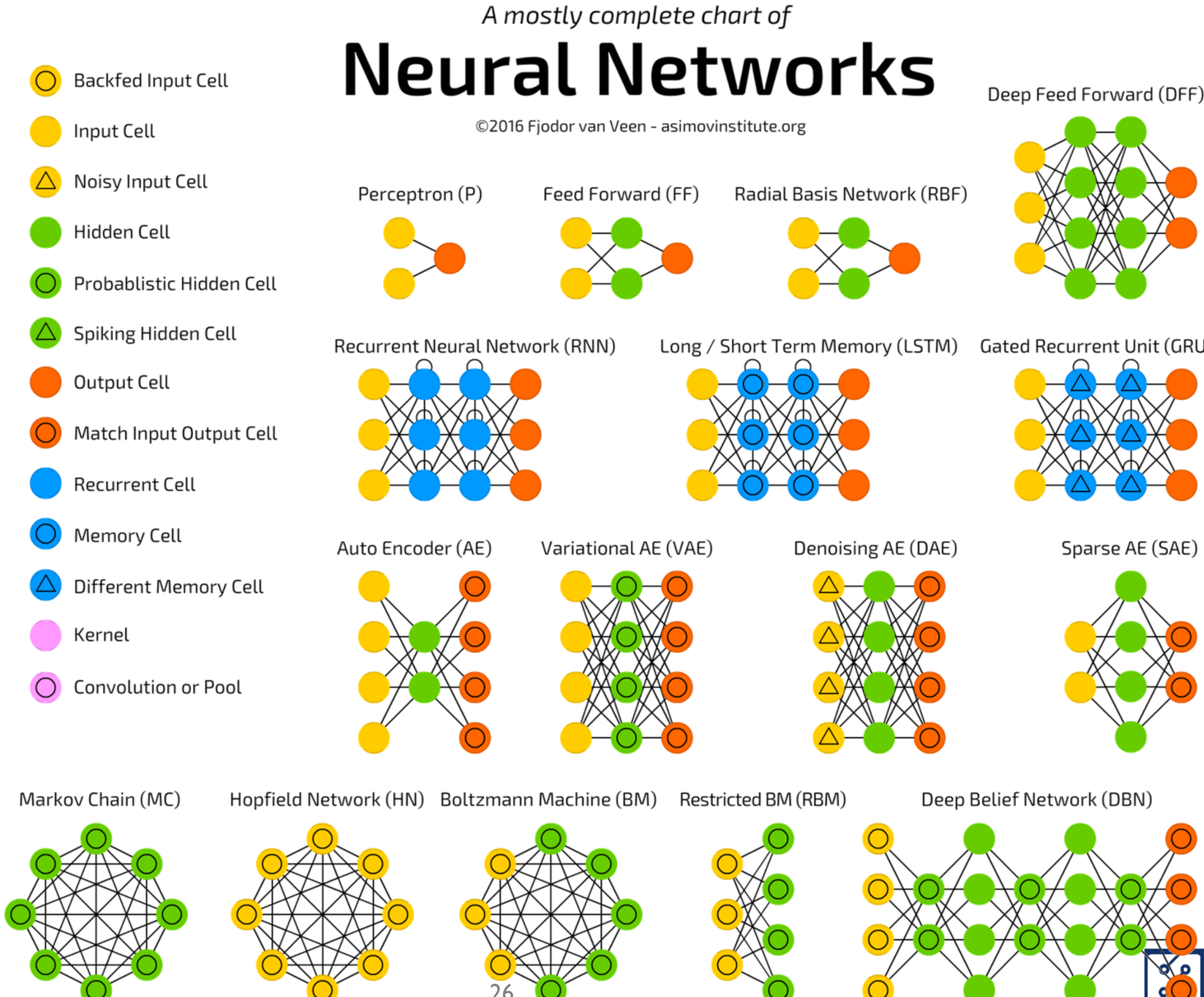
MLP: Training

- 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.



