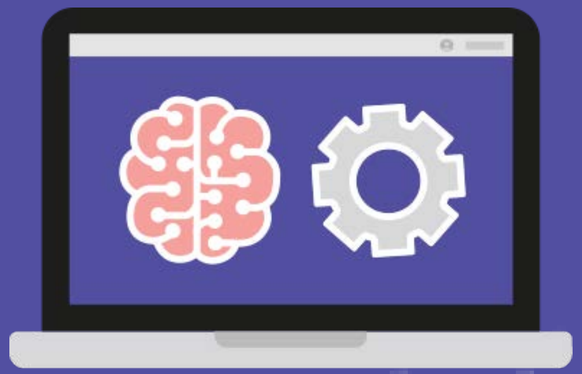
/* elice */

양재 AI School 인공지능 캠프

Lecture 13

인공신경망(ANN)과 손실함수, 역전파법



김도경 선생님

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   GD, SGD, Momentum,

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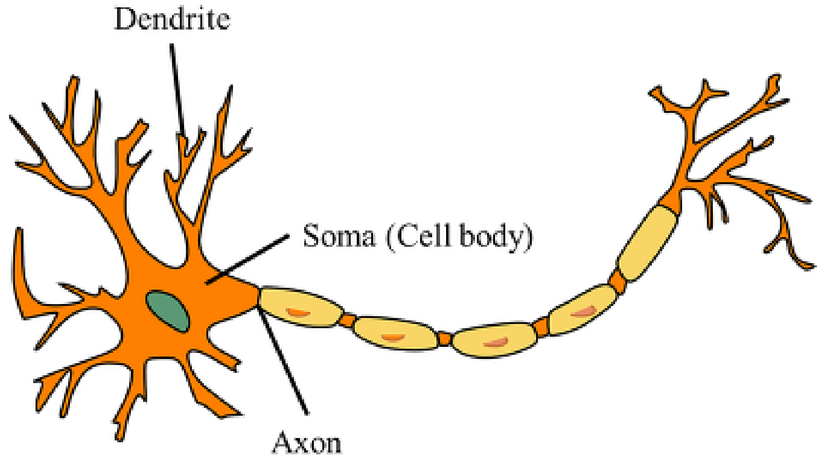
3. 역전파법(Back Propagation)
   1. 역전파법
   2. 역전파 구현

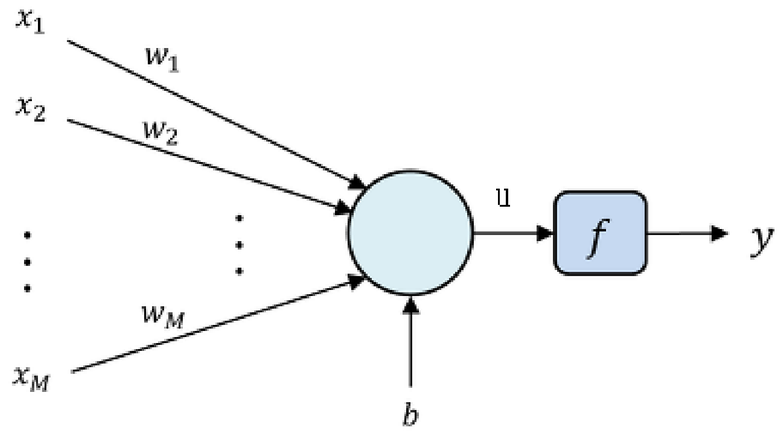
1. 인공신경망(ANN)과 손실함수

1-1. 인공신경망(ANN)

- 뇌는 신경세포(neuron)와 신경세포를 연결하는 시냅스(synapse)를 통해서 신호를 주고 받음으로써 정보를 저장하고 학습
- **인공신경망**(Artificial Neural Network)

  뇌의 학습방법을 수학적으로 모델링한 기계학습 알고리즘





$$u = \sum_{i=1}^{M} w_i x_i + b$$

$$y = f(u)$$

1-1. 인공신경망(ANN)

- 기본 용어

  x_i: 입력(Input)

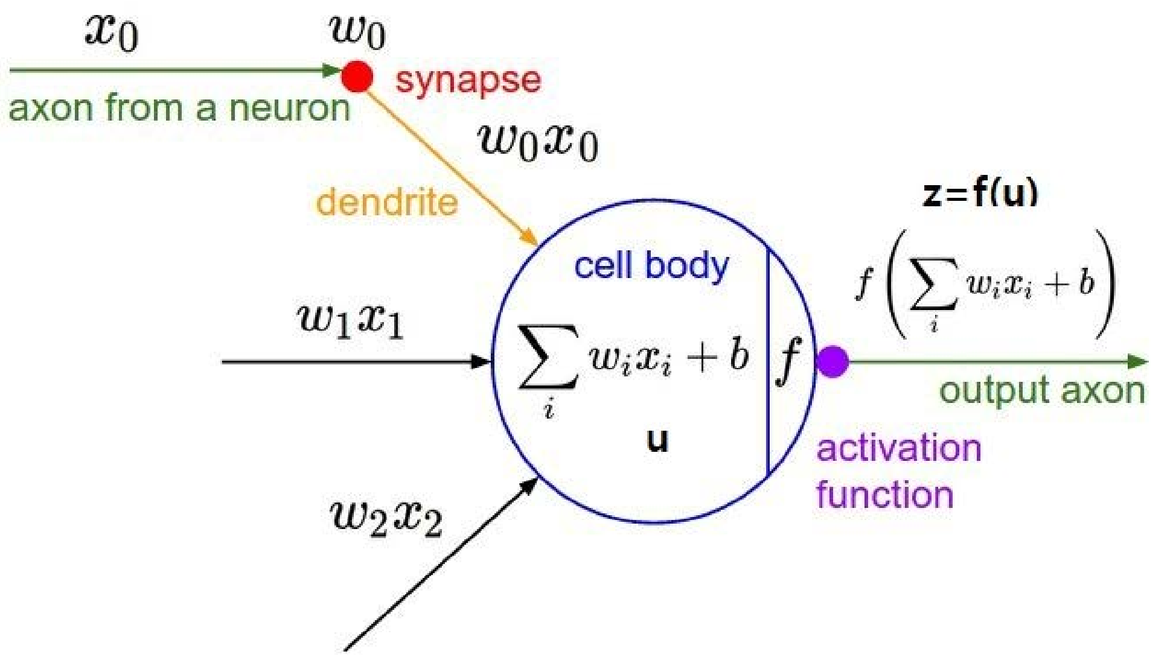
  w_i: 가중치(Weight)

  b: 편향(Bias)

  f: 활성화(Activation) 함수

  u: 선형결합(Net)

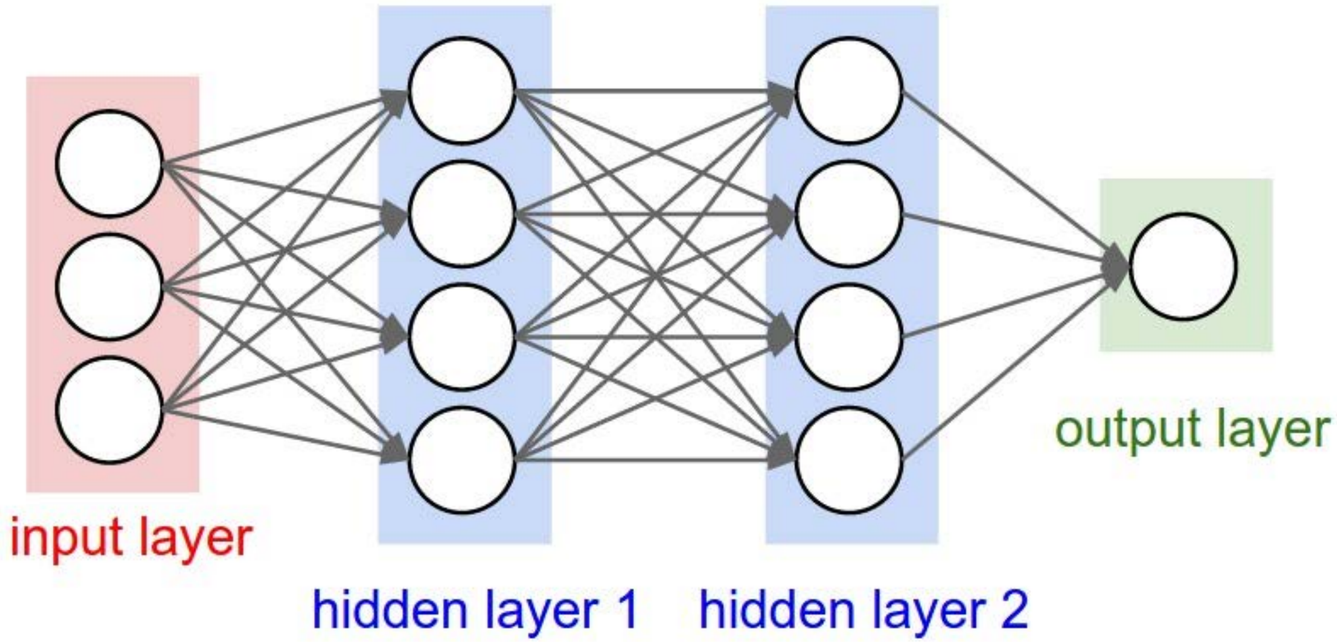
  z: 출력(Output)



