BE530 – Medical Deep Learning

- Artificial Neural Networks -

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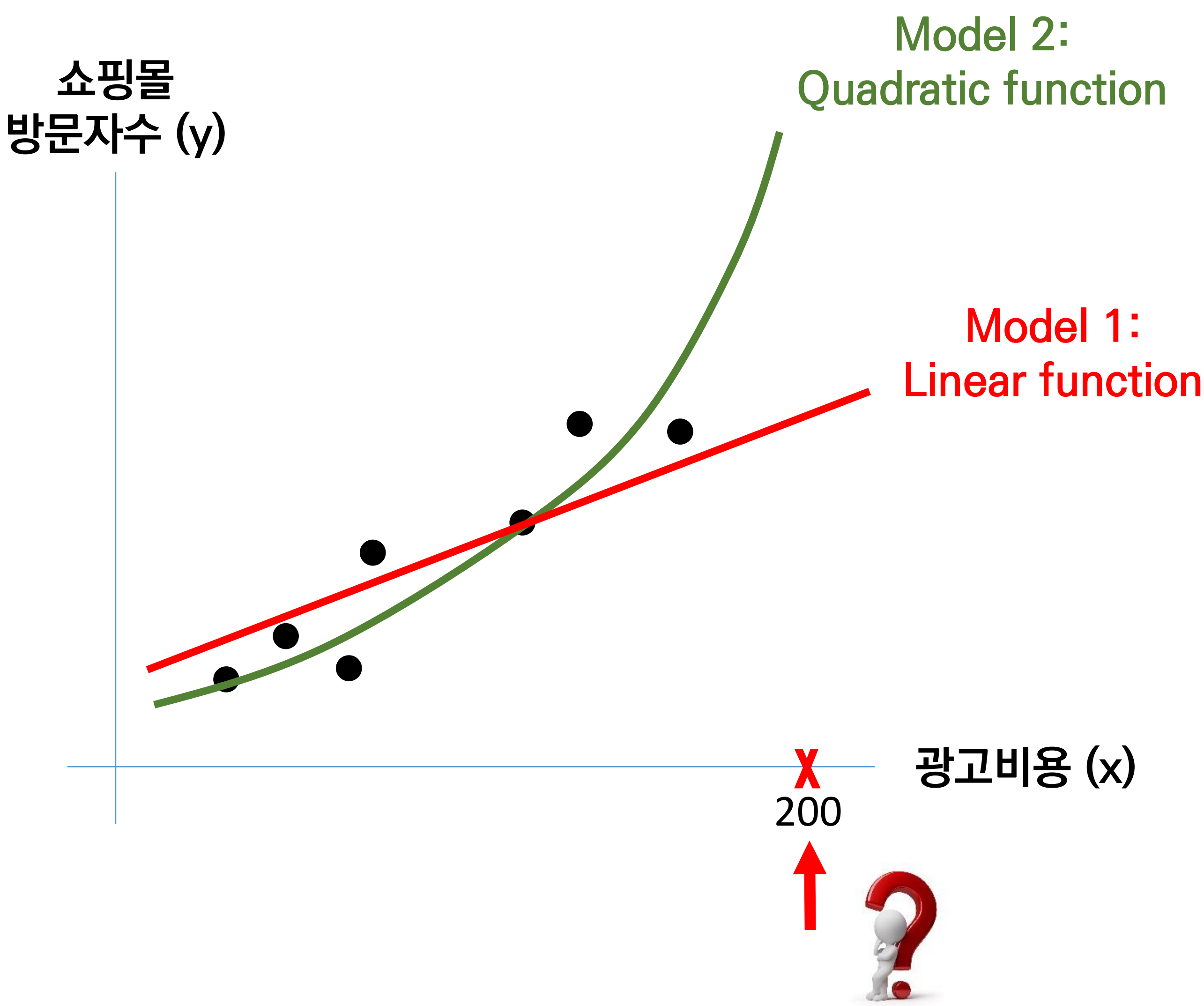
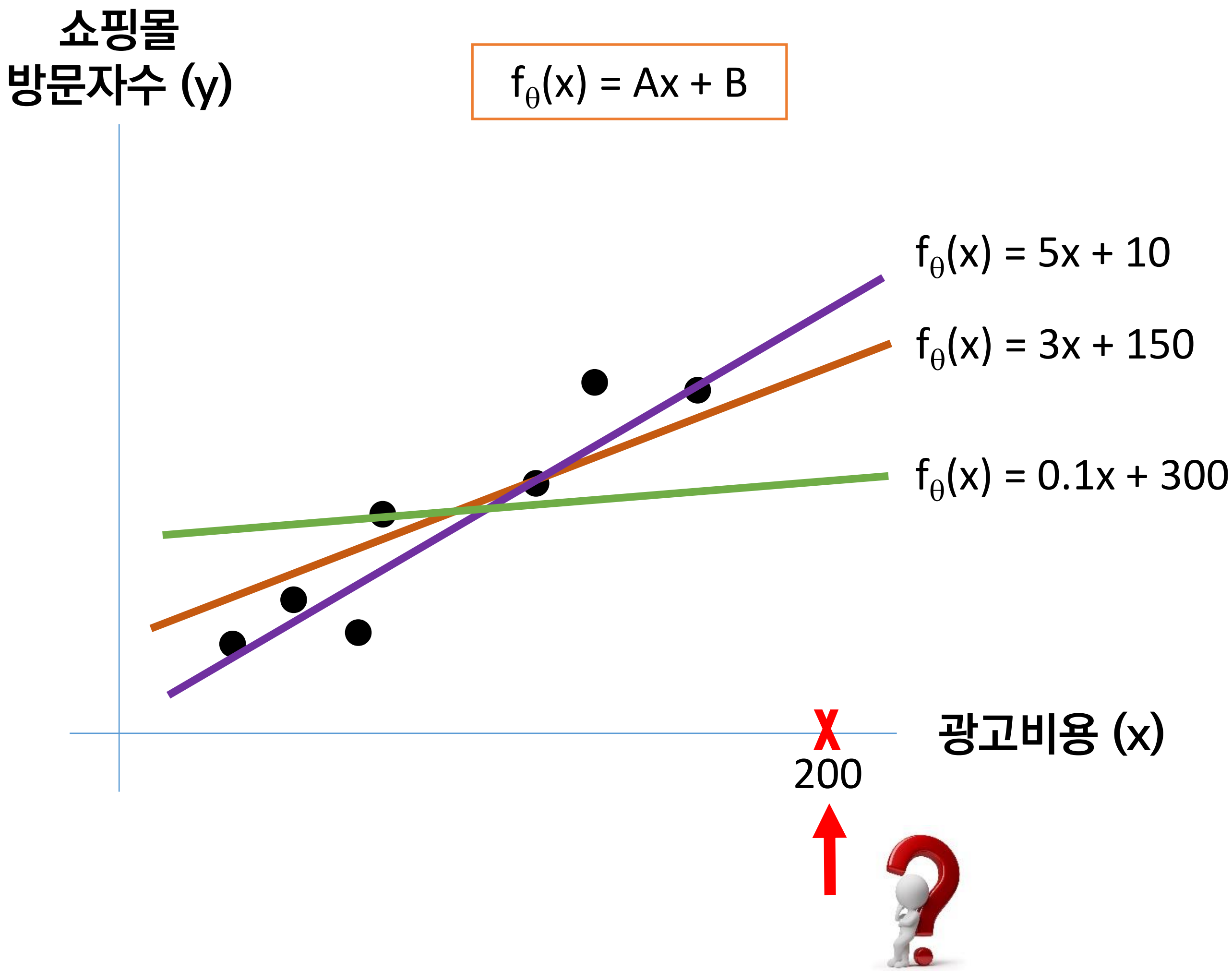
Simple Regression (1)

광고비	방문자수
58	374
70	385
81	375
84	401
95	481
107	502
113	495

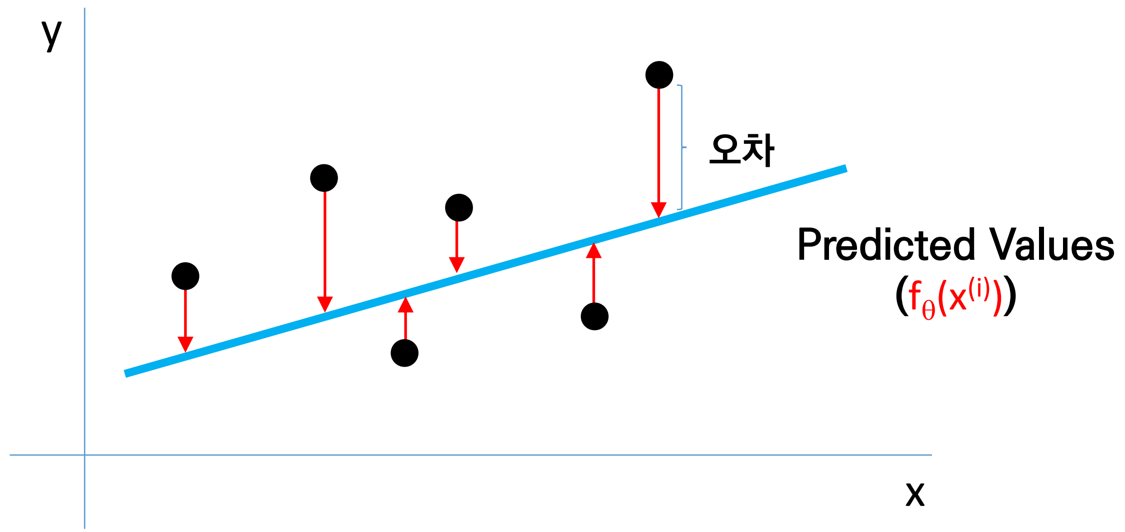


Simple Regression – (2)

광고비	방문자수
58	374
70	385
81	375
84	401
95	481
107	502
113	495



Simple Prediction – (3)



Cost Function

$$E(\theta) = \frac{1}{n}\sum_{i=1}^{n}\left(y^{(i)} - f_\theta(x^{(i)})\right)^2$$

광고비	방문자수	5x+10	3x+150	0.1x+300
58	374			
70	385			
81	375			
84	401	2401	937.57	17648.46
95	481			
107	502			
113	495			

If Deep Learning is applied

① A linear function

② $f_\theta(x) = 5x + 10$

$f_\theta(x) = 3x + 150$

$f_\theta(x) = 0.1x + 300$

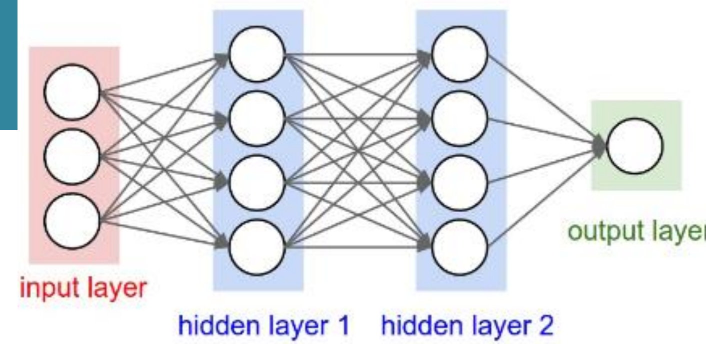
주어진 학습데이터를 이용하여
E(θ)를 최소화시키는 모델의 θ를 자동으로 찾아냄

➡ Gradient Decent Method

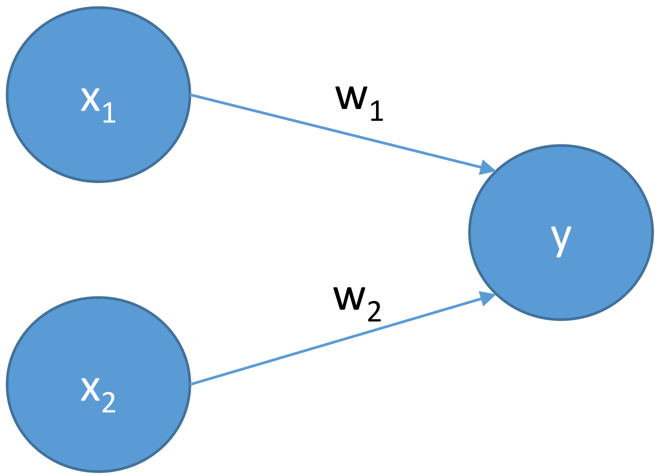
③ $$E(\theta) = \frac{1}{n}\sum_{i=1}^{n}\left(y^{(i)} - f_\theta(x^{(i)})\right)^2$$

④ $\boxed{f_\theta(x) = 3x + 150}$

Perceptron (1)



- A Perceptron with 2 inputs



$$y = \begin{cases} 0 \ (x_1 w_1 + x_2 w_2 \leq \theta) \\ 1 \ (x_1 w_1 + x_2 w_2 > \theta) \end{cases}$$

※ **가중치 (weight: w_1, w_2)**

- 각 신호(e.g., x_1, x_2)가 결과에 주는 영향력을 조절하는 요소
- 가중치가 클수록 해당 신호가 그만큼 더 중요함을 의미함

Perceptron (2)

■ Weights and Bias

$$y = \begin{cases} 0 \ (x_1 w_1 + x_2 w_2 \le \vartheta) \\ 1 \ (x_1 w_1 + x_2 w_2 > \vartheta) \end{cases} \Rightarrow y = \begin{cases} 0 \ (b + x_1 w_1 + x_2 w_2 \le 0) \\ 1 \ (b + x_1 w_1 + x_2 w_2 > 0) \end{cases}$$

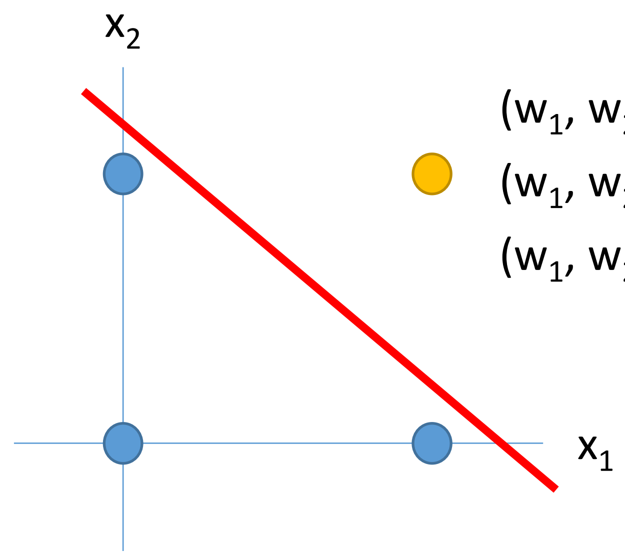
※ **가중치 (weight: w_1, w_2)**
- 각 입력 신호(e.g., x_1, x_2)가 결과에 주는 영향력을 조절하는 변수

※ **편향 (bias: b)**
- 뉴런이 얼마나 쉽게 활성화(결과로 1 출력)되는지를 조정하는 변수
- 예) b=−0.1이면 각 입력 신호와 가중치를 곱한 값들이 합이 0.1을 초과할 때만 뉴런이 활성화. b=−20.0이면 입력 신호와 가중치를 곱한 값들이 합이 20을 초과하지 않으면 뉴런이 활성화되지 않음

Perceptron (3)

