

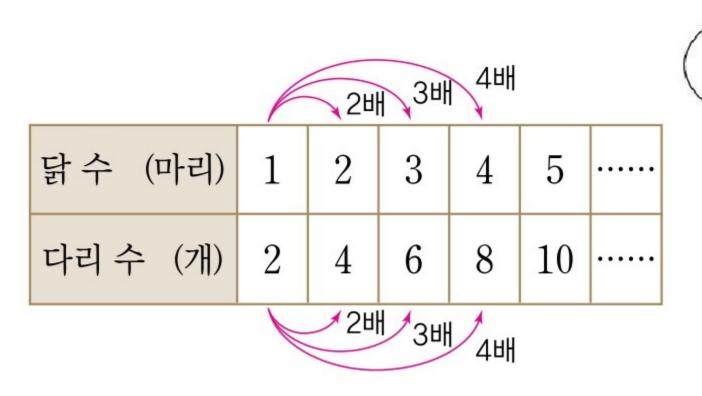
# **Logistic Regression**



#### Let's Go to the Deep Learning World!!

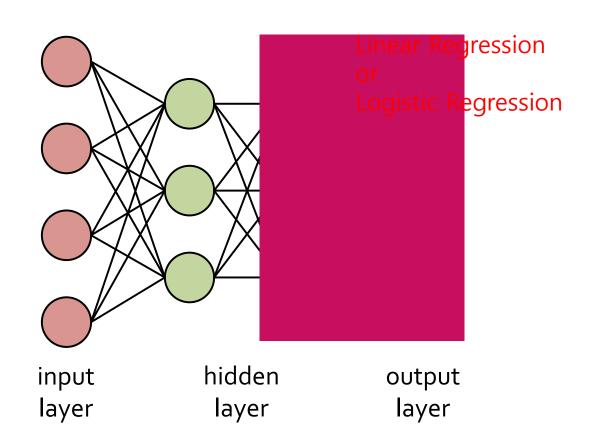
# 쉬운 것부터 시작해봅시다

# 초등학교 6학년 수학 – 정비례



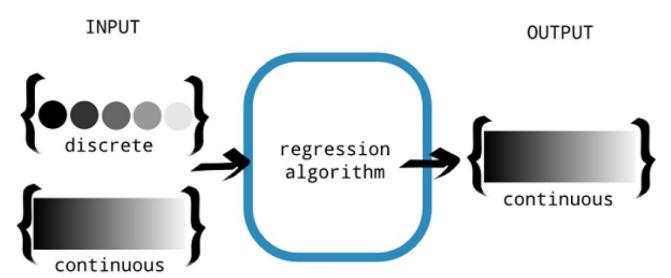


#### Deep Learning Uses Linear Regression/Logistic Regression

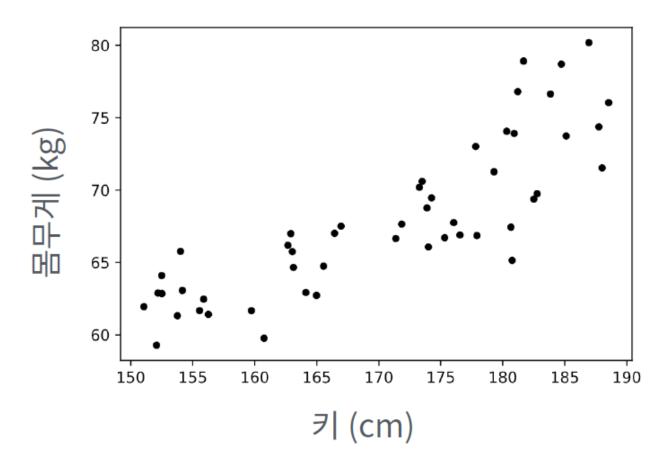


#### Regression

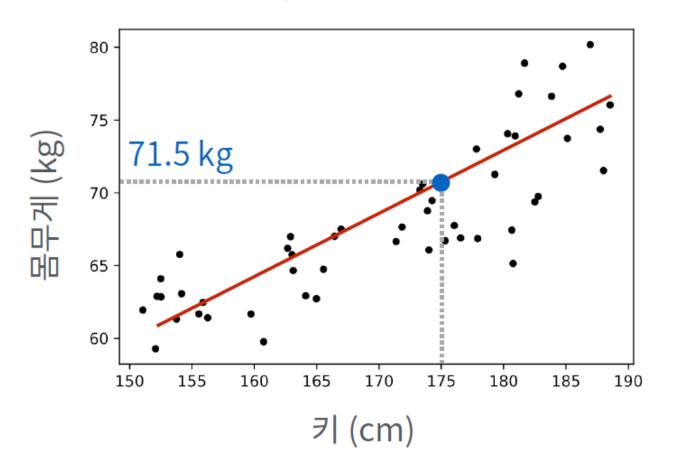
- Classification
  - Is it a dog or not? (binary)
  - What is this animal? (multi-class)
- Regression
  - What will be the stock value?  $y \in \mathbb{R}$
  - What will be the housing price?  $y \in [0, \infty)$



- 어느 학교 학생들의 신체검사 자료
- 새로 전학온 학생 A의 키가 175cm일 때 예상 몸무게는?