- 뉴런에는 선형 결합과 활성화 함수 기능이 존재
- 시냅스는 뉴런과 뉴런을 연결해주는 가중치 역할을 담당

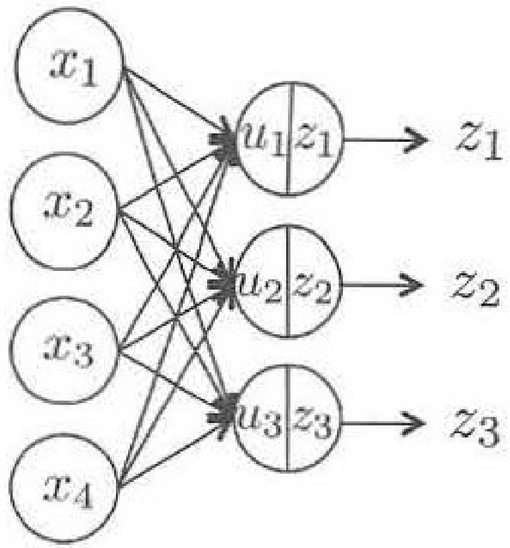
1-1. 인공신경망(ANN)

- 인공신경망은 **입력층**, **히든층**, **출력층**으로 구성
- 각 뉴런의 출력은 직접 전달되는 정보에만 의존할 뿐, 다른 정보들과는 무관
- 이 때문에 병렬처리가 가능하므로 연산속도가 매우 빠름



1-1. 인공신경망(ANN)

- 예) 1개의 레이어로 이루어진 MLP



$$u_1 = w_{11}x_1 + w_{12}x_2 + w_{13}x_3 + w_{14}x_4 + b_1$$

$$u_2 = w_{21}x_1 + w_{22}x_2 + w_{23}x_3 + w_{24}x_4 + b_2$$

$$u_3 = w_{31}x_1 + w_{32}x_2 + w_{33}x_3 + w_{34}x_4 + b_3$$

1-1. 인공신경망(ANN)

- 벡터 및 행렬 기호 도입

$$\mathbf{u} = \begin{bmatrix} u_1 \\ \vdots \\ u_J \end{bmatrix}, \ \mathbf{x} = \begin{bmatrix} x_1 \\ \vdots \\ x_I \end{bmatrix}, \ \mathbf{b} = \begin{bmatrix} b_1 \\ \vdots \\ b_J \end{bmatrix}, \ \mathbf{z} = \begin{bmatrix} z_1 \\ \vdots \\ z_J \end{bmatrix}$$

$$\mathbf{W} = \begin{bmatrix} w_{11} & \cdots & w_{1I} \\ \vdots & \ddots & \vdots \\ w_{JI} & \cdots & w_{JI} \end{bmatrix}, \ \mathbf{f}(\mathbf{u}) = \begin{bmatrix} f(u_1) \\ \vdots \\ f(u_J) \end{bmatrix}$$

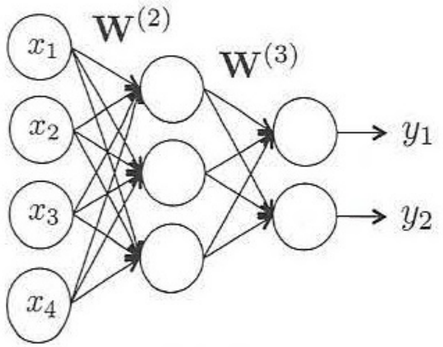
- 앞페이지의 식은 다음과 같이 간단하게 표현

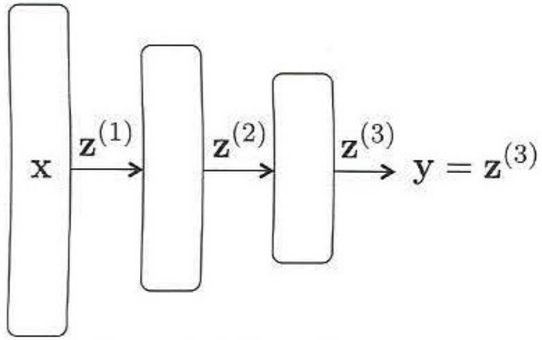
$$\mathbf{u} = \mathbf{W}\mathbf{x} + \mathbf{b}$$

$$\mathbf{z} = \mathbf{f}(\mathbf{u})$$

1-1. 인공신경망(ANN)

- 예) 2개의 레이어로 이루어진 MLP에서의 식





$$\mathbf{u}^{(2)} = \mathbf{W}^{(2)}\mathbf{x} + \mathbf{b}^{(2)}$$

$$\mathbf{z}^{(2)} = \mathbf{f}(\mathbf{u}^{(2)})$$

$$\mathbf{u}^{(3)} = \mathbf{W}^{(3)}\mathbf{z}^{(2)} + \mathbf{b}^{(3)}$$

$$\mathbf{z}^{(3)} = \mathbf{f}(\mathbf{u}^{(3)})$$

- 임의의 개수의 레이어로 이루어진 신경망에서는 $\mathbf{z}^{(1)} = \mathbf{x}$라 두면

$$\mathbf{u}^{(l+1)} = \mathbf{W}^{(l+1)}\mathbf{z}^{(l)} + \mathbf{b}^{(l+1)}$$

$$\mathbf{z}^{(l+1)} = \mathbf{f}(\mathbf{u}^{(l+1)})$$

1-2. 손실함수(Loss function)

- **손실함수(Loss or Cost function)**

  신경망에서 내놓는 결과값과 실제 결과값 사이의 차이를 정의하는 함수

- **신경망 학습의 목표**

  손실함수를 최소화하는 것

  이를 위해 SGD 등의 학습 알고리즘 사용

1-2. 손실함수(Loss function)

- 신경망의 최종출력을 $\mathbf{y} = \mathbf{z}^{(L)}$로 표기하고

  Train set을 $\mathcal{D} = \{(\mathbf{x}_1, \mathbf{d}_1), (\mathbf{x}_2, \mathbf{d}_2), \cdots, (\mathbf{x}_N, \mathbf{d}_N)\}$라 하자.

- **회귀(Regression)**

  손실함수로 제곱오차(Mean-squared error)를 사용

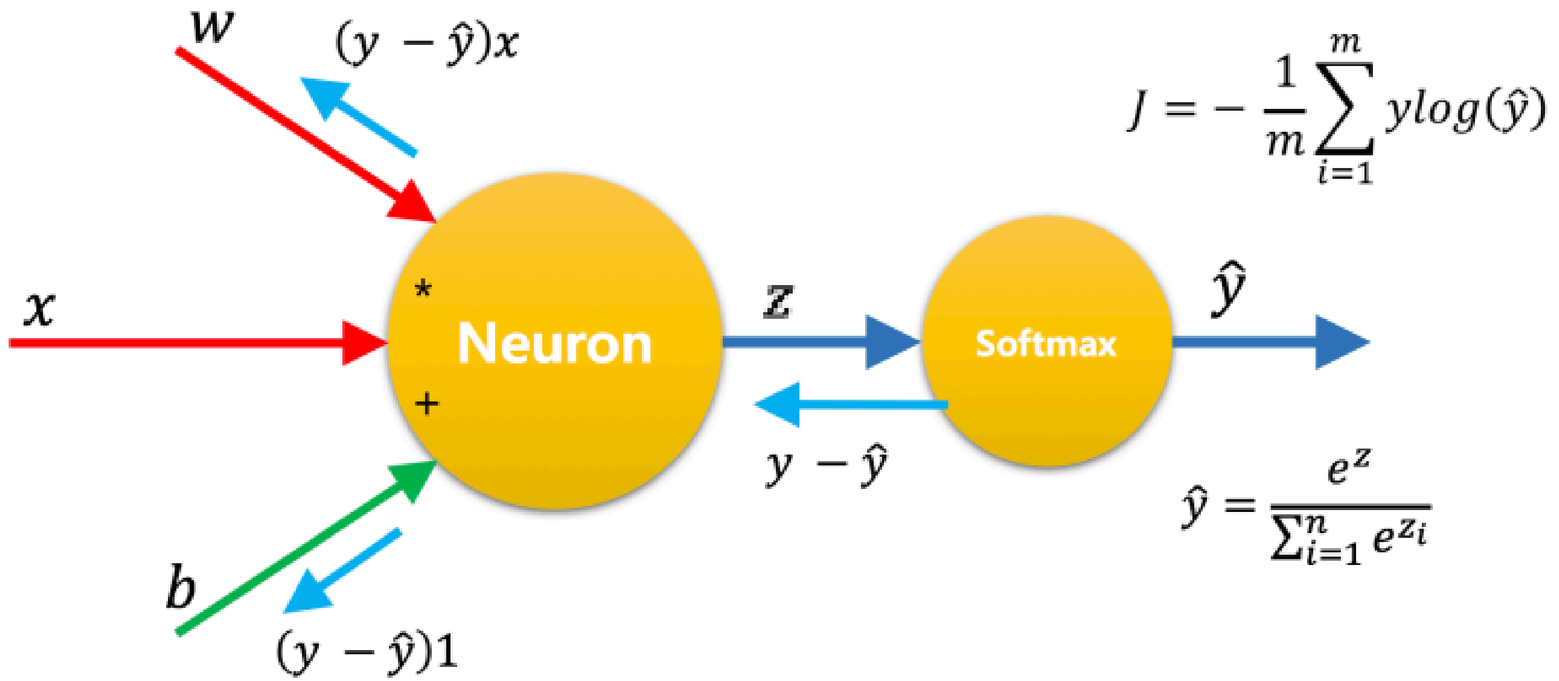
$$E(\mathbf{w}) = \frac{1}{2N}\sum_{n=1}^{N} E_n(\mathbf{w}) = \frac{1}{2N}\sum_{n=1}^{N} ||\mathbf{d}_n - \mathbf{y}(\mathbf{x}_n; \mathbf{w})||^2$$