AND gate

x_1	x_2	y
0	0	0
1	0	0
0	1	0
1	1	1



$(w_1, w_2, \theta) = (0.5, 0.5, 0.7)$

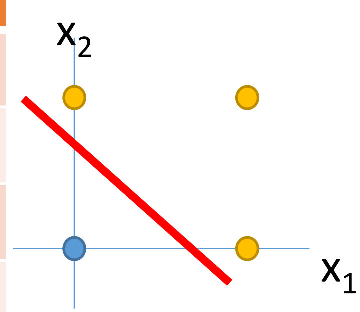
$(w_1, w_2, \theta) = (0.5, 0.5, 0.8)$

$(w_1, w_2, \theta) = (1.0, 1.0, 1.0)$

…

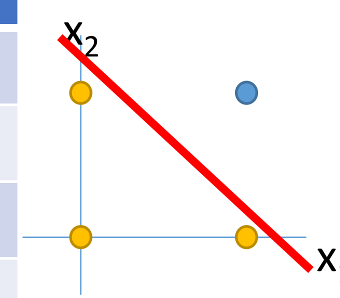
OR gate

x_1	x_2	y
0	0	0
1	0	1
0	1	1
1	1	1



NAND gate

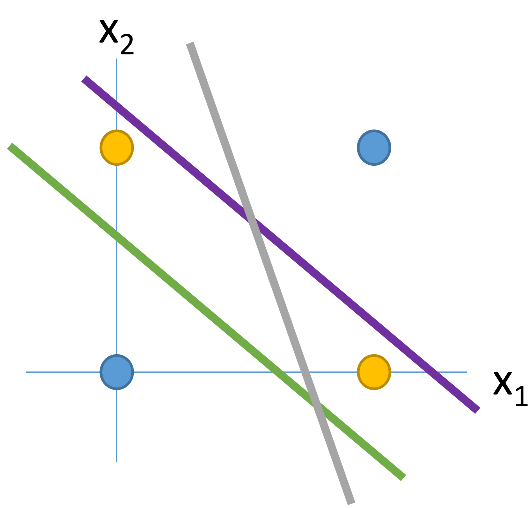
x_1	x_2	y
0	0	1
1	0	1
0	1	1
1	1	0

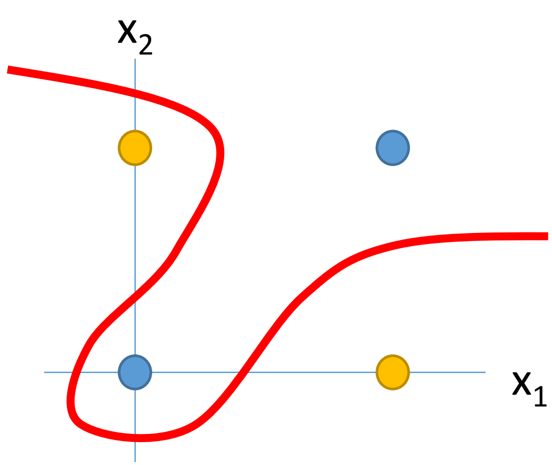


Perceptron (4)

- XOR gate
  - **Perceptron을 적용할 경우 XOR Gate에 대해 하나의 직선을 이용하여 0과 1을 구분할 수 없음**
    - Perceptron은 직선 하나로 나눈 영역에 대해서만 표현 가능

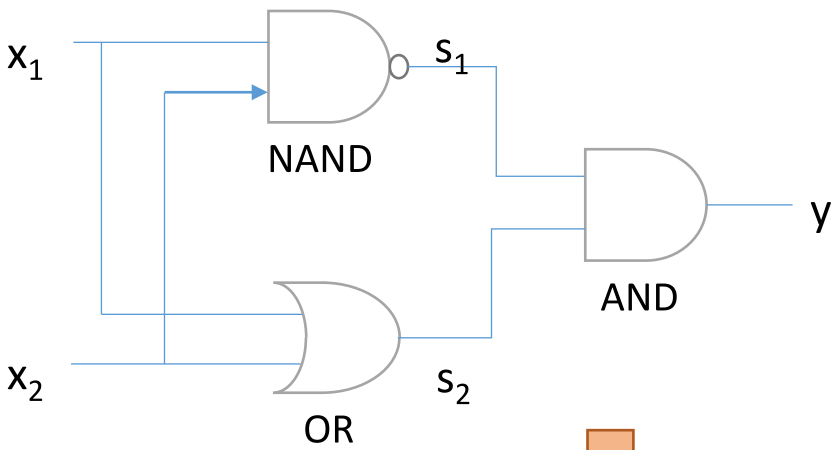
x_1	x_2	y
0	0	0
1	0	1
0	1	1
1	1	0





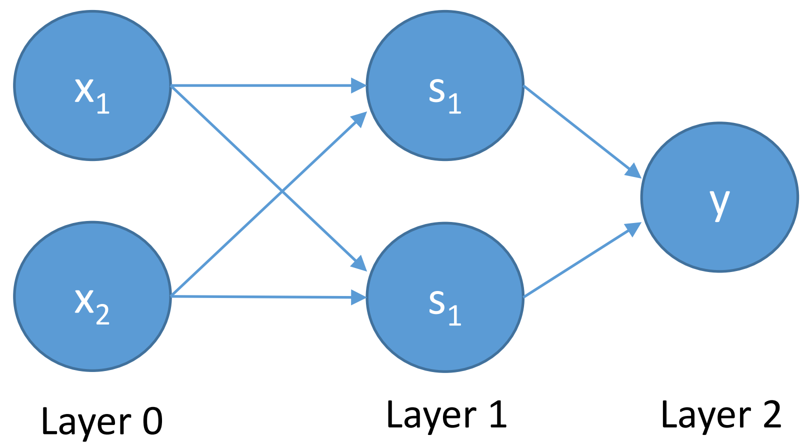
Perceptron (5)

■ Multi-layer Perceptron (MLP)



XOR Gate

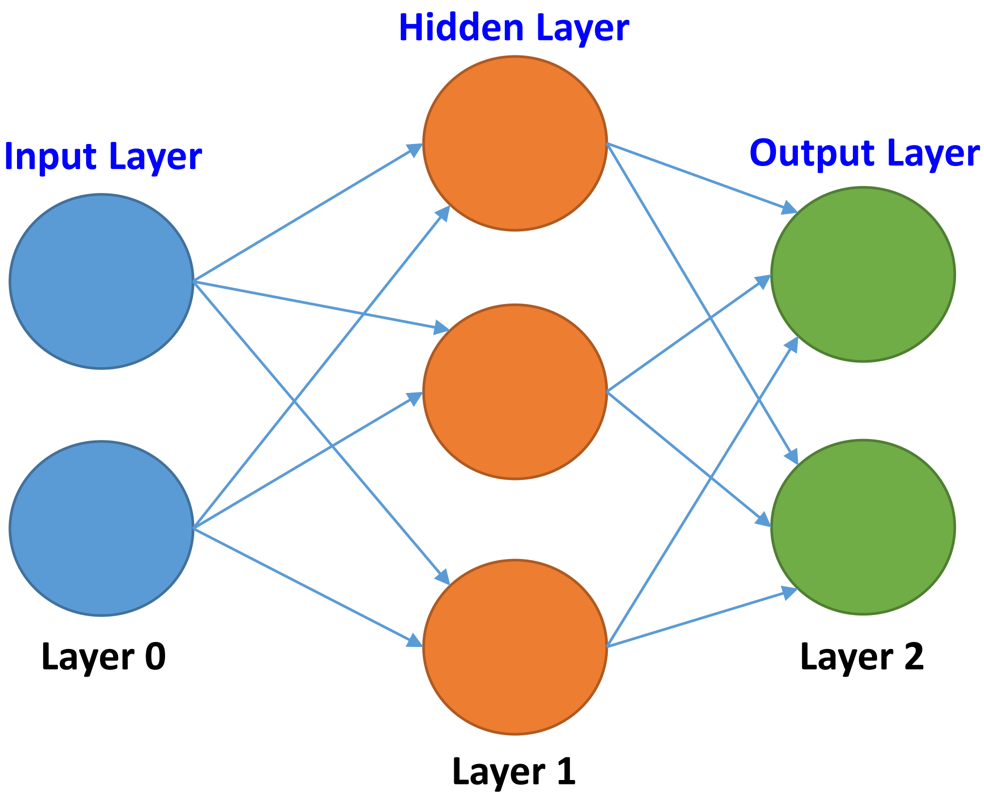
x_1	x_2	s_1	s_2	y
0	0	1	0	0
1	0	1	1	1
0	1	1	1	1
1	1	0	1	0



- Single Layer Perceptron ➔ 직선형 영역 표현
- Multi-Layer Perceptron ➔ 비선형 영역 표현

Artificial Neural Networks

- 2-Layer ANN

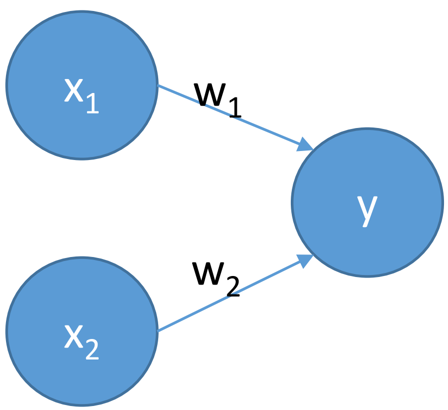


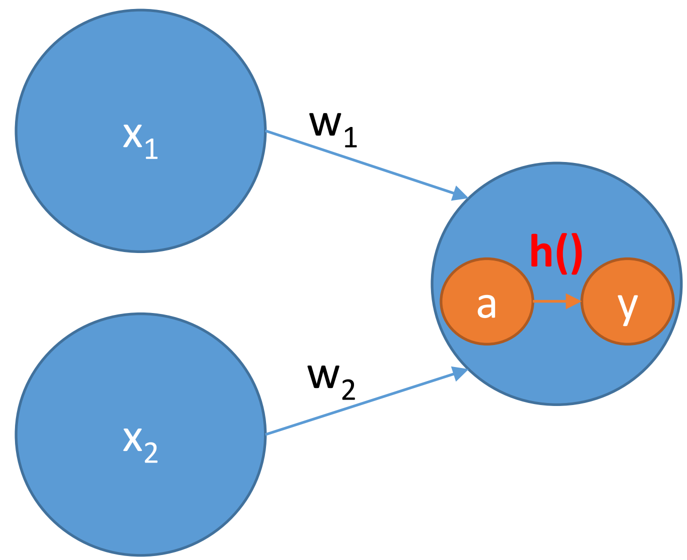
Perceptron revisited

$$y = \begin{cases} 0 \ (b + x_1w_1 + x_2w_2 \le 0) \\ 1 \ (b + x_1w_1 + x_2w_2 > 0) \end{cases}$$

$$a = b + w_1x_1 + w_2x_2$$

$$y = h(a) = \begin{cases} 0 \ (a \le 0) \\ 1 \ (a > 0) \end{cases}$$





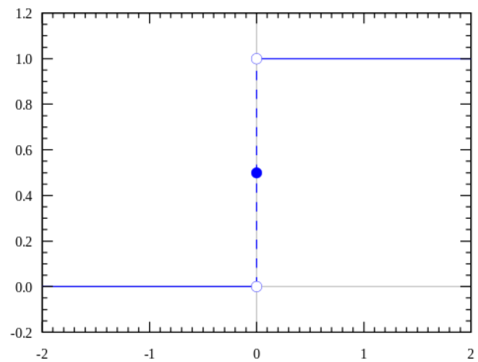
※ **h(a)**

- 활성화 함수 (Activation Function)
- 입력 신호의 총합을 출력 신호로 변환
- Ex) step, sigmoid, ReLU, …

Activation Functions

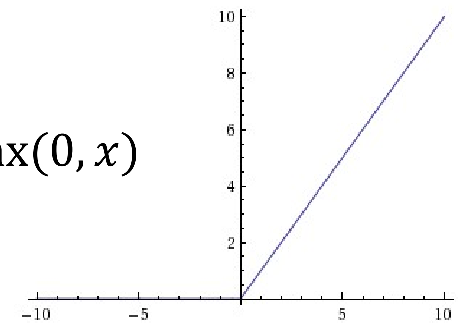
- Step function

$$f(x) = \begin{cases} 0 \ (a \leq 0) \\ 1 \ (a > 0) \end{cases}$$



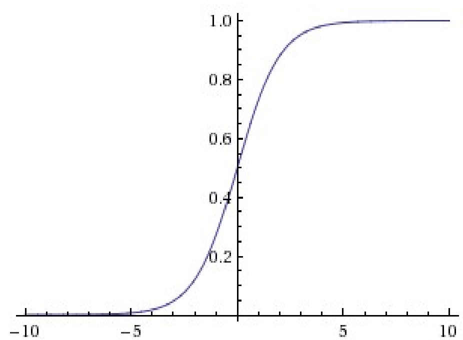
- ReLU function

$$f(x) = \max(0, x)$$



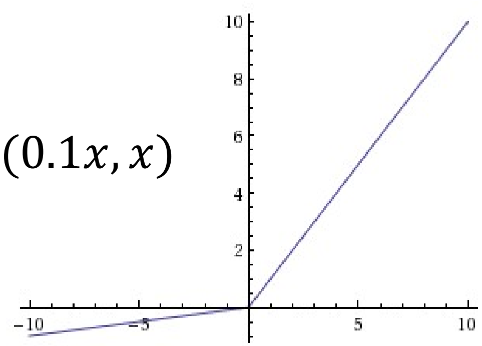
- Logistic sigmoid function

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



- Leaky ReLU function

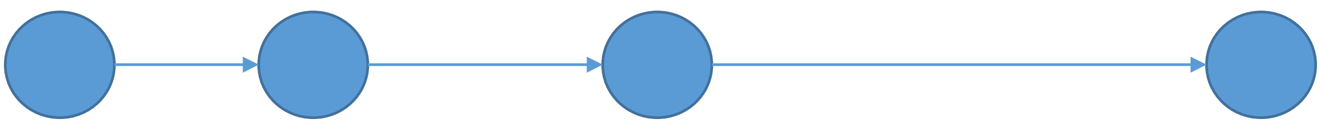
$$f(x) = \max(0.1x, x)$$



Perceptron vs. ANN

- **Perceptron과 Neural Network과의 주된 차이는 활성화 함수**
  - Perceptron ➔ step function
  - Neural networks ➔ sigmoid, ReLU, …

- **신경망에서의 활성화 함수는 비선형 함수 사용**
  - 선형 함수 사용 시 → 은닉층(Hidden Layer)을 사용하는 이점이 사라짐



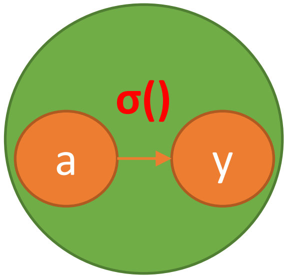
$h(a_1)=h(w_1*x)$
$=c*x$

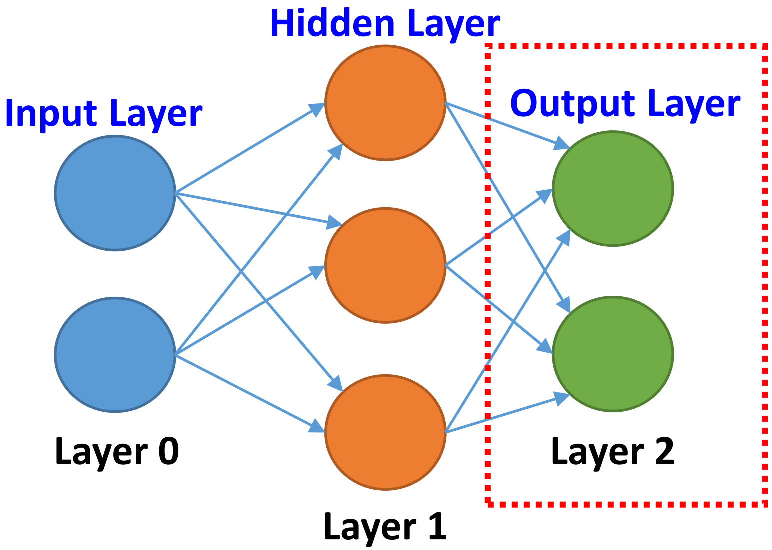
$h(a_2)=h(w_2*h(a_1))$

$y=h(a_3)=h(w_3*h(w_2*h(a_1)))=k*x$

Softmax Function

- Output Layer
  - Identity function(σ())
    - – 입력 신호 = 출력 신호





- Softmax function

$$p(c_k = 1|\boldsymbol{x}) = \frac{\exp(y_k)}{\sum_{j=1}^{C} \exp(y_j)}$$

  - 0에서 1.0사이의 출력
  - 출력의 총합 = 1.0

→ Softmax function의 출력을 『**확률**』로 해석 가능

Loss Function

■ 학습 목표

- Loss Function의 결과값을 최소화하는 가중치 매개변수 (*w*, *b*)를 찾는 것

$$\mathcal{L}(\boldsymbol{w}) = \frac{1}{N}\sum_{i=1}^{N} l(\boldsymbol{w}, \boldsymbol{x}_i, t_i) + \mathcal{R}(\boldsymbol{w})$$

N: number of training examples
$\mathcal{R}$: regularizer
$\boldsymbol{w}$: set of all parameters

■ 대표적인 손실 함수

- 평균제곱오차(MSE: Mean Squared Error) – Regression 문제

$$l = \frac{1}{2}\sum_{k}(y_k - t_k)^2 \text{ , } y_k: prediction, t_k: ground\ truth$$

