반도체소재설계
강의자료 05

한밭대학교 신소재공학과 신기현

TheMAD

Machine Learning Definition

"A computer program is said to learn from experience E with respect to some class of tasks T and performance measure P, if its performance at tasks in T, as measured by P, improves with experience E"

By Tom M. Mitchell

Machine Learning Algorithms

- Supervised learning
- Unsupervised learning
- Reinforcement learning

Supervised Learning

x ⟶ **y**

input **output**

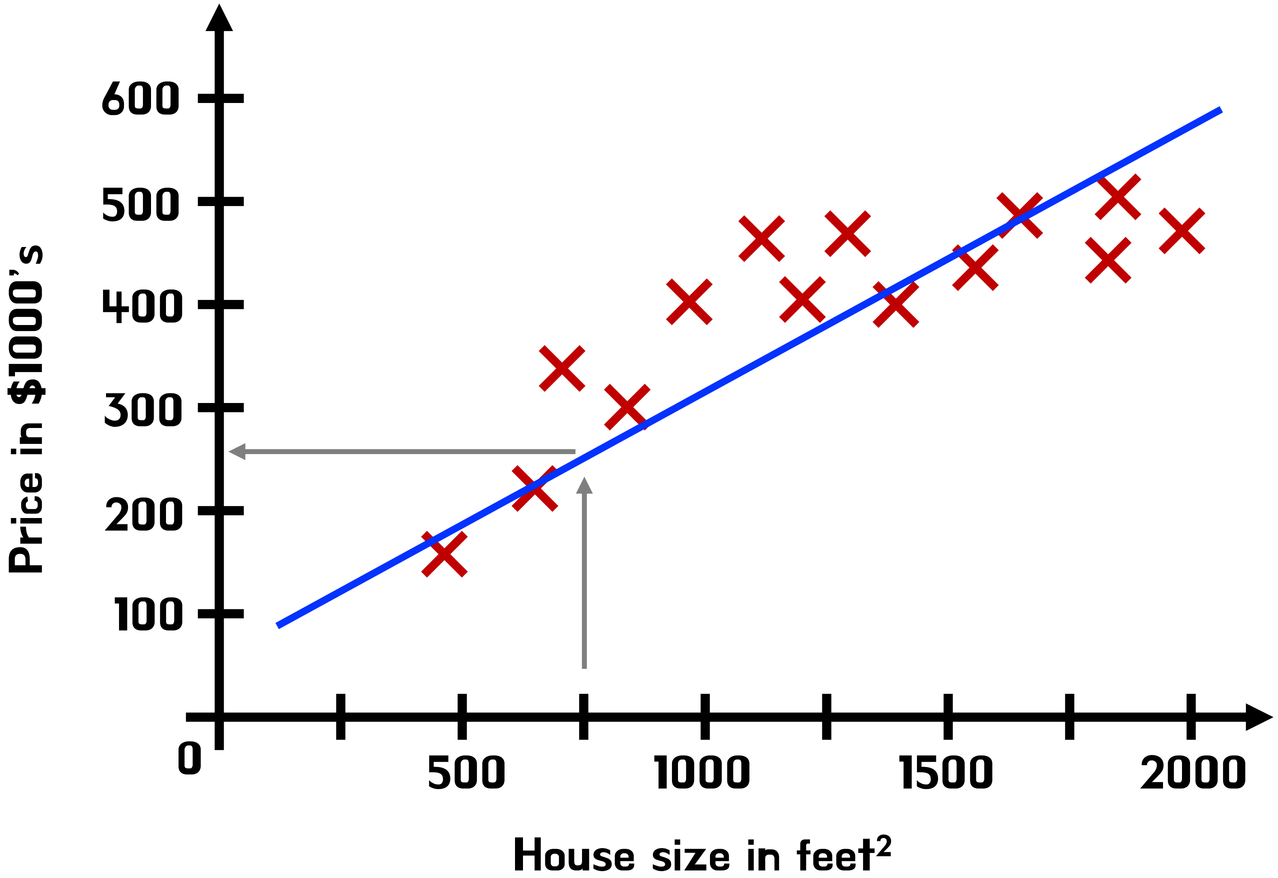
(label)

Learns from being given "right answers"

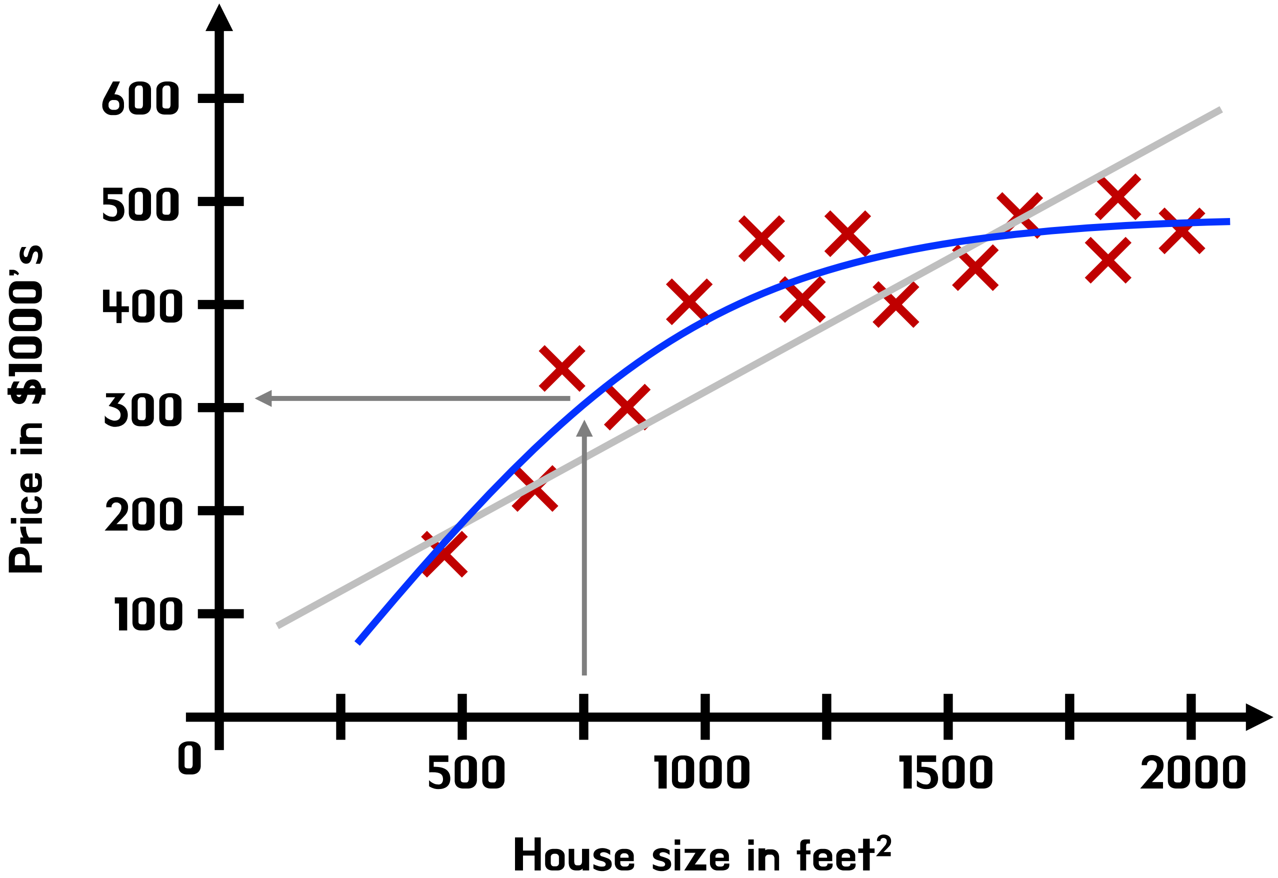
Supervised Learning

Input (x)	Output (y)	Application
email	spam? (0/1)	Spam filtering
audio	text transcripts	Speech recognition
english	spanish	Machine translation
Ad, user info.	Click ? (0/1)	Online advertising
Image, radar info.	Position of other cars	Self-driving car
Image of phone	Defect ? (0/1)	Visual inspection

Regression: Housing price prediction



Regression: Housing price prediction

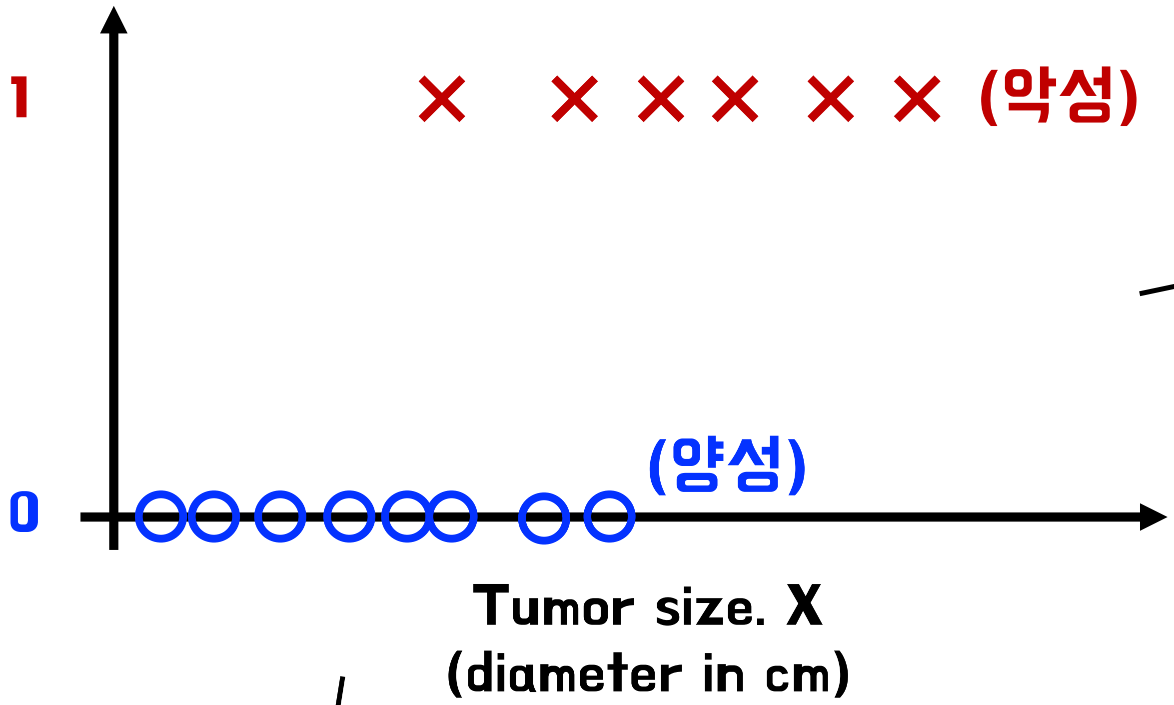


Regression

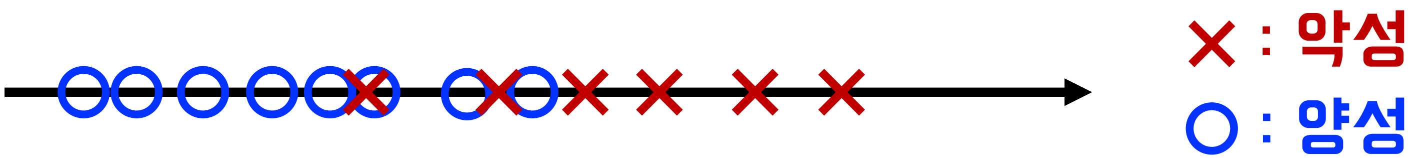
predict a number

(infinitely many possible outputs)