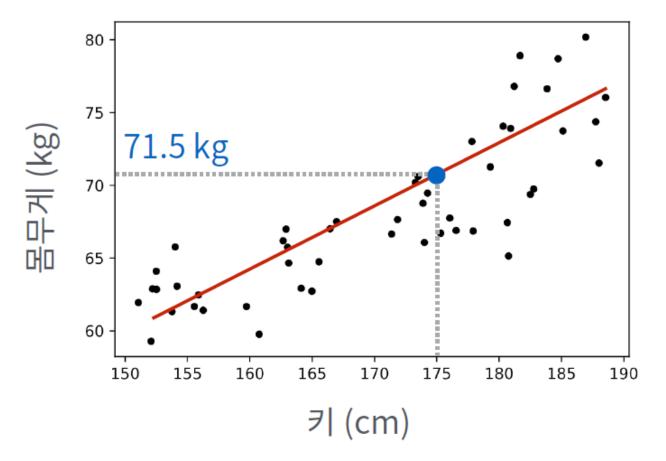


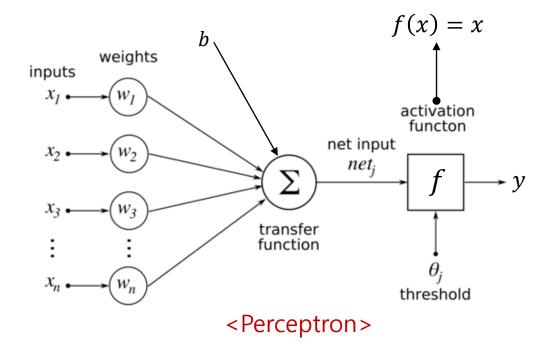
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• 선형함수(예 : 1차함수)로 주어진 data를 근사한다

• y = wx + b



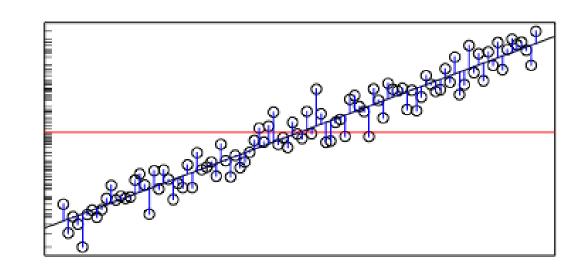


$$y = f(\mathbf{w}\mathbf{x} + \mathbf{b})$$

$$\mathbf{w} = [w_1 \ w_2 \ w_3 \ \dots \ w_n]$$

$$\mathbf{x} = [x_1 \ x_2 \ x_3 \ \dots \ x_n]^T$$

• 잘 예측했는지 측정할 척도(metric)가 필요함



$$y^* = wx + b$$
 (예측값)
$$Cost(Loss) = \sum_{i} (y_i - y_i^*)^2$$

$$= \sum_{i} (y_i - wx_i - b)^2$$

- Cost(Loss) 값을 minimize하는 w와 b를 구하면 될텐데.... 어떻게?
  - Random Search 가능????
  - Cost function을 미분해서 최솟값(미분=o이되는 점)을 찾자!

# 약간의 수학을(미분을...) 조금 해야겠습니다

# b 구하기

$$L = \sum_{i} (y_i - wx_i - b)^2$$

$$\frac{\delta L}{\delta b} = \frac{\delta \sum_{i} (y_i - wx_i - b)^2}{\delta b}$$

$$= -2\sum_{i} (y_i - wx_i - b) = ny_{avg} - nwx_{avg} - nb = 0$$

$$\therefore b = y_{avg} - wx_{avg}$$

# w구하기

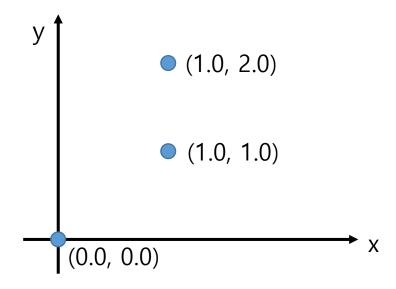
$$L = \sum_{i} (y_i - wx_i - b)^2$$

$$\frac{\delta L}{\delta w} = \frac{\delta \sum_{i} (y_i - wx_i - b)^2}{\delta w}$$

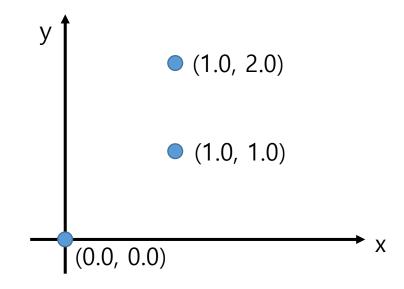
$$= -2\sum_{i} x_{i}(y_{i} - wx_{i} - b) = -2\sum_{i} x_{i}(y_{i} - wx_{i} - y_{avg} + wx_{avg})$$

$$= 0$$

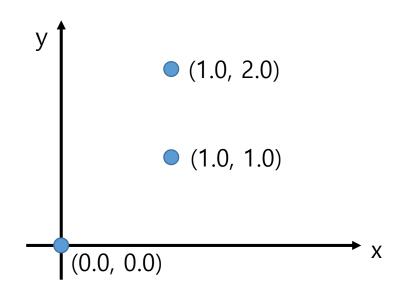
- Find the linear function(f) that best describes the given data
  - $H(x, w_0, w_1) = w_1 x + w_0$



- $H(0, w_0, w_1) \approx 0.0$
- $H(1, w_0, w_1) \approx 1.0$
- $H(1, w_0, w_1) \approx 2.0$



• 
$$L = \sum_{i} (y_i - w_1 x_i - w_0)^2$$
  
=  $(0.0 - w_1 \cdot 0.0 - w_0)^2 + (1.0 - w_1 \cdot 1.0 - w_0)^2 + (2.0 - w_1 \cdot 1.0 - w_0)^2$   
=  $2w_1^2 + 3w_0^2 - 6w_1 - 6w_0 + 4w_1w_0 + 5$ 



• 
$$\frac{\partial L}{\partial w_1} = 4w_1 + 4w_0 - 6 = 0$$
  
•  $\frac{\partial L}{\partial w_0} = 4w_1 + 6w_0 - 6 = 0$   
•  $\therefore w_1 = 1.5, w_0 = 0.0$   
• (1.0, 2.0)  
• (1.0, 1.0)

• x가 scalar값(1개)가 아니라 vector가 된다면??