- 교차 엔트로피 오차(CEE: Cross Entropy Error) – Classification 문제

$$l = -\sum_{n=1}^{N}\sum_{k=1}^{K} d_{nk} log y_k(x_n; w)$$

$$d_n = [d_{n1}, d_{n2}, \ldots, d_{nk}] \text{ /* one hot encoding*/}$$

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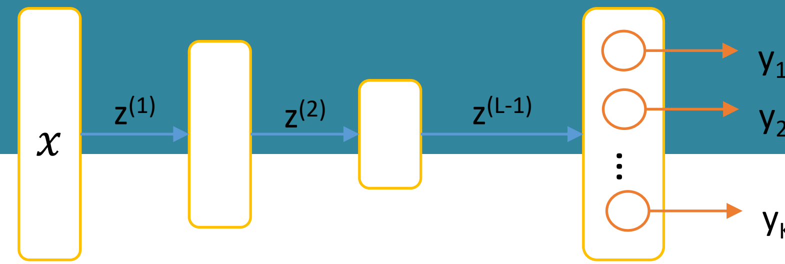
Cross Entropy Loss (1)



$$p(C_k|x) = y_k = z_k^{(L)} = \frac{\exp(u_k^{(L)})1}{\sum_{j=1}^{K} \exp(u_j^{(L)})}$$

$$d_n = [d_{n1}, d_{n2}, \ldots, d_{nK}] \text{ /* GT */}$$

$$p(d|x) = \prod_{k=1}^{K} p(C_k|x)^{d_k}$$

L(w) : 최대우도법 (maximum likelihood estimation)에 따른 w의 우도

$$L(w) = \prod_{n=1}^{N} p(d_n|x_n; w) = \prod_{n=1}^{N}\prod_{k=1}^{K} p(C_k|x)^{d_{nk}} = \prod_{n=1}^{N}\prod_{k=1}^{K} (y_k(x; w))^{d_{nk}}$$

Objective: *L(w)*를 최대화하는 w를 구할 수 있도록 학습

*L(w)*에 로그를 취하고 부호 반전

Objective: *E(w)*를 최소화하는 w를 구할 수 있도록 학습

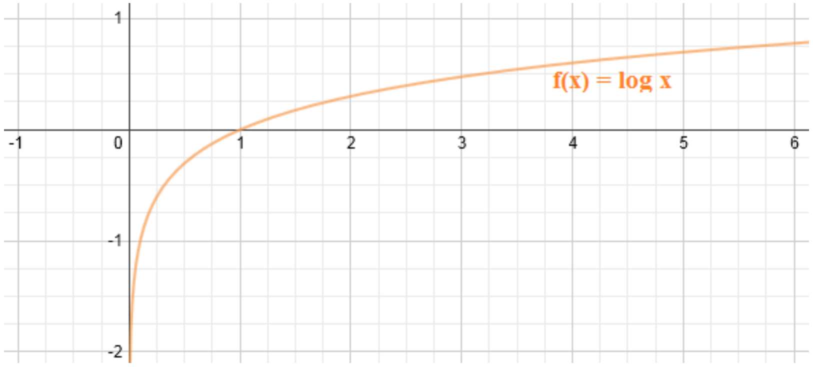
$$E(w) = -\sum_{n=1}^{N}\sum_{k=1}^{K} d_{nk}\log(y_k(x_n; w))$$

Cross Entropy Loss (2)

- Cross entropy loss with Softmax function

$$l(\boldsymbol{w}, \boldsymbol{x}, t) = -\sum_{k=1}^{C} t^{(k)} \log \underbrace{p(c_k|\boldsymbol{x})}_{\text{The output of the Softmax function}}$$

$$p(c_k = 1|\boldsymbol{x}) = \frac{\exp(y_k)}{\sum_{j=1}^{C} \exp(y_j)}$$



Gradient Descent Method (1)

- Given E(w), the gradient descent is defined as

$$\nabla E \equiv \frac{\partial E}{\partial w} = \left[\frac{\partial E}{\partial w_1}, \frac{\partial E}{\partial w_2}, \dots, \frac{\partial E}{\partial w_M}\right], M: w\text{의 성분 수}$$

- Gradient Descent Method
  - 현재의 w를 음의 기울기 방향($-\nabla E$)로 조금씩 움직이는 것을 여러 번 반복
  - 현재의 가중치를 $w^{(t)}$, 움직인 후의 가중치 $w^{(t+1)}$ 를 라고 할 때 다음과 같이 갱신

$$w^{(t+1)} = w^{(t)} - \epsilon \nabla E, \epsilon: learning\ rate$$

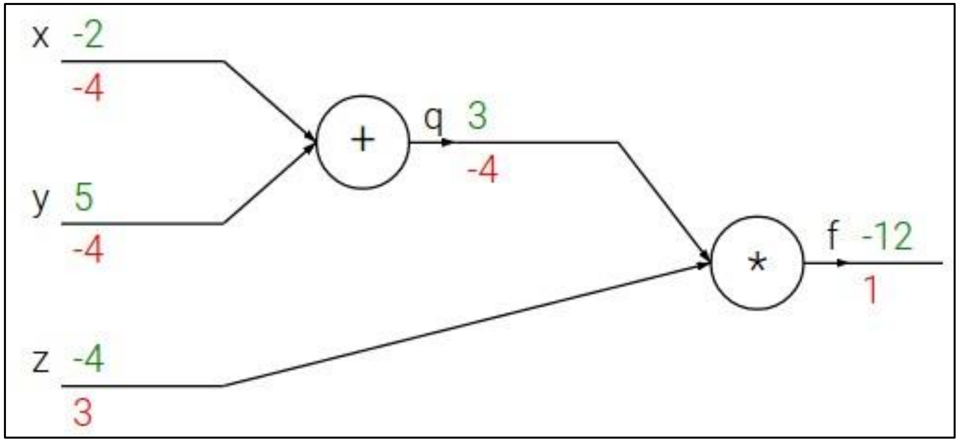
– 학습률(ϵ)을 결정하는 것은 학습에서 매우 중요한 요소

Gradient Descent Method (2)

Backpropagation (1)

$$f(x, y, z) = (x + y)z$$

e.g. x = -2, y = 5, z = -4



* Source: Stanford Univ. CS231 Lecture Notes

Backpropagation (2)

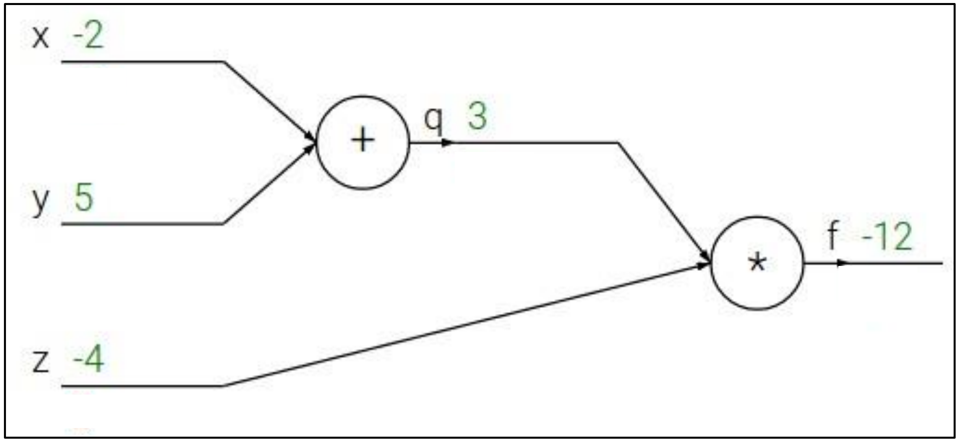
$$f(x, y, z) = (x + y)z$$

e.g. x = -2, y = 5, z = -4

$$q = x + y \qquad \frac{\partial q}{\partial x} = 1, \frac{\partial q}{\partial y} = 1$$

$$f = qz \qquad \frac{\partial f}{\partial q} = z, \frac{\partial f}{\partial z} = q$$

Want: $\frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}, \frac{\partial f}{\partial z}$



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* Source: Stanford Univ. CS231 Lecture Notes

Backpropagation (3)

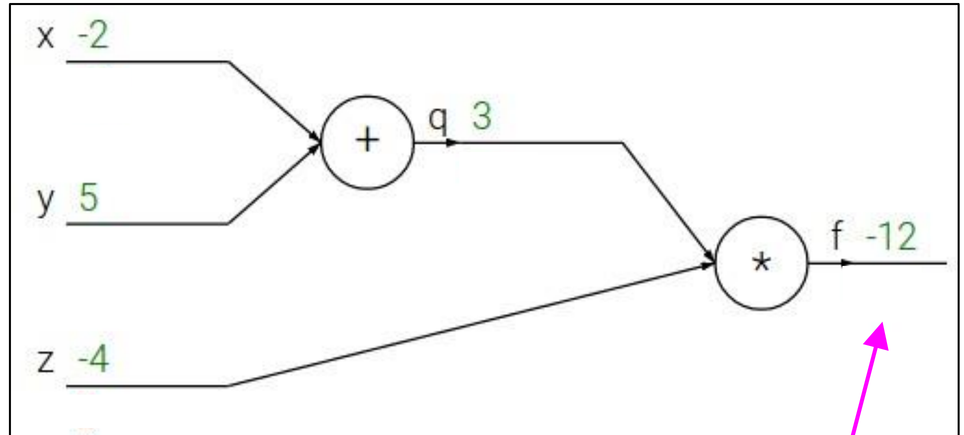
$$f(x, y, z) = (x + y)z$$

e.g. x = -2, y = 5, z = -4

$$\boxed{q = x + y \qquad \frac{\partial q}{\partial x} = 1, \frac{\partial q}{\partial y} = 1}$$

$$\boxed{f = qz \qquad \frac{\partial f}{\partial q} = z, \frac{\partial f}{\partial z} = q}$$

Want: $\frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}, \frac{\partial f}{\partial z}$



$$\boxed{\frac{\partial f}{\partial f}}$$

* Source: Stanford Univ. CS231 Lecture Notes

Backpropagation (4)

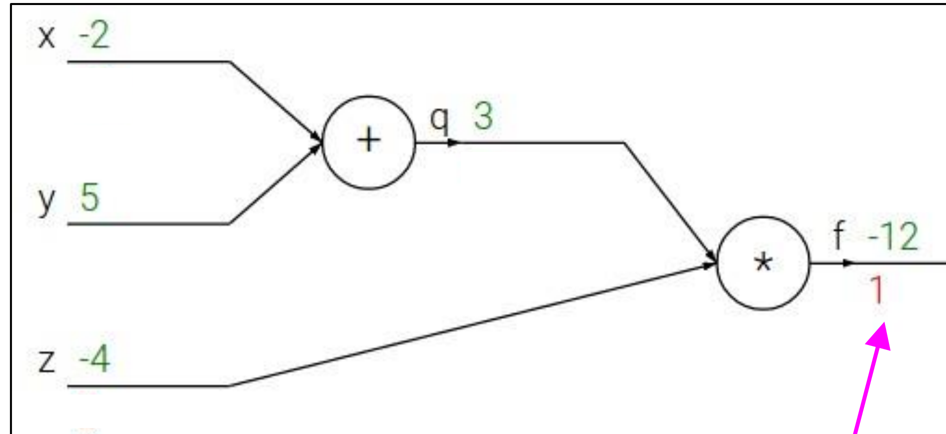
$$f(x,y,z) = (x+y)z$$

e.g. x = -2, y = 5, z = -4

$$q = x + y \qquad \frac{\partial q}{\partial x} = 1, \frac{\partial q}{\partial y} = 1$$

$$f = qz \qquad \frac{\partial f}{\partial q} = z, \frac{\partial f}{\partial z} = q$$

Want: $\frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}, \frac{\partial f}{\partial z}$



$$\frac{\partial f}{\partial f}$$

* Source: Stanford Univ. CS231 Lecture Notes

Backpropagation (5)

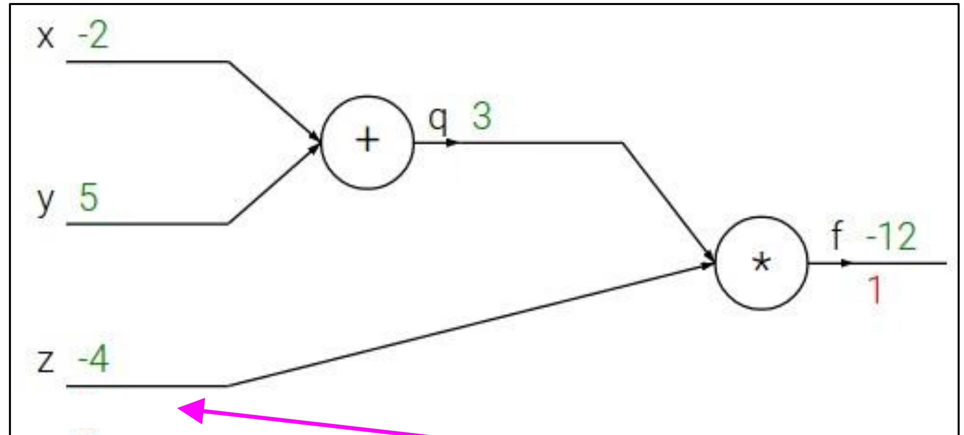
$$f(x, y, z) = (x + y)z$$

e.g. x = -2, y = 5, z = -4

$$q = x + y \qquad \frac{\partial q}{\partial x} = 1, \frac{\partial q}{\partial y} = 1$$

$$f = qz \qquad \frac{\partial f}{\partial q} = z, \frac{\partial f}{\partial z} = q$$

Want: $\frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}, \frac{\partial f}{\partial z}$



$$\frac{\partial f}{\partial z}$$

* Source: Stanford Univ. CS231 Lecture Notes

Backpropagation (6)

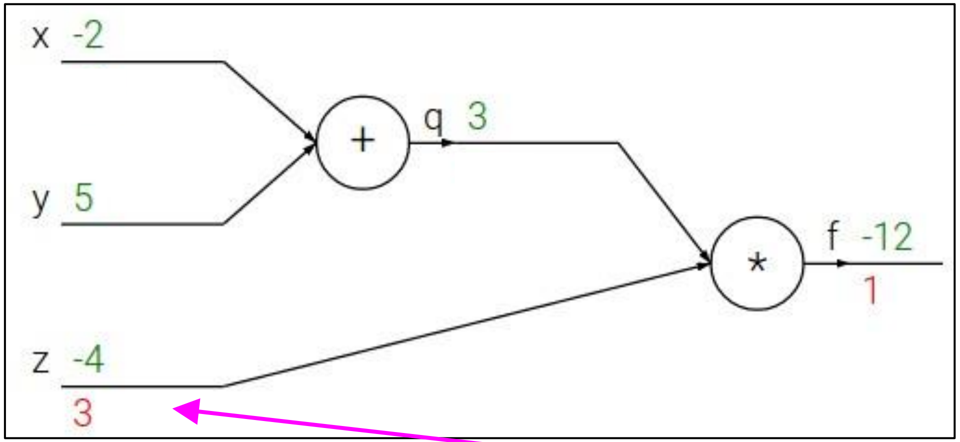
$$f(x, y, z) = (x + y)z$$

e.g. x = -2, y = 5, z = -4

$$q = x + y \qquad \frac{\partial q}{\partial x} = 1, \frac{\partial q}{\partial y} = 1$$

$$f = qz \qquad \frac{\partial f}{\partial q} = z, \frac{\partial f}{\partial z} = q$$

Want: $\frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}, \frac{\partial f}{\partial z}$



$$\frac{\partial f}{\partial z}$$

* Source: Stanford Univ. CS231 Lecture Notes

Backpropagation (7)

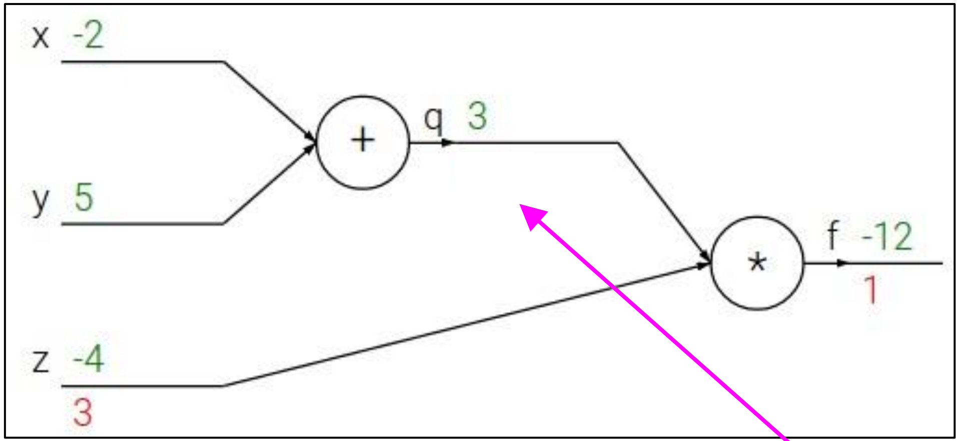
$$f(x, y, z) = (x + y)z$$

e.g. x = -2, y = 5, z = -4

$$q = x + y \qquad \frac{\partial q}{\partial x} = 1, \frac{\partial q}{\partial y} = 1$$

$$f = qz \qquad \frac{\partial f}{\partial q} = z, \frac{\partial f}{\partial z} = q$$

