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Section 6. 경사 하강 심화 이론 (Advanced Topics in Gradient Descent)

목차

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Recap from Section 5.
Gradient Descent의 기본 개념

Recap

Section 5. Gradient Descent의 기본 개념

Gradient Descent

역할: **손실 함수의 값이 최소화**하도록 **모델의 weight을 최적화하는 것**

원리:

- **경사는 손실함수가 증가하는 방향을 향한다.**
- **따라서 경사하강은 경사의 음의 방향**으로 모델의 weight을 update해주는 것이다!

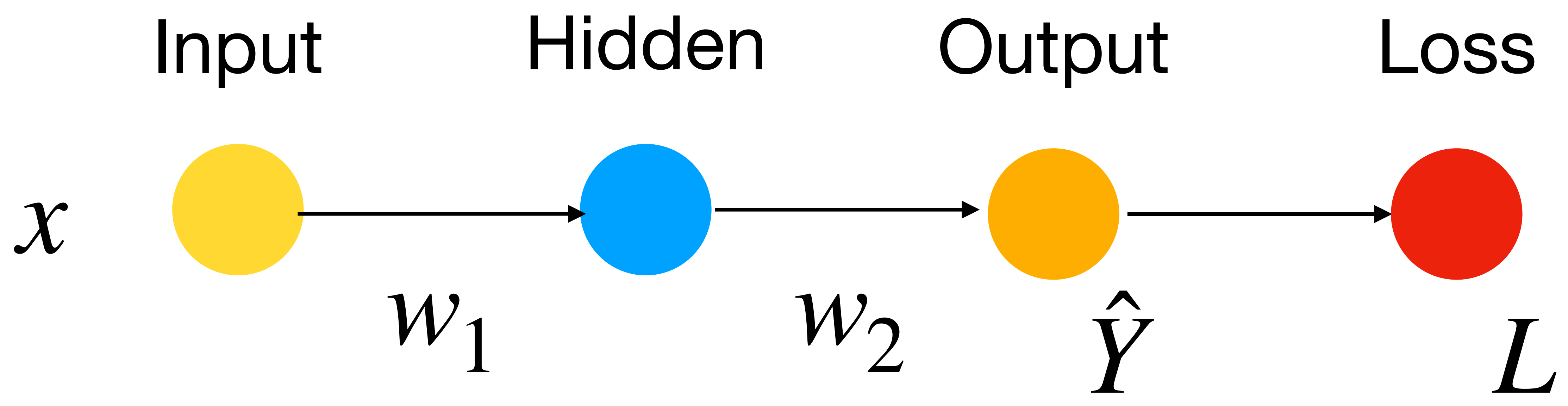
$$w \rightarrow w - \lambda \cdot \frac{dL}{dw}$$

Recap

Section 5. Gradient Descent의 기본 개념

- 하지만 이것은 variable이 하나인 (single variate input)의 간단한 예시였다.

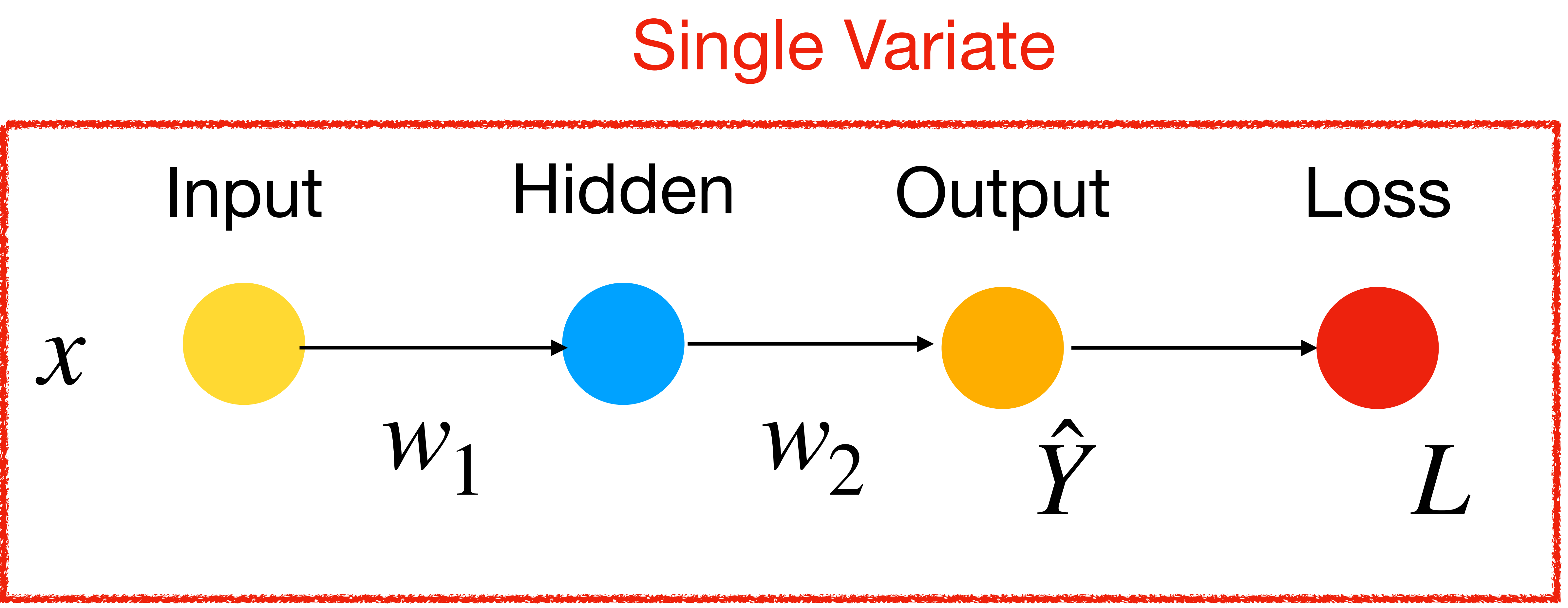
$$w \rightarrow w - \lambda \cdot \frac{dL}{dw}$$

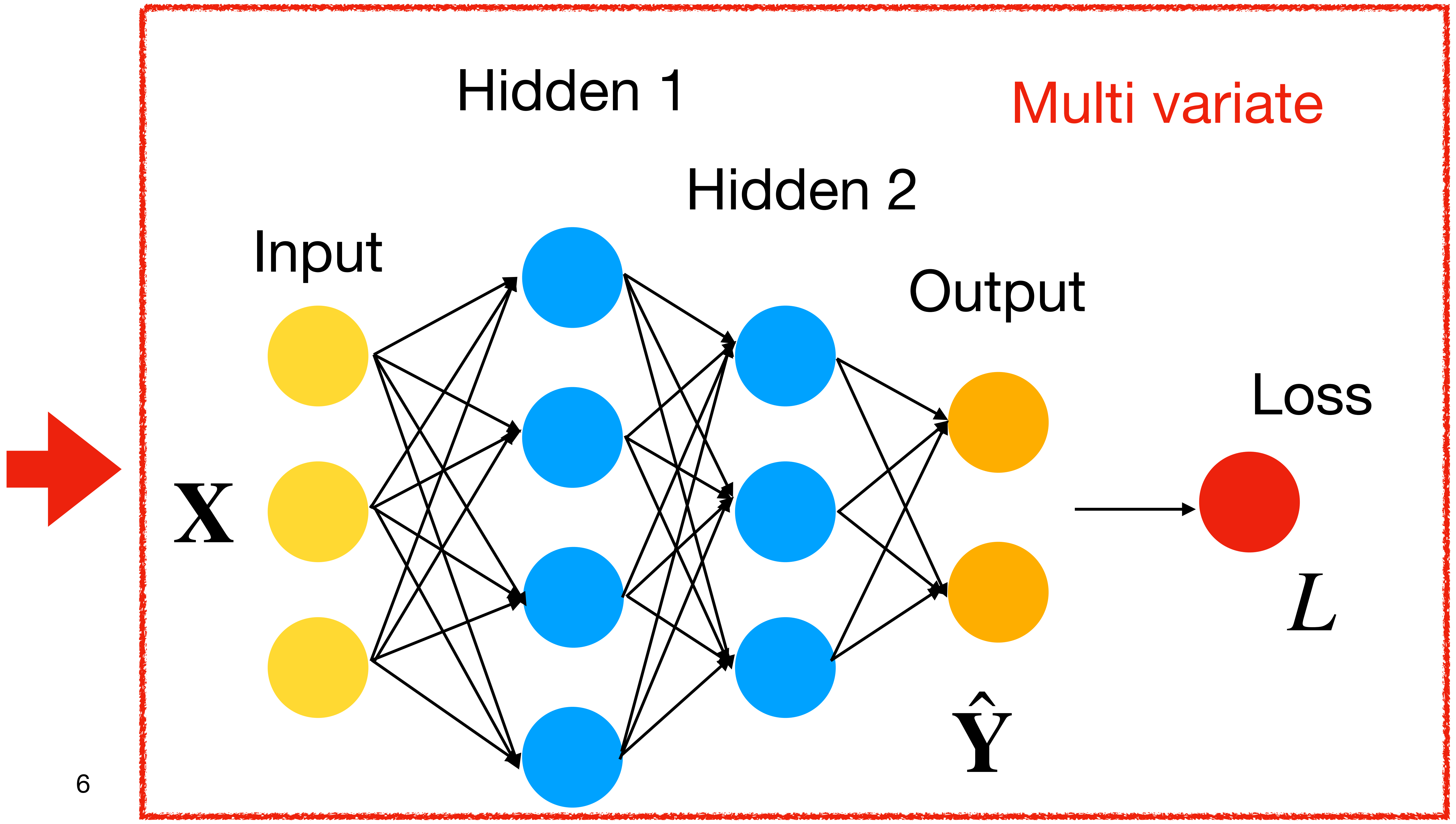


Recap

Extending from single variate to multi-variate

- 하지만 Input feature가 여러 개 (multi-variate)하거나 Hidden layer가 여러개의 neuron들로 구성되어 있으면 어떻게 할 것인가?