• Input

■ X1: Facebook 광고료

■ X2 : TV 광고료

■ X<sub>3</sub> : 신문 광고료

Output

■ 판매량

FB	TV	신문	판매량
<i>X</i> <sub>1</sub>	<i>X</i> <sub>2</sub>	<i>X</i> <sub>3</sub>	Y
230.1	37.8	69.2	22.1
44.5	39.3	45.1	10.4
17.2	45.9	69.3	9.3
151.5	41.3	58.5	18.5
180.8	10.8	58.4	12.9
8.7	48.9	75	7.2
57.5	32.8	23.5	11.8
:	:	:	

$$\mathbf{w}_{\text{lin}} = \underset{\mathbf{w} \in \mathbb{R}^{d+1}}{\operatorname{argmin}} \operatorname{E}_{\text{in}}(\mathbf{w})$$

$$= \underset{\mathbf{w} \in \mathbb{R}^{d+1}}{\operatorname{argmin}} \frac{1}{N} ||X\mathbf{w} - \mathbf{y}||^{2}$$

$$= \underset{\mathbf{w} \in \mathbb{R}^{d+1}}{\operatorname{argmin}} \frac{1}{N} (\mathbf{w}^{\top} X^{\top} X \mathbf{w} - 2 \mathbf{w}^{\top} X^{\top} \mathbf{y} + \mathbf{y}^{\top} \mathbf{y})$$

• Find w that minimize  $E_{in}(w)$  by requiring

$$\nabla E_{\rm in}(\mathbf{w}) = \mathbf{0}$$

From previous equation

$$\nabla \mathbf{E}_{\mathrm{in}}(\mathbf{w}) = \frac{2}{N} (X^{\mathsf{T}} X \mathbf{w} - X^{\mathsf{T}} \mathbf{y})$$

$$\mathbf{w}_{\text{lin}} = \underset{\mathbf{w} \in \mathbb{R}^{d+1}}{\operatorname{argmin}} \operatorname{E}_{\text{in}}(\mathbf{w})$$

$$= \underset{\mathbf{w} \in \mathbb{R}^{d+1}}{\operatorname{argmin}} \frac{1}{N} ||X\mathbf{w} - \mathbf{y}||^{2}$$

$$= \underset{\mathbf{w} \in \mathbb{R}^{d+1}}{\operatorname{argmin}} \frac{1}{N} (\mathbf{w}^{\top} X^{\top} X \mathbf{w} - 2 \mathbf{w}^{\top} X^{\top} \mathbf{y} + \mathbf{y}^{\top} \mathbf{y})$$

- Two scenarios
  - If  $X^TX$  is invertible Moore-Penrose Pseudoinverse w = y
  - If  $X^TX$  is not invertible Pseudo-inverse defined, but no unique solution

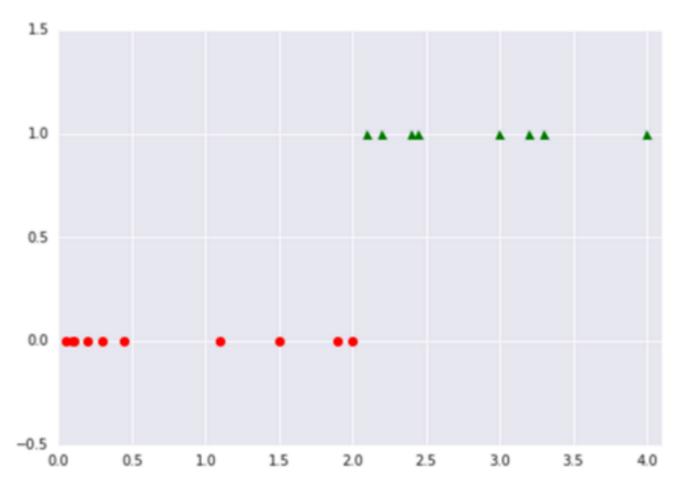
#### <Note>

 $X \in \mathbb{R}^{n \times p}$  일 때(n: sample 수, p: input vector size),

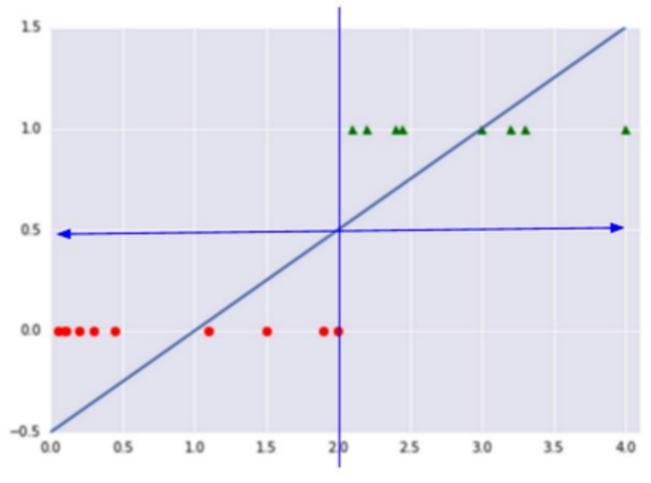
- p가 커질수록 matrix inversion 연산량이 많아짐
- p>n 이면  $X^TX$  is not invertible

### Classification도 할 수 있지 않을까요?

- 종양의 크기에 따른 양성/음성 판별 문제
  - 1 : 양성(암), o: 음성(정상)