1-2. 손실함수(Loss function)

- **분류(Classification)**

  활성화 함수로 소프트맥스(Softmax) 함수,

  손실함수로 크로스 엔트로피(Cross entropy)를 사용



2. 학습 알고리즘

2. 학습 알고리즘

- **경사하강법(Gradient Descent)**

  1. 네트워크의 parameter들을 θ 라고 했을 때, 손실함수 J(θ)의 값을 최소화하기 위해 기울기(gradient) ∇J(θ)를 이용하는 방법

  2. GD에서는 gradient의 반대 방향으로 일정 크기만큼 이동하는 것을 반복하여 손실함수의 값을 최소화하는 θ의 값을 찾음

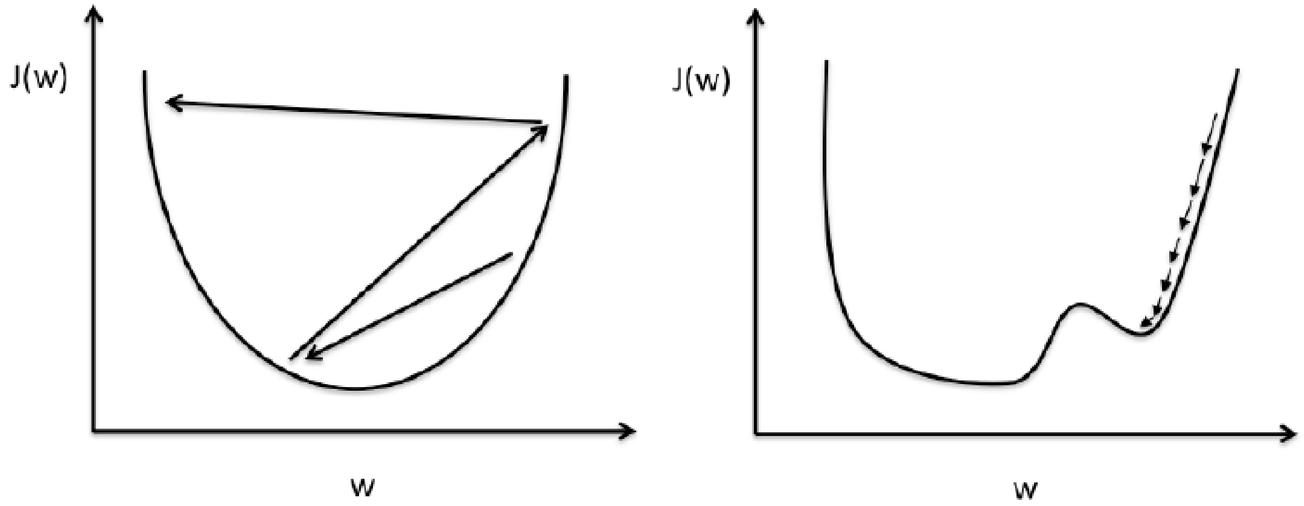
$$\theta = \theta - \eta \nabla_\theta J(\theta)$$

  3. 이 때 η는 미리 정해진 걸음의 크기(step size)로, 학습률(learning rate)이라고 함. 보통 0.01~0.001 정도를 사용

2. 학습 알고리즘

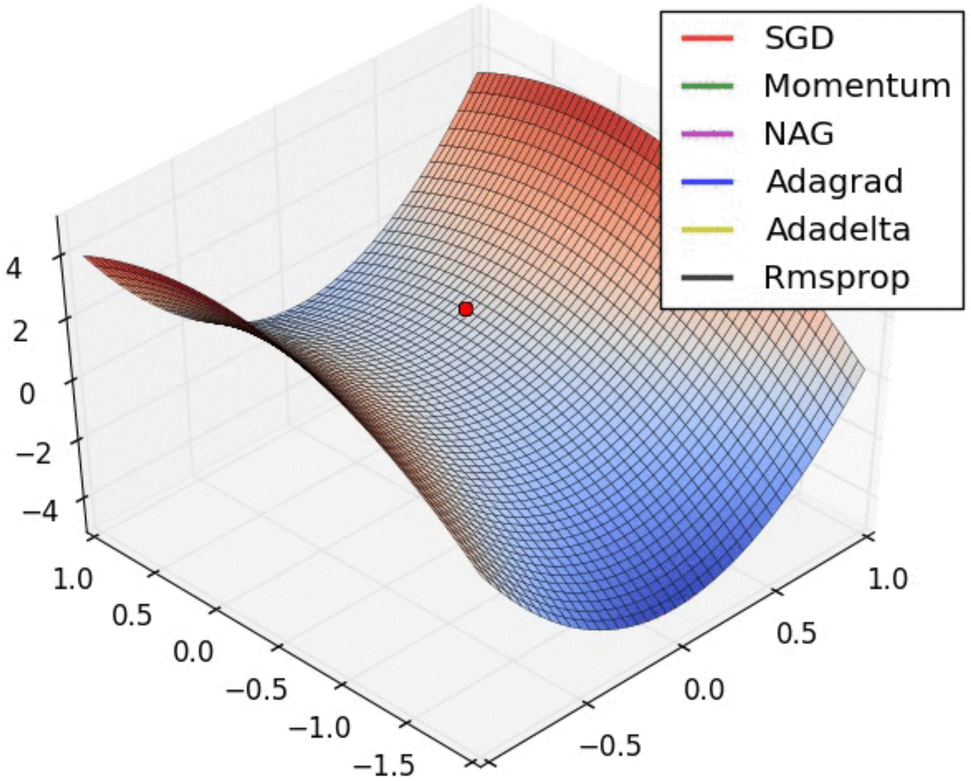
학습률(Learning rate)

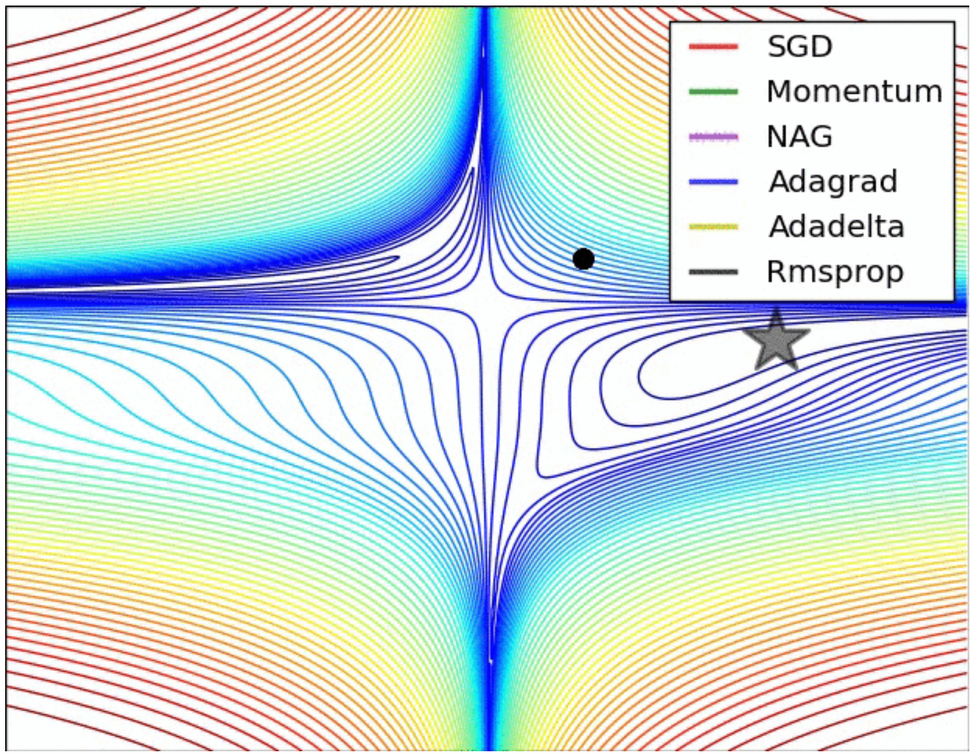
- 학습률이 너무 크면 듬성듬성하고 최소값(global minimum)을 지나쳐 갈수 있음
- 학습률이 너무 작으면 학습을 촘촘히 해서 학습속도가 느려지고 극소값(Local minimum)에 빠질 수 있음