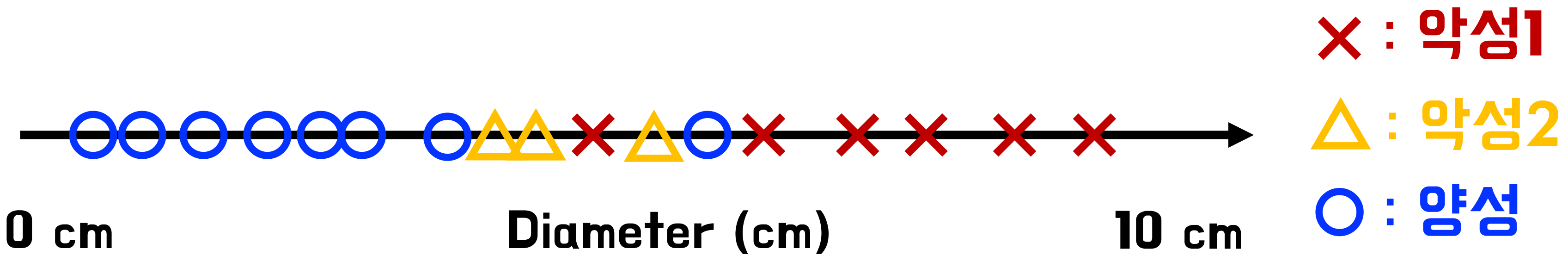
Classification: Breast cancer detection



Size	Diagnosis
2	0
5	1
1	0
7	1
6	1
⋮	⋮



Classification: Breast cancer detection

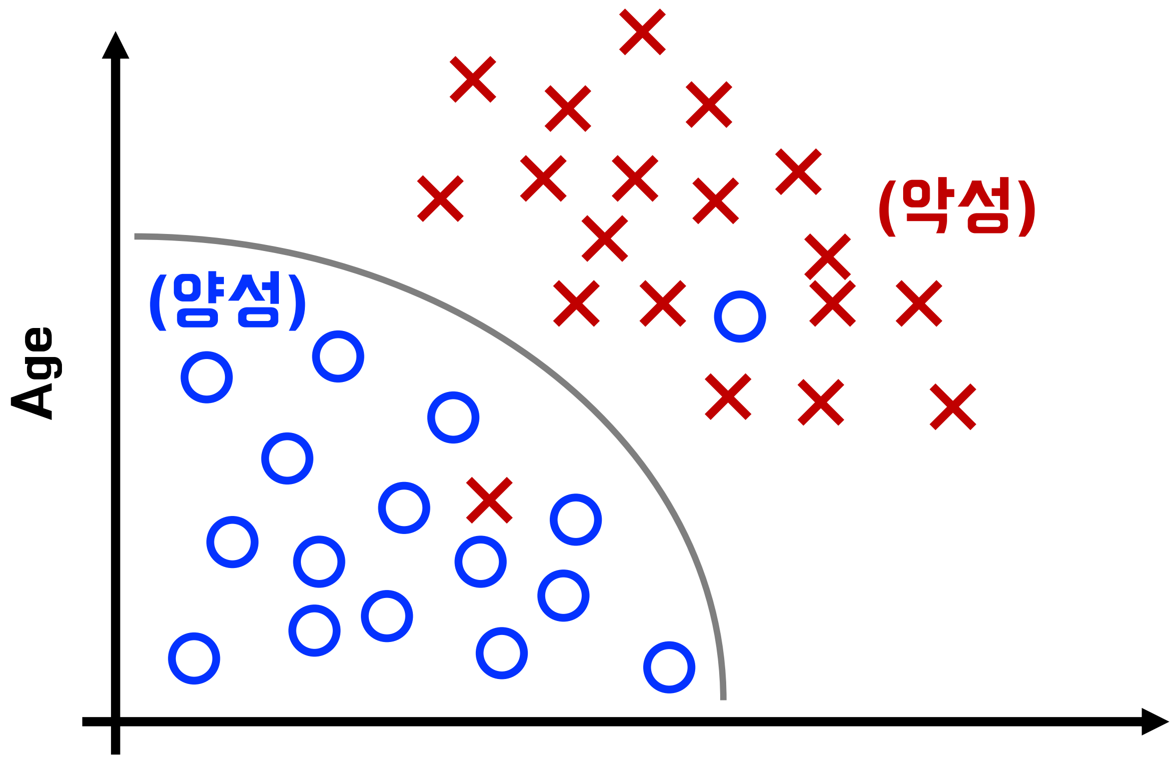


Classification

predict categoreis

(small number of possible outputs)

Two or more inputs



Many more inputs can be also available
(thickness, uniformity of size, shape)

Supervised learning

Supervised Learning

Learns from being given "right answers"

Regression

Predict a number

Infinitely many possible outputs

Classification

Predict categories

Small number of possible outputs

Unsupervised learning

Supervised learning

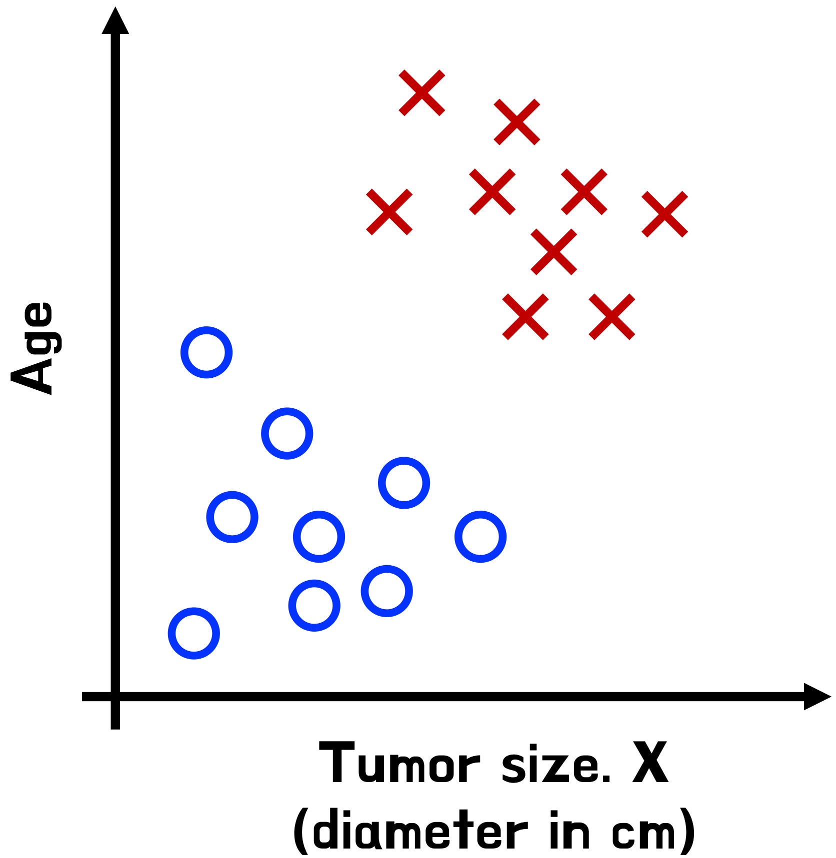
Learn from data labeled

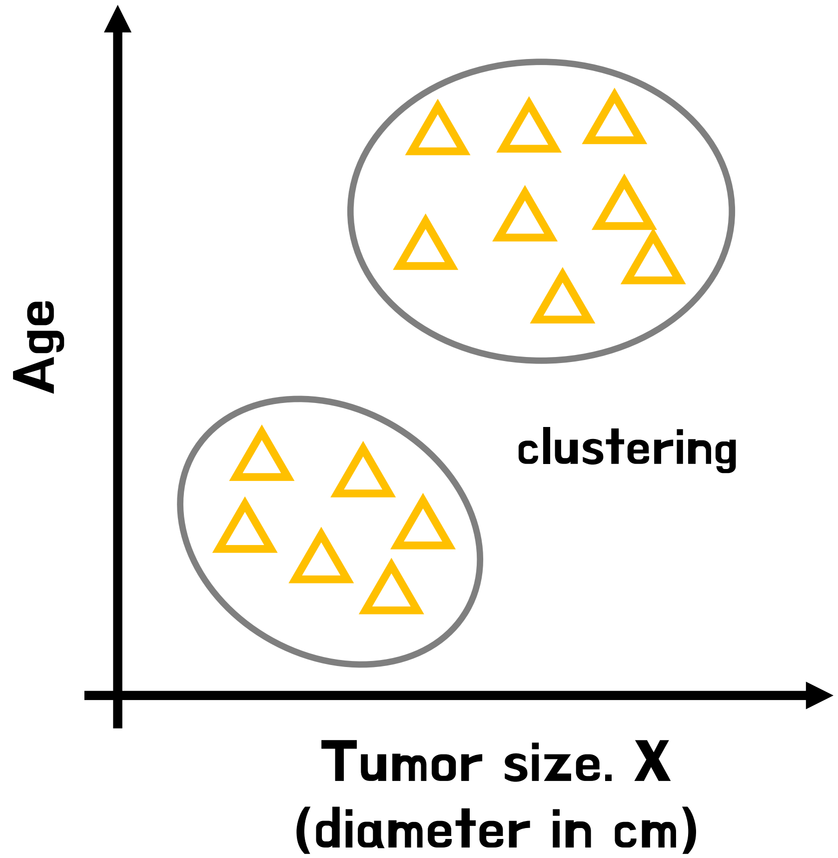
With the "right answers"

Unsupervised learning

Find something interesting

in unlabeled data

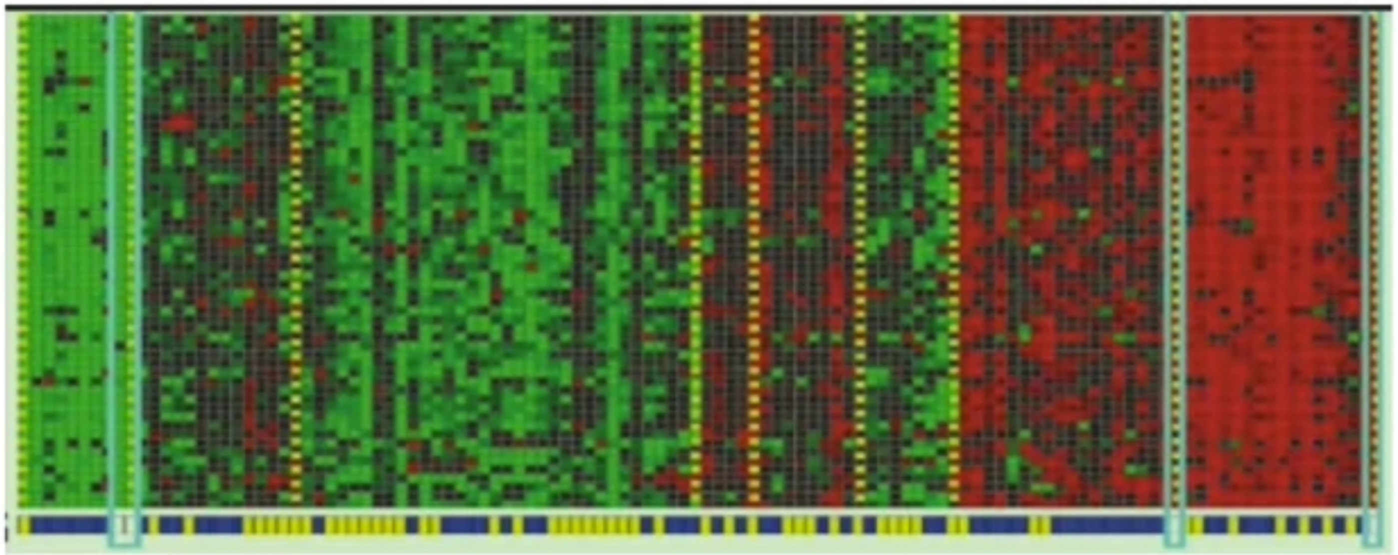




Unsupervised learning

Unsupervised learning

Genes (each row)



Individuals (each column)

Unsupervised learning

Data only comes with inputs x, but not output labels y.

