Week 3: Classification

Contents

Contents

1. Classification with Logistic Regression

Motivations

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

useful for classification

$\boxed{y \text{ can only be one of two values}}$

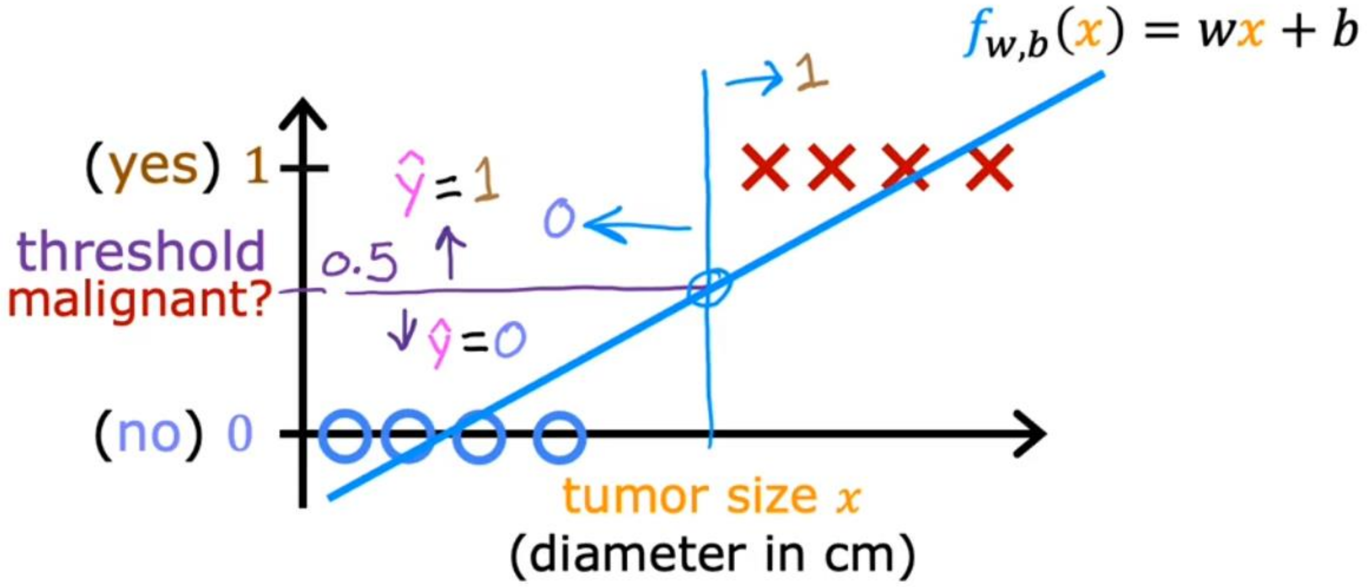
$\boxed{\text{"binary classification"}}$