2. 학습 알고리즘

- 여러 학습 알고리즘간의 **수렴속도 비교**



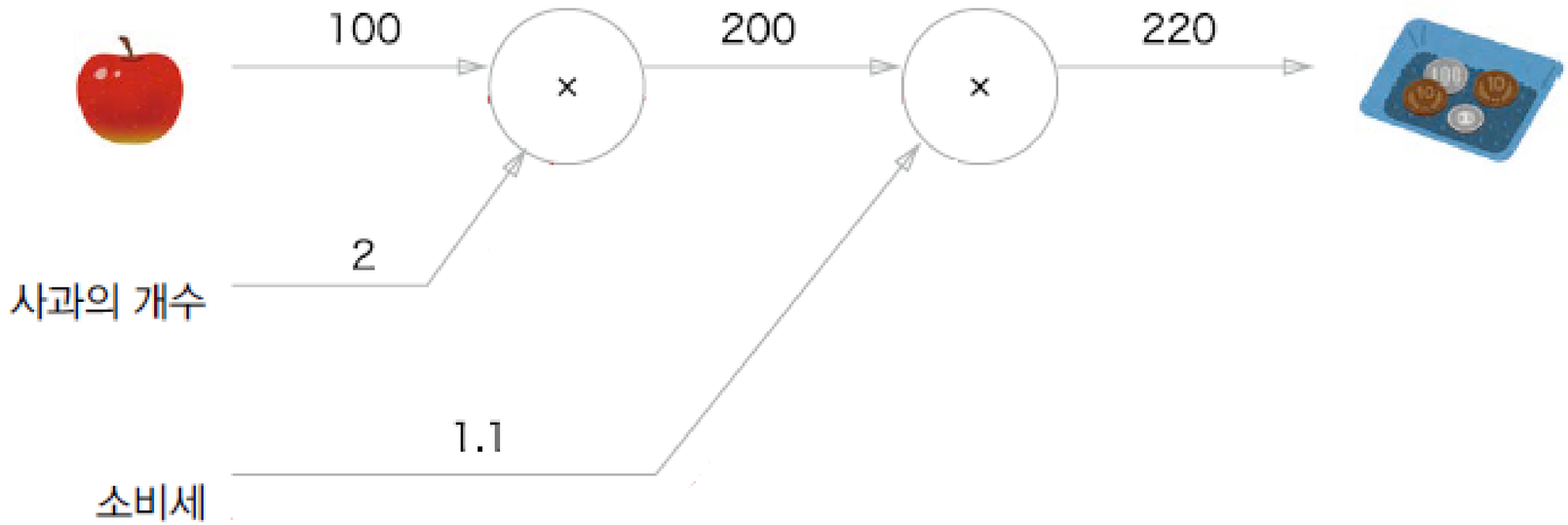


3. 역전파법(Back Propagation)

3-1. 역전파법(Back Propagation)

계산 그래프(computational graph)

- 계산 과정을 그래프로 나타낸 것
- 노드(node)와 엣지(edge)로 표현
- 노드는 연산을, 엣지는 데이터가 흘러가는 방향을 나타냄



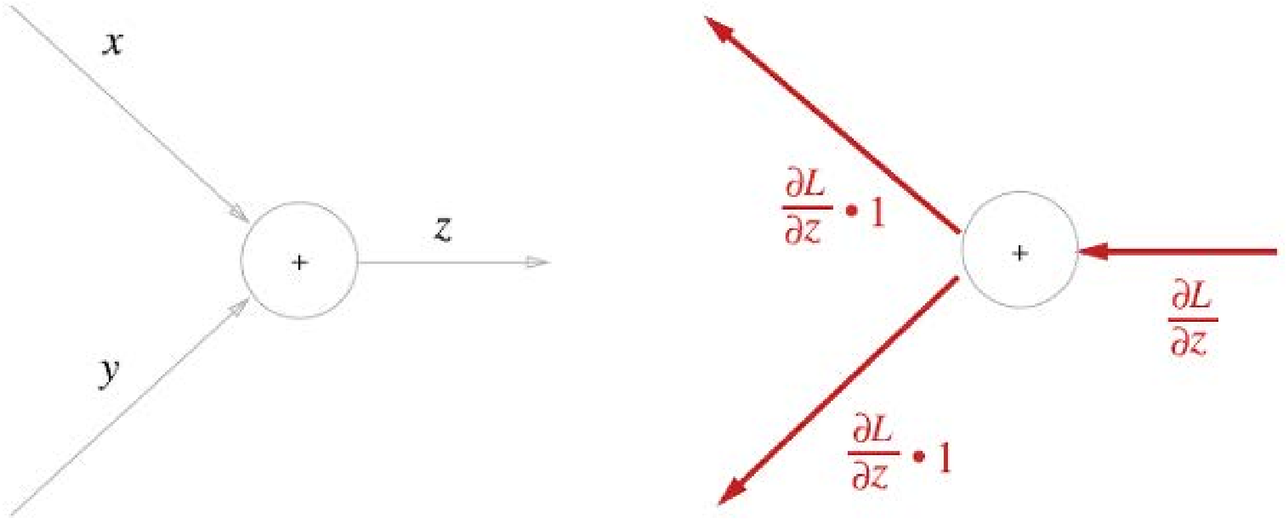
3-1. 역전파법(Back Propagation)

- 덧셈노드

$$z = x + y$$

$$\frac{\partial z}{\partial x} = 1$$

$$\frac{\partial z}{\partial y} = 1$$



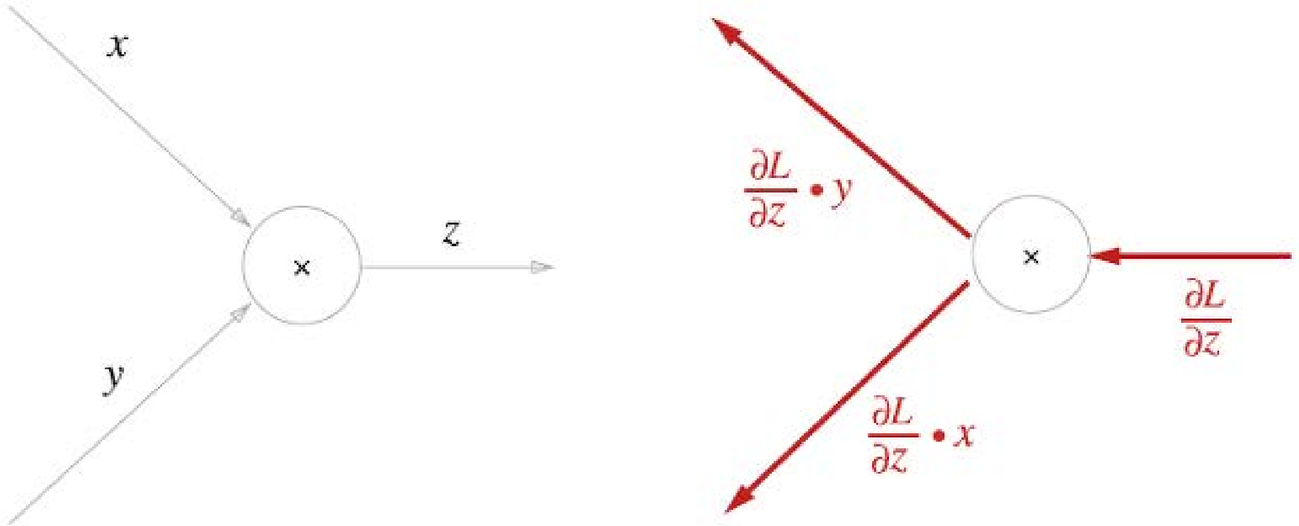
3-1. 역전파법(Back Propagation)