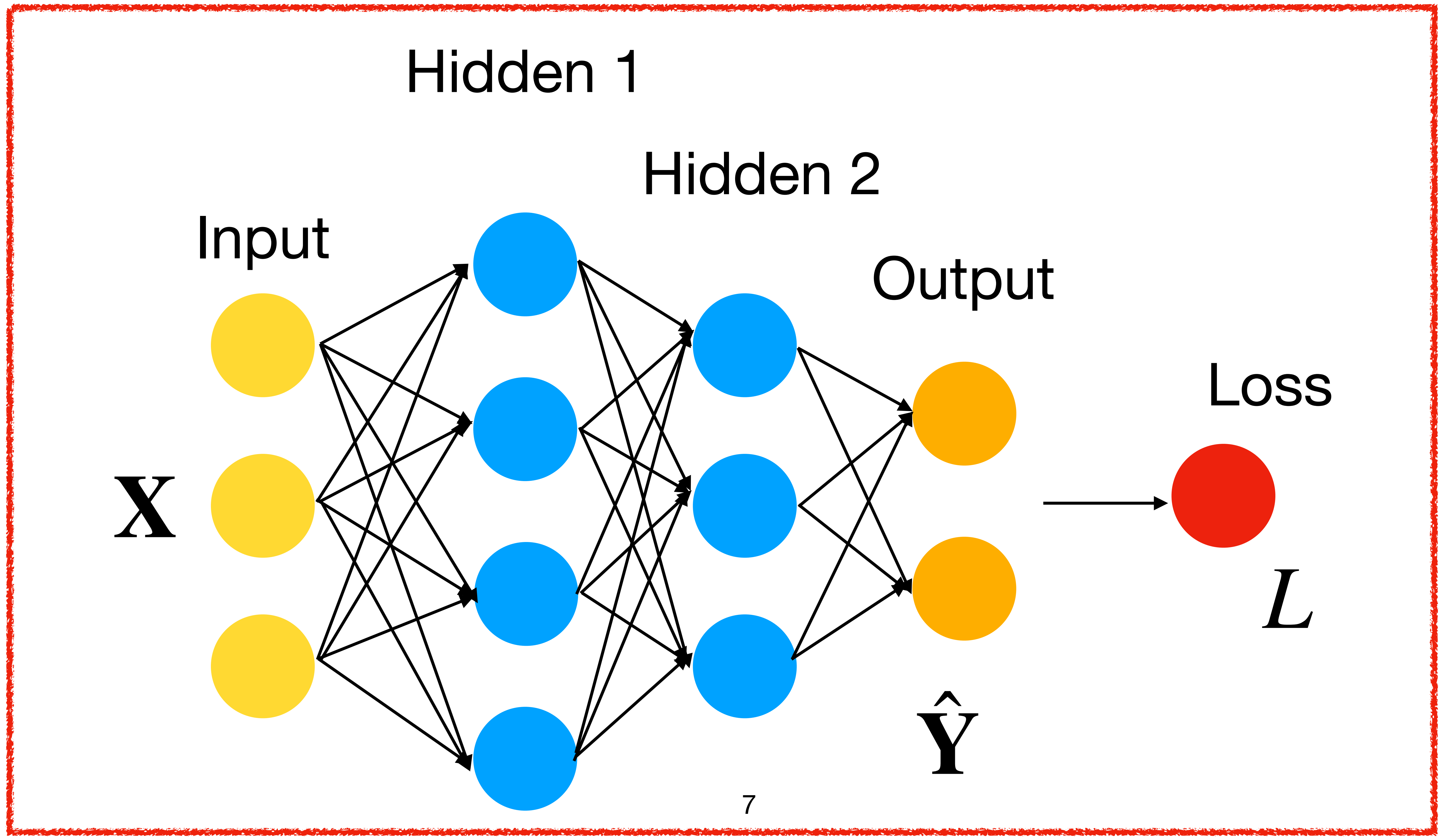




Recap

Extending from single variate to multi-variate

- 이번 시간에는 아래와 같은 Multi-variate의 경우에 대해서 살펴보자!



Multi variate

6-1. Multi-variate Multi neuron Neural Network

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Objective

학습 목표

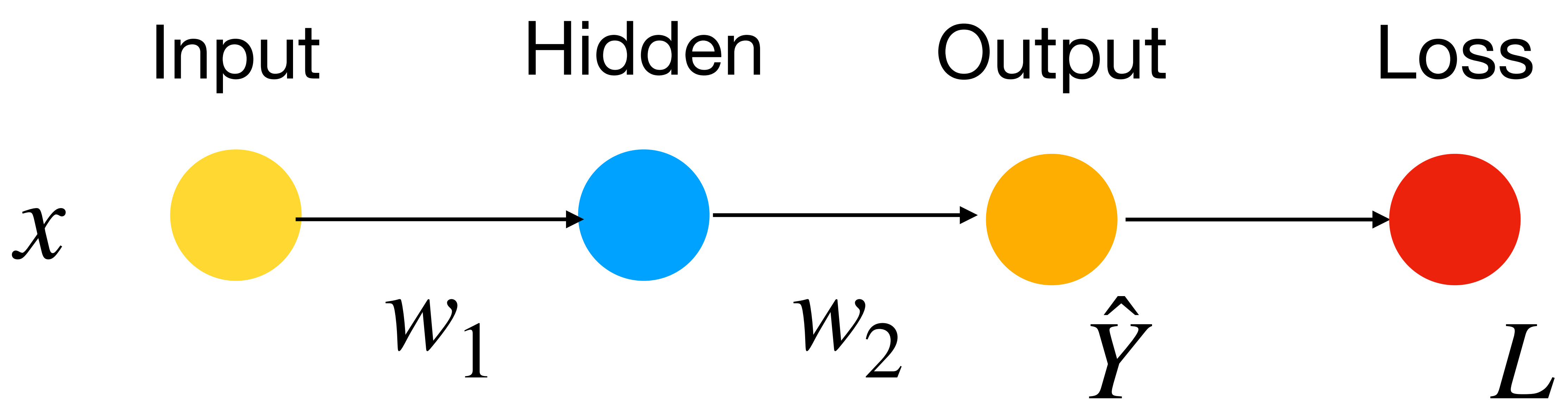
- Scalar input, single neuron으로 구성된 Neural Network을 Multi variate, Multi neuron으로 확장하기

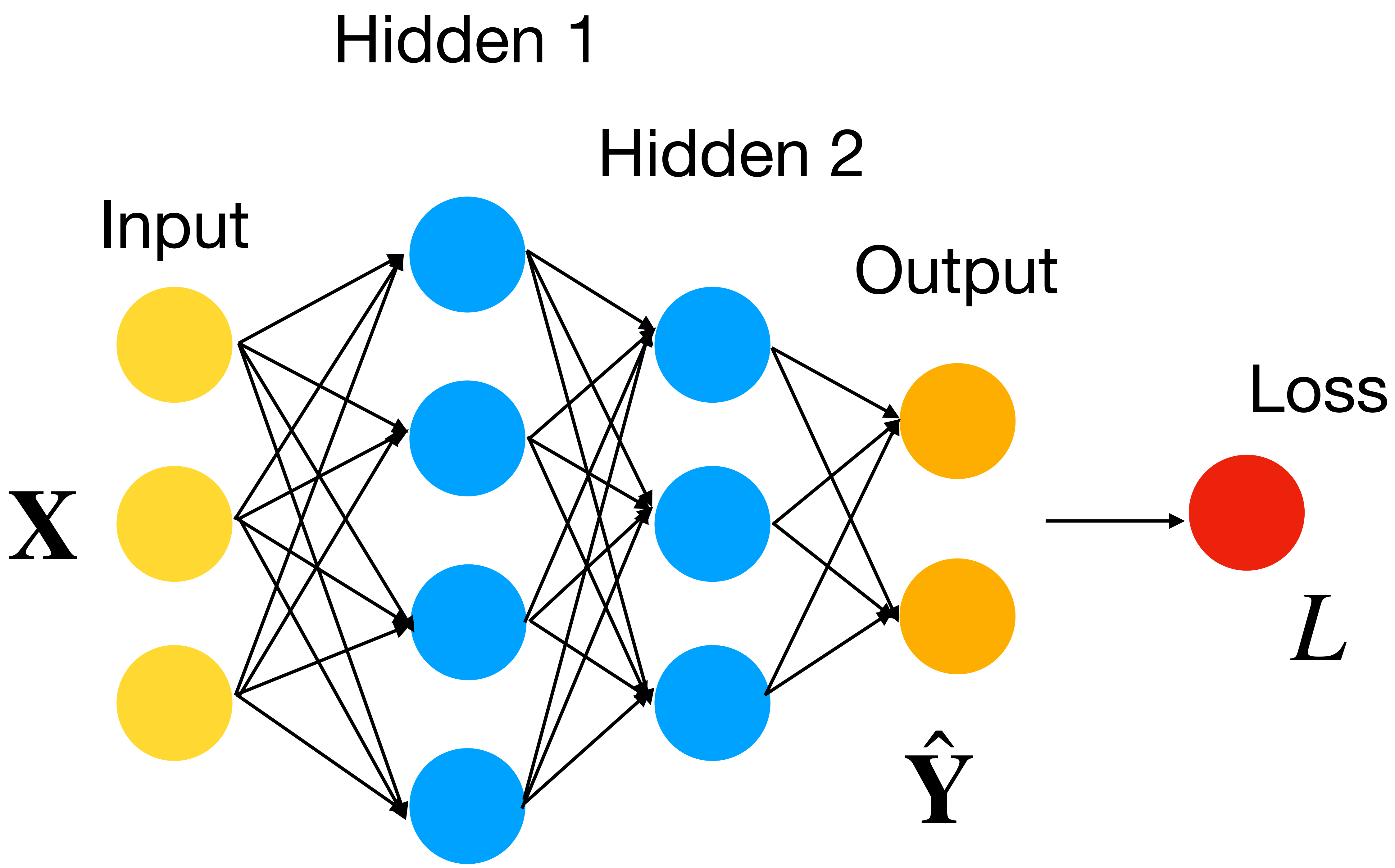
- Neural Network의 forward pass을 행렬의 곱으로 표현하기

Multi-variate Multi-neuron NN

- **여러 개의 뉴론들** $W \in \mathbb{R}^{M \times D}$로 구성된 **Layer들이 여러 개 쌓여**있고,
- **입력값이 다차원의 vector** $\mathbf{x} \in \mathbb{R}^{D}$

앞에서 고려한 매우 단순한 뉴럴넷 예제





Multi-variate Multi-neuron NN

Multivariate Case

- 예를 들어 **ResNet-50의 경우 23 million (2300만개의 weight parameter)**들로 구성됨.
- 통상적으로 input도 scalar 값이 아니라 다차원의 vector이다. (**multivariate**)
- 어떻게 하면:

$$\boxed{x, w \in \mathbb{R}^1} \rightarrow \boxed{\mathbf{x} \in \mathbb{R}^D, W \in \mathbb{R}^{M \times D}}$$

scalar input
single neuron

Multi-variate
Multi-neuron

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Single Variable, Single Neuron Neural Network Forward Pass