Want: $\frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}, \frac{\partial f}{\partial z}$



$$\frac{\partial f}{\partial q}$$

* Source: Stanford Univ. CS231 Lecture Notes

Backpropagation (8)

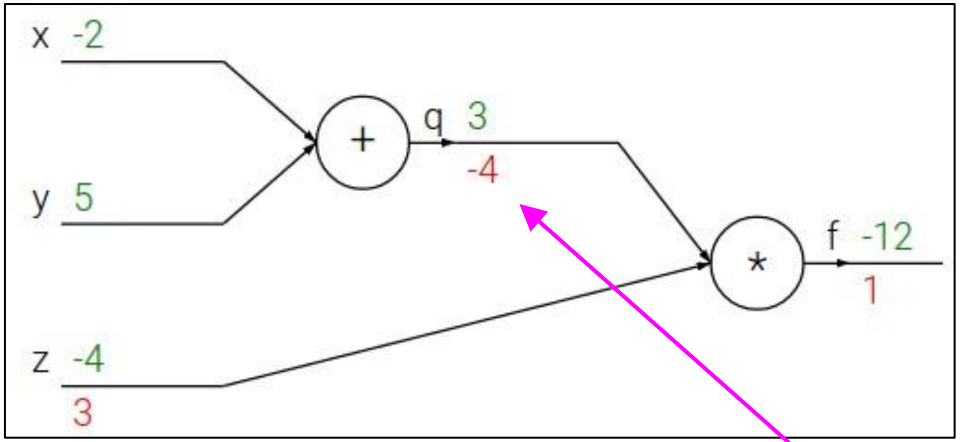
$$f(x, y, z) = (x + y)z$$

e.g. x = -2, y = 5, z = -4

$$q = x + y \qquad \frac{\partial q}{\partial x} = 1, \frac{\partial q}{\partial y} = 1$$

$$f = qz \qquad \frac{\partial f}{\partial q} = z, \frac{\partial f}{\partial z} = q$$

Want: $\frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}, \frac{\partial f}{\partial z}$



$$\frac{\partial f}{\partial q}$$

* Source: Stanford Univ. CS231 Lecture Notes

Backpropagation (9)

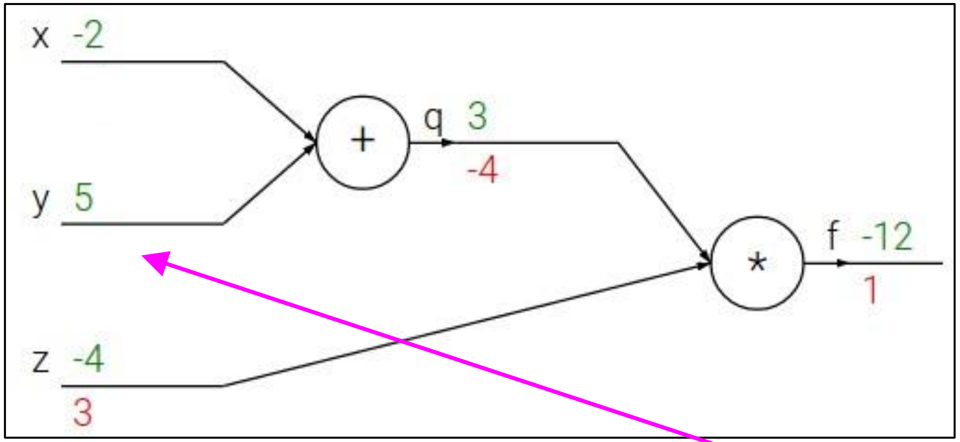
$$f(x, y, z) = (x + y)z$$

e.g. x = -2, y = 5, z = -4

$$q = x + y \qquad \frac{\partial q}{\partial x} = 1, \frac{\partial q}{\partial y} = 1$$

$$f = qz \qquad \frac{\partial f}{\partial q} = z, \frac{\partial f}{\partial z} = q$$

Want: $\frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}, \frac{\partial f}{\partial z}$



$$\boxed{\frac{\partial f}{\partial y}}$$

* Source: Stanford Univ. CS231 Lecture Notes

Backpropagation (10)

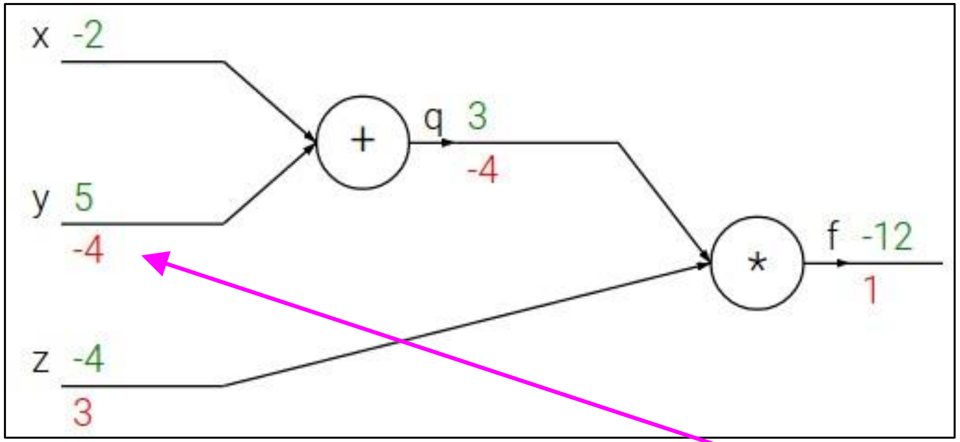
$$f(x, y, z) = (x + y)z$$

e.g. x = -2, y = 5, z = -4

$$q = x + y \qquad \frac{\partial q}{\partial x} = 1, \frac{\partial q}{\partial y} = 1$$

$$f = qz \qquad \frac{\partial f}{\partial q} = z, \frac{\partial f}{\partial z} = q$$

Want: $\frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}, \frac{\partial f}{\partial z}$



$$\frac{\partial f}{\partial y}$$

Chain rule:

$$\frac{\partial f}{\partial y} = \frac{\partial f}{\partial q} \frac{\partial q}{\partial y}$$

* Source: Stanford Univ. CS231 Lecture Notes

Backpropagation (11)

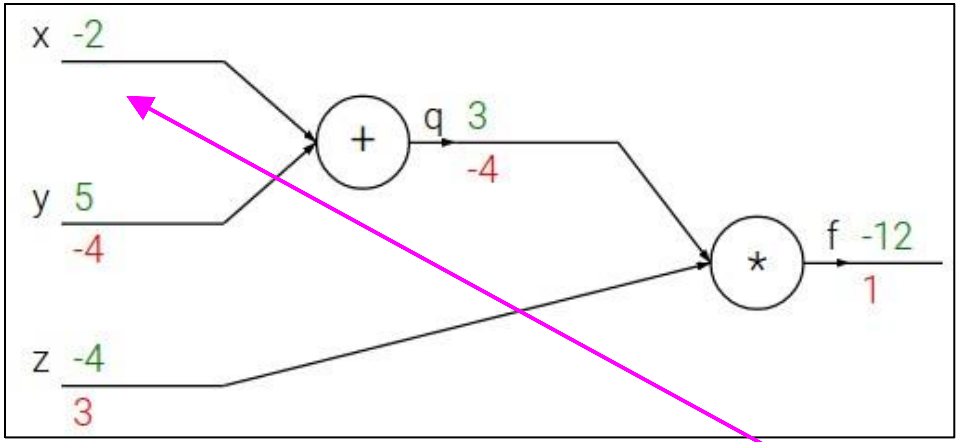
$$f(x, y, z) = (x + y)z$$

e.g. x = -2, y = 5, z = -4

$$q = x + y \qquad \frac{\partial q}{\partial x} = 1, \frac{\partial q}{\partial y} = 1$$

$$f = qz \qquad \frac{\partial f}{\partial q} = z, \frac{\partial f}{\partial z} = q$$

Want: $\frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}, \frac{\partial f}{\partial z}$



$$\boxed{\frac{\partial f}{\partial x}}$$

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* Source: Stanford Univ. CS231 Lecture Notes

Backpropagation (12)

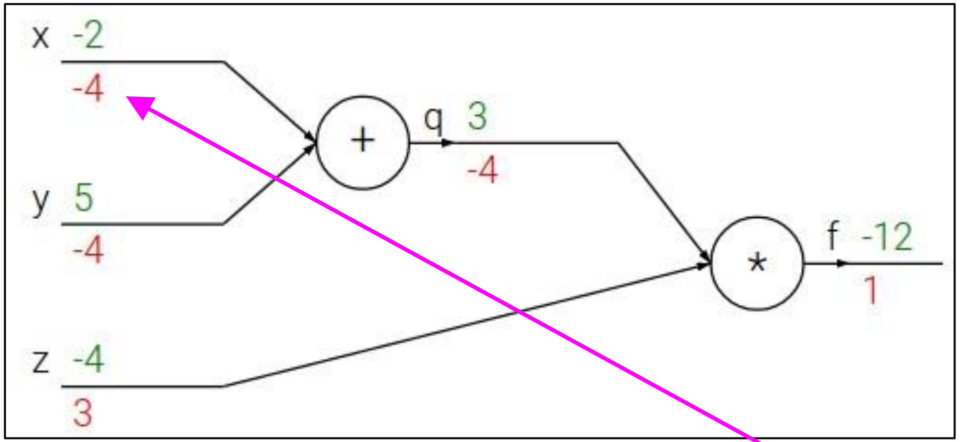
$$f(x, y, z) = (x + y)z$$

e.g. x = -2, y = 5, z = -4

$$q = x + y \qquad \frac{\partial q}{\partial x} = 1, \frac{\partial q}{\partial y} = 1$$

$$f = qz \qquad \frac{\partial f}{\partial q} = z, \frac{\partial f}{\partial z} = q$$

Want: $\frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}, \frac{\partial f}{\partial z}$



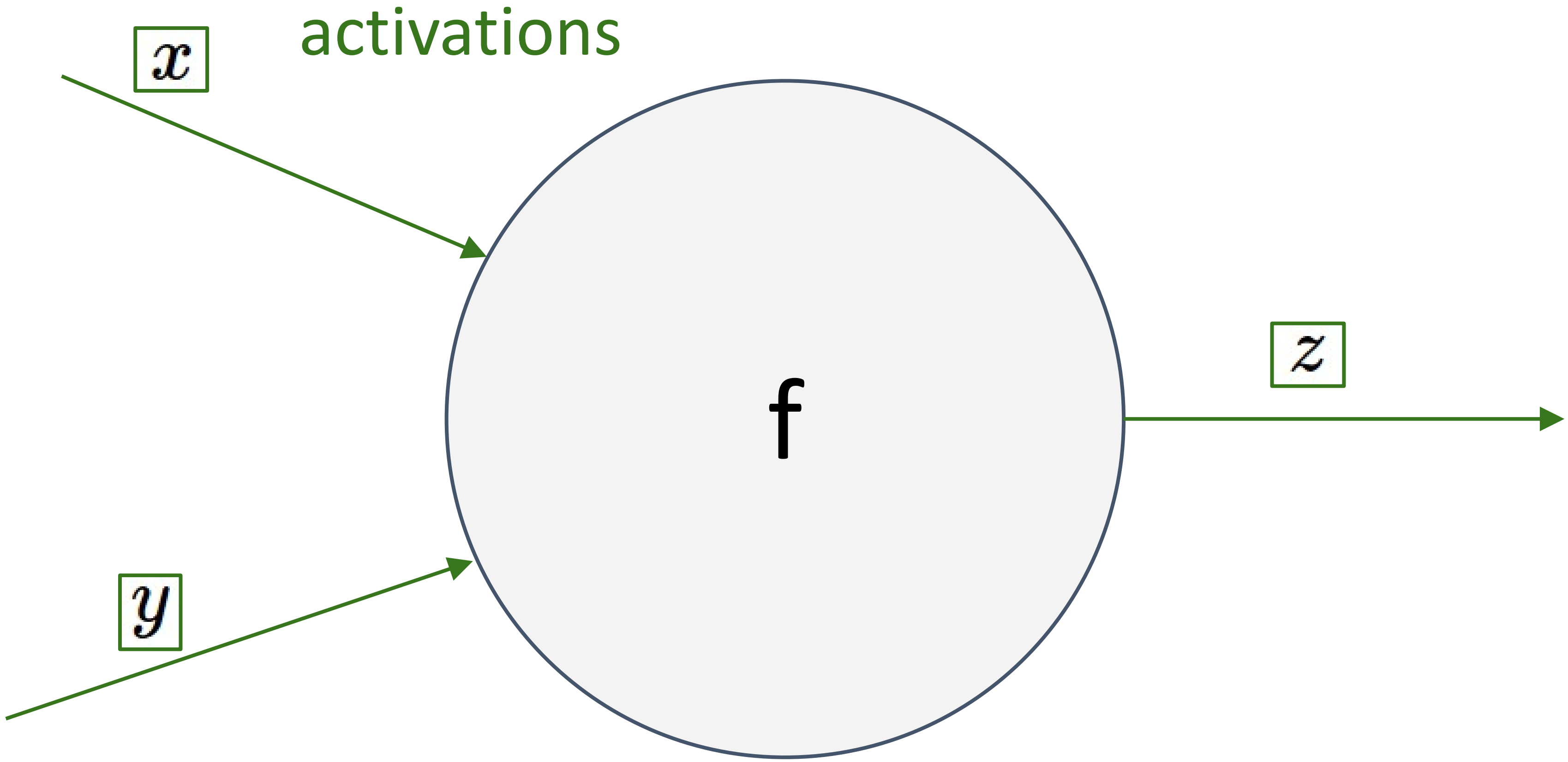
$\frac{\partial f}{\partial x}$

Chain rule:

$$\frac{\partial f}{\partial x} = \frac{\partial f}{\partial q} \frac{\partial q}{\partial x}$$

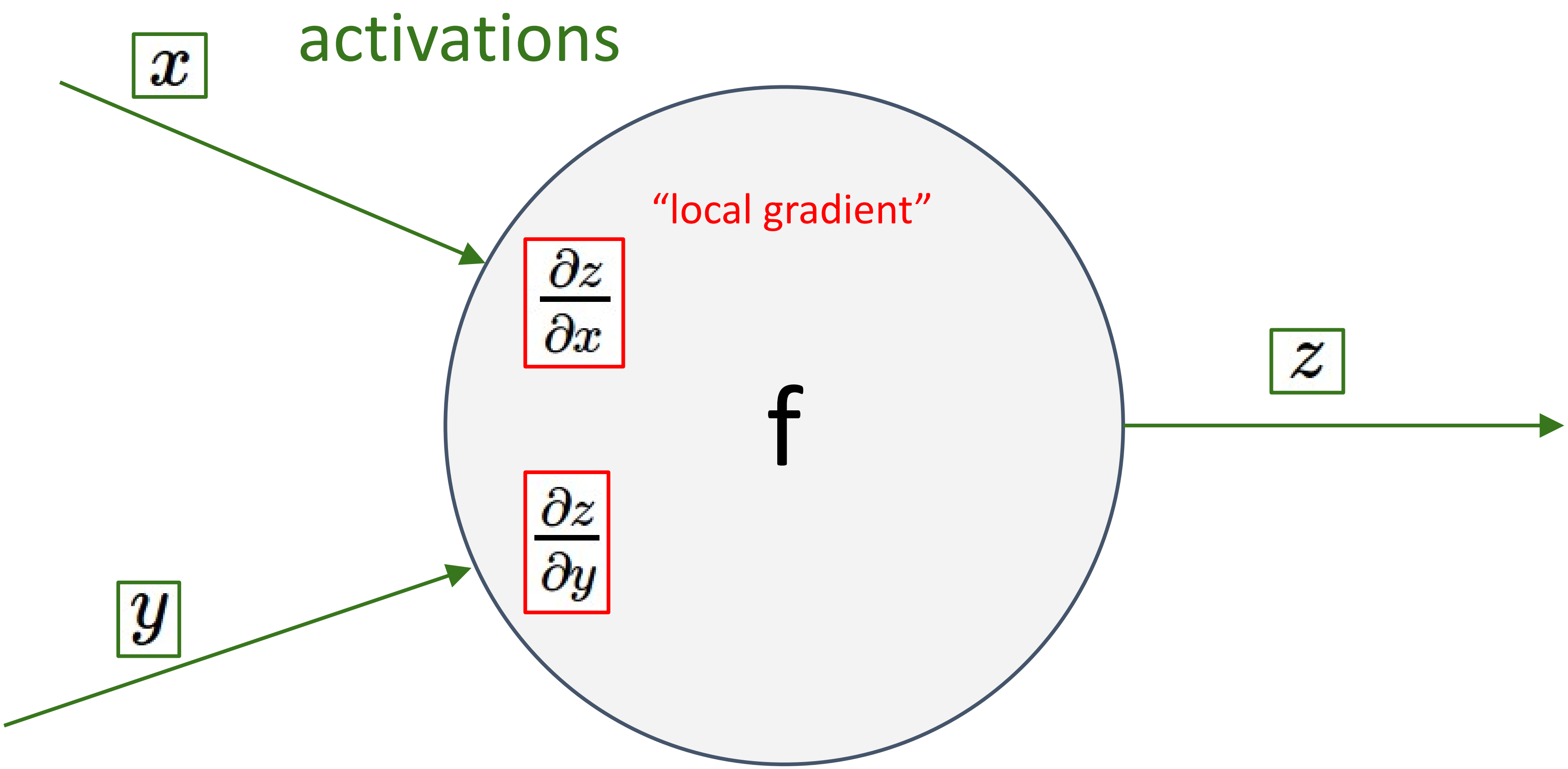
* Source: Stanford Univ. CS231 Lecture Notes