Multi-Layer Perceptron (MLP)

- Various Structure of Artificial Neural Networks



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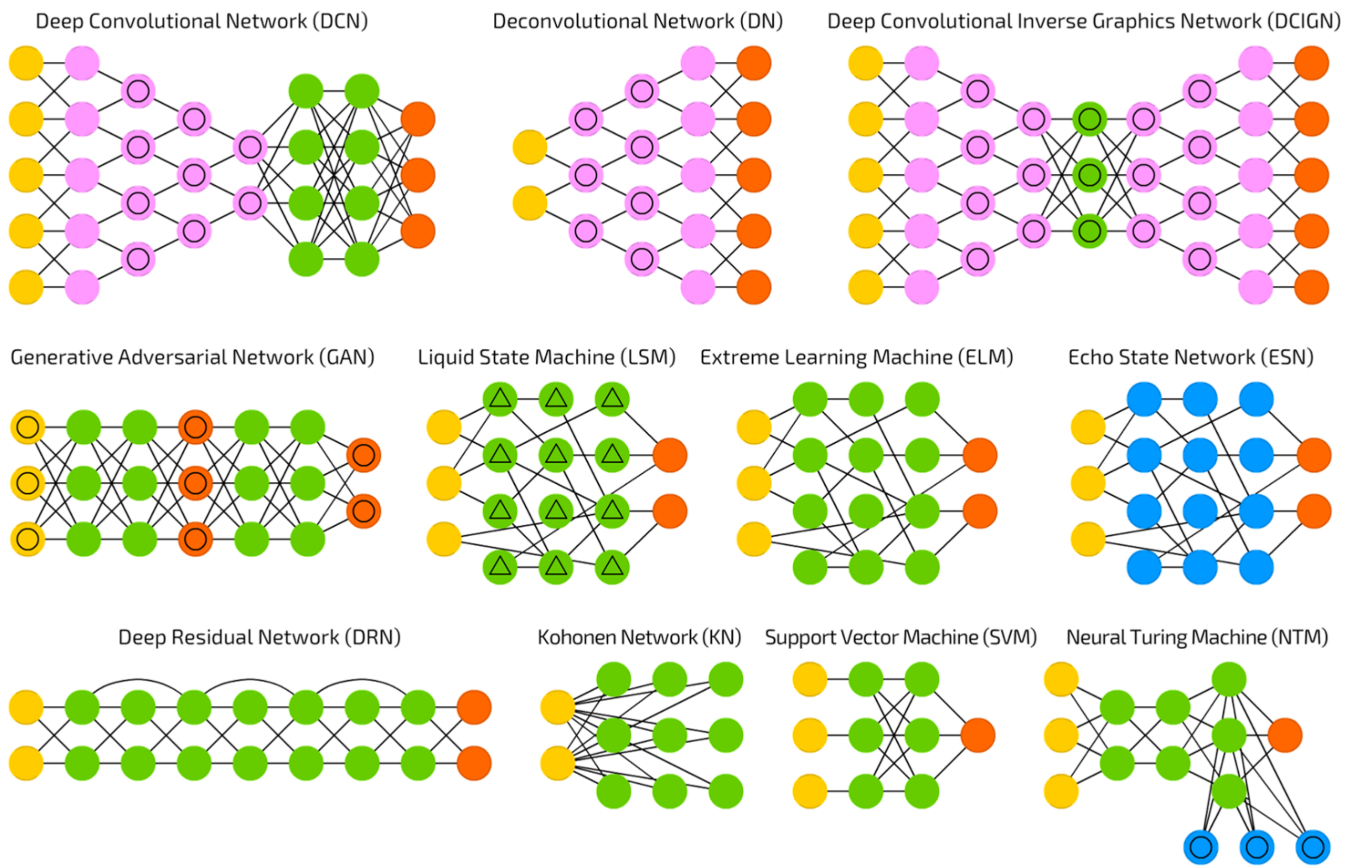