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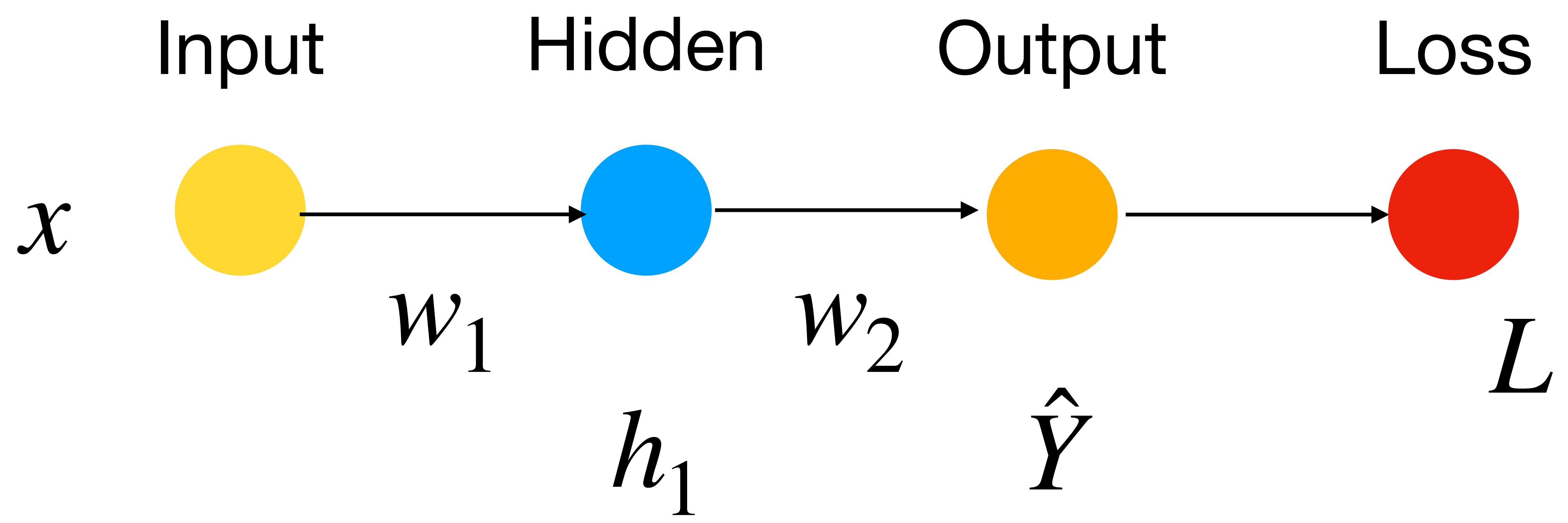
Multi-variate Multi-neuron NN

Single variate, Single Neuron의 경우

앞에서 고려한 매우 단순한 뉴럴넷 예제

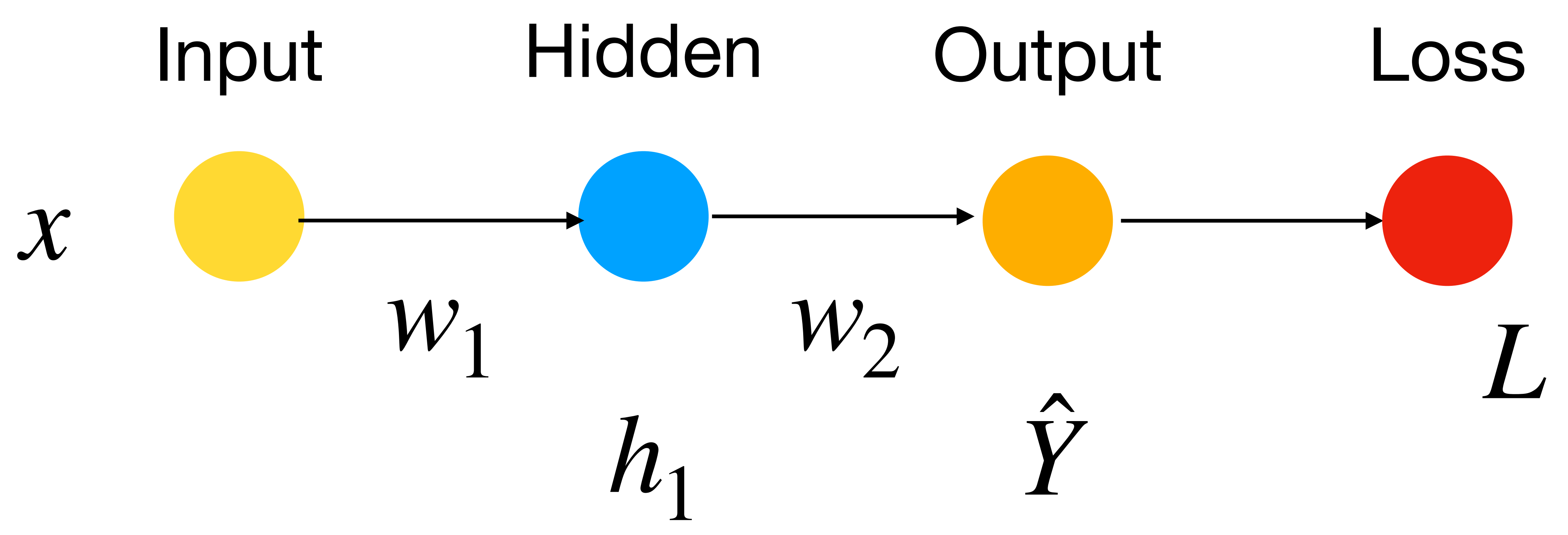


일단 편의상 Activation Function은 생략

Multi-variate Multi-neuron NN

Single variate, Single Neuron의 경우

앞에서 고려한 매우 단순한 뉴럴넷 예제



- Input → Hidden

$$h_1 = w_1 x$$

- Hidden → Output

$$\hat{Y} = w_2 h_1$$

- Output → Loss

$$L = L(Y, \hat{Y})$$

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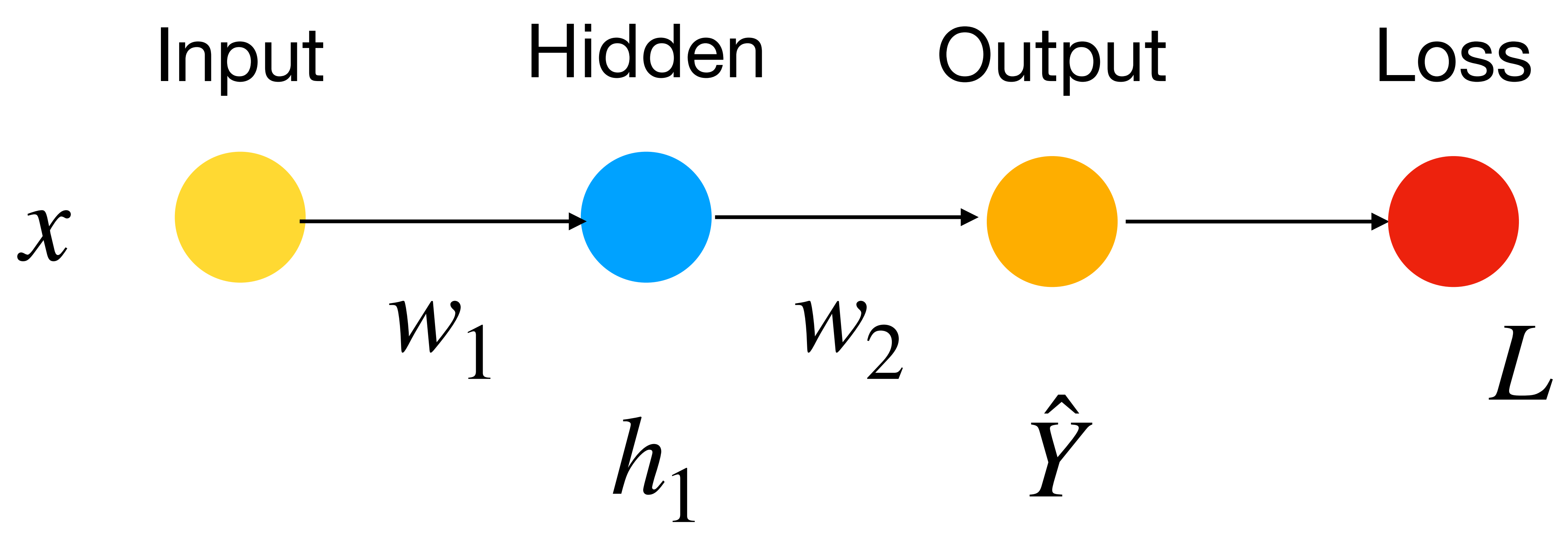
Multi-variate Multi-neuron NN

Single variate, Single Neuron의 경우

앞에서 고려한 매우 단순한 뉴럴넷 예제



- Input → Hidden

$$h_1 = w_1 x$$

- Hidden → Output

$$\hat{Y} = w_2 h_1$$

- Output → Loss

$$L = L(Y, \hat{Y})$$

단순히 scalar의 곱이다!