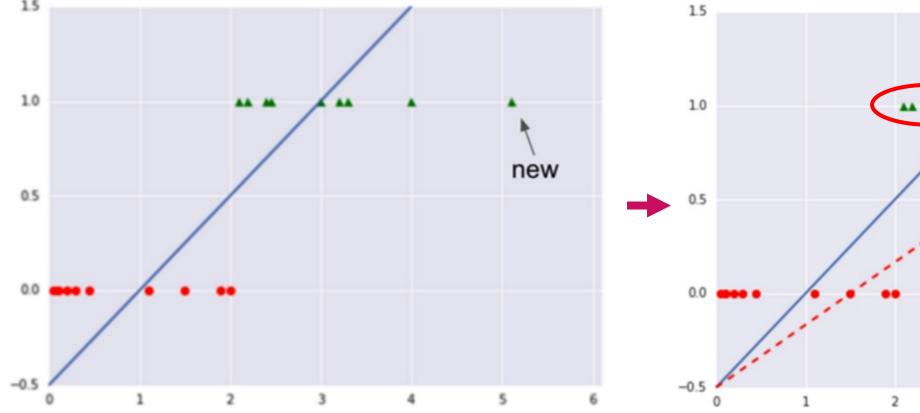


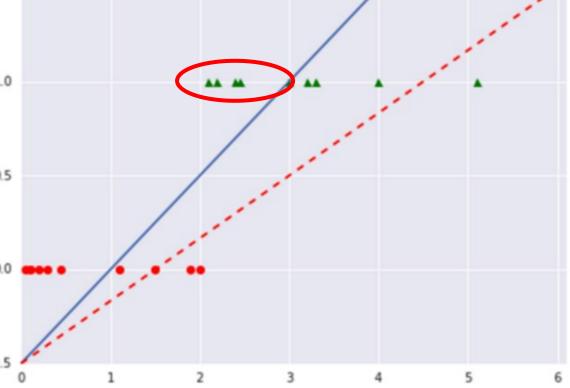
- Linear Regression으로 해봅시다
  - Regression 예측값이 o.5 이상이면 양성, o.5 이하면 음성으로 판별



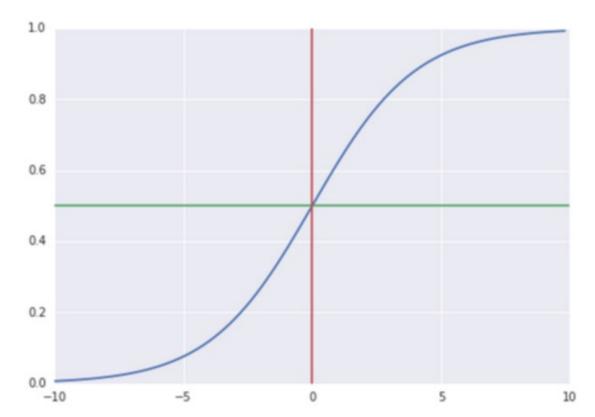
• 종양의 크기가 매우 큰 data(outlier) 가 추가된 경우







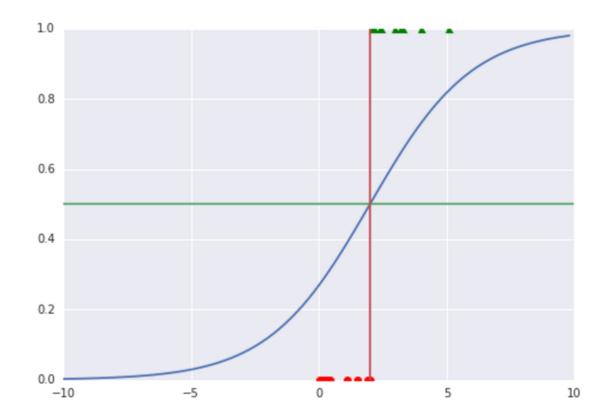
- 아주 크거나 아주 작은 data에 영향을 많이 받지 않았으면 좋겠다
- Binary classification에 맞게 o에서 1사이 값으로 나오면 좋겠다
- → Sigmoid 를 써보자



### Logistic Regression

• Linear Regression 식에 Sigmoid 함수를 통과시킨 것

$$\blacksquare H(x) = \sigma(\mathbf{w}^T \mathbf{x} + b) = \frac{1}{1 + e^{-(\mathbf{w}^T \mathbf{x} + b)}} = P(y | \mathbf{x})$$



#### Logistic Regression

• 새로운 Cost(Loss) function을 정의(maximum likelihood estimation)

$$cost(W) = -\frac{1}{m} \sum ylog(H(x)) + (1 - y)log(1 - H(x))$$

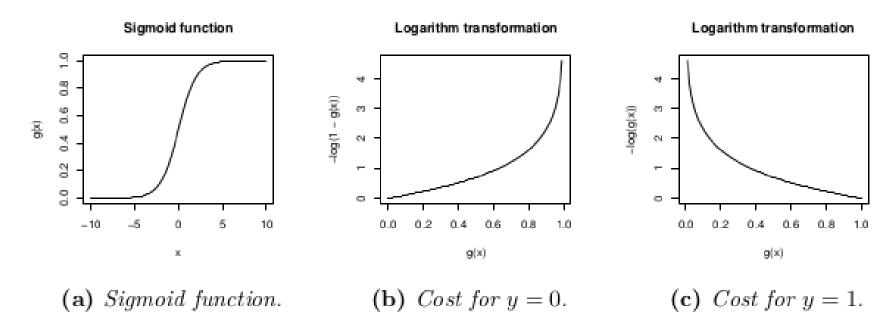


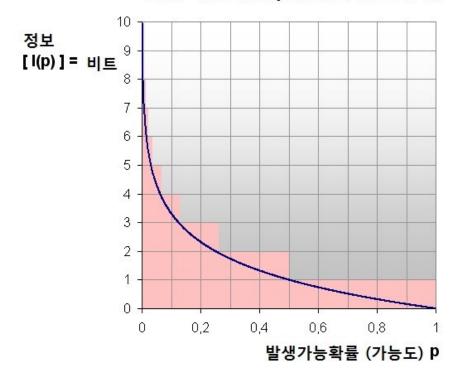
Figure B.1: Logarithmic transformation of the sigmoid function.