Algorithm has to find structure in the data.

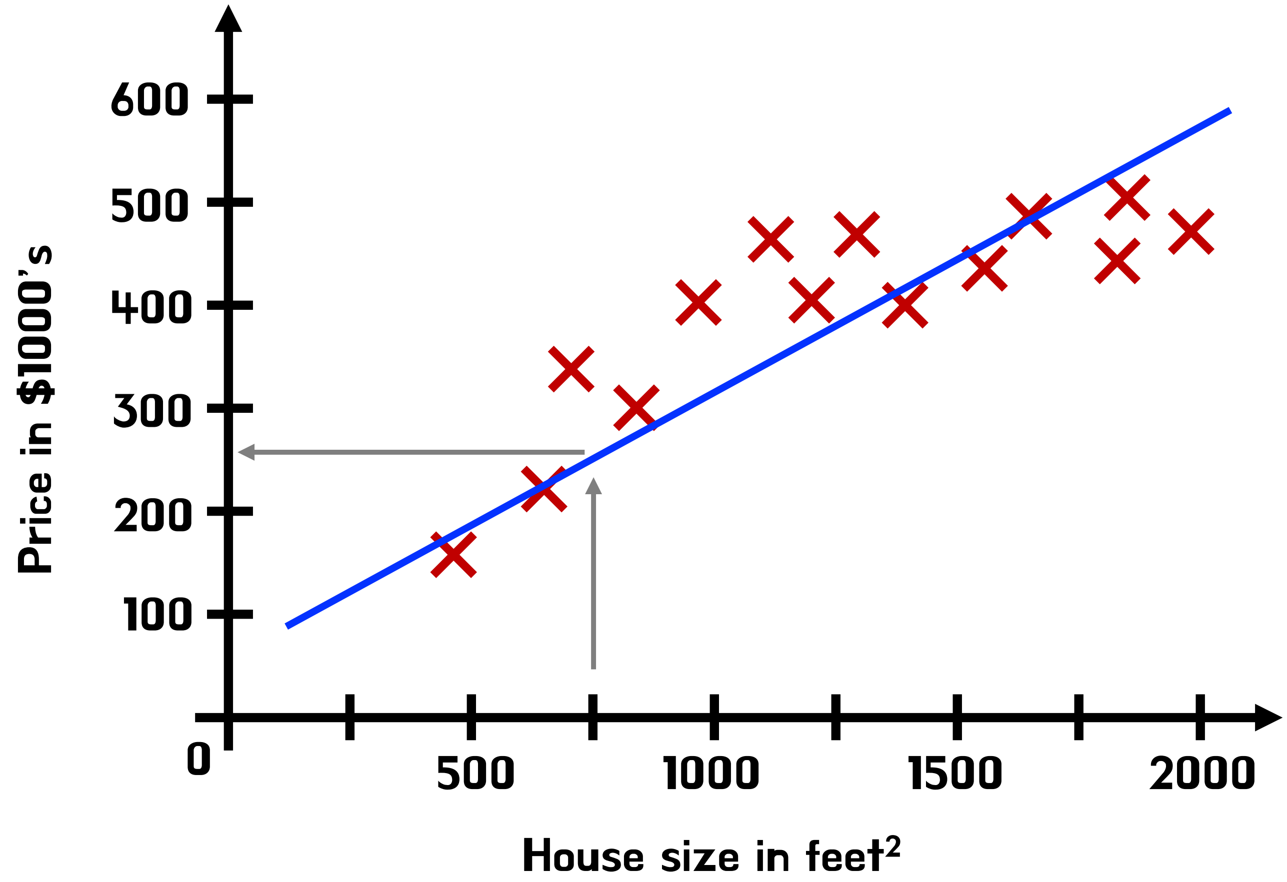
Clustering
Group similar data points together.

Dimensionality reduction (차원축소)
Compress data using fewer numbers.

Anomaly detection
Find unusual data points.

Linear Regression
(선형 회귀)

Linear regression

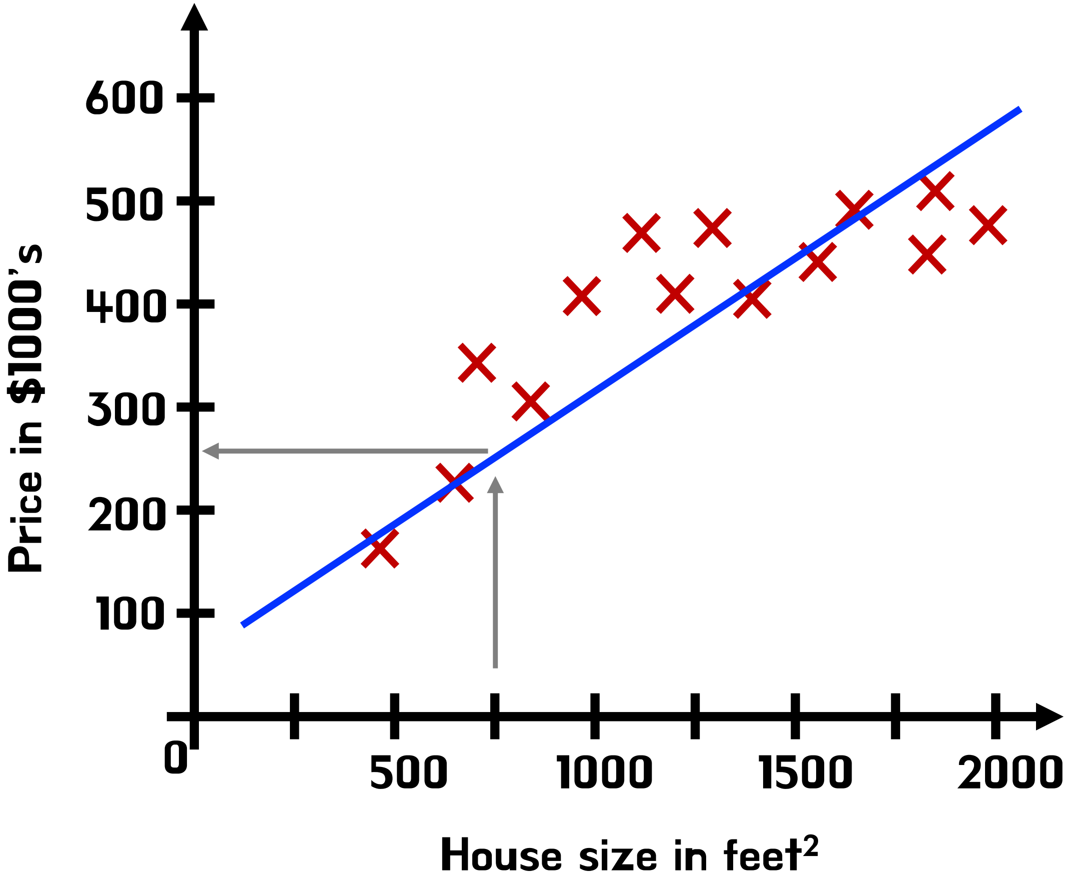


Regression model
Predicts numbers
(infinitely many possible outputs)

Supervised learning model
Data has "right answers"

Classification model
Predicts categories
(small number of possible outputs)

Linear regression



Data table

Size in feet^2	Price in $1000's
900	310
700	320
990	400
1550	406
1700	490
⋮	⋮

TheMAD

Terminology

Training set : Data used to train the model

	x Size in feet^2	y Price in $1000's
(1)	900	310
(2)	700	320
(3)	990	400
(4)	1550	406
(5)	1700	490
⋮	⋮	⋮

Test set : Data used to test the model

	Size in feet^2	Price in $1000's
(a)	980	310
(b)	1300	390
(c)	2000	500

Notation:

x = "input" variable
feature

y = "output" variable
"target" variable

m = number of training examples

(x, y) = single training example

$(x^{(i)}, y^{(i)})$ = i^{th} training example

x = 900, y = 400

(x, y) = (900, 400)

Terminology

Training set

↓

Learning algorithm

↓

$x \rightarrow f \rightarrow \hat{y}$

model

feature

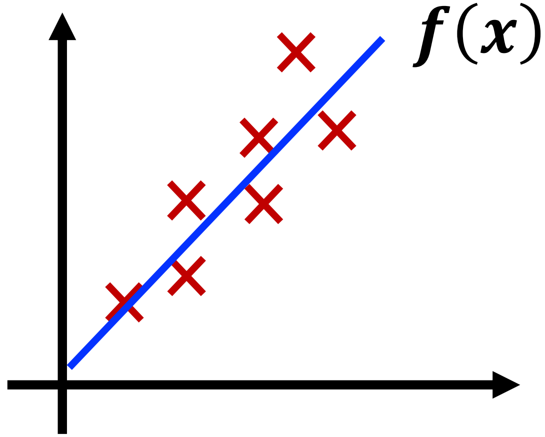
"y-hat"

Prediction

(estimated y)

How to represent f?

$$f_{w,b}(x) = f(x) = wx + b$$



$f(x) = wx + b$

Linear

Linear regression with one variable.

Univariate linear regression.