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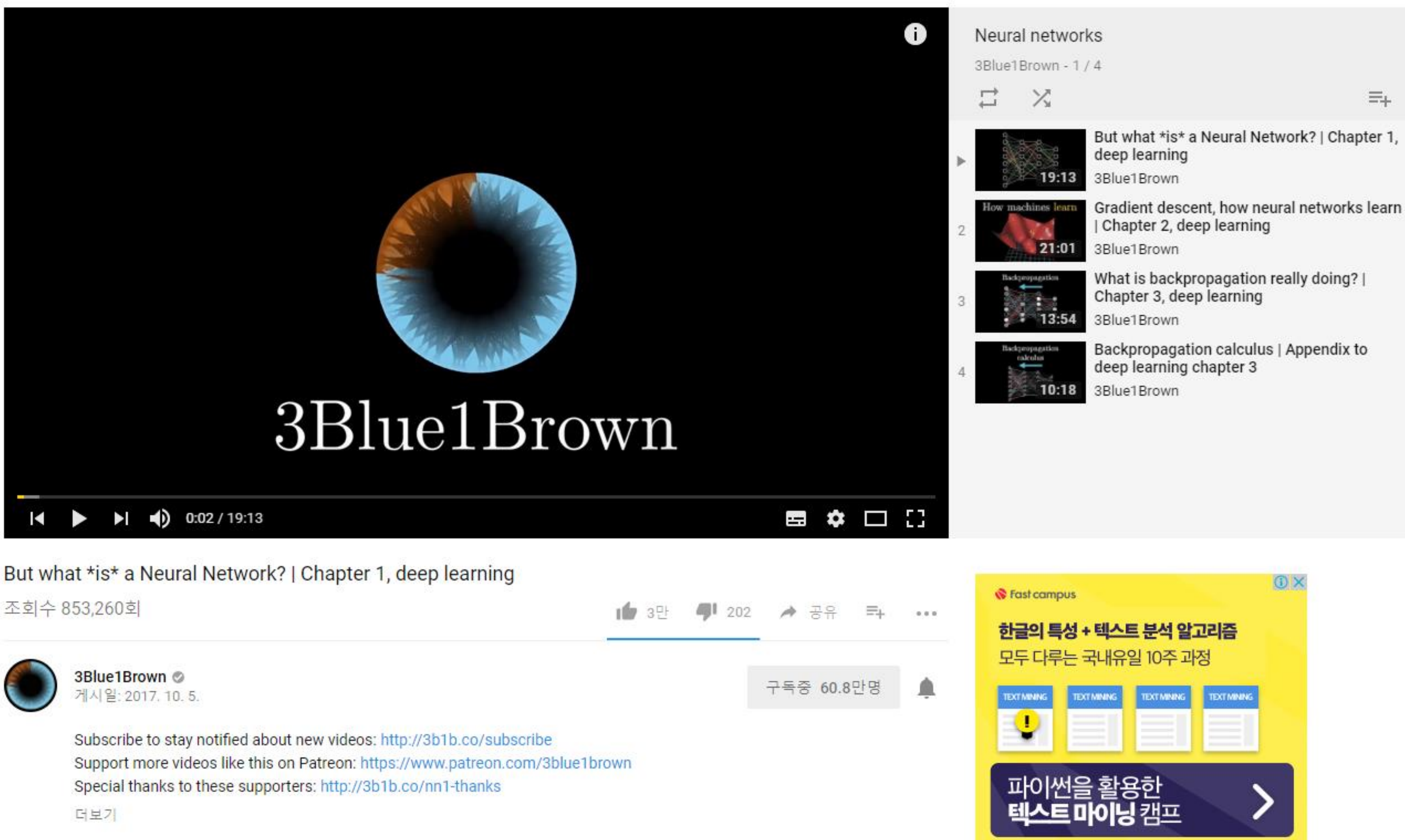
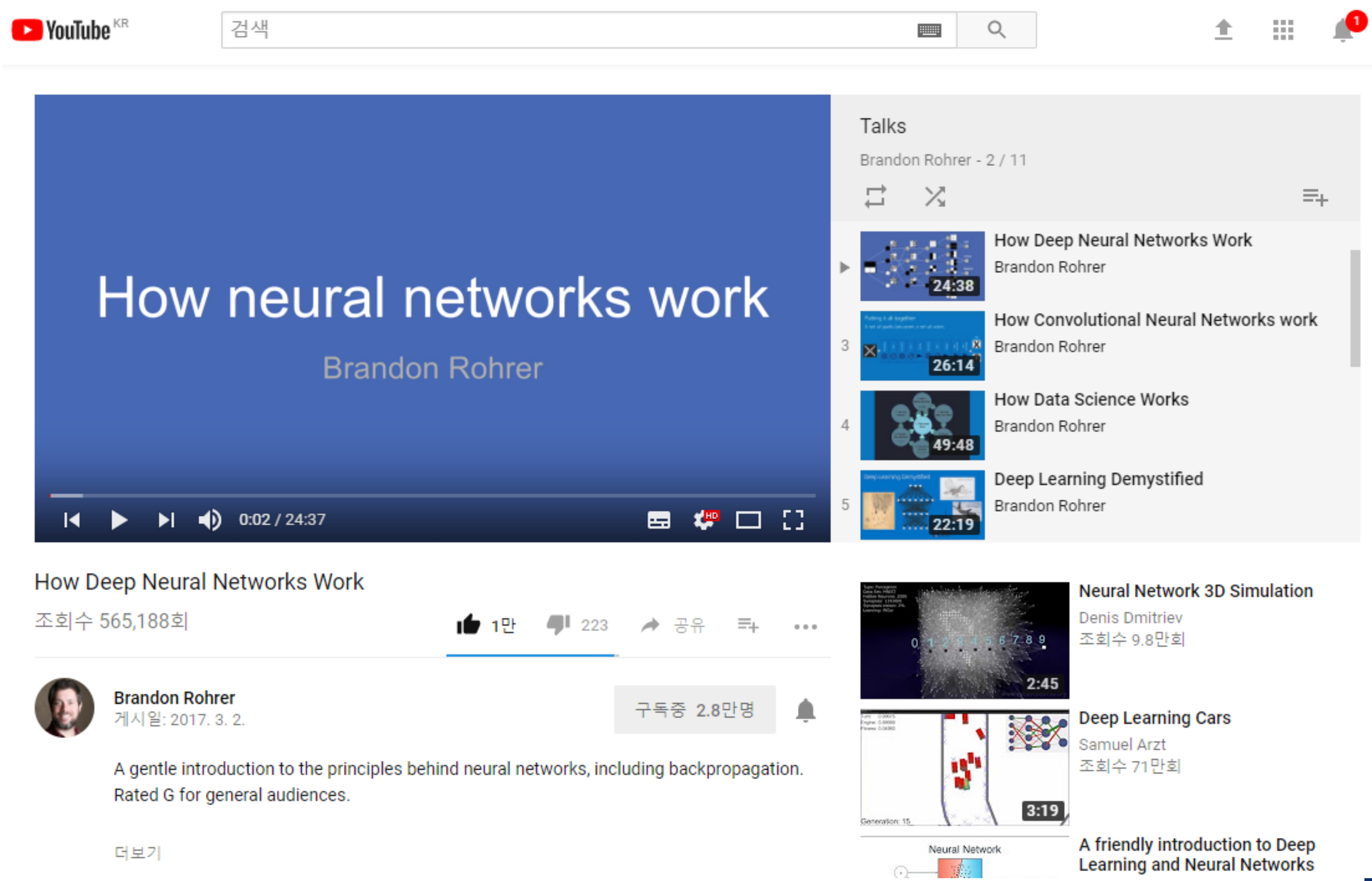
Recommended Video Lectures

- 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



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ANY
questions?