Backpropagation (13)



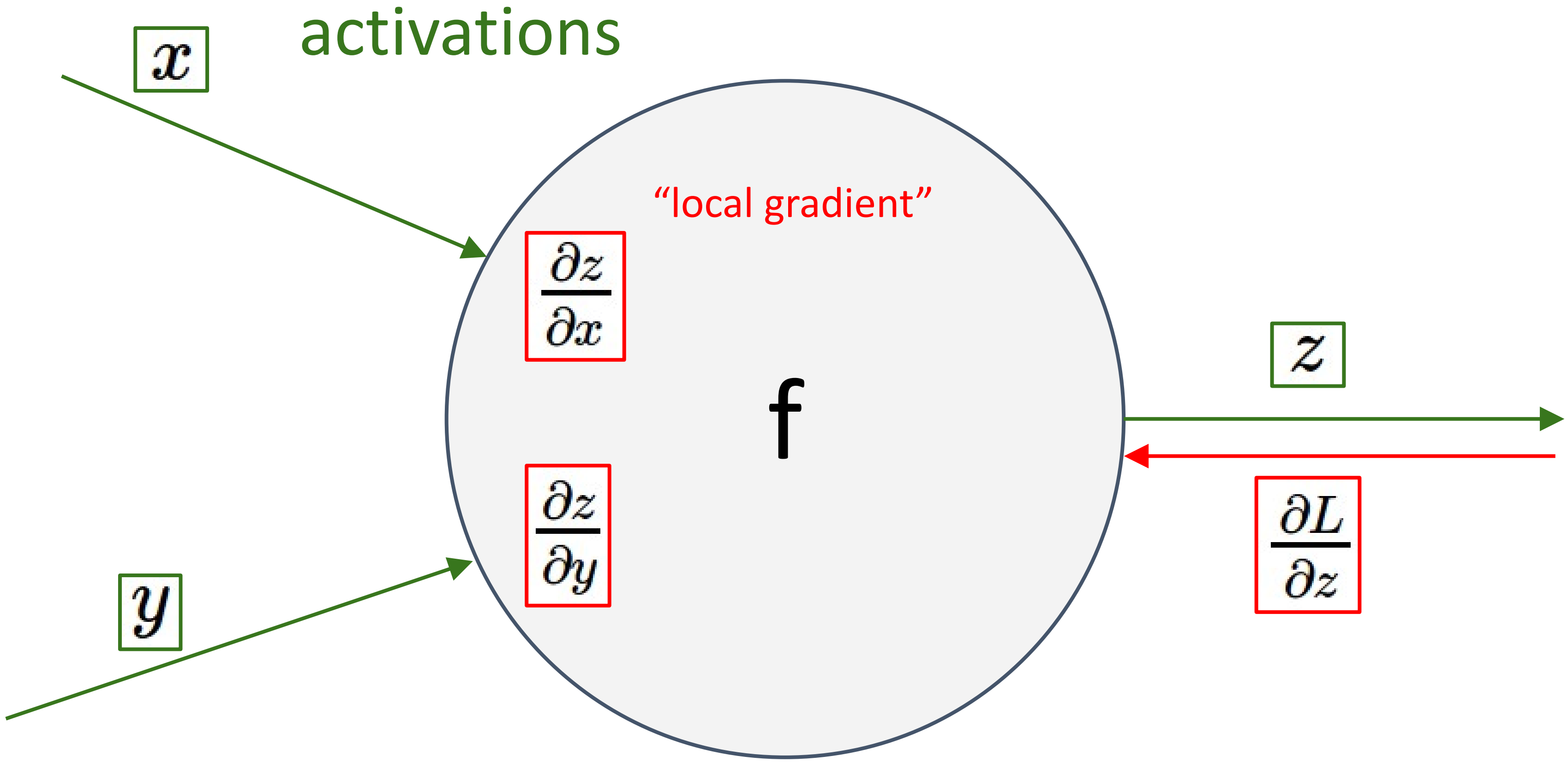
* Source: Stanford Univ. CS231 Lecture Notes

Backpropagation (14)



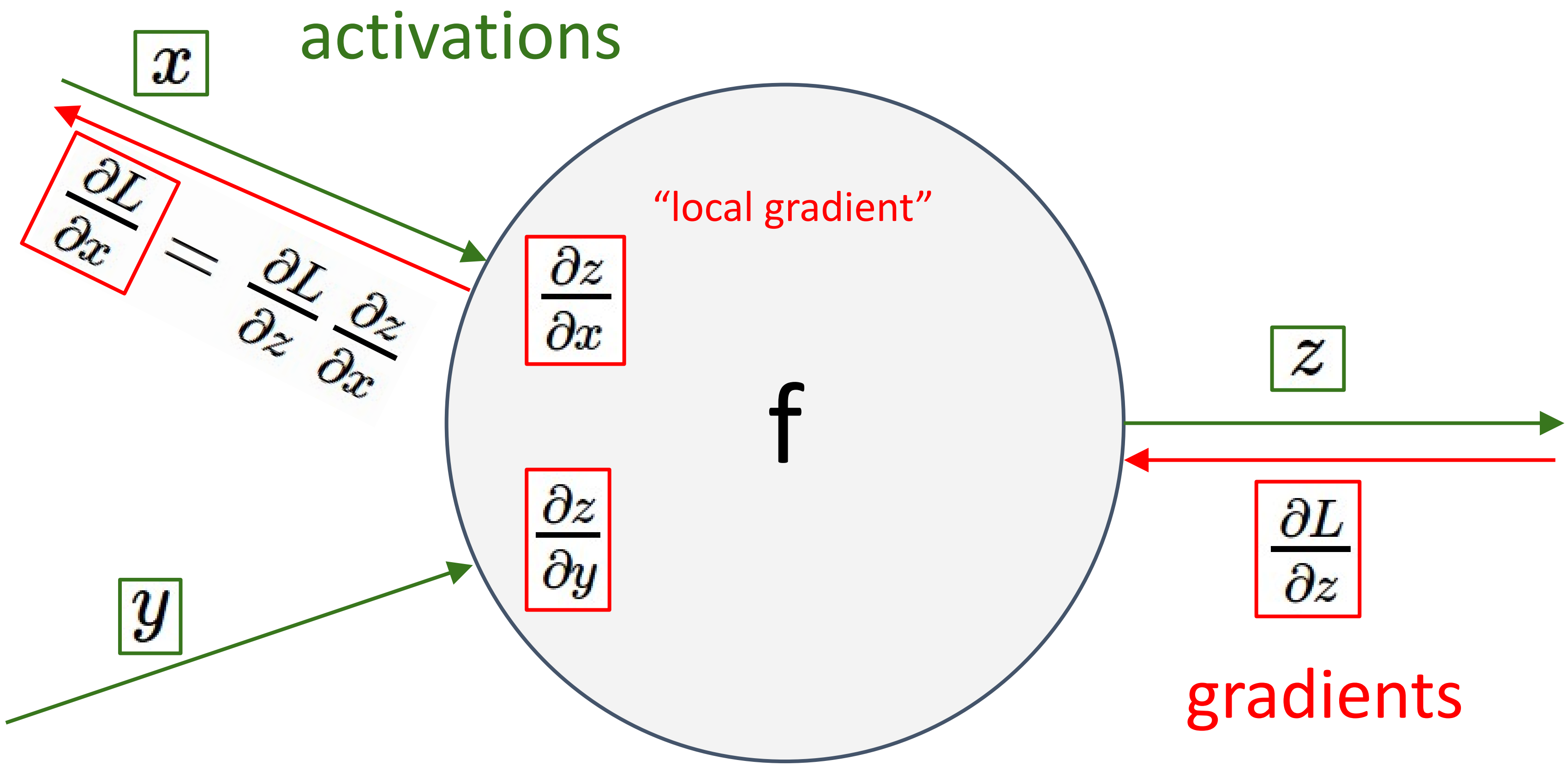
* Source: Stanford Univ. CS231 Lecture Notes

Backpropagation (15)



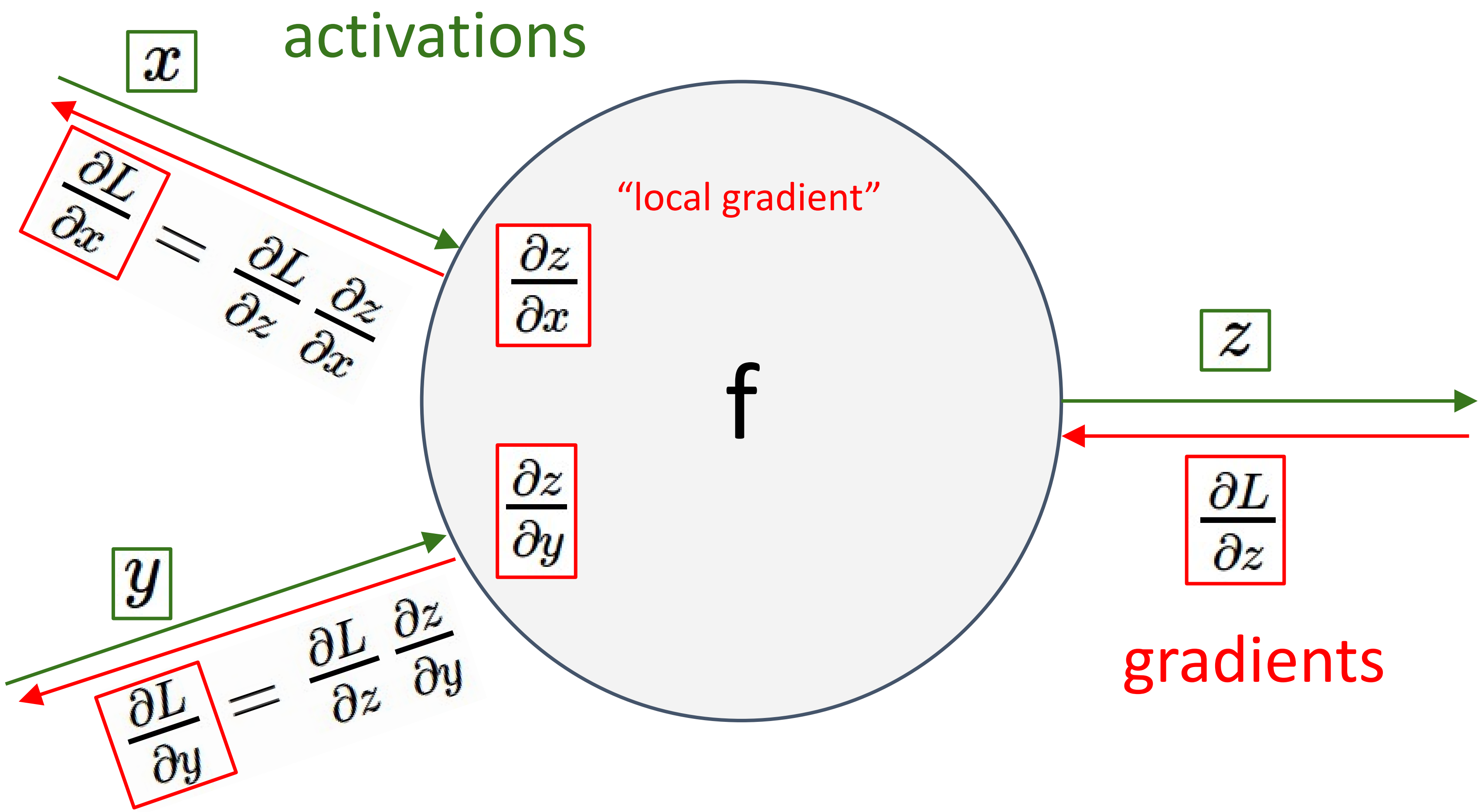
* Source: Stanford Univ. CS231 Lecture Notes

Backpropagation (16)



* Source: Stanford Univ. CS231 Lecture Notes

Backpropagation (17)



* Source: Stanford Univ. CS231 Lecture Notes

Backpropagation (18)

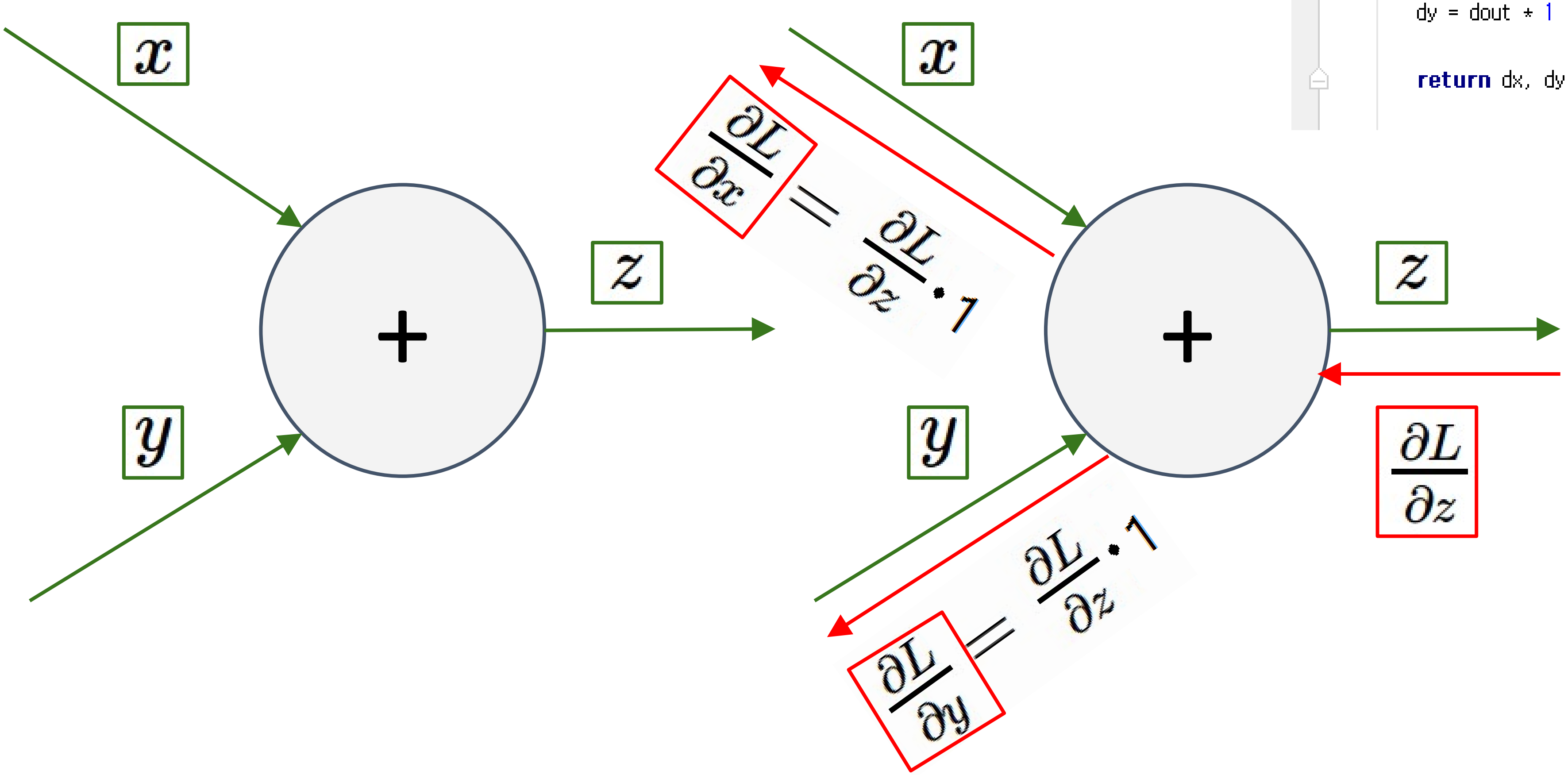
```python
class AddLayer:
    def __init__(self):
        pass

    def forward(self, x, y):
        out = x + y

        return out

    def backward(self, dout):
        dx = dout * 1
        dy = dout * 1

        return dx, dy
```