Parameters (Hyper parameters)

Training set

(feature) **(targets)**

Size in feet^2	Price in \$1000's
900	310
700	320
990	400
1550	406
1700	490
⋮	⋮

$$f(x) = wx + b$$

w, b : parameters

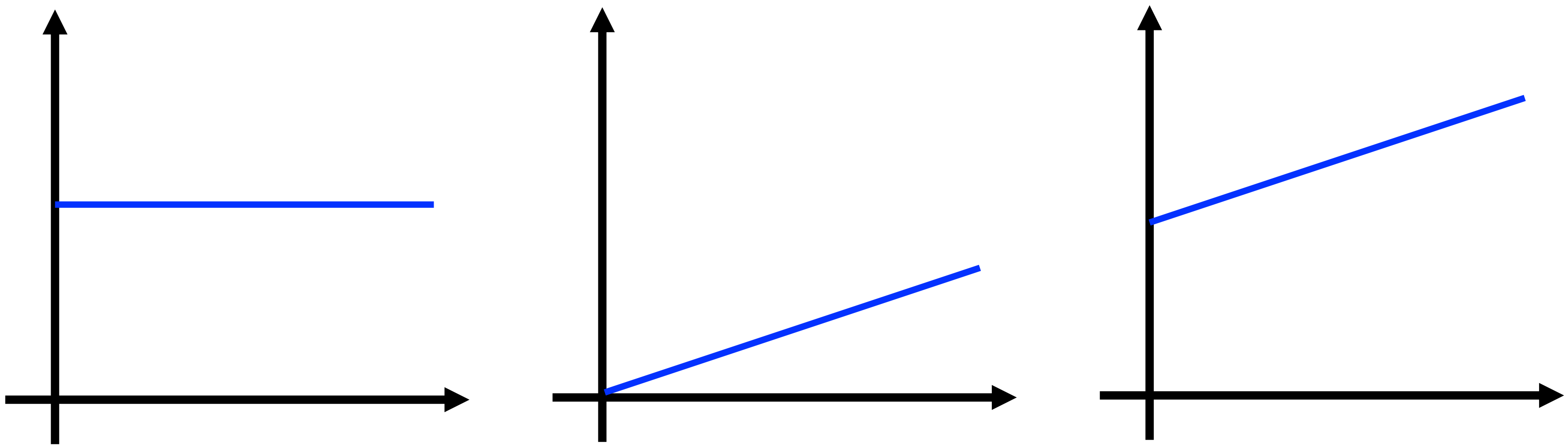
Bias

Weights

What do w, b do ?

Cost function

$$f(x) = wx + b$$

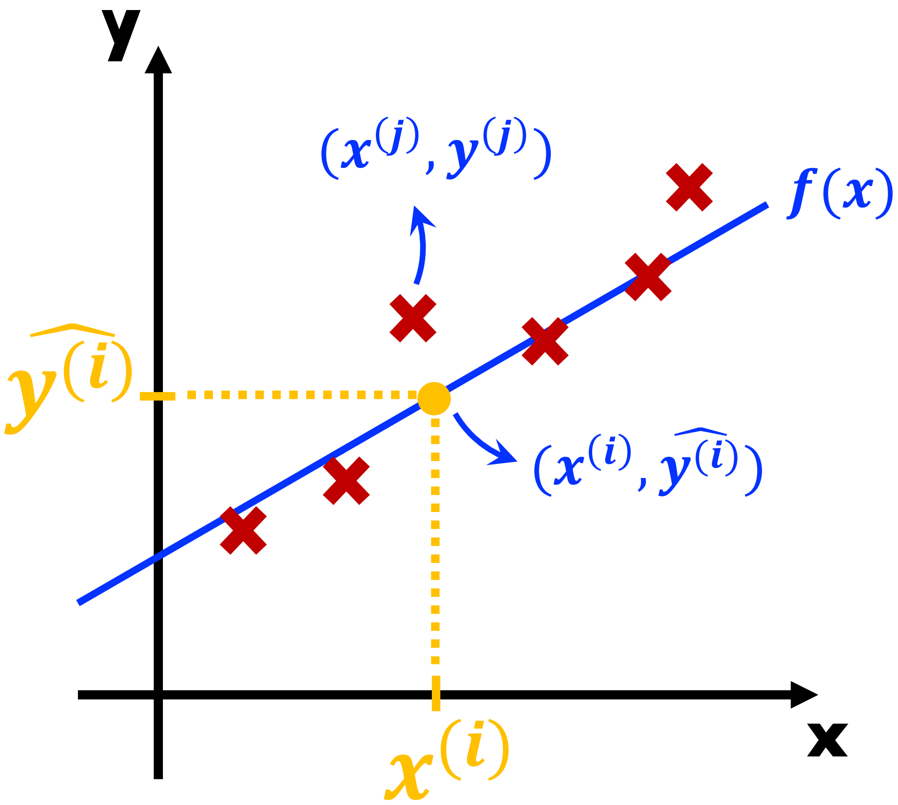


$w = 0$, $b = 1.5$

$w = 0.5$, $b = 0$

$w = 0.5$, $b = 1$

Cost function



$$\widehat{y^{(i)}} = f\left(x^{(i)}\right) = wx^{(i)} + b$$

Cost function:
Squared error cost function

$$J(w,b) = \frac{1}{2m}\sum_{i=1}^{m}\left(\widehat{y^{(i)}} - y^{(i)}\right)^2$$

error

Number of training examples (m)

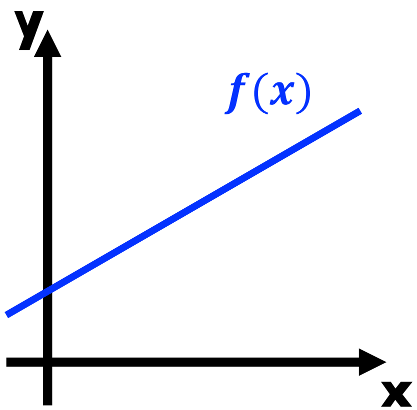
$$J(w,b) = \frac{1}{2m}\sum_{i=1}^{m}\left(f\left(x^{(i)}\right) - y^{(i)}\right)^2$$

$$J(w,b) = \frac{1}{2m}\sum_{i=1}^{m}\left(wx^{(i)} + b - y^{(i)}\right)^2$$

Cost function

Model:

$$f(x) = wx + b$$



Parameters:

$$w, b$$

Cost function:

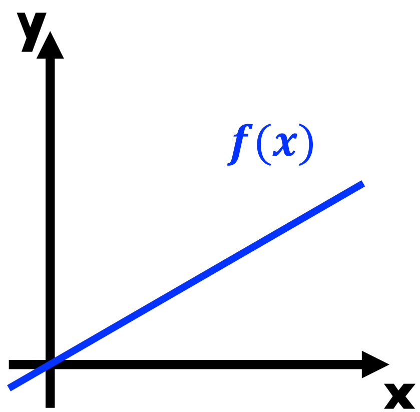
$$J(w,b) = \frac{1}{2m}\sum_{i=1}^{m}\left(f\left(x^{(i)}\right) - y^{(i)}\right)^2$$

Goal:

$$\underset{w,b}{minimize}\, J(w,b)$$

Simplified Model:

$$f(x) = wx$$



Parameters:

$$w$$

Cost function:

$$J(w) = \frac{1}{2m}\sum_{i=1}^{m}\left(f\left(x^{(i)}\right) - y^{(i)}\right)^2$$

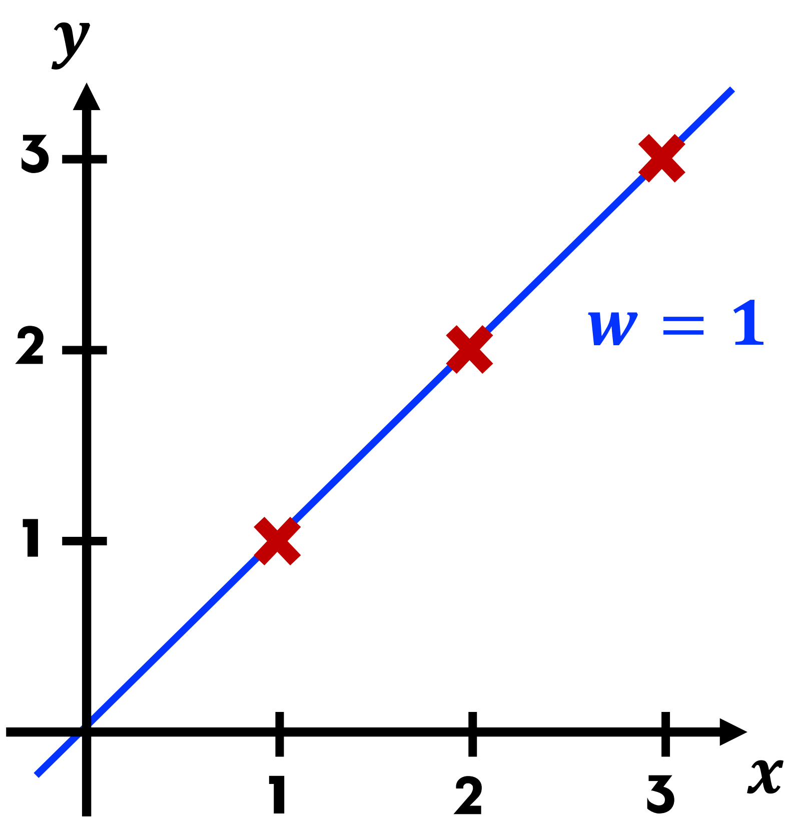
Goal:

$$\underset{w}{minimize}\, J(w)$$

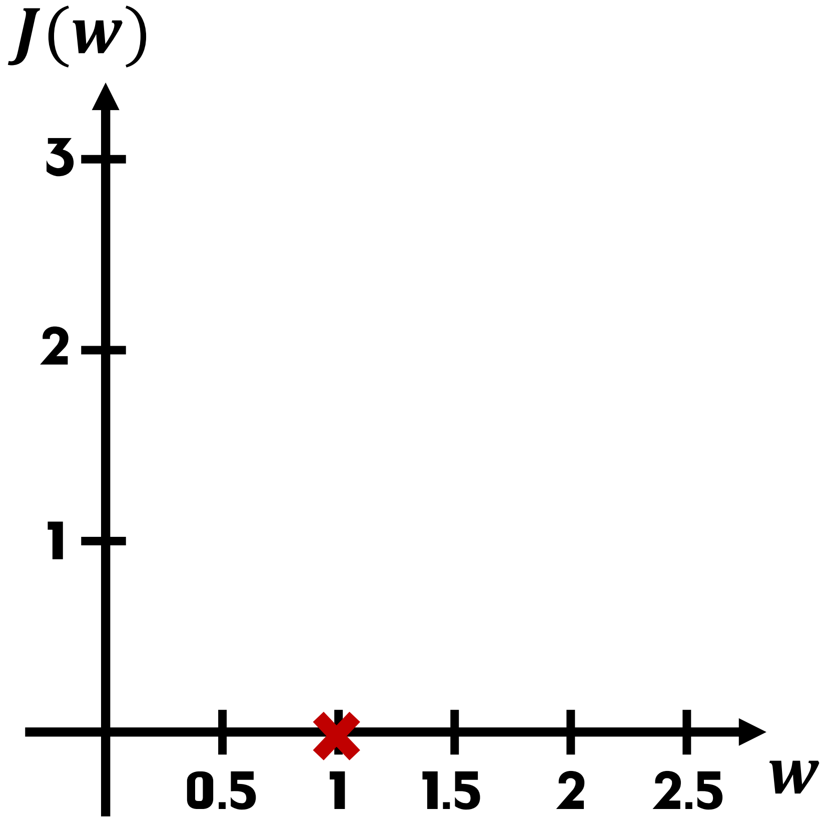
Cost function

$f_w(x)$ $J(w)$

For fixed w, function of x



Function of w

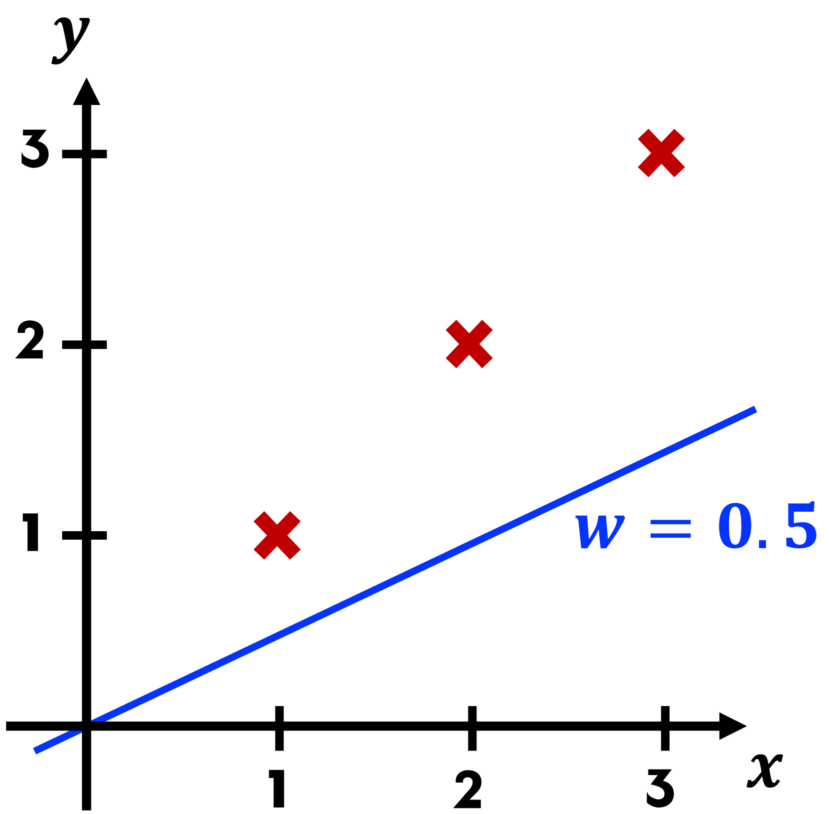


$$J(w) = \frac{1}{2m}\sum_{i=1}^{m}\left(f\left(x^{(i)}\right) - y^{(i)}\right)^2 = \frac{1}{2m}\sum_{i=1}^{m}(wx^{(i)} - y^{(i)})^2 = \frac{1}{2m}\left(0^2 + 0^2 + 0^2\right) = 0$$

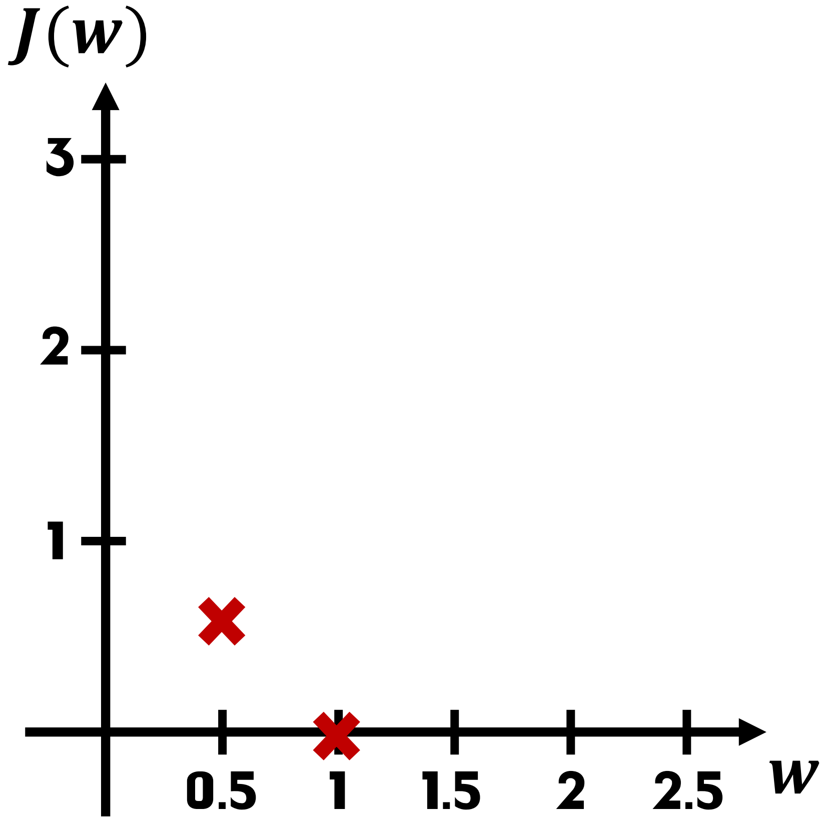
Cost function

$f_w(x)$ | $J(w)$

For fixed w, function of x



Function of w

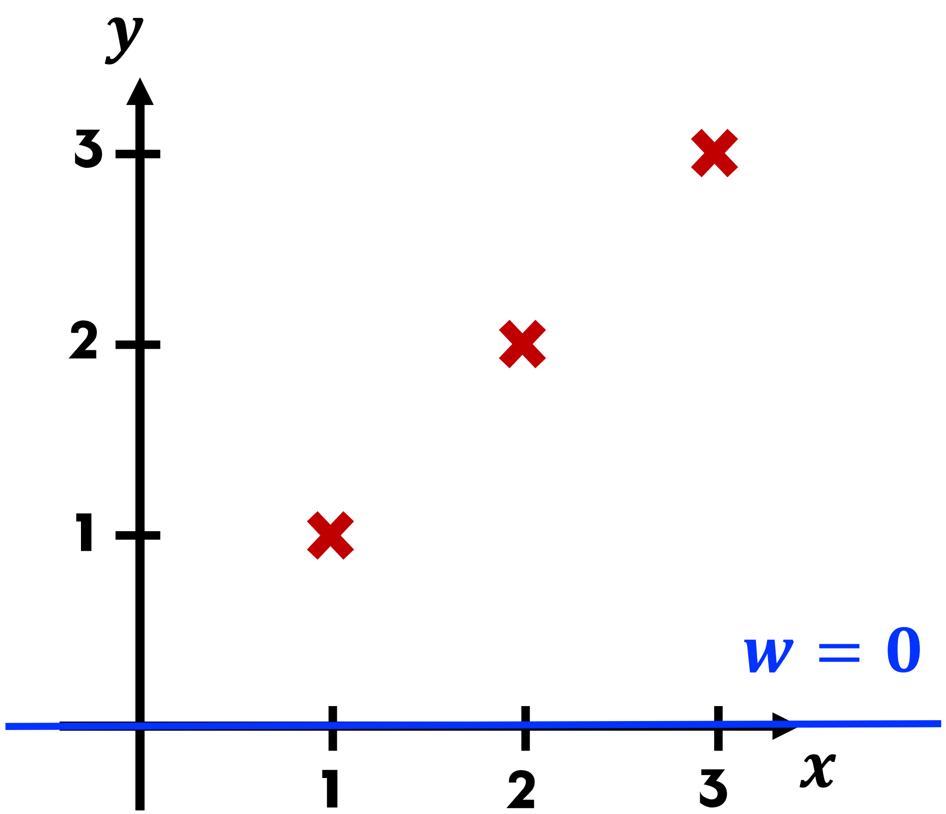


$$J(w) = \frac{1}{2m}\left((0.5-1)^2+(1-2)^2+(1.5-3)^2\right) = \frac{3.5}{6} = 0.58$$

Cost function

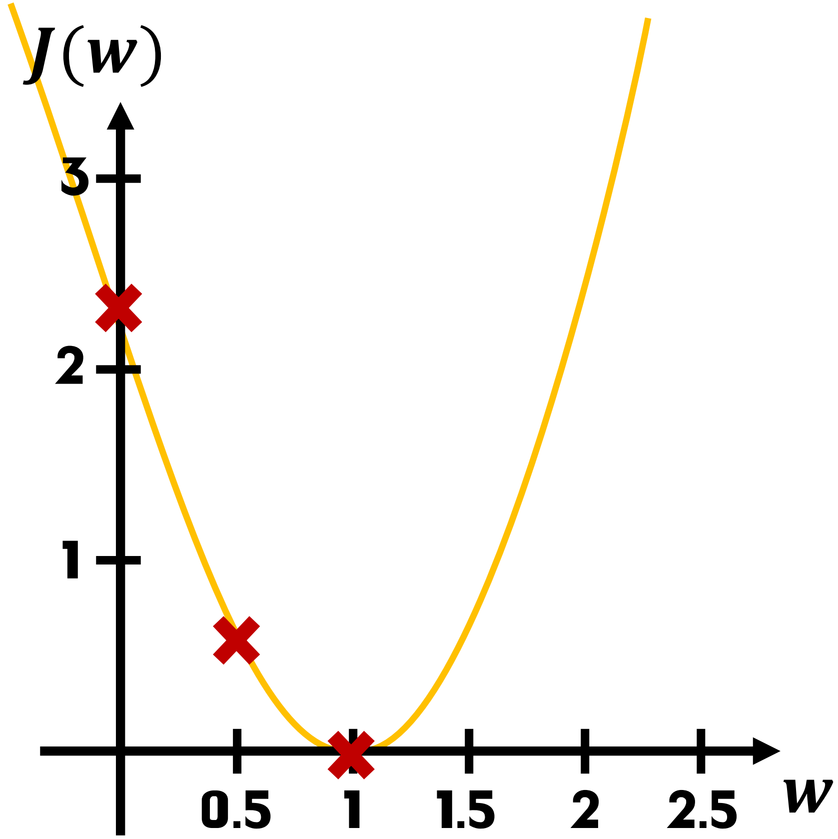
$f_w(x)$

For fixed w, function of x



$J(w)$

Function of w

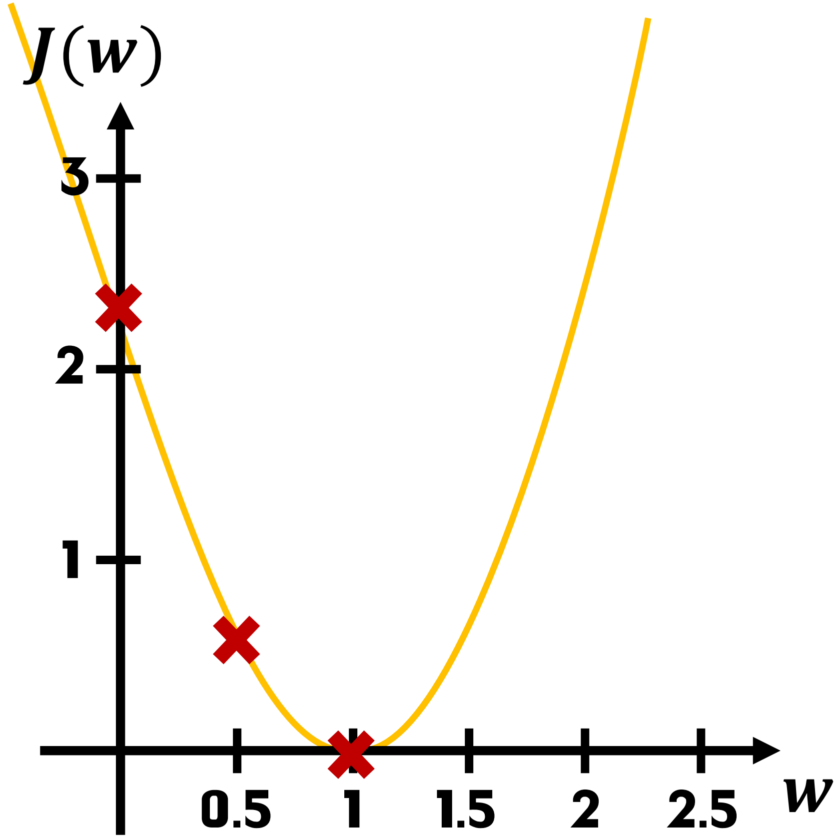


$$J(w) = \frac{1}{2m}\left((1)^2+(2)^2+(3)^2\right) = \frac{14}{6} = 2.3$$

Cost function

$J(w)$

Function of w



Goal of linear regression:

minimize $J(w)$

Choose w to minimize $J(w)$

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Logistic Regression
: classification
(로지스틱 회귀)