# entro

• Information Theory에서 Entropy란 정보량의 기댓값(평균)이다

$$\mathrm{H}(X) = \mathrm{E}[\mathrm{I}(X)] = \mathrm{E}[-\ln(\mathrm{P}(X))].$$

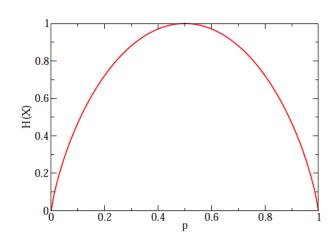
#### 발생 가능확률 p에따른 정보의 양



- 항상 일어나는 사건이라면 p=1 이고 이것이 가지고 있는 정보량은 0이다.
- 일어날 확률이 적을 수록 많은 정보를 담고 있다.

### Entropy

$$egin{aligned} &\operatorname{H}(X) = \operatorname{E}[\operatorname{I}(X)] = \operatorname{E}[-\ln(\operatorname{P}(X))]. \ &= \sum_{i=1}^n \operatorname{P}(x_i)\operatorname{I}(x_i) = -\sum_{i=1}^n \operatorname{P}(x_i)\log_b\operatorname{P}(x_i), \end{aligned}$$



Ex) 동전던지기

$$P(앞) = \frac{1}{2}$$

$$H(X) = -(0.5 * \log_2 0.5 + 0.5 * \log_2 0.5) = 0.5 + 0.5 = 1$$

이 확률 분포를 표현하기 위하여 평균 1 bit가 필요하다는 의미!

#### **Cross Entropy**

True distribution p, Model이 예측한 distribution을 q라고 하면

Cross entropy를 minimize 하는 것은 p와 q의 분포가 가까

$$\begin{split} H(p,q) &= -\sum_{i} p_{i} \log q_{i} \\ &= -\sum_{i} p_{i} \log q_{i} - \sum_{i} p_{i} \log p_{i} + \sum_{i} p_{i} \log p_{i} \\ &= H(p) + \sum_{i} p_{i} \log p_{i} - \sum_{i} p_{i} \log q_{i} \\ &= H(p) + \sum_{i} p_{i} \log \frac{p_{i}}{q_{i}} \\ &= H(p) + D_{KL}(p \parallel q) \end{split}$$

P 자체의 entropy(불변) p를 기준으로 q가 얼마나 다른가 (p의 distribution과 q의 distribution의 거리)

#### Kullback-Leibler(KL) Divergence

- 두 확률 분포간의 거리(?)를 나타냄
  - $D_{KL}(p \parallel q) = p \log \frac{p}{q} = p \log p + (-p \log q) = -H(p) + H(p,q) = H(p,q)$

p의 entropy

p, q의 cross entropy

- p는 label, q는 network output 이라고 할 경우, network의 목표는 label이 나타내는 확률 분포 p와 최대한 가까운 q를 학습하고자 하는 것임
- 일반적으로 label은 one-hot encoding 하기 때문에, 각 label의 값이 확률이라고 생각하면 p의 entropy, H(p)=0
- $D_{KL}(p \parallel q) > 0$

# Minimizing NLL

$$\mathbf{e}(h(\mathbf{x}_n), y_n) = \ln\left(1 + e^{-y_n \mathbf{w}^{\top} \mathbf{x}_n}\right)$$

We can define loss(error) function as below

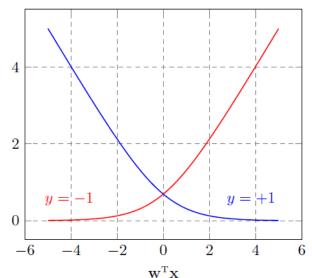
$$E_{in}(\mathbf{w}) = \frac{1}{N} \sum_{n=1}^{N} \log \left( 1 + e^{-y_n \mathbf{w}^{\top} \mathbf{x}_n} \right)$$

$$\ln\left(1 + e^{-y\mathbf{w}^{\mathrm{T}}\mathbf{x}}\right)$$

Unfortunately, not easy to manipulate analytically

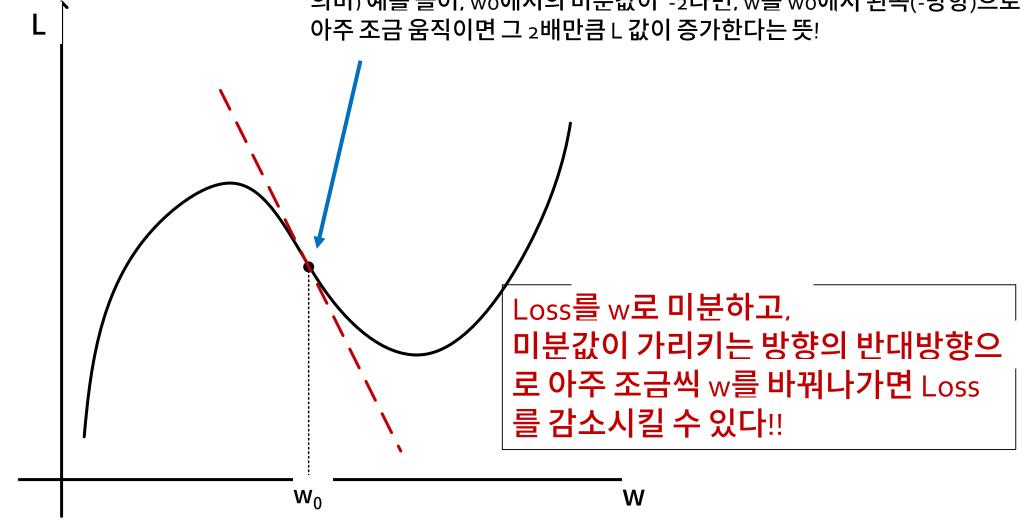
$$\nabla \mathbf{E}_{\text{in}}(\mathbf{w}) = -\frac{1}{N} \sum_{n=1}^{N} \frac{y_n \mathbf{x}_n}{1 + e^{y_n \mathbf{w}^T \mathbf{x}_n}}$$
$$= \frac{1}{N} \sum_{n=1}^{N} -y_n \mathbf{x}_n \theta(-y_n \mathbf{w}^T \mathbf{x}_n)$$

- We need iterative optimization
- Use 미분!