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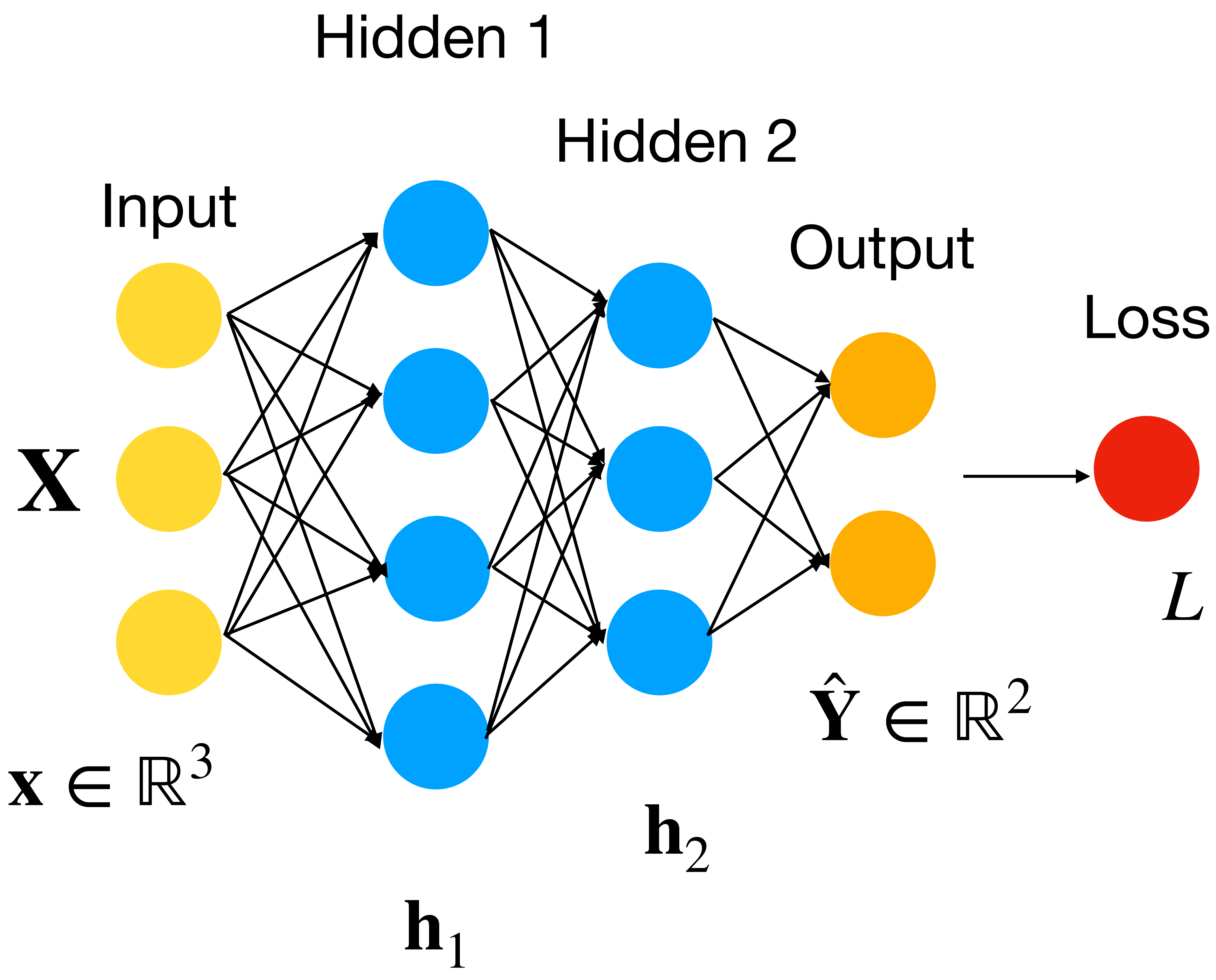
Multivariate Multi-Neuron Neural Network Forward Pass

Multi-variate Multi-neuron NN

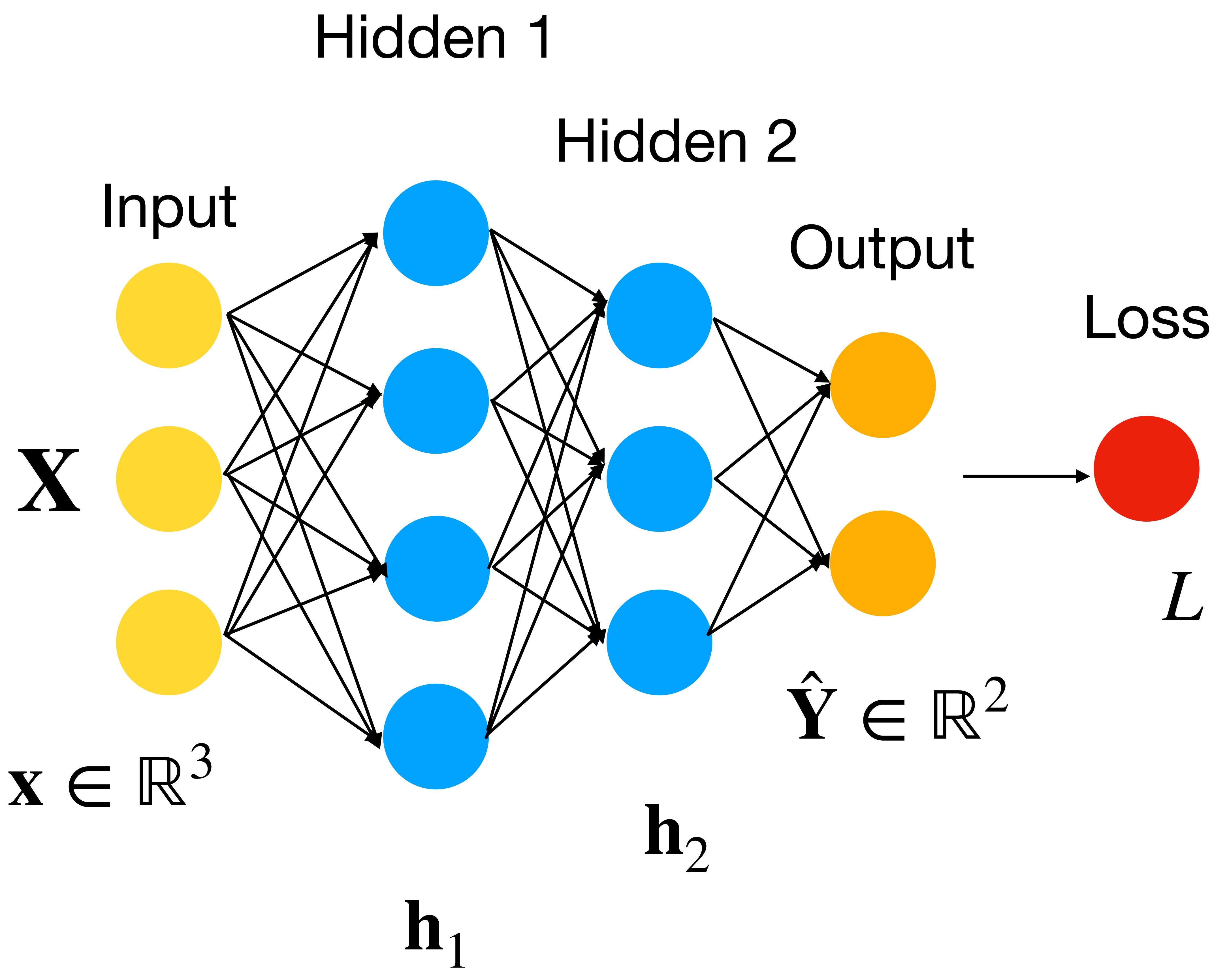
Multi variate, Multi Neuron의 경우



Multi-variate, Multi-neuron에 대해서는 forward pass을 어떻게 계산할까?

Multi-variate Multi-neuron NN

Multi variate, Multi Neuron의 경우



Multi-variate, Multi-neuron에 대해서는 forward pass을 어떻게 계산할까?

결론부터 먼저 말하면:

행렬의 곱 (Matrix Multiplication)

으로 표현할 수 있다!

왜 그렇게 되는지 살펴보자!

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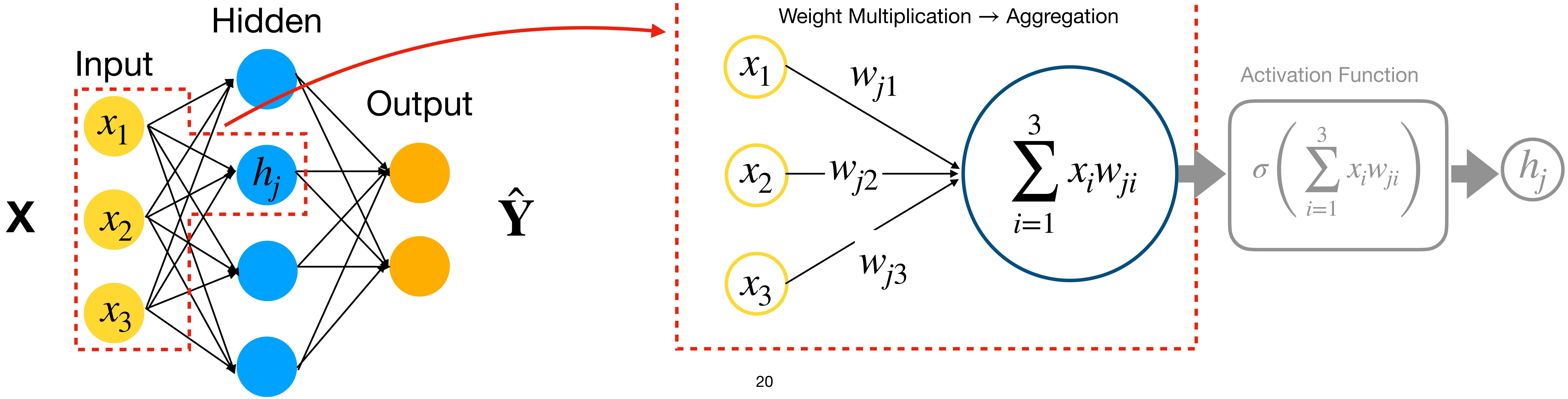
Recap from Section 2

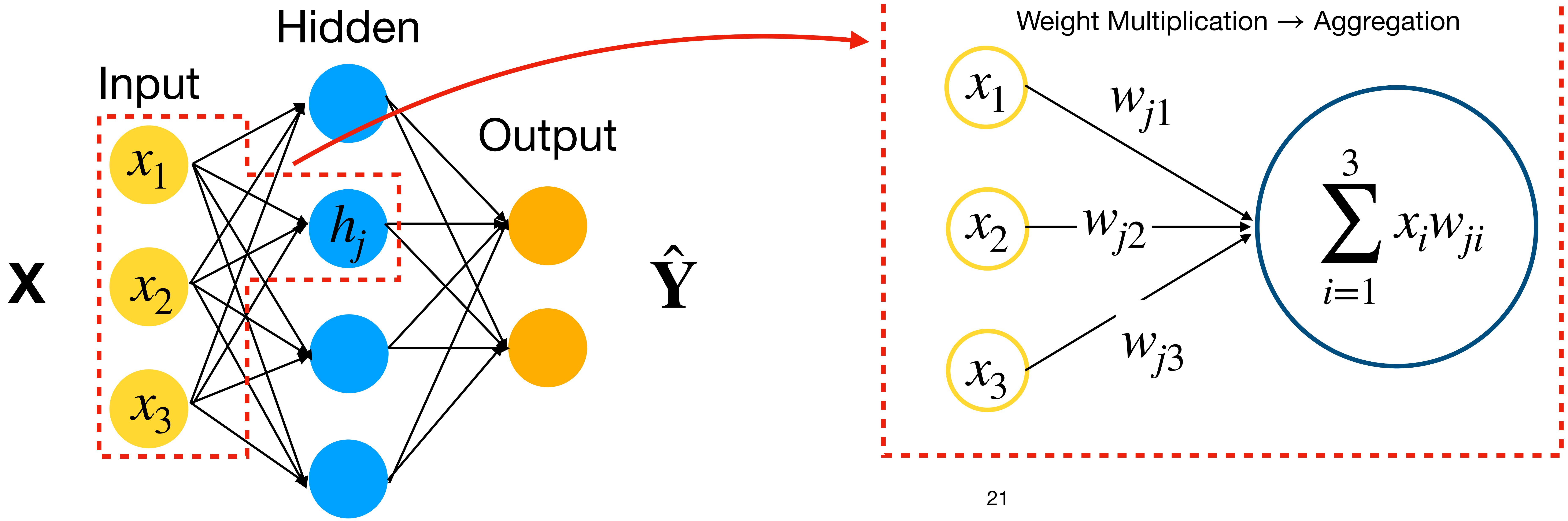
Recap from Section 2

- (일단 편의상 Activation Function에 대해서는 생략)
- $\sum_{i=1}^{3} x_i w_{ji}$: 이전 Layer의 출력값 x_i은 가중치 w_{ji} 에 곱해져서 합해진다. (weight multiplication → aggregation)