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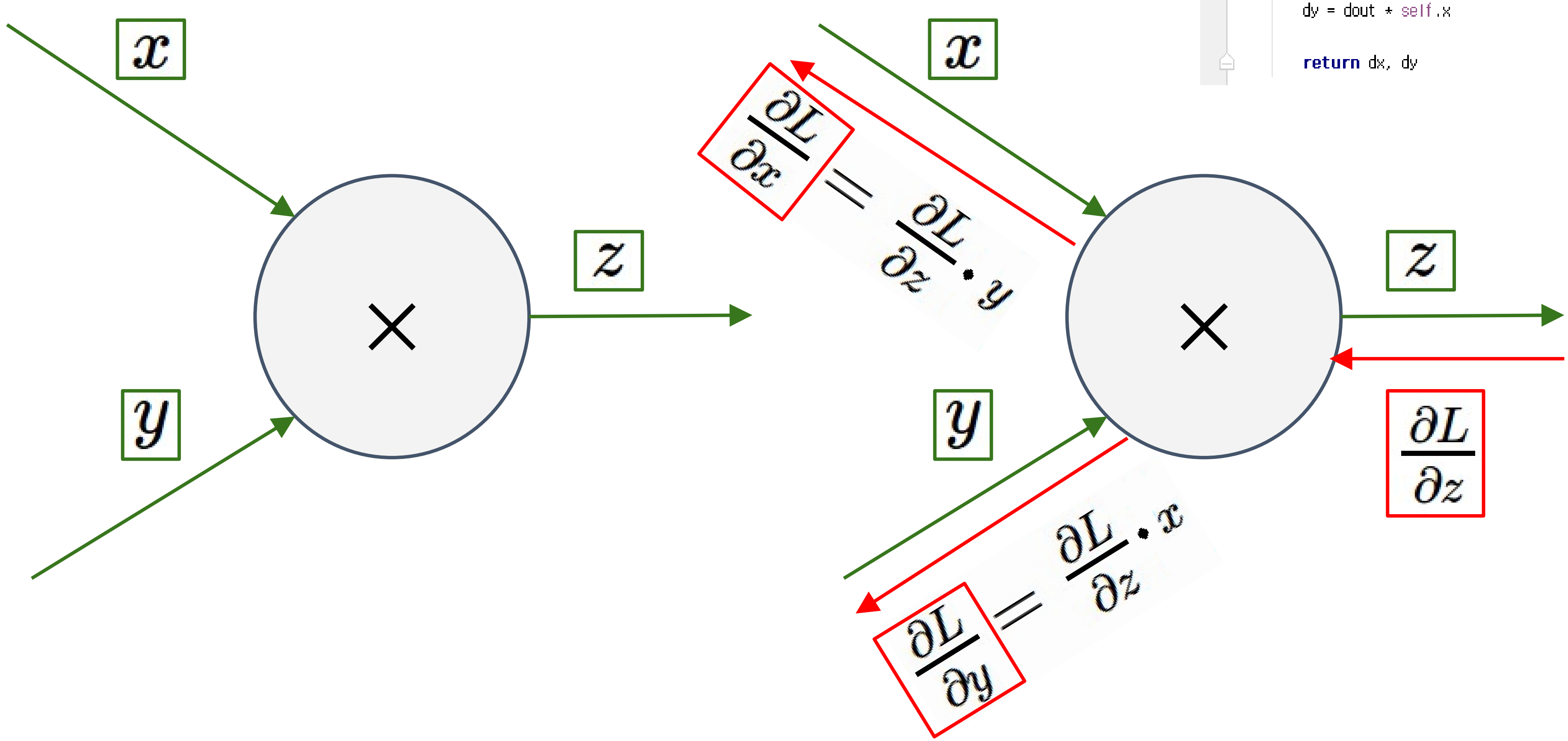
* Source: Stanford Univ. CS231 Lecture Notes

Backpropagation (19)

```python
class MulLayer:
    def __init__(self):
        self.x = None
        self.y = None

    def forward(self, x, y):
        self.x = x
        self.y = y
        out = x * y

        return out

    def backward(self, dout):
        dx = dout * self.y  # x와 y를 바꾼다.
        dy = dout * self.x

        return dx, dy
```

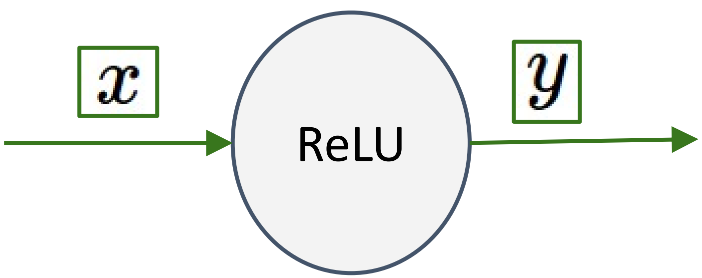


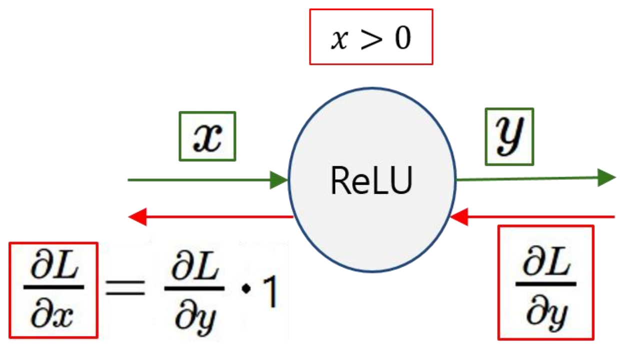
Backpropagation (20)

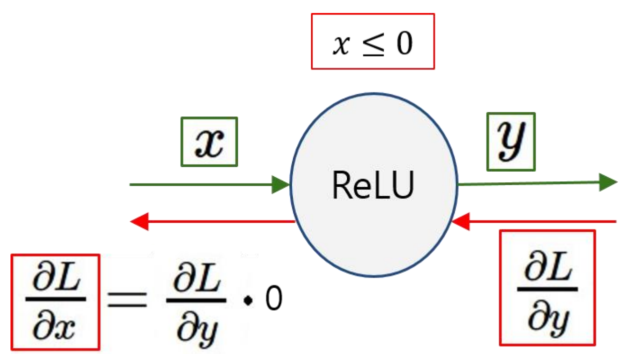
- ReLU

$$y = \begin{cases} x \ (x > 0) \\ 0 \ (x \le 0) \end{cases} \rightarrow \frac{\partial y}{\partial x} = \begin{cases} 1 \ (x > 0) \\ 0 \ (x \le 0) \end{cases}$$

```python
class ReLU:
    def __init__(self):
        self.mask = None

    def forward(self, x):
        self.mask = (x <= 0)
        out = x.copy()
        out[self.mask] = 0

        return out

    def backward(self, dout):
        dout[self.mask] = 0
        dx = dout

        return dx
```



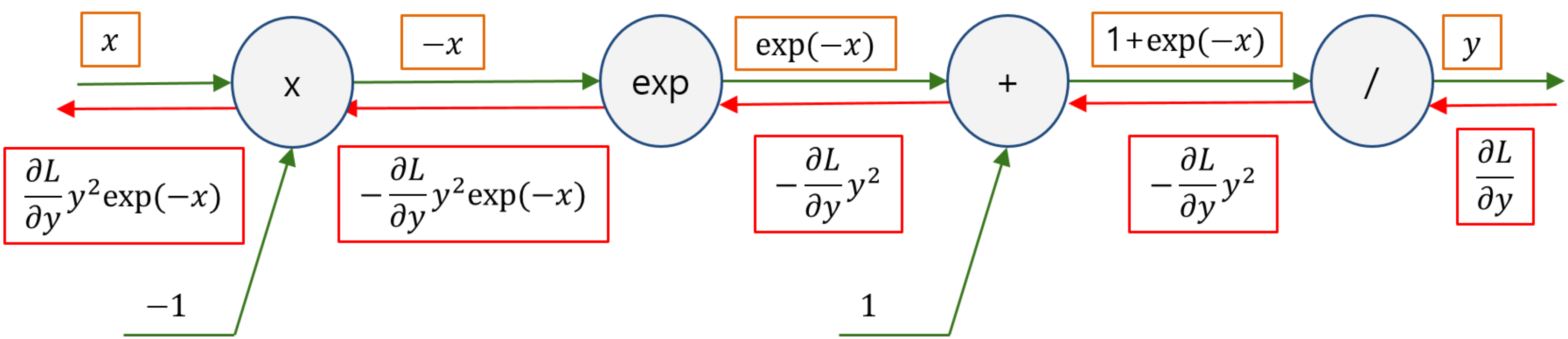




Backpropagation (21)

- Sigmoid

$$y = \frac{1}{1+\exp(-x)} \quad \rightarrow \quad \left(y = \frac{1}{x}, \frac{\partial y}{\partial x} = -\frac{1}{x^2} = -y^2\right), \left(y = \exp(x), \frac{\partial y}{\partial x} = \exp(x)\right)$$



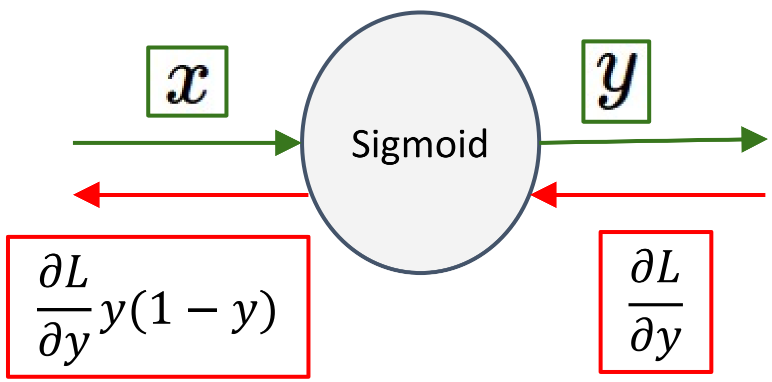
* Source: Stanford Univ. CS231 Lecture Notes

Backpropagation (22)

- Sigmoid (cont.)

$$y = \frac{1}{1+\exp(-x)}$$

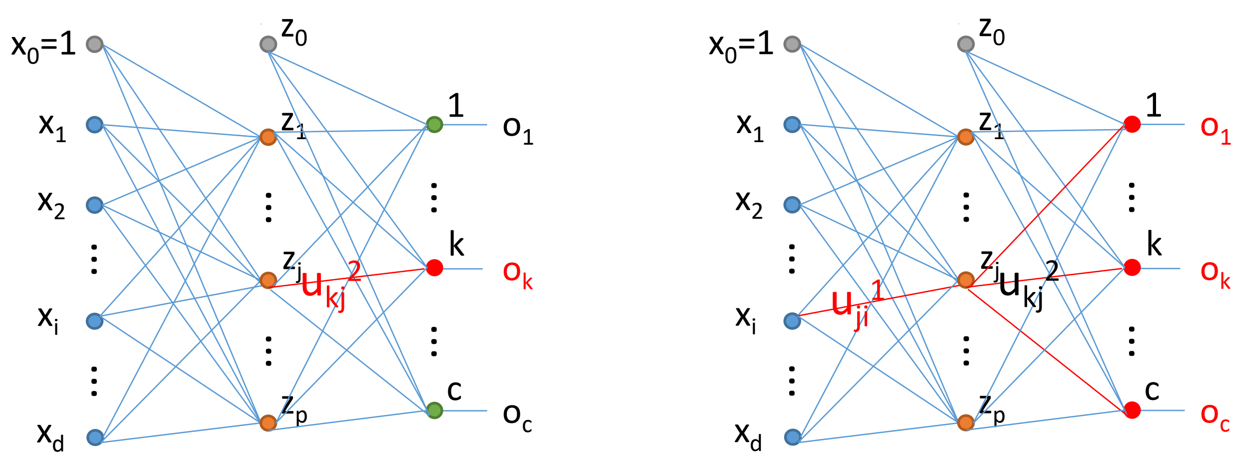
$$\frac{\partial L}{\partial y} y^2 \exp(-x) = \frac{\partial L}{\partial y} \frac{1}{(1+\exp(-x))^2} \exp(-x) = \frac{\partial L}{\partial y} \frac{1}{1+\exp(-x)} \frac{\exp(-x)}{1+\exp(-x)} = \frac{\partial L}{\partial y} y(1-y)$$




```python
class Sigmoid:
    def __init__(self):
        self.out = None

    def forward(self, x):
        out = 1 / (1+np.exp(-x))
        self.out = out

        return out

    def backward(self, dout):
        dx = dout * (1.0 - self.out)*self.out

        return dx
```

Backpropagation Example (1)

- 2-layer ANN
  - MSE Loss function: $E(\theta) = \frac{1}{2}\sum_k (y_k - t_k)^2$
  - 입력 차원 (d), 부류 개수 (c), 은닉층 노드 수 (p), one-hot encoding
  - Layer 1 가중치 행렬: U^1 ($p \times d$), Layer 2 가중치 행렬: U^2 ($c \times p$)



(a) u_{kj}^2가 미치는 영향 (b) u_{ji}^1이 미치는 영향

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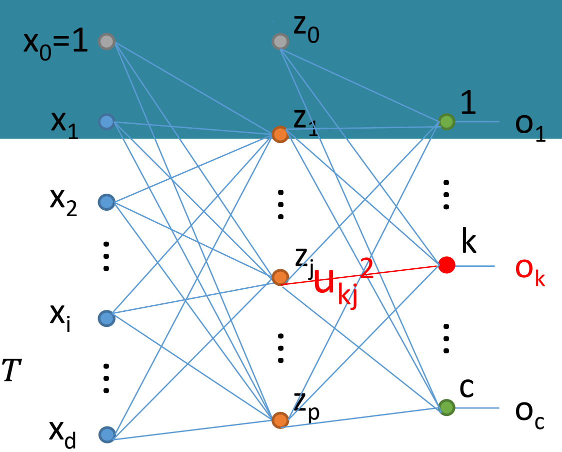
* Source: 기계학습 (오일석), 한빛아카데미

Backpropagation Example (2)



$$o_k = \tau(osum_k), k = 1, 2, \dots, c$$

$$osum_k = u_k^2 \times z,\ u_k^2 = \left(u_{k0}^2, u_{k1}^2, \dots, u_{kp}^2\right), z = (1, z_1, z_2, \dots, z_p)^T$$

$$\frac{\partial E}{\partial u_{kj}^2} = \frac{\partial(0.5\|y - f(U^1, U^2)\|_2^2)}{\partial u_{kj}^2}$$

$$= \frac{\partial(0.5\sum_{q=1}^{c}(y_q - o_q)^2)}{\partial u_{kj}^2} = \frac{\partial(0.5(y_k - o_k)^2)}{\partial u_{kj}^2}$$

$$= -(y_k - o_k)\frac{\partial(o_k)}{\partial u_{kj}^2} = -(y_k - o_k)\frac{\partial\tau(osum_k)}{\partial u_{kj}^2}$$

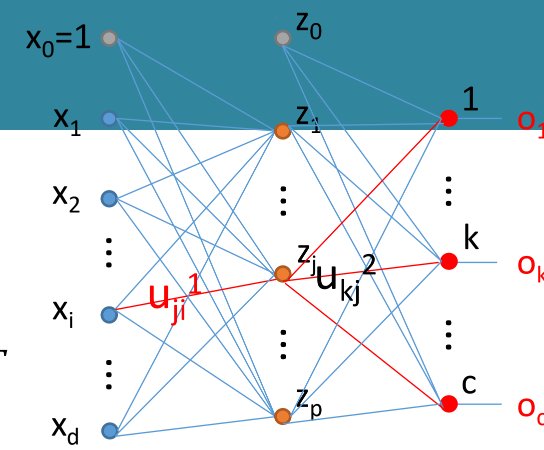
$$= -(y_k - o_k)\tau'(osum_k)\frac{\partial(osum_k)}{\partial u_{kj}^2}$$

$$= -(y_k - o_k)\tau'(osum_k)z_j$$

$$\boxed{\begin{aligned} &\delta_k = (y_k - o_k)\tau'(osum_k), 1 \le k \le c \\ &\frac{\partial E}{\partial u_{kj}^2} = -\delta_k z_j, 0 \le j \le p, 1 \le k \le c \end{aligned}}$$