- 곱셈노드

$$z = xy$$

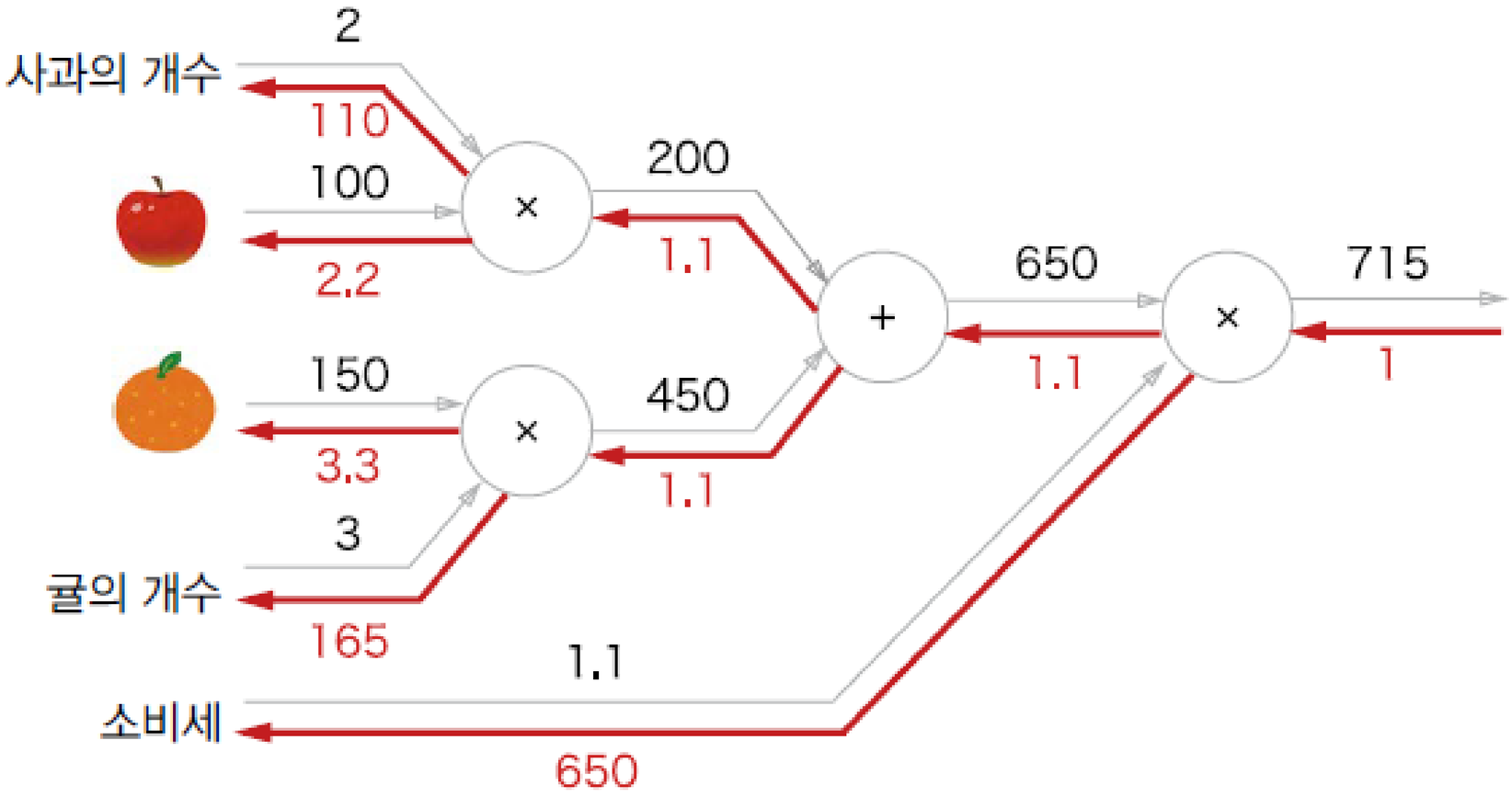
$$\frac{\partial z}{\partial x} = y$$

$$\frac{\partial z}{\partial y} = x$$



3-1. 역전파법(Back Propagation)

- **계산그래프에서의 역전파**



3-1. 역전파법(Back Propagation)

- **합성함수 미분법(Chain rule) 1**

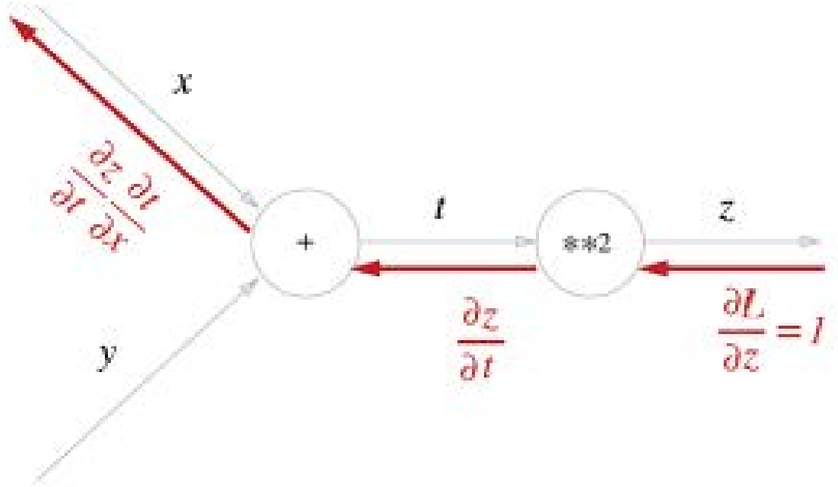
$$t = x + y$$

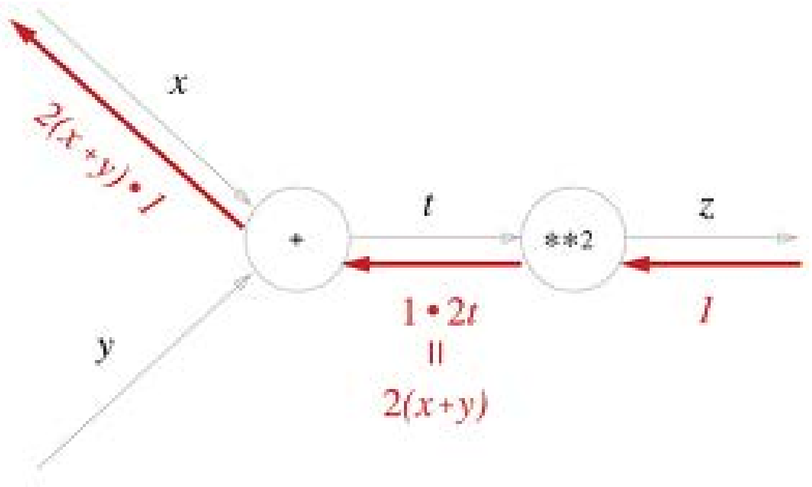
$$z = t^2$$

$$\frac{\partial z}{\partial t} = 2t$$

$$\frac{\partial t}{\partial x} = 1$$

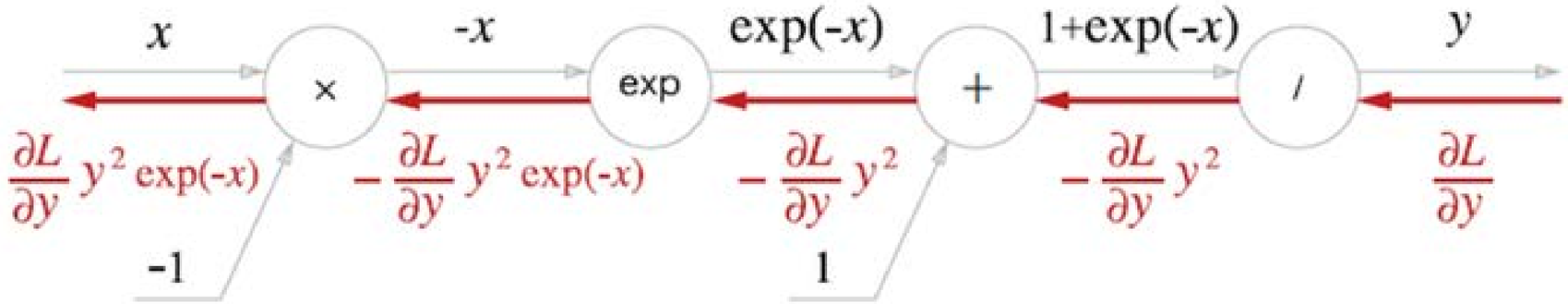
$$\frac{\partial z}{\partial x} = \frac{\partial z}{\partial t}\frac{\partial t}{\partial x} = 2t \cdot 1 = 2(x+y)$$