Classification

Question	Answer "y"	
Is this email spam ?	no	yes
Is the transaction fraudulent?	no	yes
Is the tumor malignant?	no	yes

false true

0 1

y can only be one of two values

"binary classification"

= category

Negative class

≠ "bad"

absence

Positive class

≠ "good"

presence

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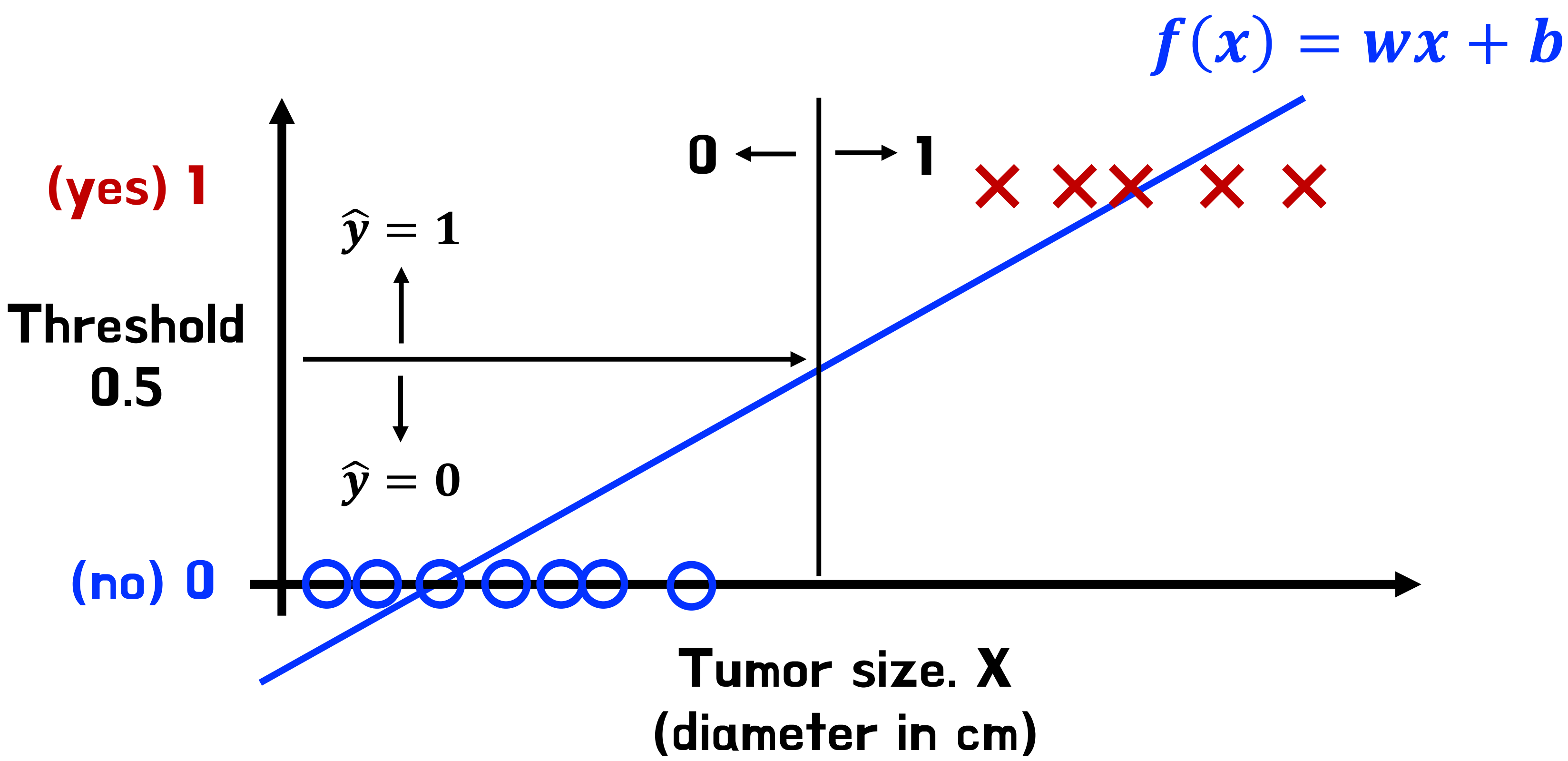
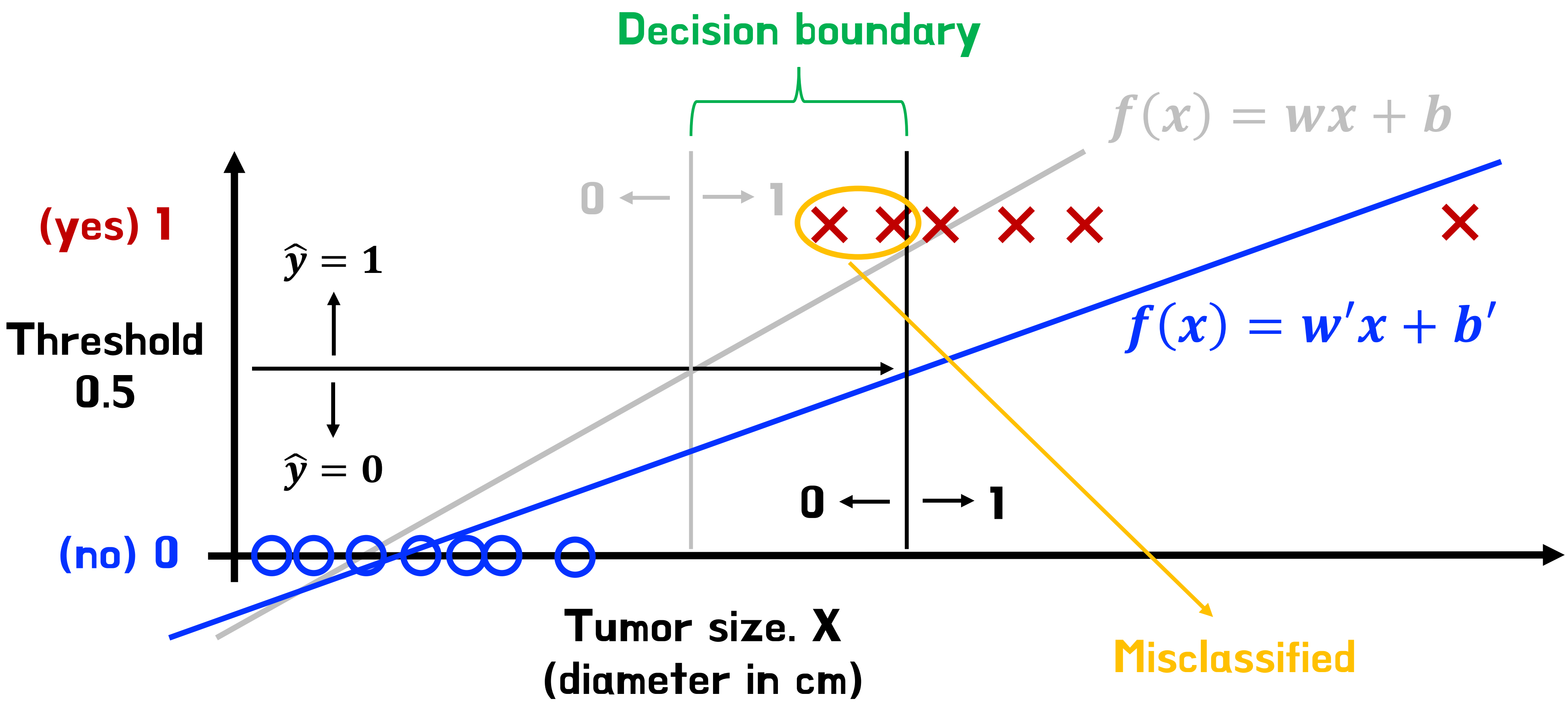
Linear regression