Recap from Section 2

- 참고로 w_{ji}에서
  - j 은 현재 Hidden layer에서 j 번째 뉴론을 의미
  - i 은 이전 layer에서 i 번째 뉴론을 의미

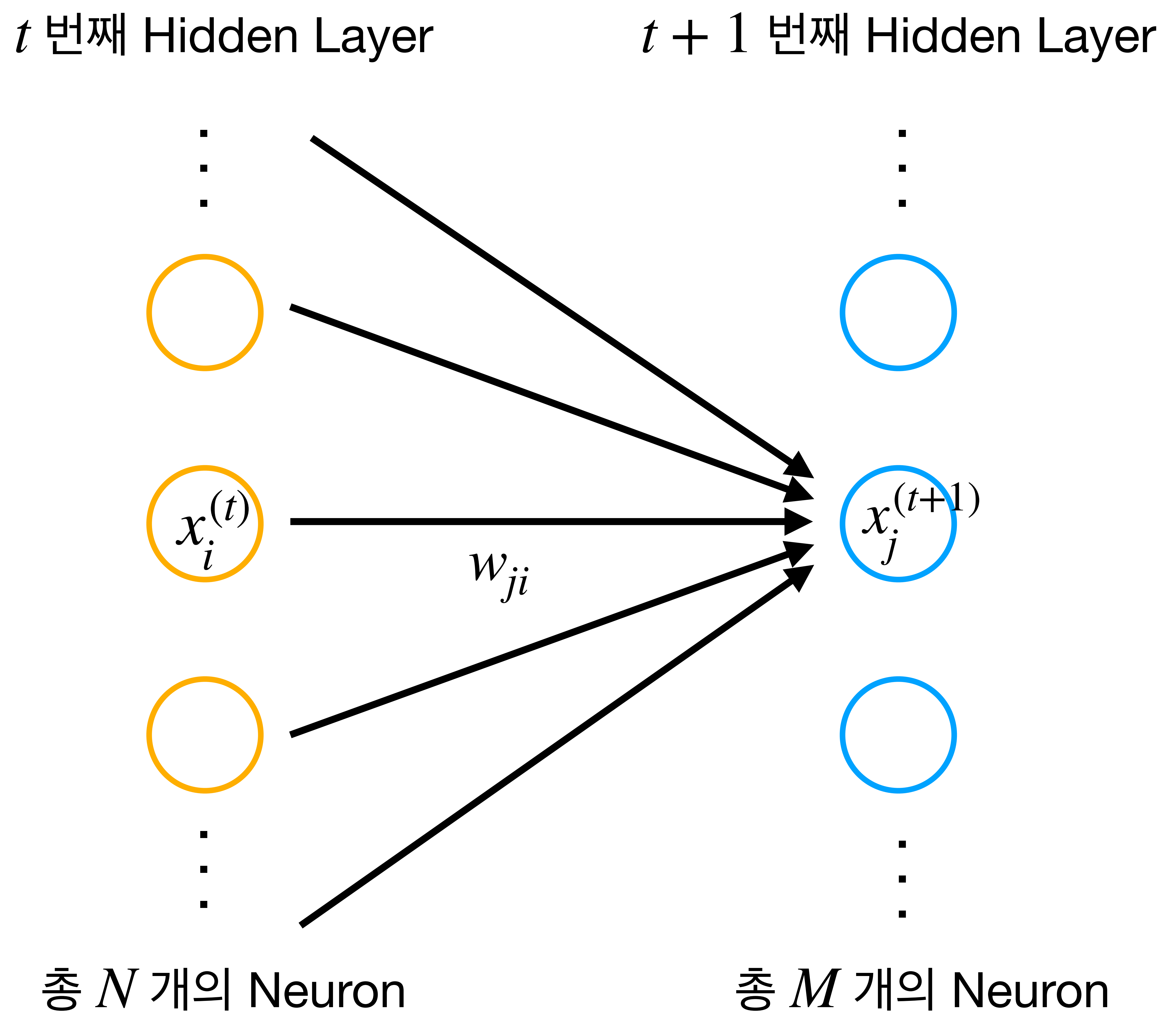


Forward Pass as Matrix Multiplication

Forward Pass

$$x_j^{(t+1)} = \sum_{i=1}^{N} w_{ji} x_i^{(t)}$$

$$= w_{j1}x_1 + w_{j2}x_2 + \cdots + w_{jN}x_N$$

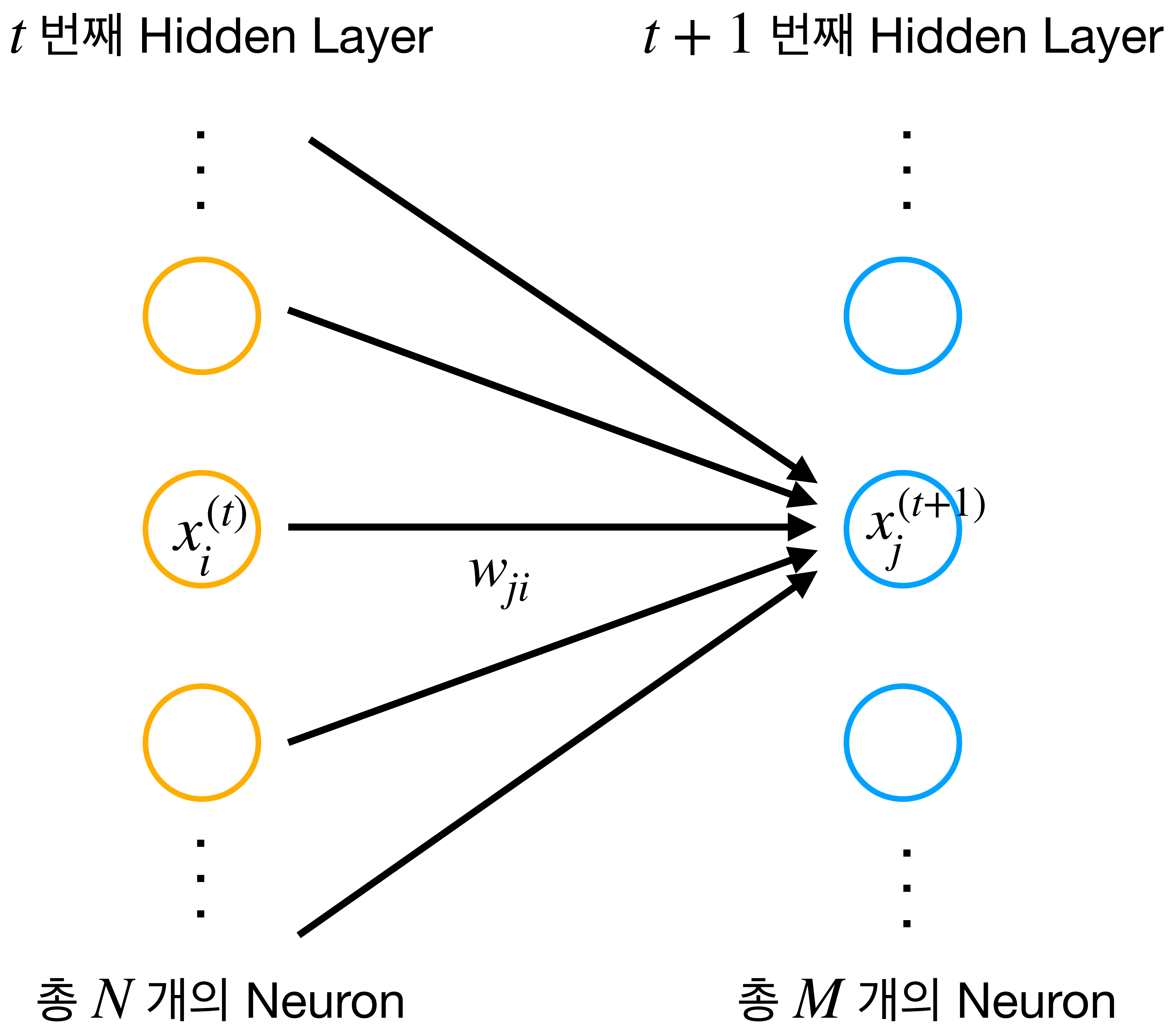


Forward Pass

$$x_j^{(t+1)} = \sum_{i=1}^{N} w_{ji} x_i^{(t)}$$

$$\boxed{= w_{j1}x_1 + w_{j2}x_2 + \cdots + w_{jN}x_N}$$

Vector의 내적으로 표현할 수 있다!