* Source: 기계학습 (오일석), 한빛아카데미

Backpropagation Example (3)



$$z_j = \tau(zsum_j), j = 1, 2, \dots, p$$

$$zsum_j = u_j^1 \times x,\ u_j^1 = (u_{j0}^1, u_{j1}^1, \dots, u_{jd}^1),\ x = (1, x_1, x_2, \dots, x_d)^T$$

$$\frac{\partial E}{\partial u_{ji}^1} = \frac{\partial(0.5\|y - f(U^1, U^2)\|_2^2)}{\partial u_{ji}^1}$$

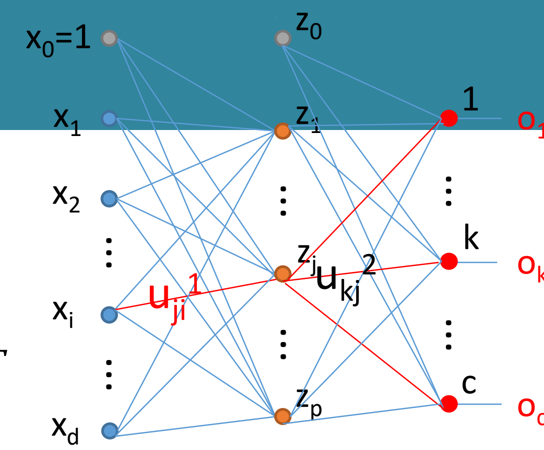
$$= \frac{\partial(0.5\sum_{q=1}^{c}(y_q - o_q)^2)}{\partial u_{ji}^1} = -\sum_{q=1}^{c}(y_q - o_q)\frac{\partial(o_q)}{\partial u_{ji}^1}$$

$$= -\sum_{q=1}^{c}(y_q - o_q)\,\tau'(osum_q)\frac{\partial(osum_q)}{\partial u_{ji}^1}$$

$$= -\sum_{q=1}^{c}(y_q - o_q)\,\tau'(osum_q)\frac{\partial(osum_q)}{\partial z_j}\frac{\partial(z_j)}{\partial u_{ji}^1}$$

$$= -\sum_{q=1}^{c}(y_q - o_q)\,\tau'(osum_q)u_{qj}^2\frac{\partial(z_j)}{\partial u_{ji}^1}$$

Backpropagation Example (3)



$$z_j = \tau(zsum_j), j = 1, 2, \dots, p$$

$$zsum_j = u_j^1 \times x,\ u_j^1 = (u_{j0}^1, u_{j1}^1, \dots, u_{jd}^1),\ x = (1, x_1, x_2, \dots, x_d)^T$$

$$= -\sum_{q=1}^{c} (y_q - o_q)\,\tau'(osum_q) u_{qj}^2 \frac{\partial (z_j)}{\partial u_{ji}^1}$$

$$= -\sum_{q=1}^{c} (y_q - o_q)\,\tau'(osum_q) u_{qj}^2 \tau'(zsum_j) x_i$$

$$= -\tau'(zsum_j) x_i \underbrace{\sum_{q=1}^{c} (y_q - o_q)\,\tau'(osum_q) u_{qj}^2}_{\delta_q}$$

$$\boxed{\begin{aligned} \delta_k &= (y_k - o_k)\tau'(osum_k), 1 \le k \le c \\ \frac{\partial E}{\partial u_{kj}^2} &= -\delta_k z_j, 0 \le j \le p, 1 \le k \le c \end{aligned}}$$

$$\boxed{\begin{aligned} \eta_j &= \tau'(zsum_j) \sum_{q=1}^{c} \delta_q u_{qj}^2, 1 \le j \le p \\ \frac{\partial E}{\partial u_{ji}^1} &= -\eta_j x_i, 0 \le i \le d, 1 \le j \le p \end{aligned}}$$

Training Process (1)

- 배치 학습 (batch learning)
  - 모든 훈련 샘플에 대해 계산되는 $E_n(w)$의 합을 오차함수로 사용

$$E(w) = \sum_{n=1}^{N} E_n(w)$$

- 확률적 경사 하강법 (SGD: Stochastic Gradient Descent)
  - 샘플의 일부, 극단적으로는 샘플 하나만을 사용하여 가중치 업데이트 수행
  - DNN에서는 배치 학습보다는 SGD를 더 많이 사용

Training Process (2)

▪ Minibatch

- 샘플 한 개 단위가 아니라 몇 개의 샘플을 하나의 작은 집합으로 묶은 단위 (e.g., minibatch)로 가중치 업데이트 수행

$$E(w) = \frac{1}{N_t}\sum_{n \in D_t}^{N} E_n(w)\,, N_t = |D_t|$$

- 일반적으로 $D_t(t = 1, 2, \ldots)$는 학습 시작 전에 결정하여 고정
  - 미니배치의 크기는 대체로 10~100개 샘플 전후로 결정하는 경우가 많음
  - 클래스의 수가 10~100개 정도이면서 클래스의 출현 빈도가 서로 같을 경우 분류하려는 클래스 수와 같은 크기의 미니배치를 생성하는 것이 좋음
  - 클래스 수가 그 이상인 경우 샘플을 랜덤으로 섞은 후에 미니배치를 분할

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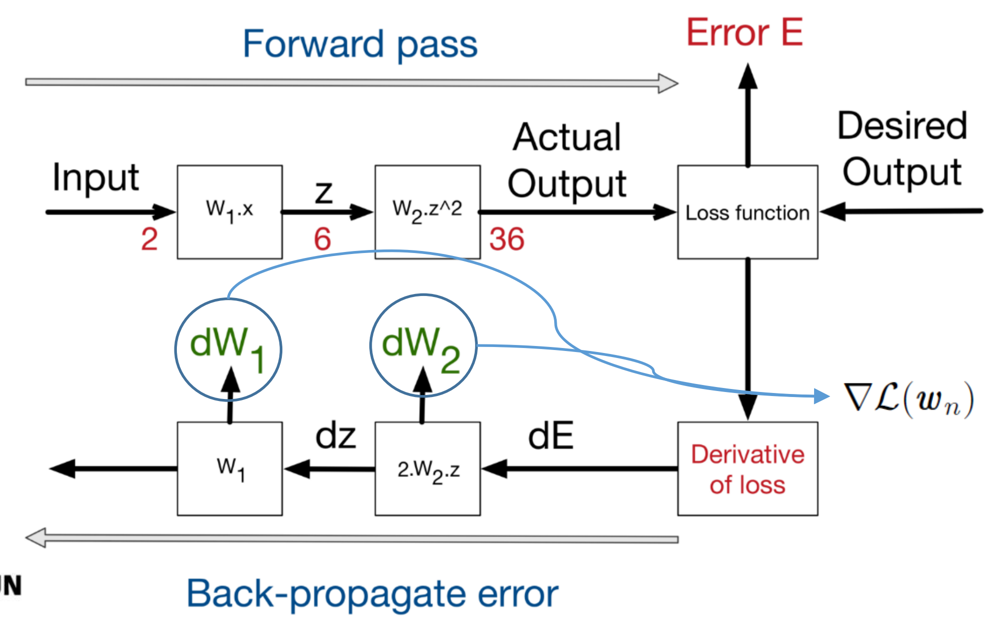
Training Process (3)

- The objective of training process

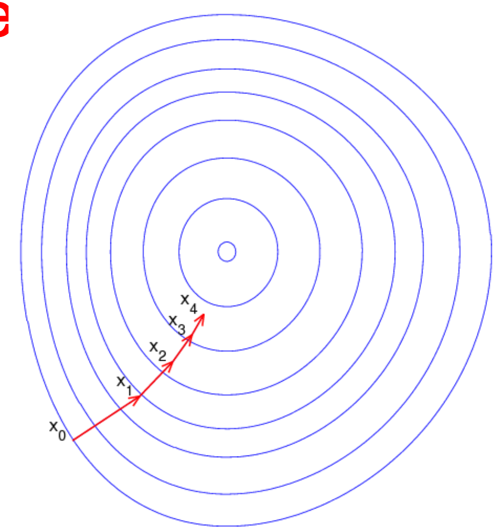
$$\boldsymbol{w}^* = \operatorname*{argmin}_{\boldsymbol{w}} \frac{1}{N}\sum_{i=1}^{N} l(\boldsymbol{w}, \boldsymbol{x}_i, t_i) + \mathcal{R}(\boldsymbol{w})$$

- At each iteration, we need to compute

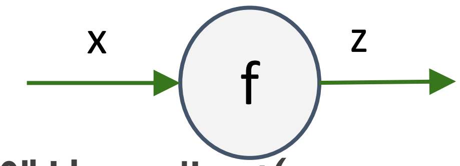
$$\boldsymbol{w}_{n+1} = \boldsymbol{w}_n - \gamma_n \nabla \mathcal{L}(\boldsymbol{w}_n)$$



$$\nabla \mathcal{L}(\boldsymbol{w}_n) = \frac{1}{N}\sum_{i=1}^{N} \nabla l(\boldsymbol{w}_n, \boldsymbol{x}_i, t_i) + \nabla \mathcal{R}(\boldsymbol{w}_n)$$

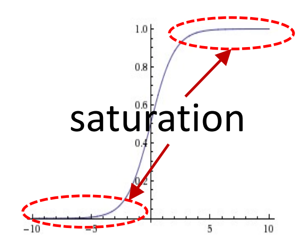


Vanishing Gradient Program (1)



- Vanishing Gradient란?
  - NN의 depth가 깊어지게 되면 $w_{n+1} = w_n - \alpha \times \nabla f(= \frac{\partial f}{\partial x})$ 에서 gradient(e.g., $\frac{\partial f}{\partial x}$)가 아주 작은 값을 가지게 되며, 따라서 Input Layer에 가까운 Layer일 수록 w에 변화가 거의 없어지게 됨
- Why does it happen?
  - $\frac{\partial L}{\partial x} = \frac{\partial z}{\partial x}\frac{\partial L}{\partial z}$가 되며 이 중 하나의 항이라도 0에 가까울수록 $\frac{\partial L}{\partial x}$는 0에 가까워지며 결과적으로 $\alpha \times \nabla f$ 이 0에 가까워짐에 따라 w_{n+1}과 w_n이 변화가 없게 됨
  - Sigmoid 함수를 사용하게 될 경우 함수가 saturation이 되는 부분에서는 기울기의 변화가 거의 없으며 따라서 $\frac{\partial z}{\partial x}$(e.g., local gradient)가 0에 가깝게 됨
  - Output Layer에서 가까운 neuron이 항상 1에 가까운 값을 낼 경우, 즉 Saturation 될 경우 그 neuron과 연결된 앞쪽 Layer에서 사용되는 w는 거의 변화가 없어지게 됨

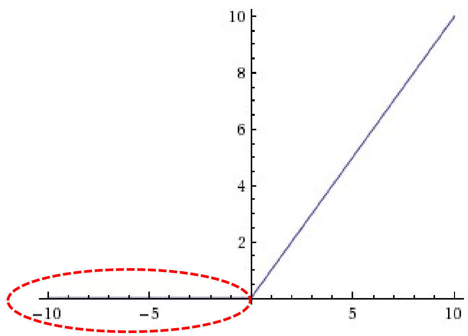
  ➔ Error의 Backpropagation이 제대로 이루어지지 않음



Vanishing Gradient Problem (2)

ReLU 함수를 사용할 경우

- ReLU는 x가 0보다 큰 경우 선형적으로 증가하기 때문에 $\frac{\partial z}{\partial x}$(e.g., local gradient)가 0이 되는 경우는 발생하지 않음. 따라서 gradient가 0에 근접하는 경우는 발생하지 않음
- 그러나 특정 neuron이 선택되지 않는 경우 (즉, ReLU의 output이 0이 발생하는 구간)에는 local gradient, 즉 $\frac{\partial z}{\partial x} = 0$이 됨. 따라서 해당 neuron과 연결된 앞쪽 neuron의 경우 gradient가 항상 0이 되기 때문에 w에 변화가 발생하지 않음



Parameter Updates (1)

- SGD

$$W \leftarrow W - \eta \frac{\partial L}{\partial W}$$

- Momentum

$$v \leftarrow \alpha v - \eta \frac{\partial L}{\partial W}$$

$$W \leftarrow W + v$$

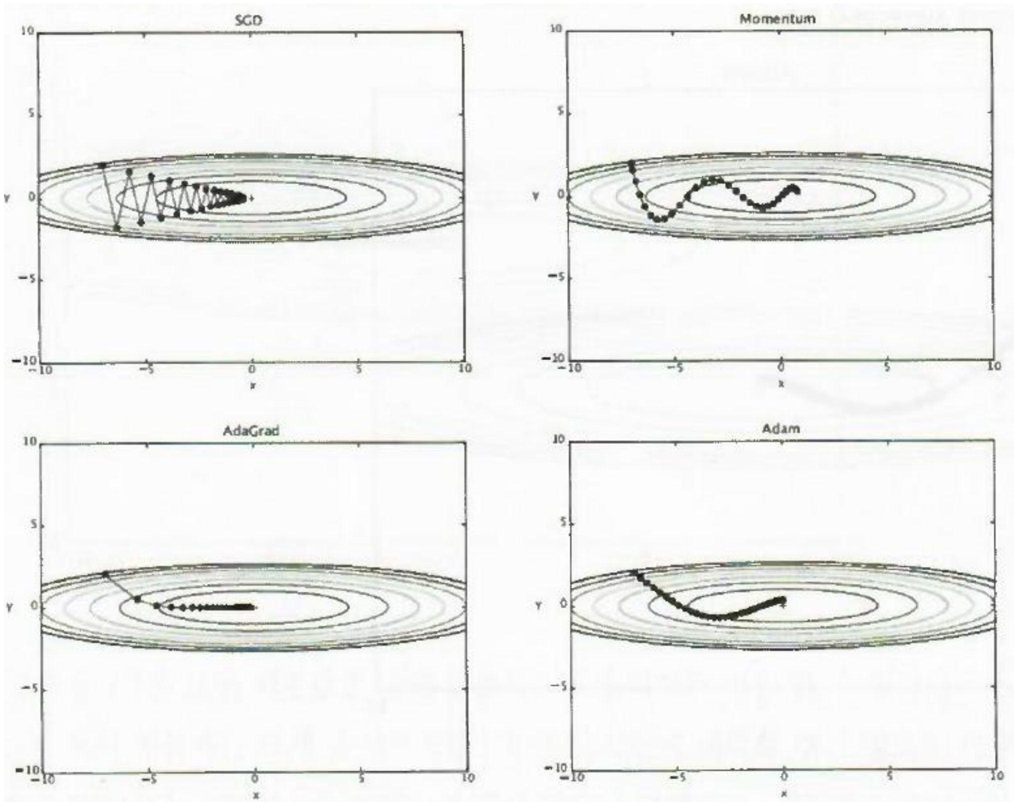
- AdaGrad
  - 각각의 매개변수를 대상으로 학습률 감소(learning rate decay) 적용