If $f(x) < 0.5 \rightarrow \hat{y} = 0$

If $f(x) \geq 0.5 \rightarrow \hat{y} = 1$

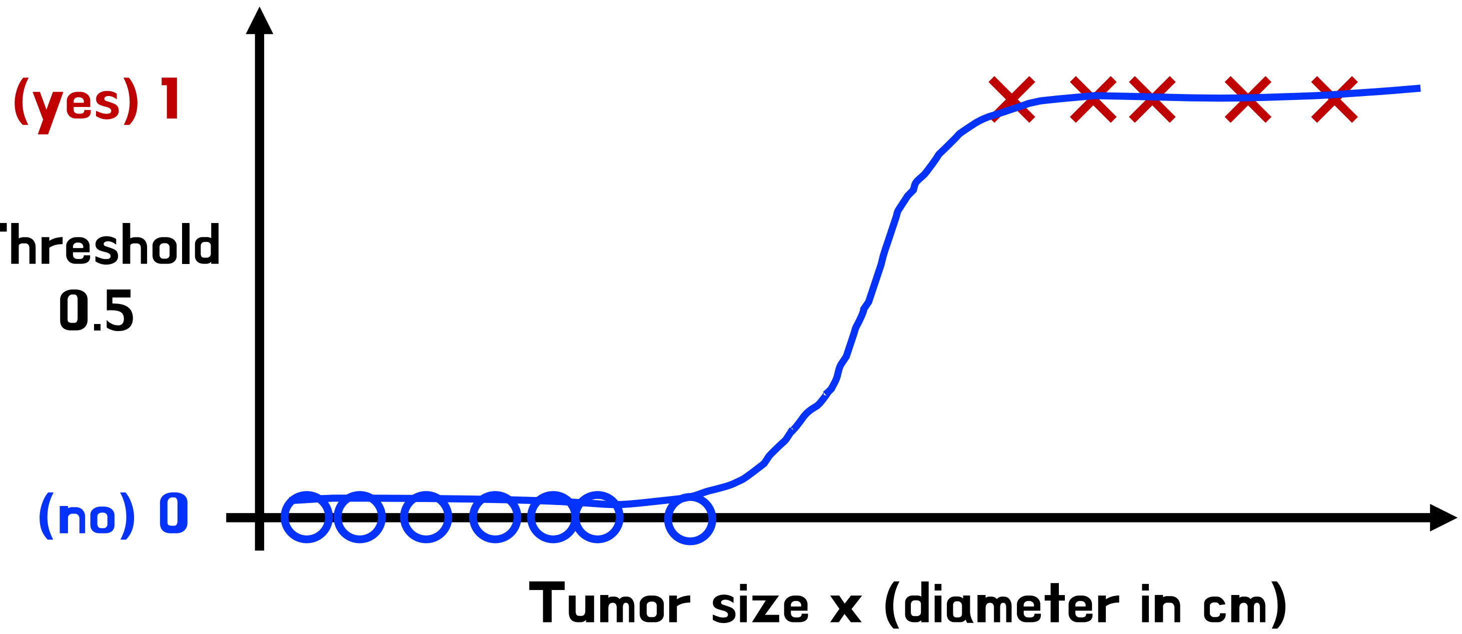
Linear regression

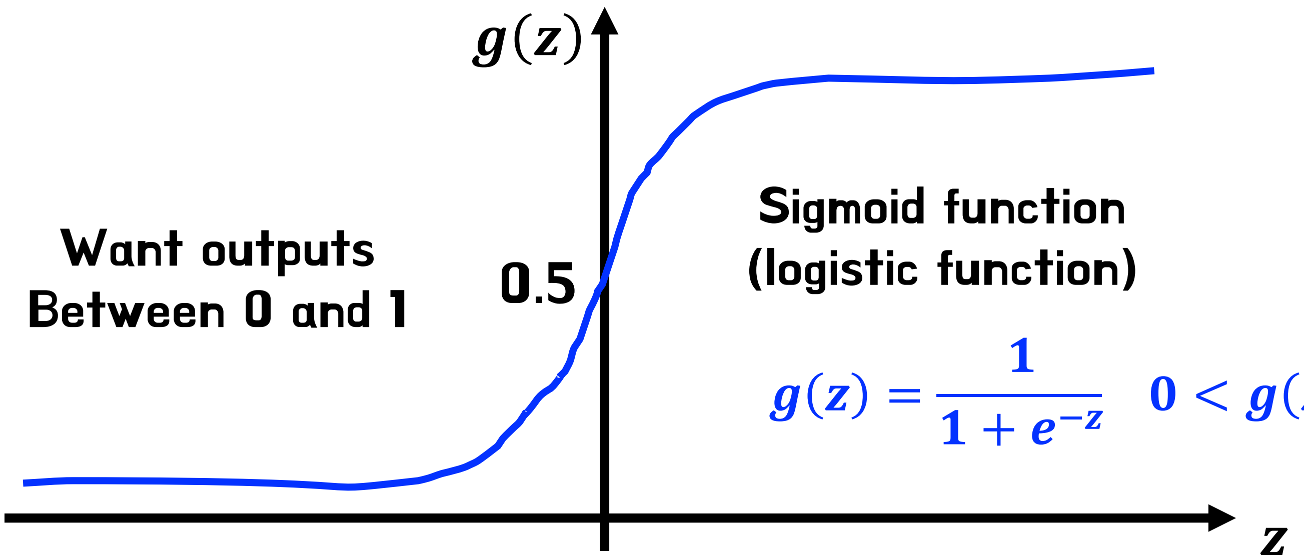


If $f(x) < 0.5 \rightarrow \hat{y} = 0$

If $f(x) \geq 0.5 \rightarrow \hat{y} = 1$

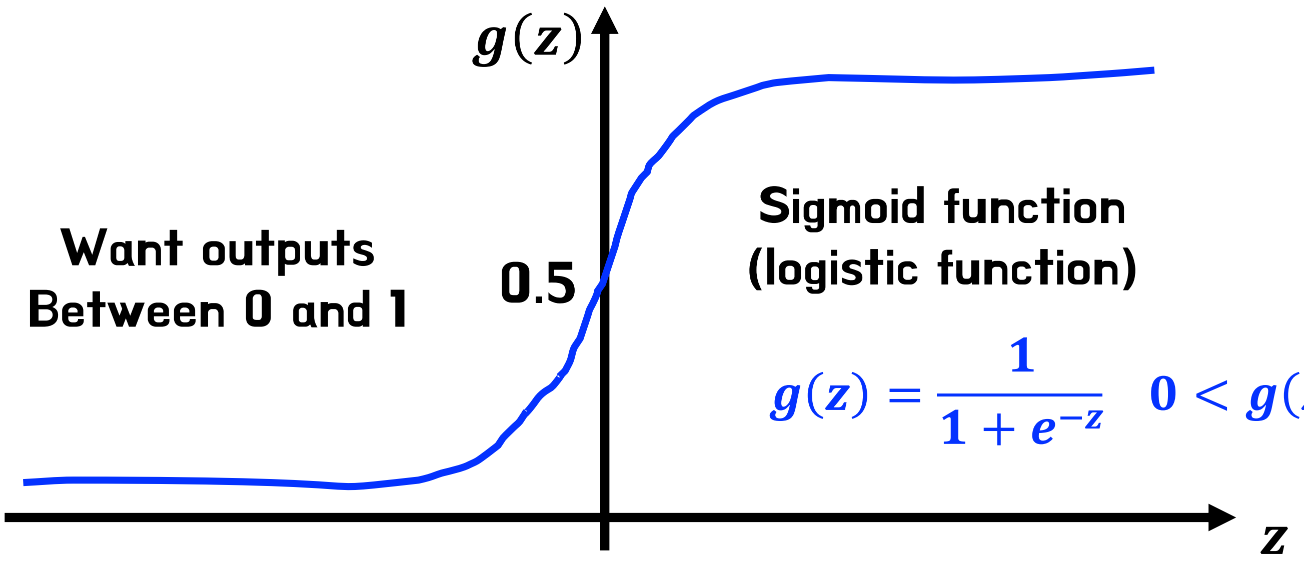
Logistic regression





$$g(z) = \frac{1}{1 + e^{-z}} \quad 0 < g(z) < 1$$

Logistic regression



Want outputs
Between 0 and 1

Sigmoid function
(logistic function)

$$g(z) = \frac{1}{1+e^{-z}} \quad 0 < g(z) < 1$$

$$f_{w,b}(x) = wx + b$$

in linear regression

$$z = wx + b$$

$$f_{w,b}(x) = g(wx+b) = \frac{1}{1+e^{-(wx+b)}}$$

$$= z$$

$$g(z) = \frac{1}{1+e^{-z}}$$

"Logistic regression"

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Logistic regression

$$f_{w,b}(x) = \frac{1}{1 + e^{-(wx+b)}}$$

"probability" that class is 1

Example:

x is "tumor size"

y is 0 (양성)

or 1 (악성)

$$f_{w,b}(x) = 0.7$$

70% chance that y is 1

$$f_{w,b}(x) = P(y = 1 | x; w, b)$$

Probability that y is 1,

given input x, parameters w , b

$$P(y = 0) + P(y = 1) = 1$$

Logistic regression

$$f_{w,b}(x) = g(wx + b) = \frac{1}{1 + e^{-(wx+b)}}$$

$$= P(y = 1 \mid x; w, b)$$

Is $f_{w,b}(x) \geq 0.5$? **Yes:** $\hat{y} = 1$ **No:** $\hat{y} = 0$

When is $f_{w,b}(x) \geq 0.5$?