Forward Pass

행렬의 곱 Recap

$$\begin{pmatrix} w_{j1} & \dots & w_{ji} & \dots & w_{jN} \end{pmatrix} \begin{pmatrix} x_1^{(t)} \\ \dots \\ x_i^{(t)} \\ \dots \\ x_N^{(t)} \end{pmatrix} = w_{j1}x_1^{(t)} + \cdots + w_{ji}x_i^{(t)} + \cdots + w_{jN}x_N^{(t)}$$

Forward Pass

행렬의 곱 Recap

$$\begin{pmatrix} \boxed{w_{j1}} & \cdots & w_{ji} & \cdots & w_{jN} \end{pmatrix} \begin{pmatrix} \boxed{x_1^{(t)}} \\ \cdots \\ x_i^{(t)} \\ \cdots \\ x_N^{(t)} \end{pmatrix} = \boxed{w_{j1}x_1^{(t)}} + \cdots + w_{ji}x_i^{(t)} + \cdots + w_{jN}x_N^{(t)}$$

Forward Pass

행렬의 곱 Recap

$$\begin{pmatrix} w_{j1} & \cdots & \boxed{w_{ji}} & \cdots & w_{jN} \end{pmatrix} \begin{pmatrix} x_1^{(t)} \\ \cdots \\ \boxed{x_i^{(t)}} \\ \cdots \\ x_N^{(t)} \end{pmatrix} = w_{j1}x_1^{(t)} + \cdots + \boxed{w_{ji}x_i^{(t)}} + \cdots + w_{jN}x_N^{(t)}$$

Forward Pass

행렬의 곱 Recap

$$\begin{pmatrix} w_{j1} & \dots & w_{ji} & \dots & \boxed{w_{jN}} \end{pmatrix} \begin{pmatrix} x_1^{(t)} \\ \dots \\ x_i^{(t)} \\ \dots \\ \boxed{x_N^{(t)}} \end{pmatrix} = w_{j1}x_1^{(t)} + \cdots + w_{ji}x_i^{(t)} + \cdots + \boxed{w_{jN}x_N^{(t)}}$$

Forward Pass

행렬의 곱 Recap

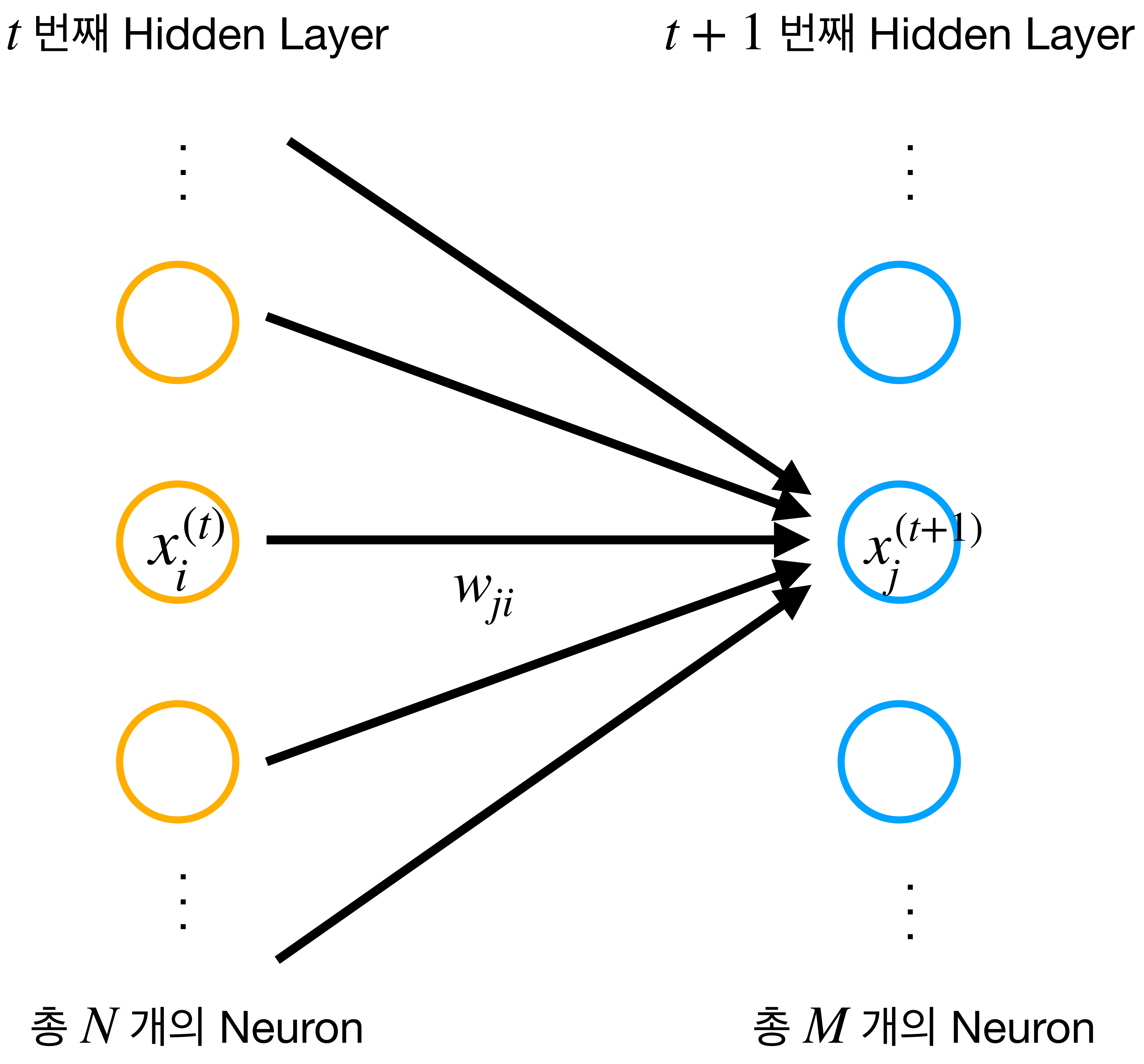
$$\begin{pmatrix} w_{j1} & \dots & w_{ji} & \dots & w_{jN} \end{pmatrix} \begin{pmatrix} x_1^{(t)} \\ \dots \\ x_i^{(t)} \\ \dots \\ x_N^{(t)} \end{pmatrix} = w_{j1}x_1^{(t)} + \cdots + w_{ji}x_i^{(t)} + \cdots + w_{jN}x_N^{(t)}$$

$$= \sum_{i=1}^{N} w_{ji}x_i^{(t)}$$

Forward Pass

행렬의 곱 Recap

이것은 t+1 번째 Hidden layer에서 j 번째 neuron에 해당된다.
나머지 1~M개의 neuron에 대해서도 확장해보자!

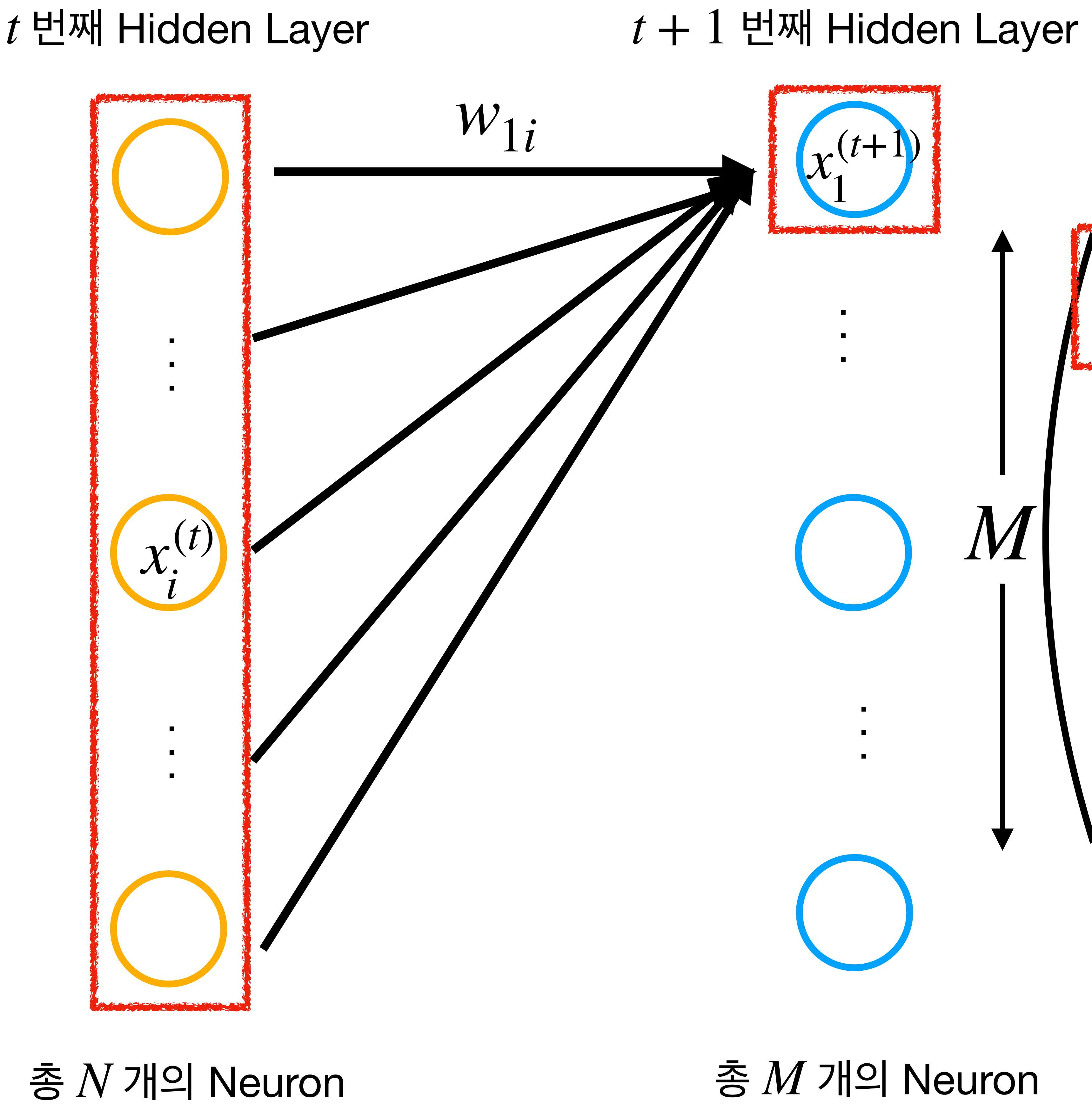


$$\boxed{\begin{pmatrix} w_{j1} & \dots & w_{ji} & \dots & w_{jN} \end{pmatrix}} \begin{pmatrix} x_1^{(t)} \\ \dots \\ x_i^{(t)} \\ \dots \\ x_N^{(t)} \end{pmatrix} = \sum_{i=1}^{N} w_{ji} x_i^{(t)} = x_j^{(t+1)}$$