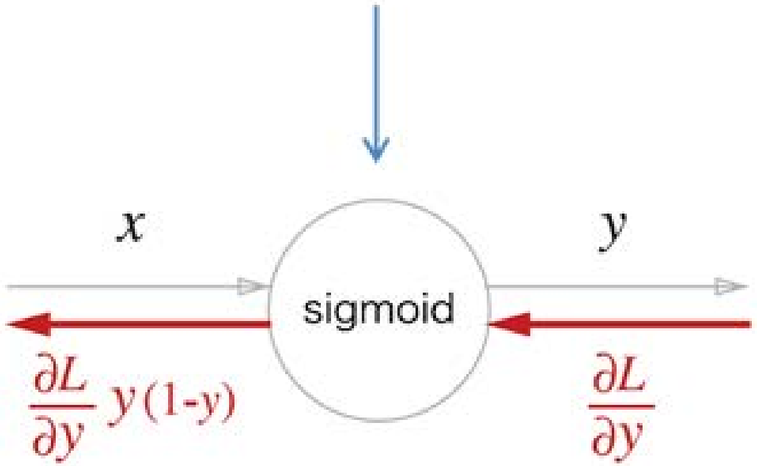




3-1. 역전파법(Back Propagation)

- 시그모이드 함수의 역전파



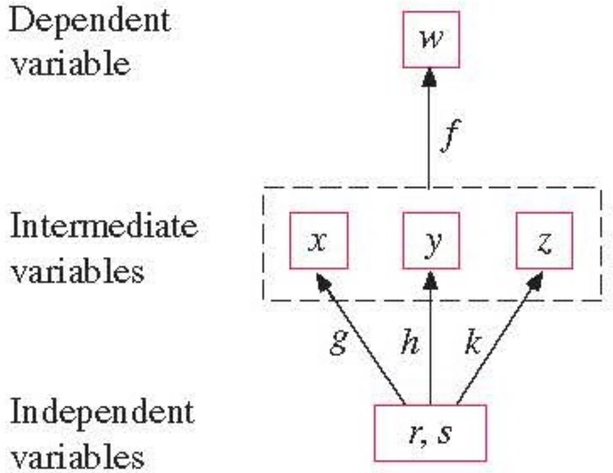


$$y = \frac{1}{1 + \exp(-x)}$$

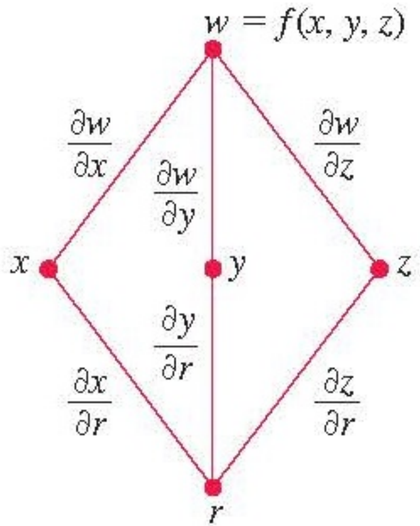
$$\begin{aligned}\frac{\partial L}{\partial y} y^2 exp(-x) &= \frac{\partial L}{\partial y} \frac{1}{(1 + exp(-x))^2} \exp(-x) \\ &= \frac{\partial L}{\partial y} \frac{1}{1 + exp(-x)} \frac{exp(-x)}{1 + exp(-x)} \\ &= \frac{\partial L}{\partial y} y(1 - y)\end{aligned}$$

3-1. 역전파법(Back Propagation)

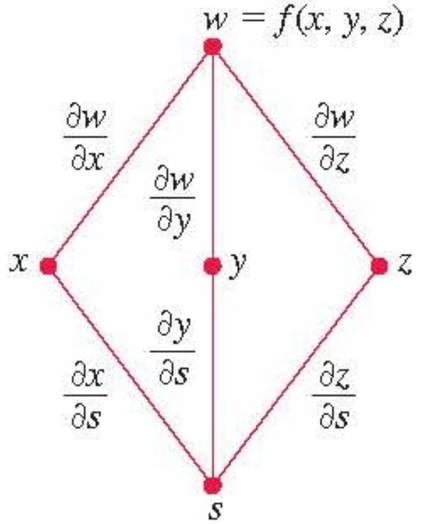
- **합성함수 미분법(Chain rule) 2**



$$w = f(g(r, s), h(r, s), k(r, s))$$



$$\frac{\partial w}{\partial r} = \frac{\partial w}{\partial x}\frac{\partial x}{\partial r} + \frac{\partial w}{\delta y}\frac{\partial y}{\partial r} + \frac{\partial w}{\partial z}\frac{\partial z}{\partial r}$$



$$\frac{\partial w}{\partial s} = \frac{\partial w}{\partial x}\frac{\partial x}{\partial s} + \frac{\partial w}{\partial y}\frac{\partial y}{\partial s} + \frac{\partial w}{\partial z}\frac{\partial z}{\partial s}$$

3-1. 역전파법(Back Propagation)

- **연습문제**

$$u = x^2 + 2y$$

$$x = r\sin t, \qquad y = \sin^2 t$$

일 때 $\frac{\partial u}{\partial r}, \frac{\partial u}{\partial t}$를 구하여라.

3-1. 역전파법(Back Propagation)

- **정답**

$$\frac{\partial u}{\partial r} = \frac{\partial u}{\partial x}\frac{\partial x}{\partial r} + \frac{\partial u}{\partial y}\frac{\partial y}{\partial r} = (2x)(\sin(t)) + (2)(0) = 2r\sin^2(t),$$

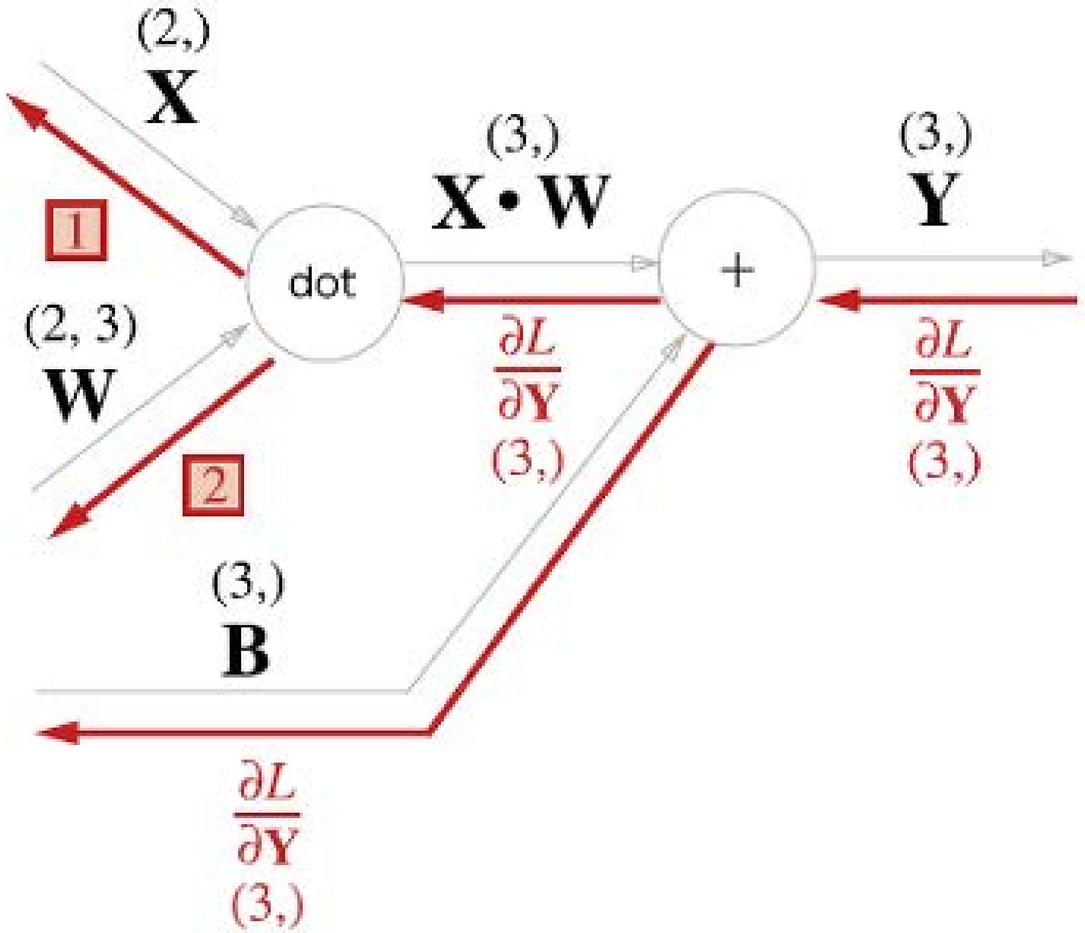
$$\begin{aligned}\frac{\partial u}{\partial t} &= \frac{\partial u}{\partial x}\frac{\partial x}{\partial t} + \frac{\partial u}{\partial y}\frac{\partial y}{\partial t} \\ &= (2x)(r\cos(t)) + (2)(2\sin(t)\cos(t)) \\ &= (2r\sin(t))(r\cos(t)) + 4\sin(t)\cos(t) \\ &= 2(r^2+2)\sin(t)\cos(t) \\ &= (r^2+2)\sin(2t).\end{aligned}$$