$$g(z) \geq 0.5$$

$$z \geq 0$$

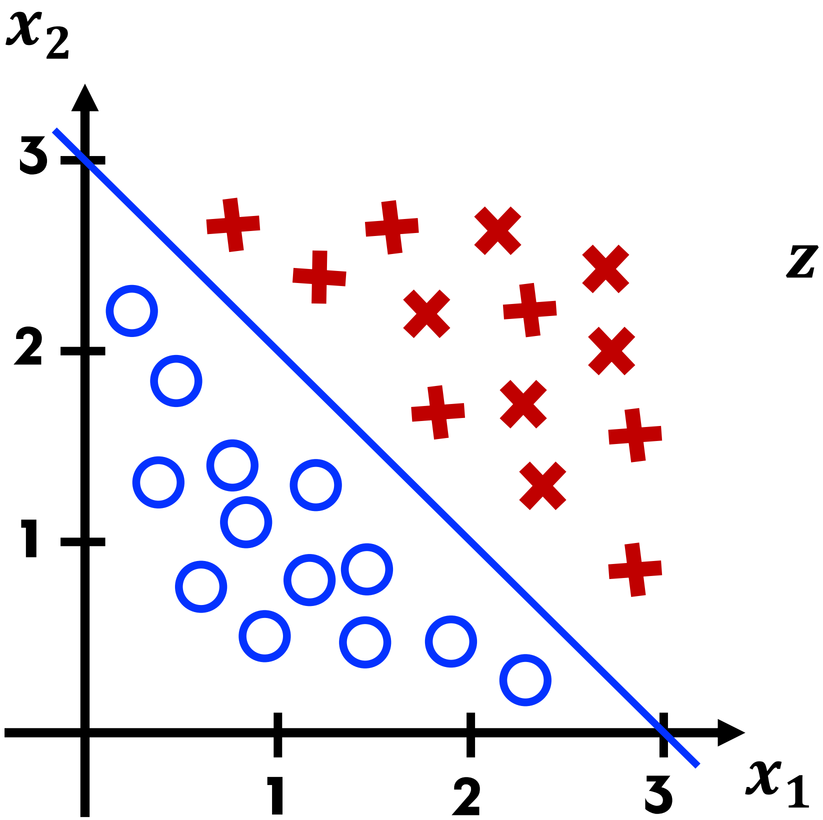
$$wx + b \geq 0 \qquad wx + b < 0$$

$$\hat{y} = 1 \qquad \hat{y} = 0$$

Decision boundary

$$f_{w,b}(x) = g(z) = g(w_1 x_1 + w_2 x_2 + b)$$

$w_1 = 1 \quad w_2 = 1 \quad b = -3$



$$z = wx + b = 0$$

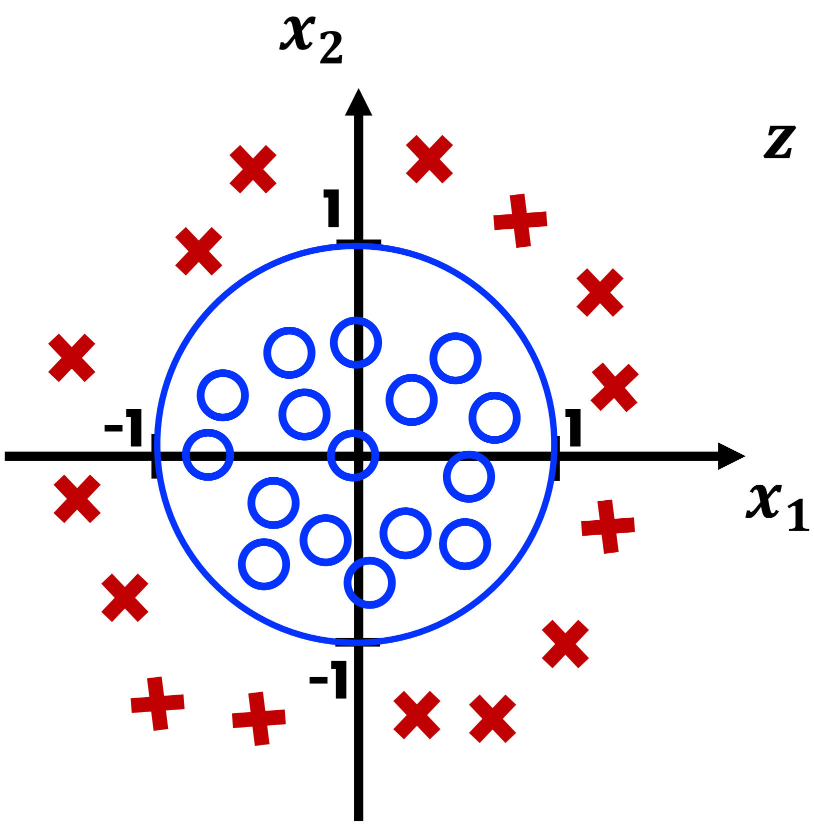
$$= x_1 + x_2 - 3 = 0$$

$$x_1 + x_2 = 3$$

Non-linear decision boundaries

$$f_{w,b}(x) = g(z) = g(w_1 x_1{}^2 + w_2 x_2{}^2 + b)$$

$w_1 = 1$, $w_2 = 1$, $b = -1$



$$z = x_1{}^2 + x_2{}^2 - 1 = 0$$

$$x_1{}^2 + x_2{}^2 = 1$$

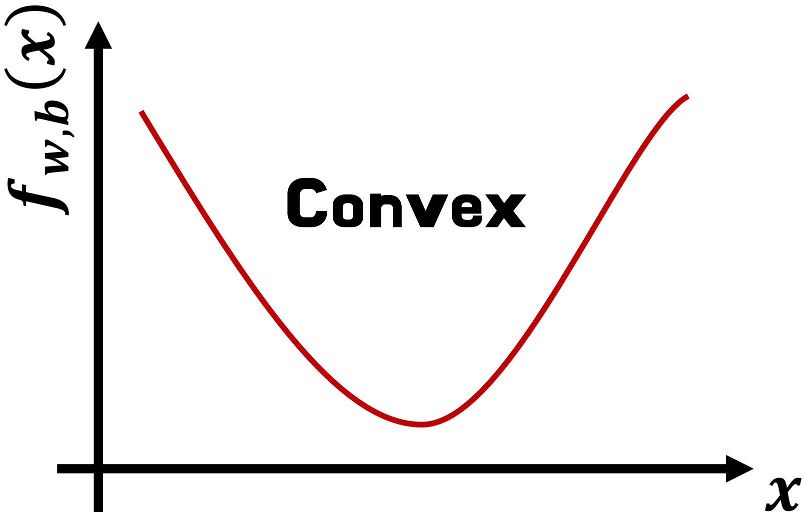
Squared error cost

$$J(w,b) = \frac{1}{m}\sum_{i=1}^{m}\frac{1}{2}\left(f(x^{(i)}) - y^{(i)}\right)^2$$

$$= L\left(f\left(x^{(i)}\right), y^{(i)}\right) \quad \textbf{Loss}$$

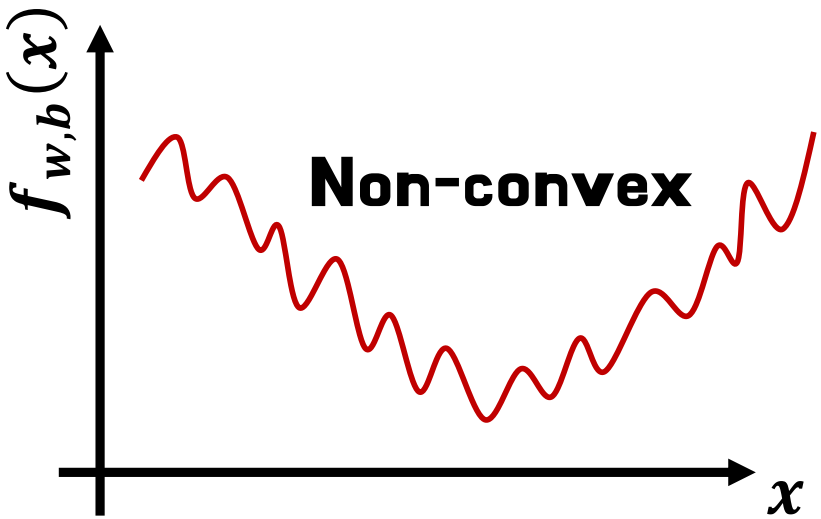
Linear regression

$$f_{w,b}(x) = wx + b$$



Logistic regression

$$f_{w,b}(x) = \frac{1}{1 + e^{-(wx+b)}}$$



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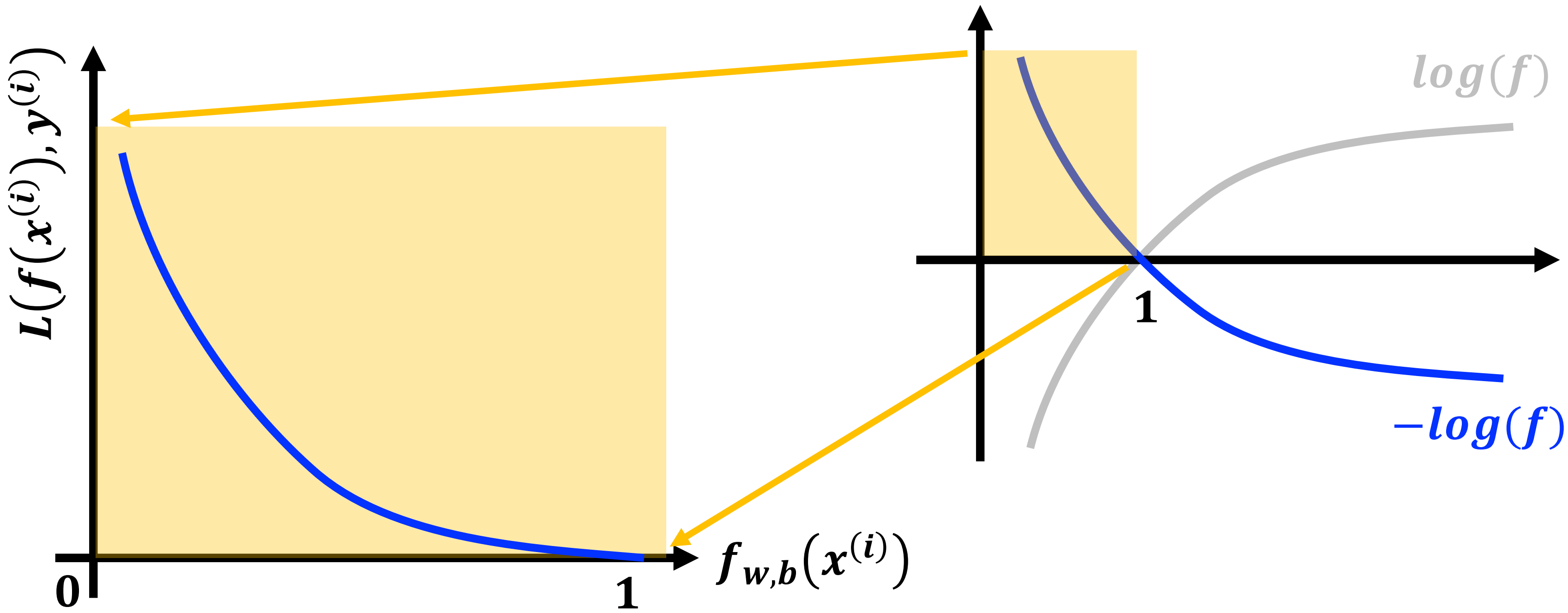
Loss function

$$L\left(f\left(x^{(i)}\right), y^{(i)}\right) = \begin{cases} -log\left(f_{w,b}\left(x^{(i)}\right)\right) & if \;\; y^{(i)} = 1 \\ -log\left(1 - f_{w,b}\left(x^{(i)}\right)\right) & if \;\; y^{(i)} = 0 \end{cases}$$

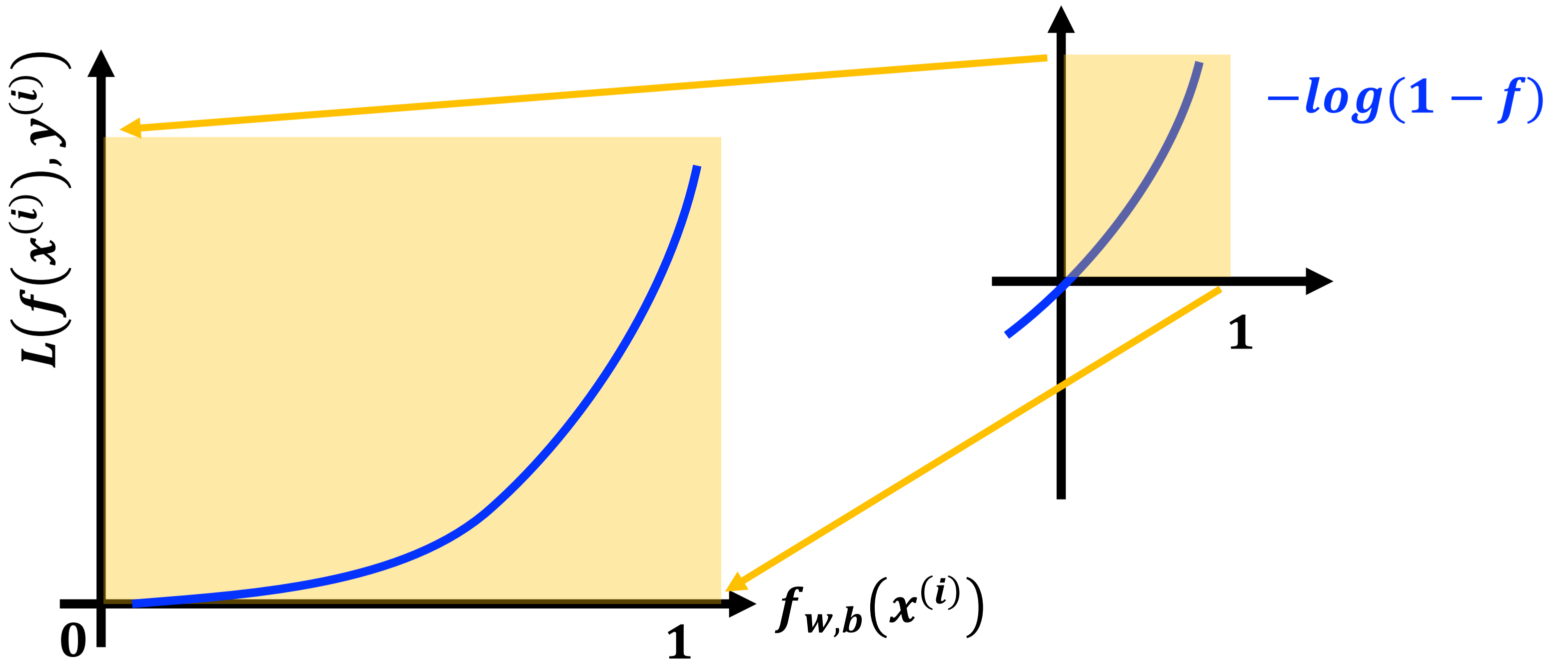


As $f_{w,b}\left(x^{(i)}\right)$ → 1 then loss → 0

As $f_{w,b}\left(x^{(i)}\right)$ → 0 then loss → infinite

Loss function

$$L\left(f\left(x^{(i)}\right), y^{(i)}\right) = \begin{cases} -log\left(f_{w,b}\left(x^{(i)}\right)\right) & if\ \ y^{(i)} = 1 \\ -log\left(1 - f_{w,b}\left(x^{(i)}\right)\right) & if\ \ y^{(i)} = 0 \end{cases}$$



As $f_{w,b}\left(x^{(i)}\right)$ → 1 then loss → infinite

As $f_{w,b}\left(x^{(i)}\right)$ → 0 then loss → 0