Forward Pass

행렬의 곱 Recap

$$\mathbf{x}^{(t+1)} = W\mathbf{x}^{(t)}$$



$$\overbrace{\begin{pmatrix} w_{11} & \cdots & w_{1i} & \cdots & w_{1N} \\ w_{j1} & \cdots & w_{ji} & \cdots & w_{jN} \\ w_{M1} & \cdots & w_{Mi} & \cdots & w_{MN} \end{pmatrix}}^{N} \begin{pmatrix} x_1^{(t)} \\ \cdots \\ x_i^{(t)} \\ \cdots \\ x_N^{(t)} \end{pmatrix} = \begin{pmatrix} \sum_{i=1}^{N} w_{1i}x_i^{(t)} \\ \cdots \\ \sum_{i=1}^{N} w_{ji}x_i^{(t)} \\ \cdots \\ \sum_{i=1}^{N} w_{Mi}x_i^{(t)} \end{pmatrix} = \begin{pmatrix} x_1^{(t+1)} \\ \cdots \\ x_j^{(t+1)} \\ \cdots \\ x_N^{(t+1)} \end{pmatrix}$$

M

$$W \in \mathbb{R}^{M\times N} \qquad \mathbf{x}^{(t)} \in \mathbb{R}^{N} \qquad \mathbf{x}^{(t+1)} \in \mathbb{R}^{M}$$

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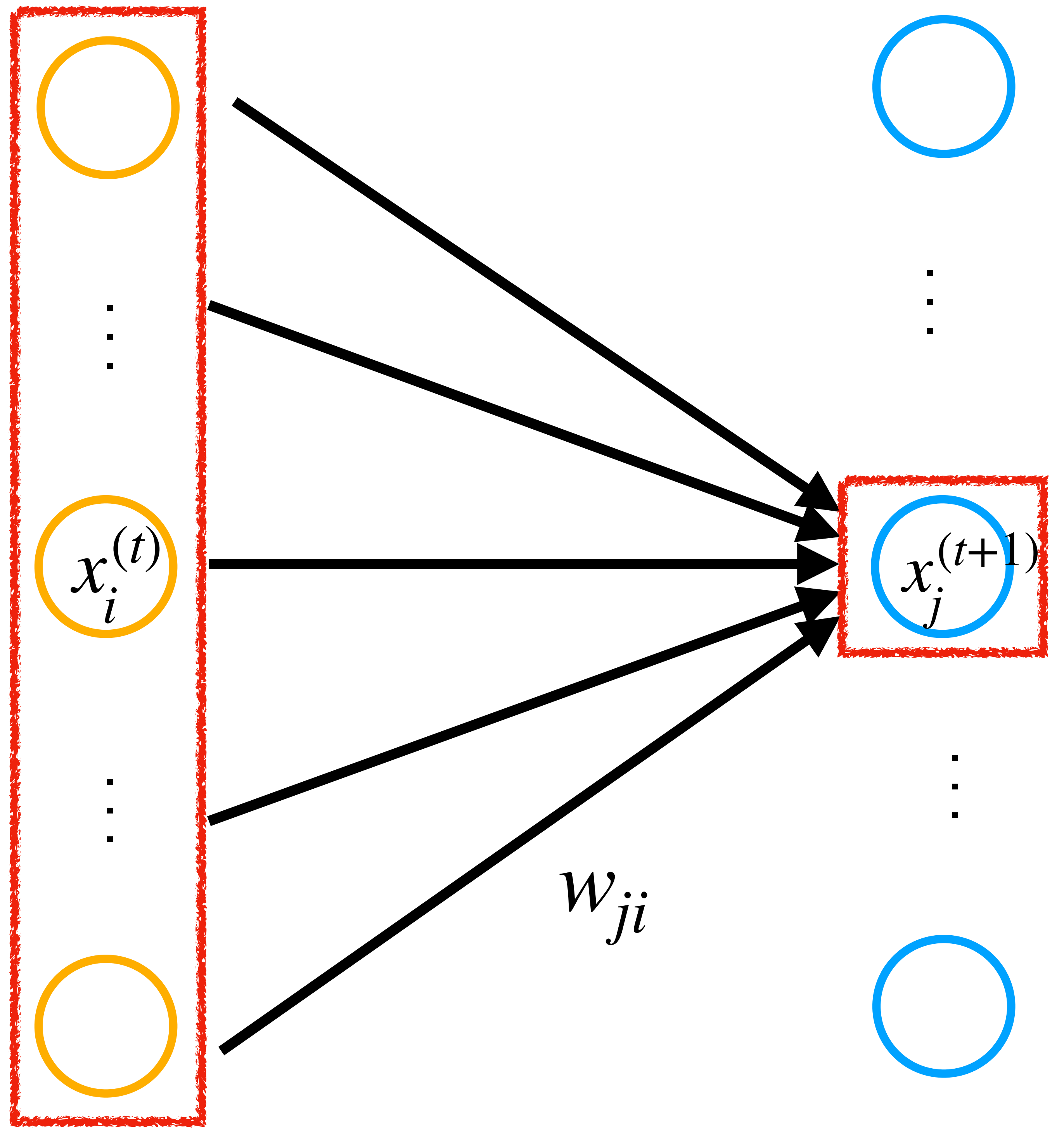
Forward Pass

행렬의 곱 Recap

$$\mathbf{x}^{(t+1)} = W\mathbf{x}^{(t)}$$

t 번째 Hidden Layer

$t+1$ 번째 Hidden Layer



총 N 개의 Neuron

총 M 개의 Neuron

$$\begin{pmatrix} w_{11} & \cdots & w_{1i} & \cdots & w_{1N} \\ & & & & \\ \boxed{w_{j1}} & \boxed{\cdots} & \boxed{w_{ji}} & \boxed{\cdots} & \boxed{w_{jN}} \\ & & & & \\ w_{M1} & \cdots & w_{Mi} & \cdots & w_{MN} \end{pmatrix} \begin{pmatrix} x_1^{(t)} \\ \cdots \\ x_i^{(t)} \\ \cdots \\ x_N^{(t)} \end{pmatrix} = \begin{pmatrix} \sum_{i=1}^{N} w_{1i} x_i^{(t)} \\ \cdots \\ \boxed{\sum_{i=1}^{N} w_{ji} x_i^{(t)}} \\ \cdots \\ \sum_{i=1}^{N} w_{Mi} x_i^{(t)} \end{pmatrix} = \begin{pmatrix} x_1^{(t+1)} \\ \cdots \\ \boxed{x_j^{(t+1)}} \\ \cdots \\ x_N^{(t+1)} \end{pmatrix}$$

$$W \in \mathbb{R}^{M \times N} \qquad \mathbf{x}^{(t)} \in \mathbb{R}^{N} \qquad \mathbf{x}^{(t+1)} \in \mathbb{R}^{M}$$

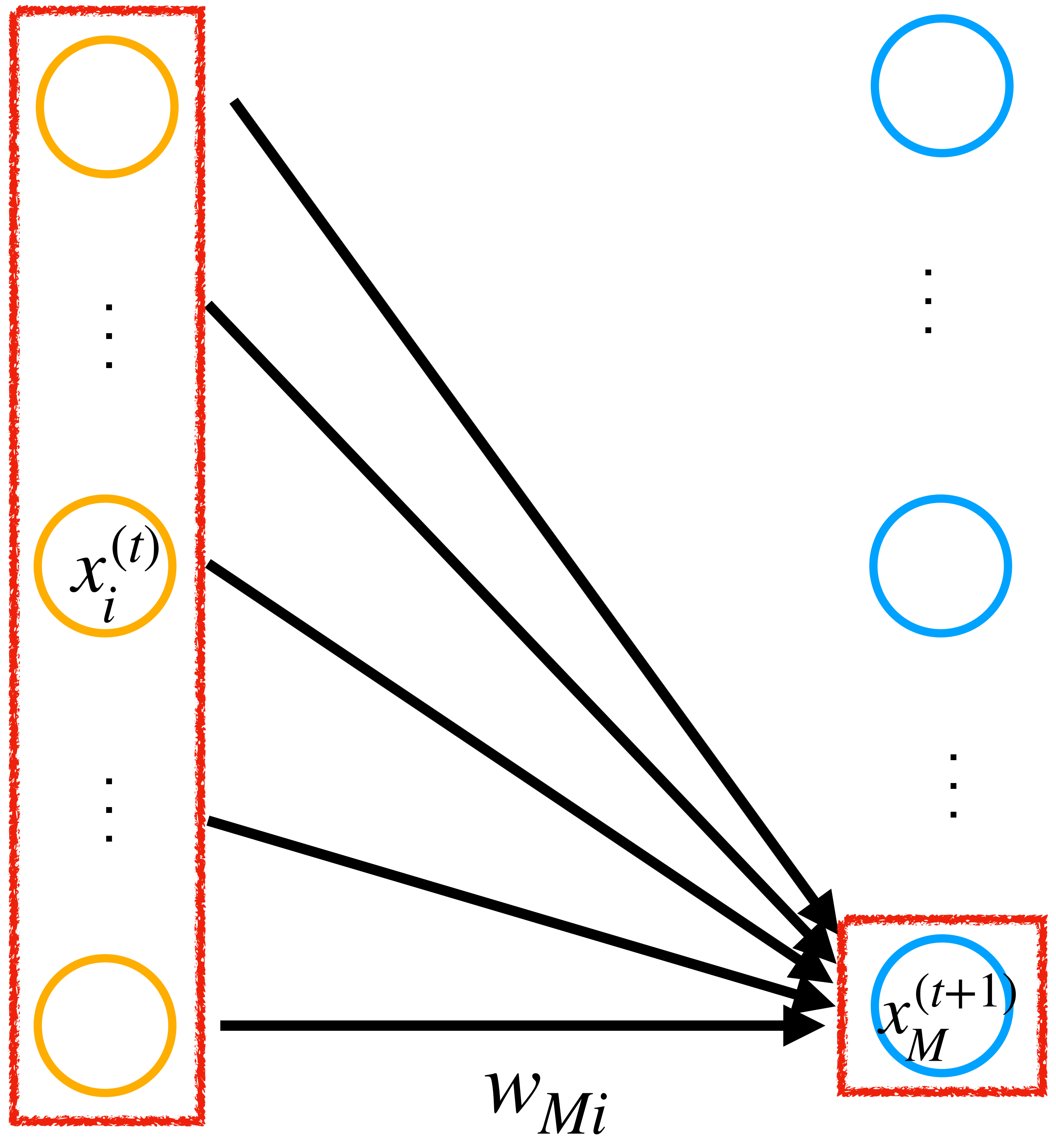
Forward Pass

행렬의 곱 Recap

$$\mathbf{x}^{(t+1)} = W\mathbf{x}^{(t)}$$

t 번째 Hidden Layer

$t+1$ 번째 Hidden Layer



총 N 개의 Neuron

총 M 개의 Neuron

$$\begin{pmatrix} w_{11} & \cdots & w_{1i} & \cdots & w_{1N} \\ w_{j1} & \cdots & w_{ji} & \cdots & w_{jN} \\ \boxed{w_{M1} \quad \cdots \quad w_{Mi} \quad \cdots \quad w_{MN}} \end{pmatrix} \boxed{\begin{pmatrix} x_1^{(t)} \\ \cdots \\ x_i^{(t)} \\ \cdots \\ x_N^{(t)} \end{pmatrix}} = \begin{pmatrix} \sum_{i=1}^{N} w_{1i}x_i^{(t)} \\ \cdots \\ \sum_{i=1}^{N} w_{ji}x_i^{(t)} \\ \boxed{\sum_{i=1}^{N} w_{Mi}x_i^{(t)}} \end{pmatrix} = \begin{pmatrix} x_1^{(t+1)} \\ \cdots \\ x_j^{(t+1)} \\ \cdots \\ \boxed{x_N^{(t+1)}} \end{pmatrix}$$