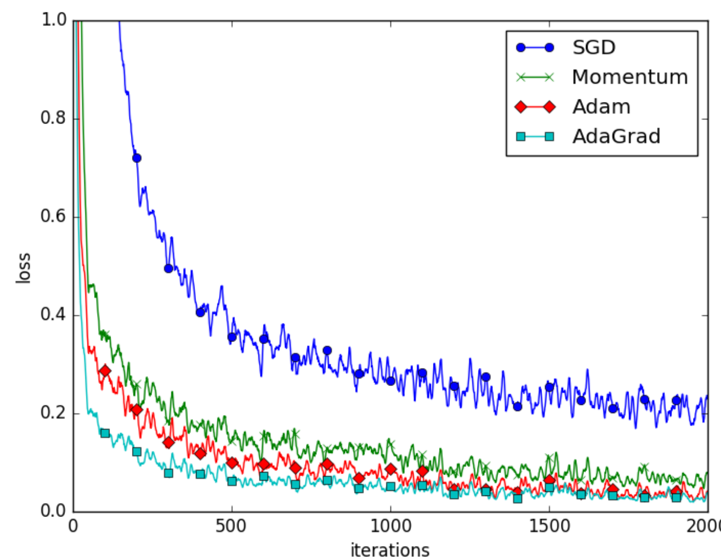
$$h \leftarrow h + \frac{\partial L}{\partial W} \cdot \frac{\partial L}{\partial W}$$

$$W \leftarrow W + \eta \frac{1}{\sqrt{h}} \frac{\partial L}{\partial W}$$

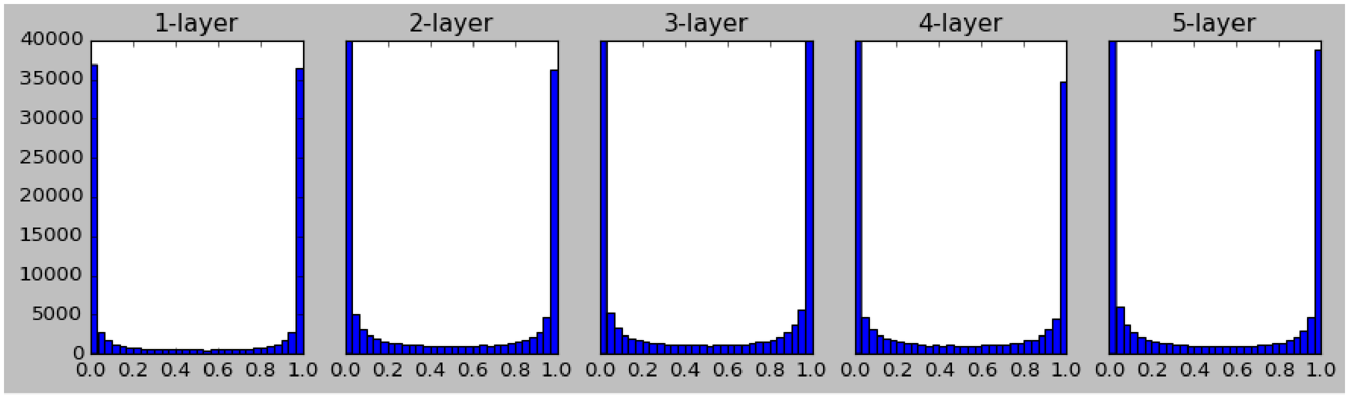
- Adam
  - Momentum + AdaGrad

Parameter Updates (2)

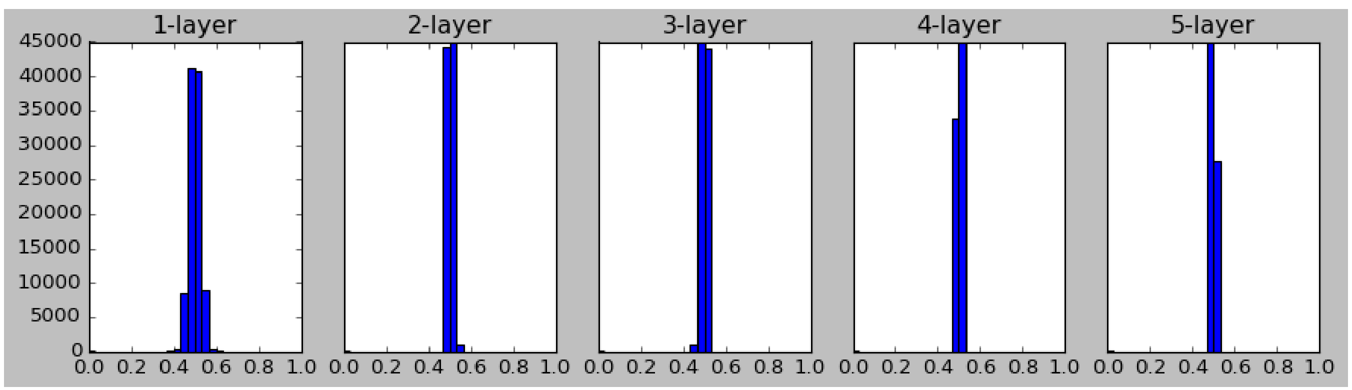




Initialization (1)



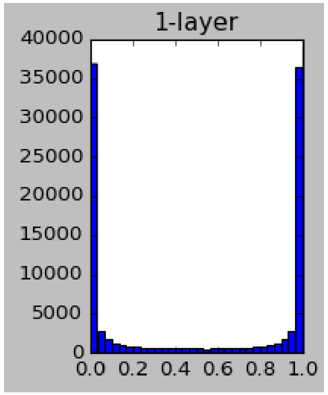
가중치를
표준편차가 1인
정규분포로
초기화할 때의 각
층의 활성화값
분포



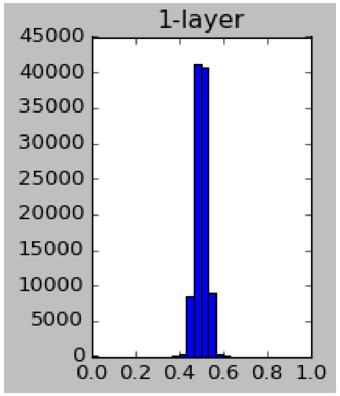
가중치를
표준편차가 0.01인
정규분포로
초기화할 때의 각
층의 활성화값
분포

Initialization (2)

- **각 층의 활성화값 (활성화 함수의 출력 데이터)은 적당히 골고루 분포되어야 함**
  - 층과 층 사이에 적당하게 다양한 데이터가 흐르게 해야 신경망 학습이 효율적으로 이루어짐
  - 반대로 치우친 데이터가 흐르면 기울기 소실이나 표현력 제한 문제에 빠져 학습이 잘 이루어지지 않는 경우 발생



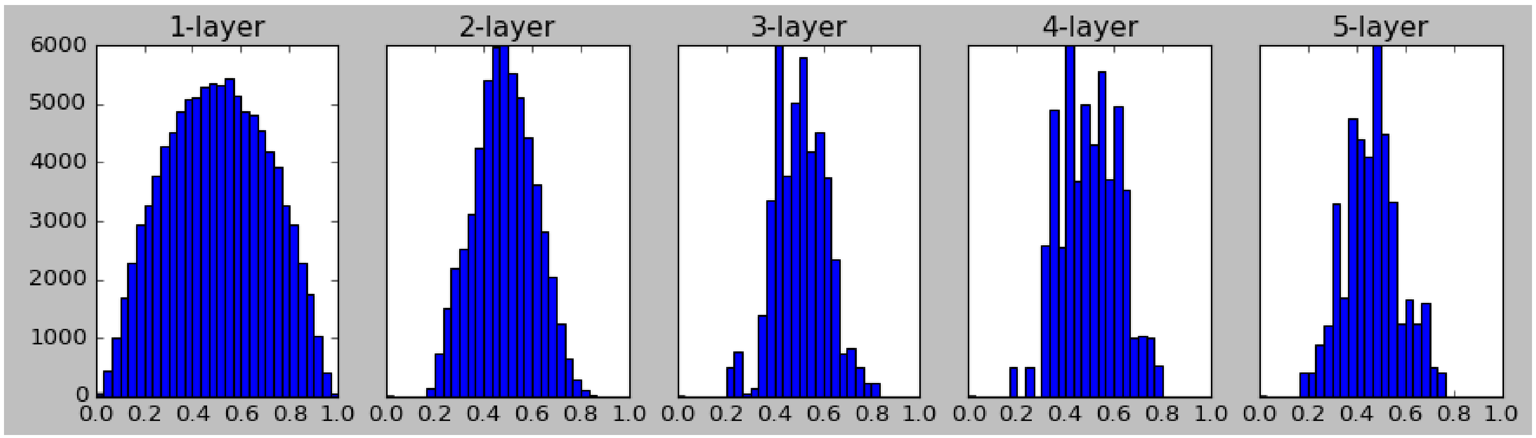
데이터가 0과 1에 치우쳐지게 분포
→ Sigmoid 함수의 Saturation Point
→ Vanishing Gradient 문제 발생



다수의 뉴런의 유사한 값 출력
→ 뉴런을 여러 개 둔 의미가 없어짐
(100개의 뉴런이 같은 값을 가질 경우
1개의 뉴런으로 구성하는 것과 동일

Initialization (3)

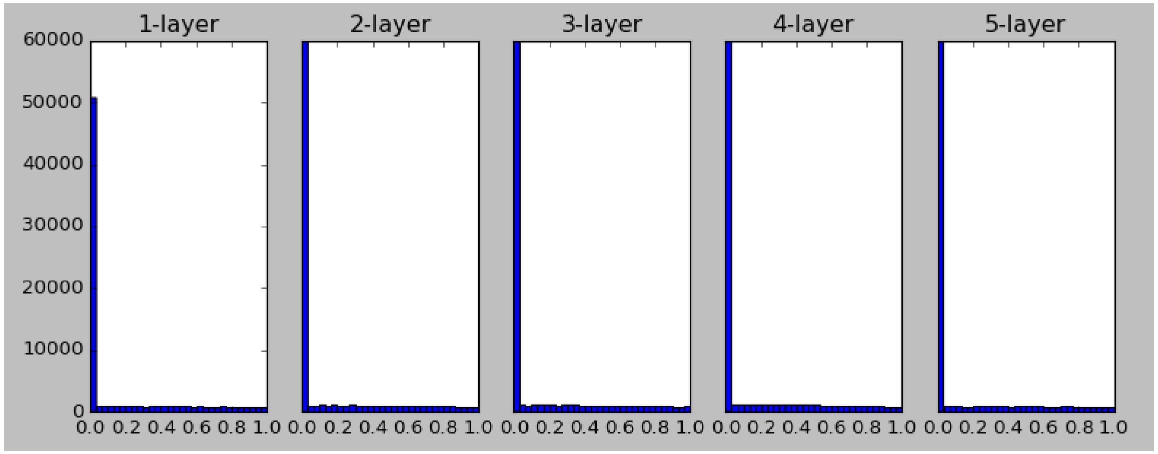
- Xavier Initialization
  - 표준편차가 ($^1/_{\sqrt{n}}$)인 정규 분포로 가중치 초기값 설정 (n: 앞 층의 노드 수)



  - Sigmoid, tanh 등 활성화 함수가 선형일 때 사용 (좌우 대칭 형태이므로 중앙 부근이 선형으로 볼 수 있음

Initialization (4)

- He Initialization
  - 표준편차가 ($1/\sqrt{n/2}$)인 정규 분포로 가중치 초기값 설정 (n: 앞 층의 노드 수)



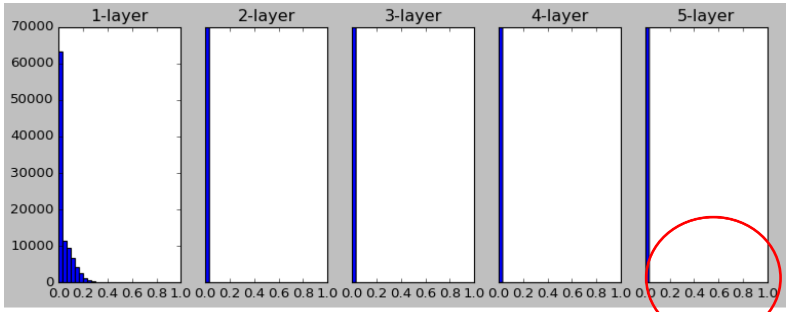
  - 활성화 함수로 ReLU 함수를 사용할 때 사용

Initialization (5)

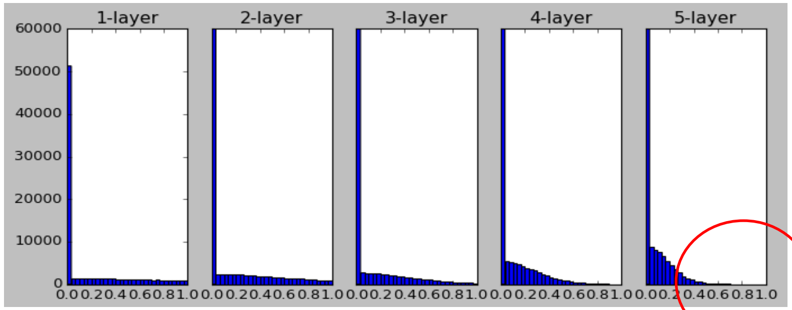
- Bias Initialization
  - Bias는 0으로 초기화하는 것이 보편적
  - ReLU를 사용할 경우 0.01과 같은 작은 값으로 초기화하면 성능 향상 효과가 있다는 보고도 있으나 모든 경우 그렇지는 않음

Initialization (6)

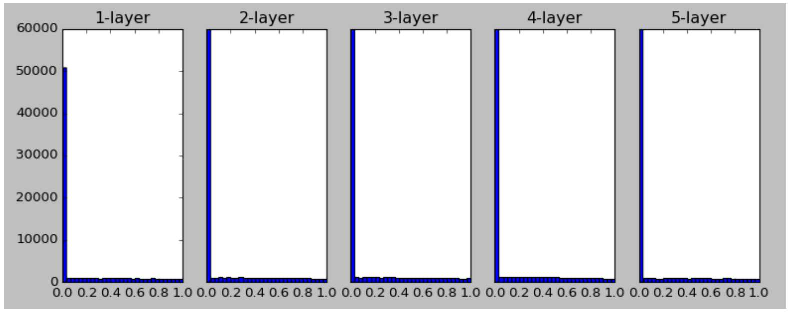
- 활성화 함수로 ReLU를 사용한 경우 가중치 초기값에 따른 활성화값 분포 변화



[표준편차가 0.01인 정규분포]()
→ 역전파 시 가중치의 기울기 역시 작아짐
→ 학습이 거의 이루어지지 않음



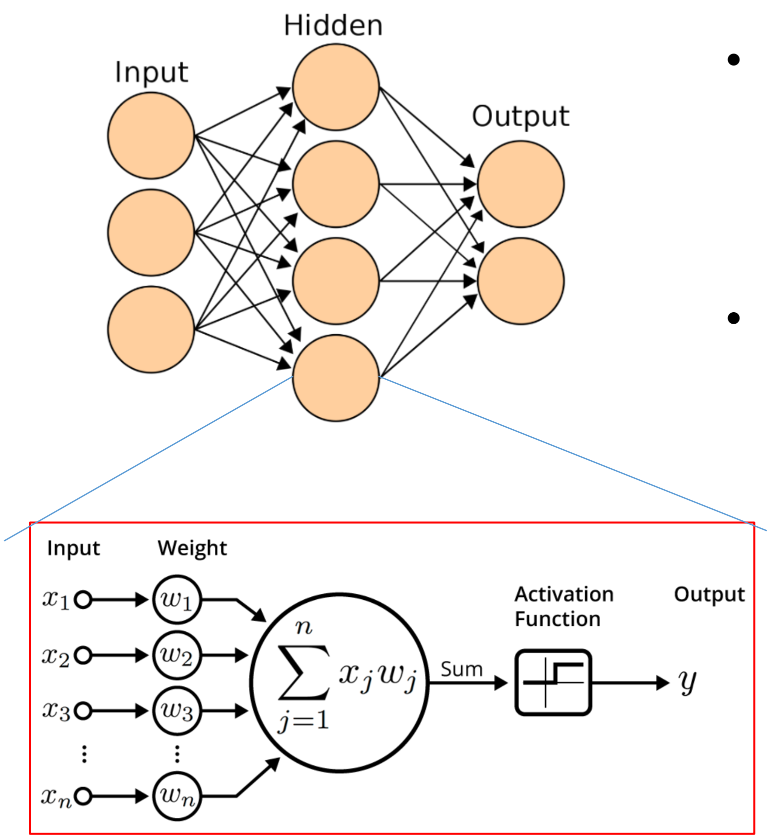
[Xavier 초기값]()
→ Vanishing Gradient 문제 발생 가능



[He 초기값]()
→ 층이 깊어져도 분포가 모든 층에서 균일하게 분포

Wrap-Up

■ Multi-Layer Perceptron



- 학습 목표 → Loss function

$$\mathcal{L}(\boldsymbol{w}) = \frac{1}{N}\sum_{i=1}^{N} l(\boldsymbol{w}, \boldsymbol{x}_i, t_i) + \mathcal{R}(\boldsymbol{w})$$

- 학습 방법 → Gradient Descent Method

$$W \leftarrow W - \eta \frac{\partial L}{\partial W}$$

References

- CS231n: Convolutional Neural Networks for Visual Recognition, http://cs231n.stanford.edu/
- 라온피플 머신러닝 아카데미, https://laonple.blog.me/
- 밑바닥부터 시작하는 딥러닝, 한빛미디어
- 기초 수학으로 이해하는 머신러닝 알고리즘, 위키북스
- 딥러닝 제대로 시작하기, 제이펍
- 기계학습, 한빛아카데미


ANY
QUESTIONS?