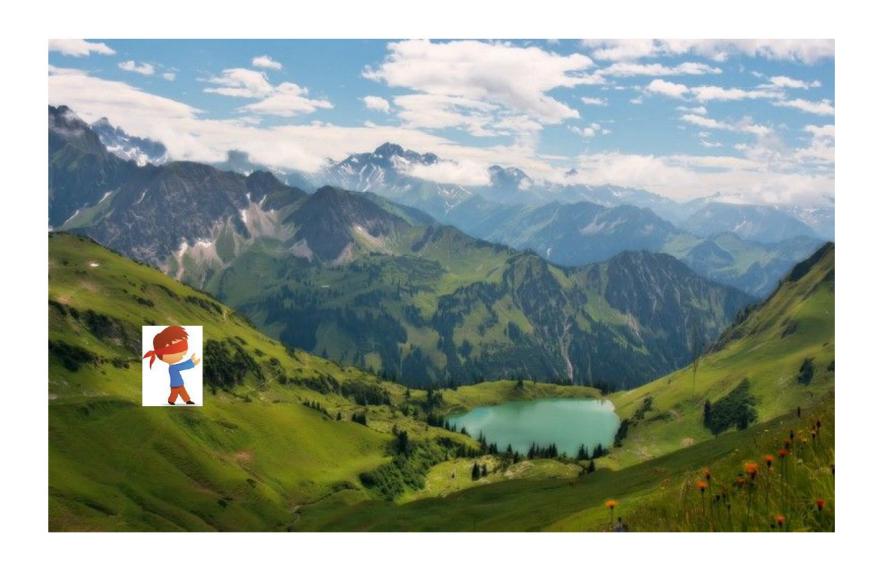


#### 미분??

w=w¸에서의 미분값 = 이 점에서의 접선의 기울기 의미) 예를 들어, wo에서의 미분값이 -2라면, w를 wo에서 왼쪽(-방향)으로 아주 조금 움직이면 그 2배만큼 L 값이 증가한다는 뜻!



#### **Gradient Descent**

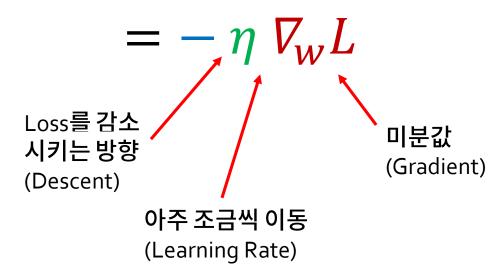


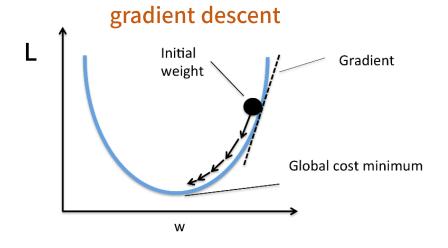
### **Gradient Descent**

# Loss Function의 미분(Gradient)를 이용하여 weight를 update하는 방법

$$w_{new} = w_{old} - \eta \nabla_{w} L$$

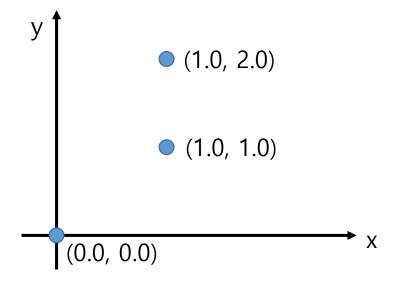
Weight update =  $w_{new} - w_{old}$ 





### Linear Regression Again

- Find the linear function(f) that best describes the given data
  - $H(x, w_0, w_1) = w_1 x + w_0$



$$L = \sum_{i} (y_i - w_1 x_i - w_0)^2$$

$$= (0.0 - w_1 \cdot 0.0 - w_0)^2 + (1.0 - w_1 \cdot 1.0 - w_0)^2 + (2.0 - w_1 \cdot 1.0 - w_0)^2$$

$$= 2w_1^2 + 3w_0^2 - 6w_1 - 6w_0 + 4w_1 w_0 + 5$$

## Solving Linear Regression Using GD

- Choose a small value for  $\eta$  such as  $\eta=0.1$
- Randomly select  $w_0^0 = 1, w_1^0 = 1$ , initially
- Repeat