$W \in \mathbb{R}^{M\times N}$ $\quad$ $\mathbf{x}^{(t)} \in \mathbb{R}^{N}$ $\quad$ $\mathbf{x}^{(t+1)} \in \mathbb{R}^{M}$

Forward Pass

$$\begin{pmatrix} w_{j1} & \dots & w_{ji} & \dots & w_{jN} \end{pmatrix} \begin{pmatrix} x_1^{(t)} \\ \dots \\ x_i^{(t)} \\ \dots \\ x_N^{(t)} \end{pmatrix} = x_j^{(t+1)}$$

정리하자면:

$$\boxed{x_j^{(t+1)}} = \sum_{i=1}^{N} \boxed{w_{ji}} \boxed{x_i^{(t)}}$$

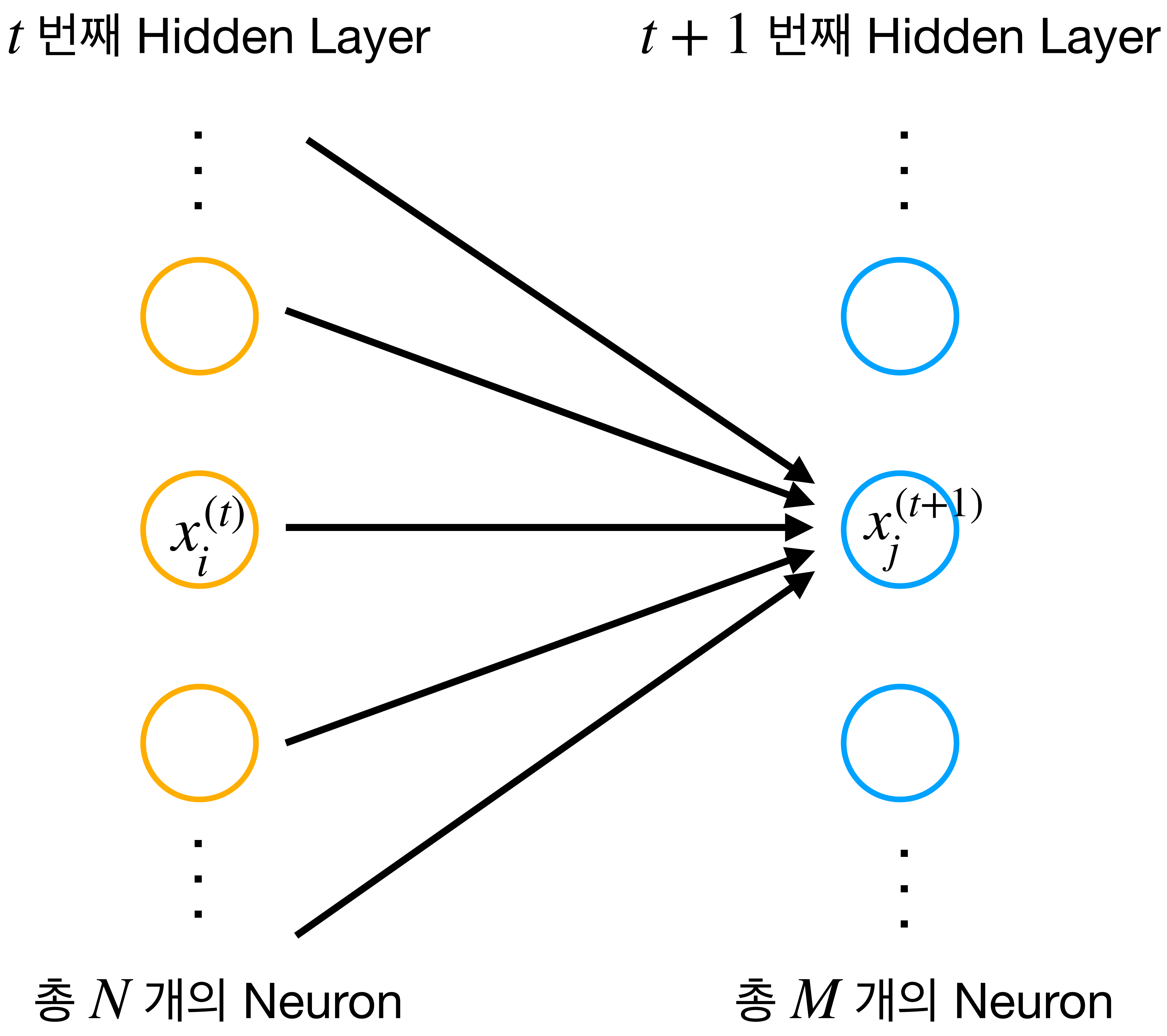
Weight Matrix	Input vector		Output vector

column = N개

$$\begin{array}{l} \\ \text{row} = \text{M개} \end{array} \begin{pmatrix} w_{11} & \dots & w_{1i} & \dots & w_{1N} \\ & & \dots & & \\ w_{j1} & \dots & w_{ji} & \dots & w_{jN} \\ & & \dots & & \\ w_{M1} & \dots & w_{Mi} & \dots & w_{MN} \end{pmatrix} \begin{pmatrix} x_1^{(t)} \\ \dots \\ x_i^{(t)} \\ \dots \\ x_N^{(t)} \end{pmatrix} = \begin{pmatrix} x_1^{(t+1)} \\ \dots \\ \boxed{x_j^{(t+1)}} \\ \dots \\ x_M^{(t+1)} \end{pmatrix}$$

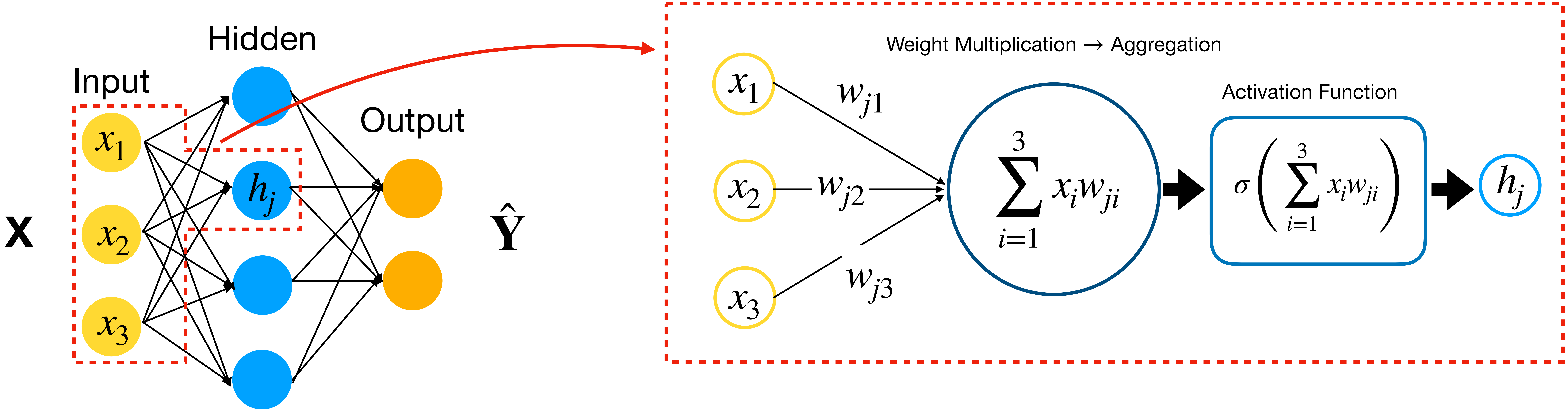
M x N matrix — N vector — M vector

Forward Pass



즉, (Activation function이 제외된) Neural Network은 단순히 matrix의 곱이다!

$$\mathbf{x}^{(t+1)} = W\mathbf{x}^{(t)}$$



만약에 Activation Function을 포함한다면,

$$\mathbf{h} = \sigma(W\mathbf{x})$$

Activation Function도 포함하는 경우

$$\boxed{x_j^{(t+1)}} = \sigma\left(\sum_{i=1}^{N} \boxed{w_{ji}}\boxed{x_i^t}\right) \rightarrow \mathbf{x}^{(t+1)} = \sigma\left(W\mathbf{x}^{(t)}\right)$$

Weight Matrix | **Input vector** | **Output vector**

$$\sigma\left(\begin{pmatrix} w_{11} & \cdots & w_{1i} & \cdots & w_{1N} \\ & & \cdots & & \\ w_{j1} & \cdots & w_{ji} & \cdots & w_{jN} \\ & & \cdots & & \\ w_{M1} & \cdots & w_{Mi} & \cdots & w_{MN} \end{pmatrix} \begin{pmatrix} x_1^{(t)} \\ \cdots \\ x_i^{(t)} \\ \cdots \\ x_N^{(t)} \end{pmatrix}\right) = \begin{pmatrix} \sigma\left(\sum_{i=1}^{N} w_{1i}x_i^{(t)}\right) \\ \cdots \\ \sigma\left(\sum_{i=1}^{N} w_{ji}x_i^{(t)}\right) \\ \cdots \\ \sigma\left(\sum_{i=1}^{N} w_{Mi}x_i^{(t)}\right) \end{pmatrix} = \begin{pmatrix} x_1^{(t+1)} \\ \cdots \\ x_j^{(t+1)} \\ \cdots \\ x_M^{(t+1)} \end{pmatrix}$$