3-1. 역전파법(Back Propagation)

- **행렬연산과 역전파**

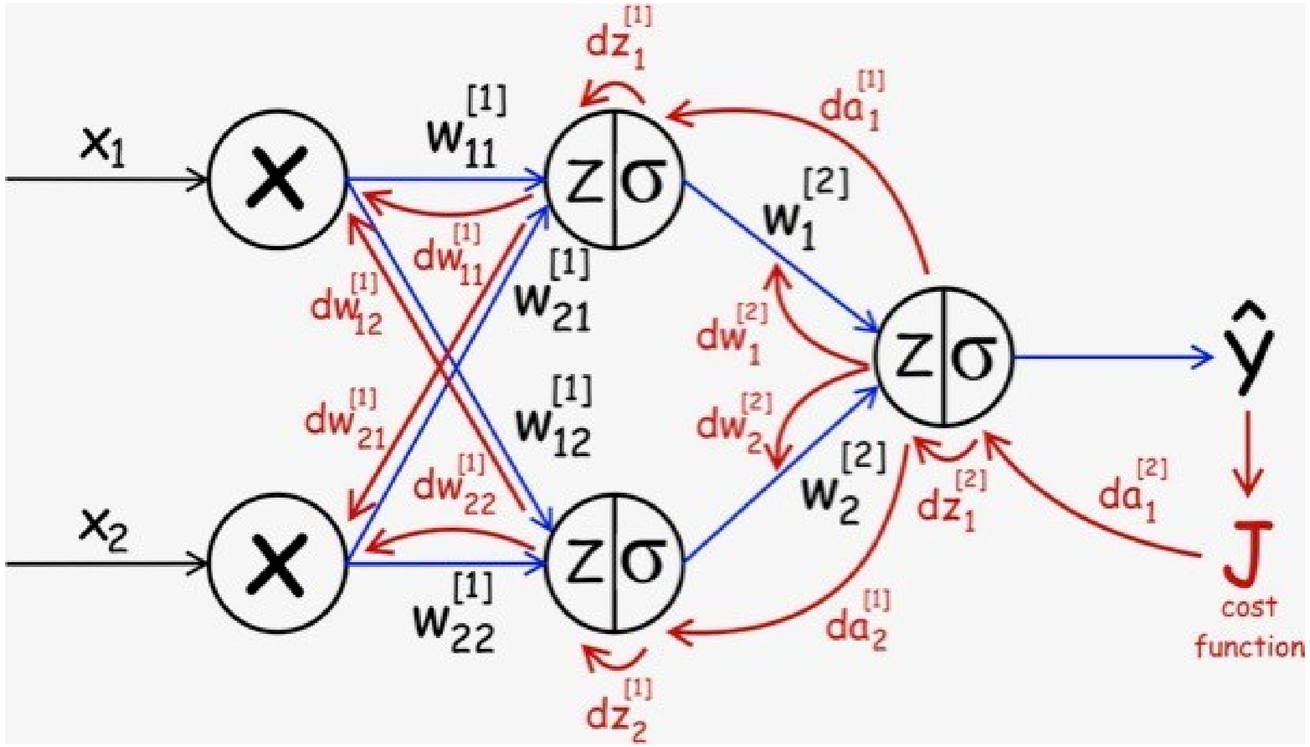
$$\boxed{1}\quad \underset{(2,)}{\frac{\partial L}{\partial \mathbf{X}}} = \underset{(3,)}{\frac{\partial L}{\partial \mathbf{Y}}}\ \underset{(3,2)}{\mathbf{W}^{\mathrm{T}}}$$

$$\boxed{2}\quad \underset{(2,3)}{\frac{\partial L}{\partial \mathbf{W}}} = \underset{(2,1)}{\mathbf{X}^{\mathrm{T}}}\ \underset{(1,3)}{\frac{\partial L}{\partial \mathbf{Y}}}$$



3-2. 역전파 구현

- binary 분류용 2-layer Neural Net에 대한 역전파



3-2. 역전파 구현

- binary 분류용 2-layer Neural Net에 대한 역전파

$$
\begin{aligned}
Z^{[1]} &= W^{[1]} X + b^{[1]} \\
A^{[1]} &= \sigma(Z^{[1]}) \\
Z^{[2]} &= W^{[2]} A^{[1]} + b^{[2]} \\
\hat{y} &= A^{[2]} = \sigma(Z^{[2]})
\end{aligned}
$$

$$
\begin{aligned}
W^{[1]} &=: W^{[1]} - \alpha \frac{dJ}{dW^{[1]}} \\
b^{[1]} &=: b^{[1]} - \alpha \frac{dJ}{db^{[1]}} \\
W^{[2]} &=: W^{[2]} - \alpha \frac{dJ}{dW^{[2]}} \\
b^{[2]} &=: b^{[2]} - \alpha \frac{dJ}{db^{[2]}}
\end{aligned}
$$

3-2. 역전파 구현

- **binary 분류용 2-layer Neural Net에 대한 역전파**

$$J = -\frac{1}{n}\left(Y log\left(A^{[2]}\right) - (1-Y)\, log\left(1 - A^{[2]}\right)\right)$$

$$\frac{dJ}{dW^{[2]}} = \left[-\frac{Y}{A^{[2]}} + \frac{1-Y}{1-A^{[2]}}\right]\left[A^{[2]}(1-A^{[2]})\right]\left[A^{[2]}\right]$$

$$\begin{aligned}\frac{dJ}{db^{[2]}} &= \frac{dJ}{dA^{[2]}}\frac{dA^{[2]}}{dZ^{[2]}}\frac{dZ^{[2]}}{db^{[2]}} \\ &= \left[A^{[2]} - Y\right]\left[1\right] \\ &= \left[A^{[2]} - Y\right] \\ &= dZ^{[2]}\end{aligned}$$

3-2. 역전파 구현

- binary 분류용 2-layer Neural Net에 대한 역전파

$$
\begin{aligned}
\frac{dJ}{dW^{[1]}} &= \frac{dJ}{dA^{[2]}}\frac{dA^{[2]}}{dZ^{[2]}}\frac{dZ^{[2]}}{dA^{[1]}}\frac{dA^{[1]}}{dZ^{[1]}}\frac{dZ^{[1]}}{dW^{[1]}} \\
&= \frac{dJ}{dZ^{[2]}}\frac{dZ^{[2]}}{dA^{[1]}}\frac{dA^{[1]}}{dZ^{[1]}}\frac{dZ^{[1]}}{dW^{[1]}} \\
&= \left[A^{[2]}-Y\right]\left[W^{[2]}\right]\left[g'\left(Z^{[1]}\right)\right]\left[A^{[0]}\right] \\
&= dZ^{[2]}W^{[2]}g'\left(Z^{[1]}\right)A^{[0]} \\
&= dZ^{[1]}A^{[0]}
\end{aligned}
$$

$$
\begin{aligned}
\frac{dJ}{db^{[1]}} &= \frac{dJ}{dA^{[2]}}\frac{dA^{[2]}}{dZ^{[2]}}\frac{dZ^{[2]}}{dA^{[1]}}\frac{dA^{[1]}}{dZ^{[1]}}\frac{dZ^{[1]}}{db^{[1]}} \\
&= \frac{dJ}{dZ^{[2]}}\frac{dZ^{[2]}}{dA^{[1]}}\frac{dA^{[1]}}{dZ^{[1]}}\frac{dZ^{[1]}}{db^{[1]}} \\
&= \left[A^{[2]}-Y\right]\left[W^{[2]}\right]\left[g'\left(Z^{[1]}\right)\right]\left[1\right] \\
&= dZ^{[2]}W^{[2]}g'\left(Z^{[1]}\right) \\
&= dZ^{[1]}
\end{aligned}
$$

- 즉, 다음 layer의 gradient 값들을 이용해 이전 layer의 gradient 값을 구할수 있다. (병렬연산 가능)