$$w_0^{t+1} = w_0^t - \eta(4w_1^t + 6w_0^t - 6)$$
  
$$w_1^{t+1} = w_1^t - \eta(4w_1^t + 4w_0^t - 6)$$

$$\frac{\partial L}{\partial w_1} = 4w_1 + 4w_0 - 6 = 0$$

$$\frac{\partial L}{\partial w_0} = 4w_1 + 6w_0 - 6 = 0$$

## Solving Linear Regression Using GD

$$w_0^0 = 1$$
  
 $w_1^0 = 1$ 

$$w_0^1 = 1 - 0.1(4 \times 1 + 6 \times 1 - 6) = 0.6$$
  
 $w_1^1 = 1 - 0.1(4 \times 1 + 4 \times 1 - 6) = 0.8$ 

$$w_0^2 = 0.6 - 0.1(4 \times 0.8 + 6 \times 0.6 - 6) = 0.54$$
  
 $w_1^2 = 0.8 - 0.1(4 \times 0.8 + 4 \times 0.6 - 6) = 0.84$ 

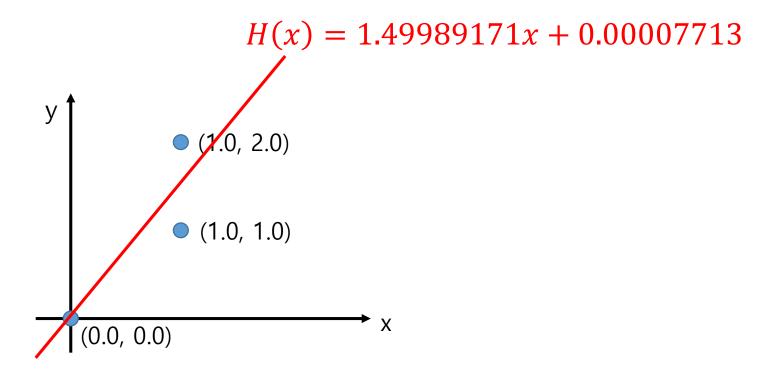
$$w_0^3 = 0.54 - 0.1(4 \times 0.84 + 6 \times 0.54 - 6) = 0.480$$
  
 $w_1^3 = 0.84 - 0.1(4 \times 0.84 + 4 \times 0.54 - 6) = 0.888$ 

## Solving Linear Regression Using GD

$$w_0^4 = 0.480 - 0.1(4 \times 0.888 + 6 \times 0.480 - 6) = 0.4368$$
  
 $w_1^4 = 0.888 - 0.1(4 \times 0.888 + 4 \times 0.480 - 6) = 0.9408$ 

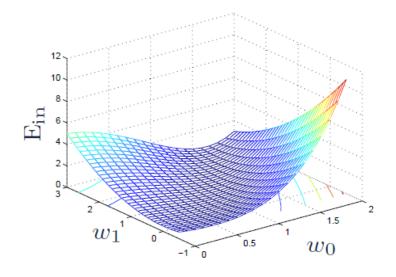
...

$$w_0^{100} = 0.00007713$$
  
 $w_1^{100} = 1.49989171$ 

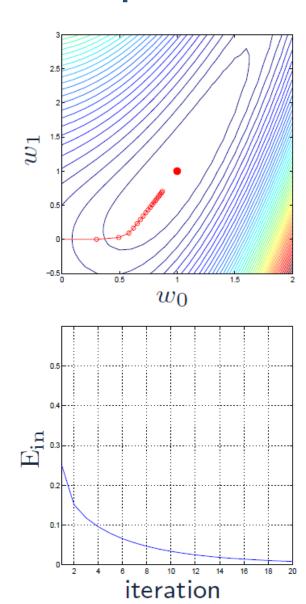


## Gradient Decent Example

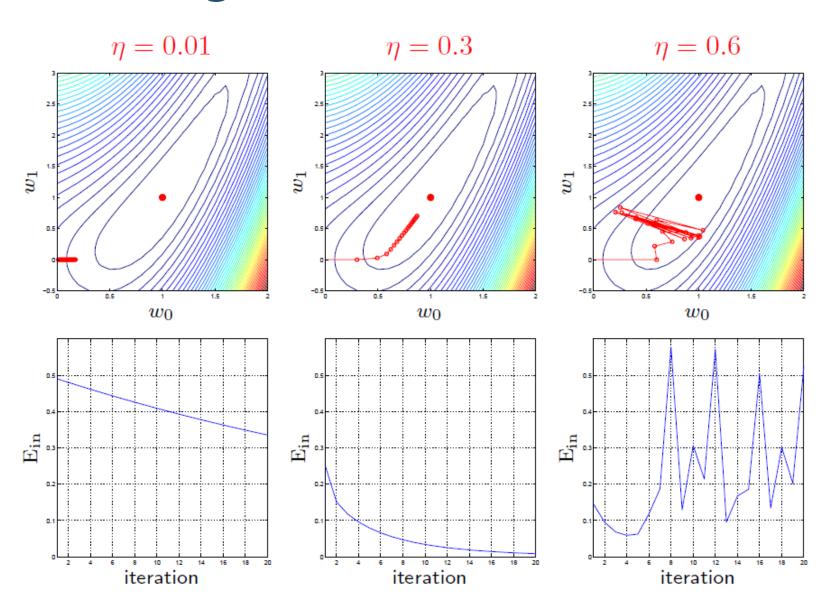
► Global minimum 0 at (1,1)



- ► Start at (0,0)
  - # iterations (steps) = 20
  - $\bullet \ \ {\rm step \ size} \ \eta = 0.3$

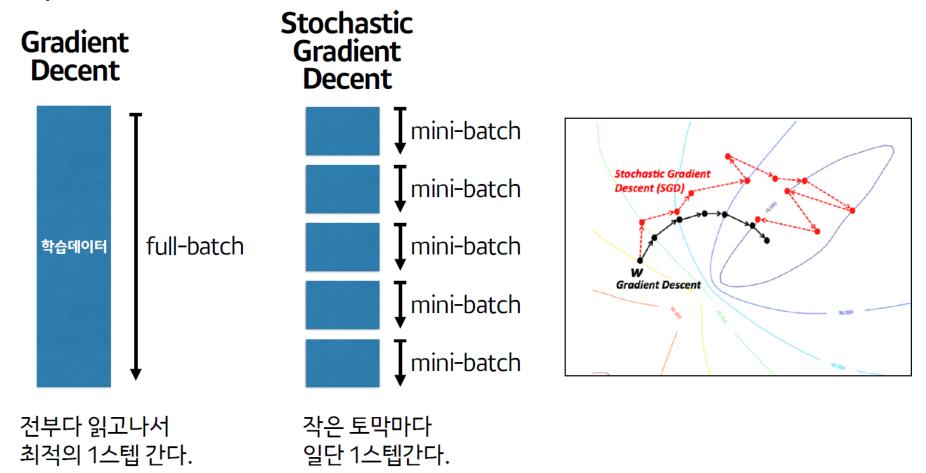


## Learning Rate



### Stochastic Gradient Descent, Mini-batch Training

• Data가 너무 많아서 한번에 다 넣고 학습하면 시간도 오래걸리고, memory도 부족하게 됨



### Learning Rate & Mini-Batch



**Mini-Batch size:** Number of training instances the network evaluates per weight update step.

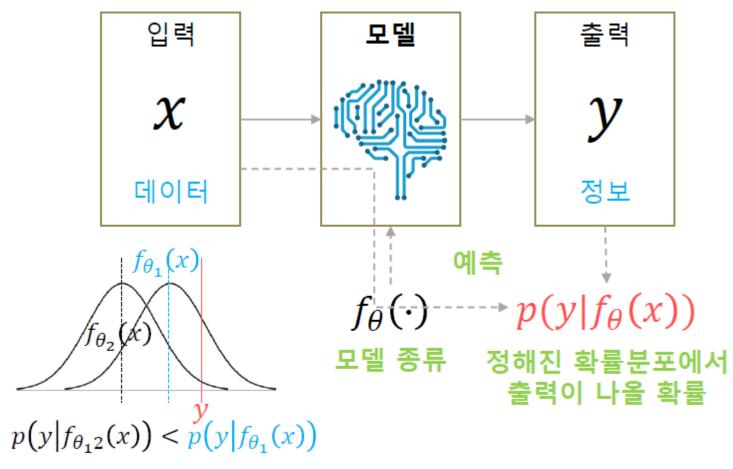
- Larger batch size = more computational speed
- Smaller batch size = (empirically) better generalization

"Training with large minibatches is bad for your health. More importantly, it's bad for your test error. Friends don't let friends use minibatches larger than 32."

- Yann LeCun

Revisiting Small Batch Training for Deep Neural Networks (2018)

"when increasing the batch size, a linear increase of the learning rate  $\eta$  with the batch size m is required to keep the mean SGD weight update per training example constant"



$$\theta^* = \underset{\theta}{\operatorname{argmin}} [-\log(p(y|f_{\theta}(x)))]^{\text{주어진 데이터를 제일 질 설명하는 모델 찾기}}$$

#### Maximum Likelihood Estimation

#### i.i.d Condition on $p(y|f_{\theta}(x))$

Assumption 1 : Independence

All of our data is independent of each other

$$p(y|f_{\theta}(x)) = \prod_{i} p_{D_i}(y|f_{\theta}(x_i))$$

Assumption 2: Identical Distribution

Our data is identically distributed

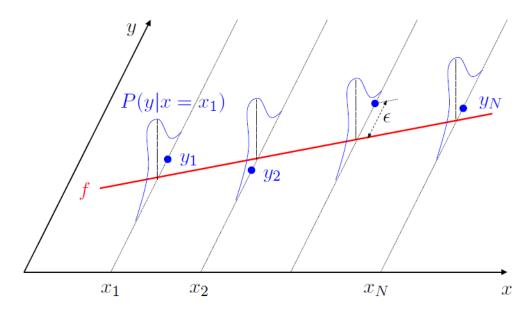
$$p(y|f_{\theta}(x)) = \prod_{i} p(y|f_{\theta}(x_i))$$

Negative Log-Likelihood(NLL)

$$-\log(p(y|f_{\theta}(x))) = -\sum_{i}\log(p(y_{i}|f_{\theta}(x_{i})))$$

- Linear Regression
  - Training data is considered as the set of iid samples from underlying probabilistic model:

 $y_i = \theta^T x_i + \epsilon_i$ , where  $\epsilon_i$  follows Gaussian distribution  $\epsilon_i \sim N(0, \sigma^2)$ 



• Models predict the mean of Gaussian distribution( $\mu_i$ )

- Logistic Regression
  - Training data is considered as the set of iid samples which follows Bernoulli distribution:

$$p(x) = p^{x}(1-p)^{(1-x)}$$

• Models predict the probability  $p(y = 1 | x, \theta)$  directly

### Minimize Negative Log-Likelihod

#### Univariate cases

$$-\log(p(y_i|f_{\theta}(x_i)))$$

#### Gaussian distribution

$$f_{\theta}(x_i) = \mu_i, \sigma_i = 1$$

$$p(y_i|\mu_i, \sigma_i) = \frac{1}{\sqrt{2\pi}\sigma_i} \exp\left(-\frac{(y_i - \mu_i)^2}{2\sigma_i^2}\right)$$

$$\log(p(y_i|\mu_i,\sigma_i)) = \log\frac{1}{\sqrt{2\pi}\sigma_i} - \frac{(y_i - \mu_i)^2}{2\sigma_i^2}$$

$$-\log(p(y_i|\mu_i)) = -\log\frac{1}{\sqrt{2\pi}} + \frac{(y_i - \mu_i)^2}{2}$$

$$-\log(p(y_i|\mu_i)) \propto \frac{(y_i - \mu_i)^2}{2} = \frac{(y_i - f_\theta(x_i))^2}{2}$$

#### Mean Squared Error

#### Bernoulli distribution

$$f_{\theta}(x_i) = p_i$$

$$p(y_i|p_i) = p_i^{y_i}(1-p_i)^{1-y_i}$$

$$\log(p(y_i|p_i)) = y_i \log p_i + (1 - y_i) \log(1 - p_i)$$

$$-\log(p(y_i|p_i)) = -[y_i \log p_i + (1 - y_i) \log(1 - p_i)]$$

Cross-entropy