3-2. 역전파 구현

- **binary 분류용 L-layer Neural Net에 대한 역전파**
  - Initialize $W^{[1]}..W^{[L]}, b^{[1]}...b^{[L]}$
  - Set $A^{[0]} = X$ (Input) , $L =$ Total Layers
  - Loop epoch = 1 to max iteration
    - Forward Propagation
      - Loop $l = 1$ to $L - 1$
        - $Z^{[l]} = W^{[l]} A^{[l-1]} + b^{[l]}$
        - $A^{[l]} = g\left(b^{[l]}\right)$
        - Save $A^{[l]}, W^{[l]}$ in memory for later use
      - $Z^{[L]} = W^{[L]} A^{[L-1]} + b^{[L]}$
      - $A^{[L]} = \sigma\left(Z^{[L]}\right)$
    - Cost $J = -\frac{1}{n}\left(Y log\left(A^{[2]}\right) - (1 - Y)\, log\left(1 - A^{[2]}\right)\right)$

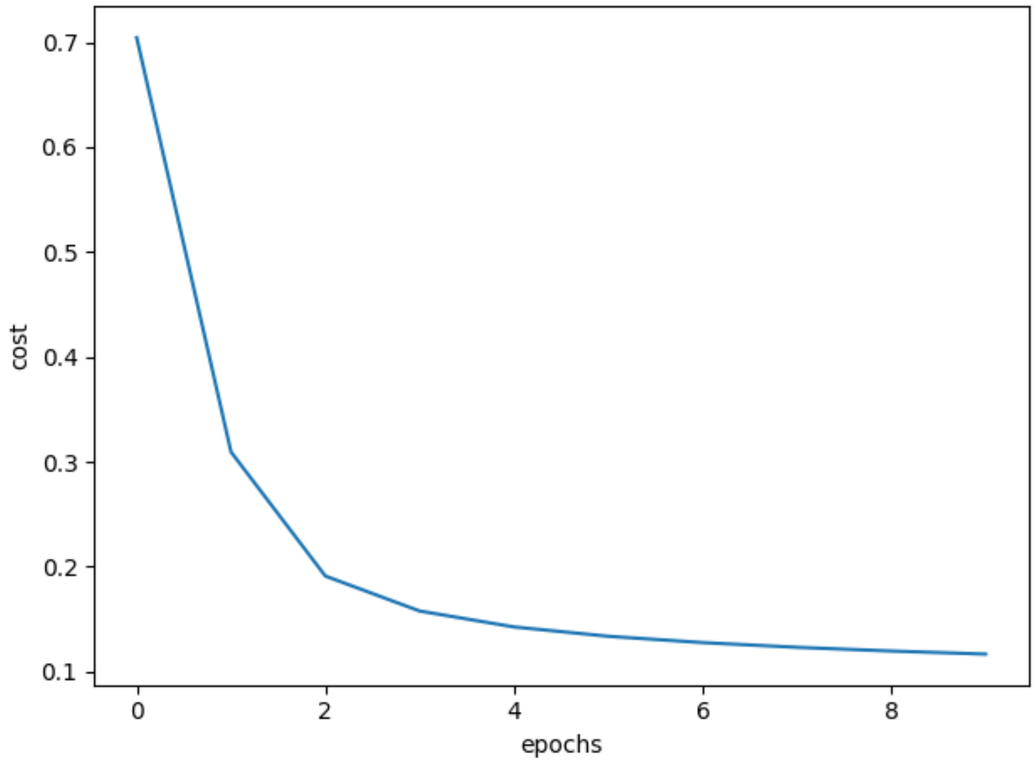
3-2. 역전파 구현

- **binary 분류용 L-layer Neural Net에 대한 역전파**
  - Backward Propagation
    - $dA^{[L]} = -\frac{Y}{A^{[L]}} + \frac{1-Y}{1-A^{[L]}}$
    - $dZ^{[L]} = dA^{[L]}\sigma'\left(dA^{[L]}\right)$
    - $dW^{[L]} = dZ^{[L]}dA^{[L-1]}$
    - $db^{[L]} = dZ^{[L]}$
    - $dA^{[L-1]} = dZ^{[L]}W^{[L]}$
    - Loop $l = L-1$ to 1
      - $dZ^{[l]} = dA^{[l]}g'\left(dA^{[l]}\right)$
      - $dW^{[l]} = dZ^{[l]}dA^{[l-1]}$
      - $db^{[l]} = dZ^{[l]}$
      - $dA^{[l-1]} = dZ^{[l]}W^{[l]}$
  - Update W and b
    - Loop $l = 1$ to L
      - $W^{[l]} = W^{[l]} - \alpha . dW^{[l]}$
      - $b^{[l]} = b^{[l]} - \alpha . db^{[l]}$

3-2. 역전파 구현

- **binary 분류용 2-layer Neural Net에 대한 역전파**

  MNIST의 5와 8을 이진분류로 1,000회 돌렸을 때의 손실함수



3-2. 역전파 구현

- **binary 분류용 2-layer Neural Net에 대한 역전파**

```
def backward(self, X, Y, store):
        derivatives = {}
        store["A0"] = X.T
        A = store["A" + str(self.L)]
        dA = -np.divide(Y, A) + np.divide(1 - Y, 1 - A)
        dZ = dA * self.sigmoid_derivative(store["Z" + str(self.L)])
        dW = dZ.dot(store["A" + str(self.L - 1)].T) / self.n
        db = np.sum(dZ, axis=1, keepdims=True) / self.n
        dAPrev = store["W" + str(self.L)].T.dot(dZ)
        derivatives["dW" + str(self.L)] = dW
        derivatives["db" + str(self.L)] = db
            ...
        return derivatives
```

3-2. 역전파 구현

- **binary 분류용 2-layer Neural Net에 대한 역전파**

Forward Propagation – Layer 1:

$$
\begin{aligned}
X &= (11272, 784) \\
W^{[1]} &= (196, 784) \\
b^{[1]} &= (196, 1) \\
A^{[0]} &= X^T \\
&= (784, 11272) \\
Z^{[1]} &= W^{[1]} A^{[0]} + b^{[1]} \\
&= (196, 784) * (784, 11272) + (196, 1) \\
&= (196, 11272) + (196, 1) \\
&= (196, 11272) \\
A^{[1]} &= g\left(Z^{[1]}\right) \\
&= (196, 11272)
\end{aligned}
$$

MNIST 데이터셋의 Train set 6만개 중 5와 8만을 뽑아낸 것의 개수: 11,272

히든 레이어에 존재하는 노드의 수: 196

3-2. 역전파 구현

- **binary 분류용 2-layer Neural Net에 대한 역전파**

Forward Propagation - Layer 2:

$$
\begin{aligned}
W^{[2]} &= (1, 196) \\
b^{[2]} &= (1, 1) \\
Z^{[2]} &= W^{[2]} A^{[1]} + b^{[2]} \\
&= (1, 196) * (196, 11272) + (1, 1) \\
&= (1, 11272) + (1, 1) \\
&= (1, 11272) \\
A^{[2]} &= g\left(Z^{[2]}\right) \\
&= (1, 11272)
\end{aligned}
$$

3-2. 역전파 구현

- **binary 분류용 2-layer Neural Net에 대한 역전파**

Backward Propagation - Layer 2:

$$
\begin{aligned}
Y^T &= (1, 11272) \\
dA^{[2]} &= -\frac{Y^T}{A^{[2]}} + \frac{1 - Y^T}{1 - A^{[2]}} \\
&= (1, 11272) \\
dZ^{[2]} &= dA^{[2]} g'(Z^{[2]}) \\
&= (1, 11272) * (1, 11272) \\
&= (1, 11272) \\
dW^{[2]} &= dZ^{[2]} \left(A^{[1]}\right)^T \\
&= (1, 11272) * (11272, 196) \\
&= (1, 196) \\
db^{[2]} &= dZ^{[2]} \\
&= (1, 1) \\
dA^{[1]} &= \left(W^{[2]}\right)^T dZ^{[2]} \\
&= (196, 1) * (1, 11272) \\
&= (196, 11272)
\end{aligned}
$$

3-2. 역전파 구현

- **binary 분류용 2-layer Neural Net에 대한 역전파**

Backward Propagation - Layer 1:

$$
\begin{aligned}
dZ^{[1]} &= dA^{[1]} g'(Z^{[1]}) \\
&= (196, 11272) * (196, 11272) \\
&= (196, 11272) \\
dW^{[1]} &= dZ^{[1]} \left(A^{[0]} \right)^T \\
&= (196, 11272) * (11272, 784) \\
&= (196, 784) \\
db^{[1]} &= dZ^{[1]} \\
&= (196, 1)
\end{aligned}
$$

참고자료

1. 인공신경망
   https://untitledtblog.tistory.com/141

2. 학습 알고리즘
   http://shuuki4.github.io/deep%20learning/2016/05/20/Gradient-Descent-Algorithm-Overview.html

3. 역전파
   1. https://excelsior-cjh.tistory.com/171
   2. http://www.adeveloperdiary.com/data-science/machine-learning/understand-and-implement-the-backpropagation-algorithm-from-scratch-in-python/

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