class = category

"negative class" ≠ "bad" absence

"positive class" ≠ "good" presence

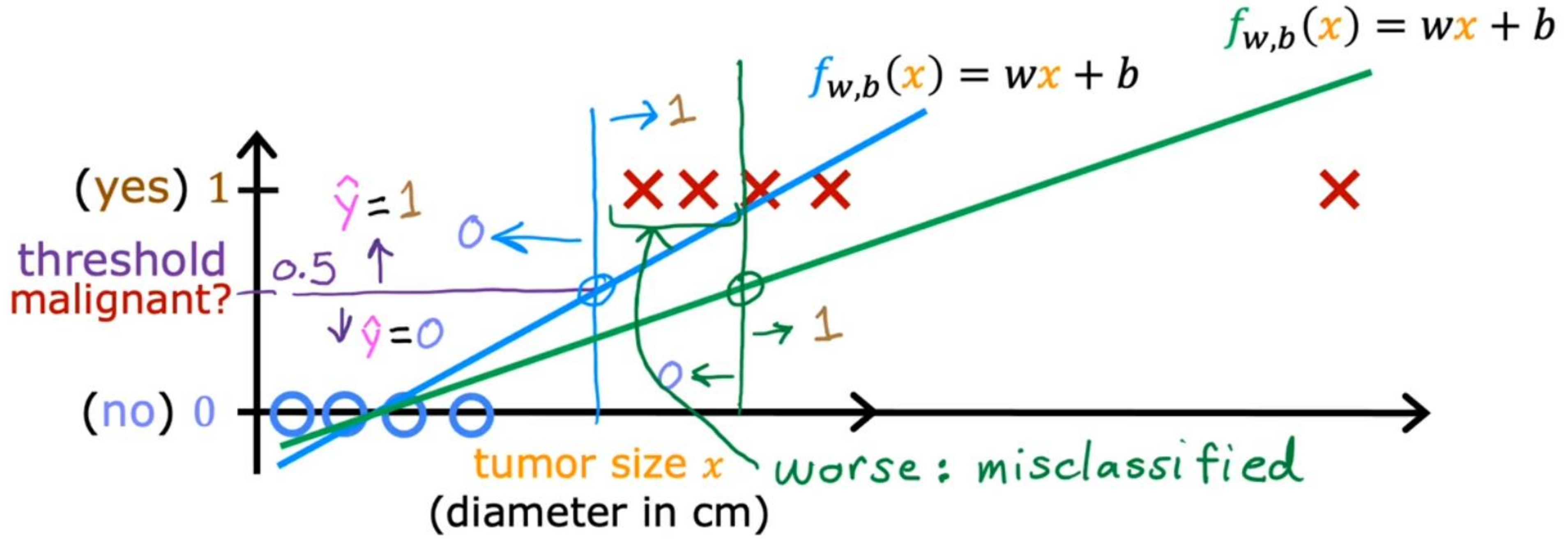
Motivations



if $f_{w,b}(x) < 0.5 \rightarrow \hat{y} = 0$

if $f_{w,b}(x) \geq 0.5 \rightarrow \hat{y} = 1$

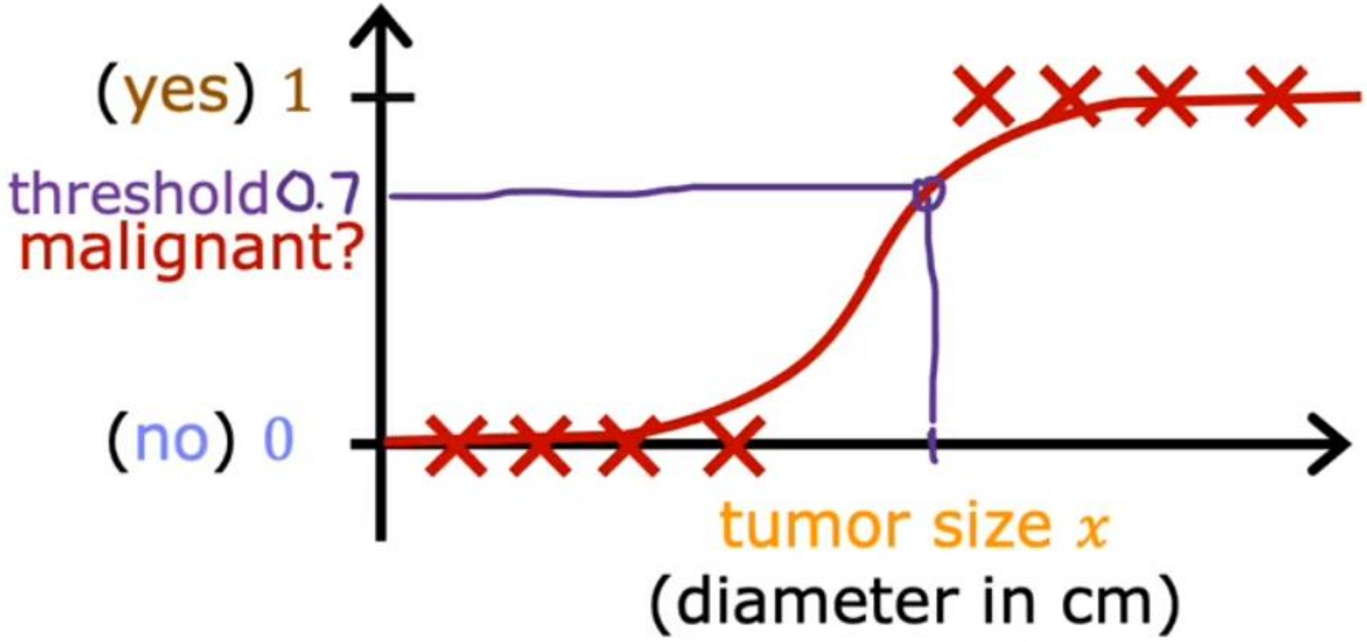
Motivations



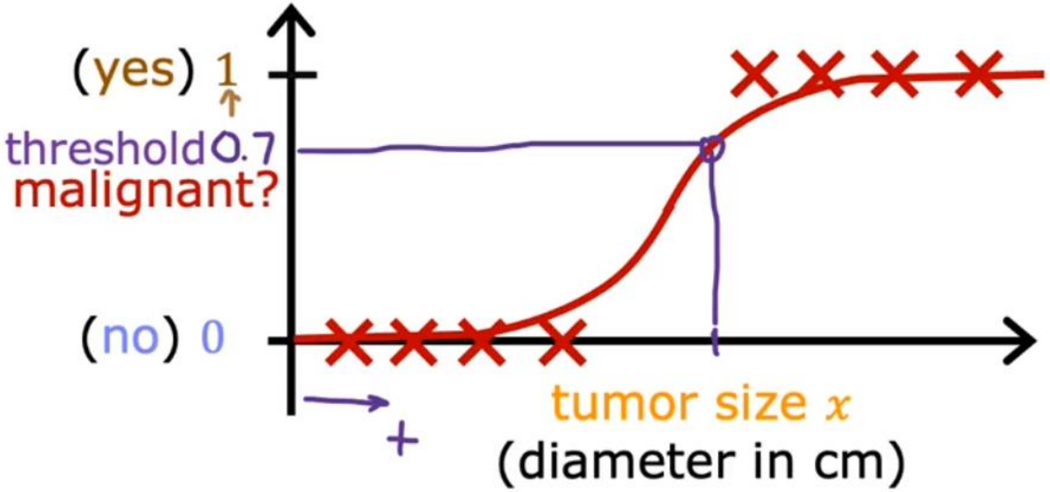
if $f_{w,b}(x) < 0.5 \rightarrow \hat{y} = 0$

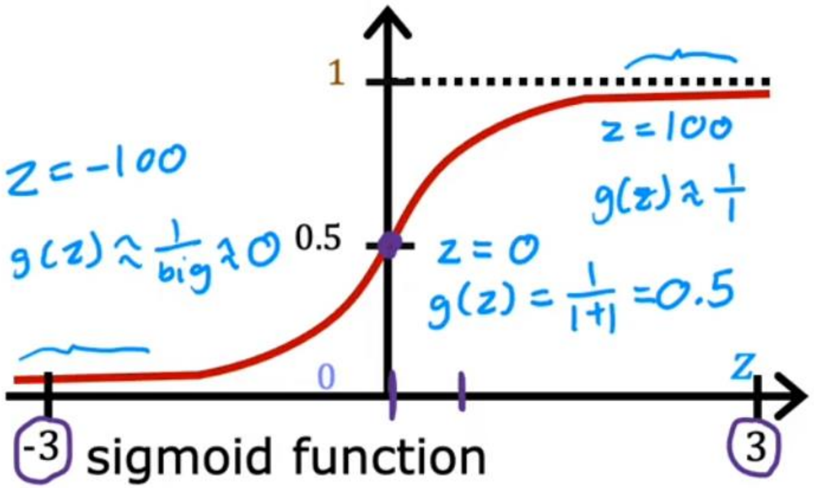
if $f_{w,b}(x) \geq 0.5 \rightarrow \hat{y} = 1$

Logistic Regression



Logistic Regression





sigmoid function

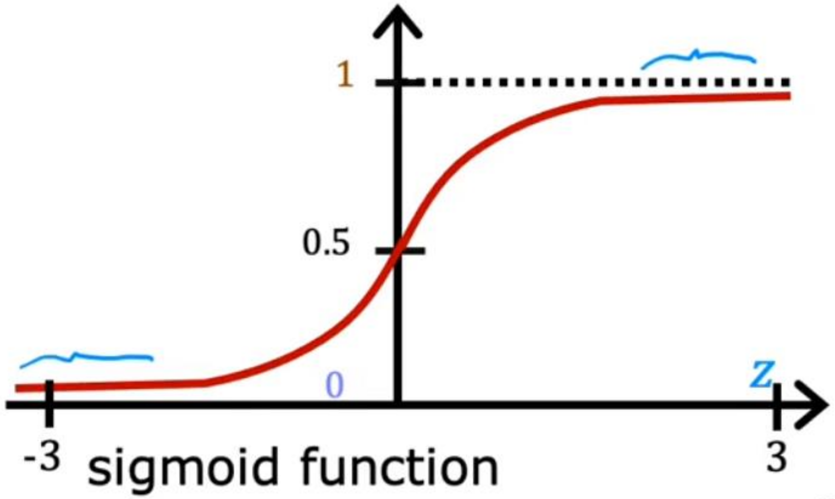
logistic function

outputs between 0 and 1

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

Logistic Regression

Want outputs between 0 and 1



sigmoid function

logistic function

outputs between 0 and 1

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

$f_{\vec{w},b}(\vec{x})$

$$\boxed{z = \vec{w} \cdot \vec{x} + b}$$

$$\downarrow$$

$$z$$

$$\downarrow$$

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

$$f_{\vec{w},b}(\vec{x}) = g(\underbrace{\vec{w} \cdot \vec{x} + b}_{z}) = \frac{1}{1 + e^{-(\vec{w}\cdot\vec{x}+b)}}$$

"logistic regression"

Logistic Regression

Interpretation of logistic regression output

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

"probability" that class is 1

Example:

x is "tumor size"
y is 0 (not malignant)
or 1 (malignant)

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

70% chance that y is 1

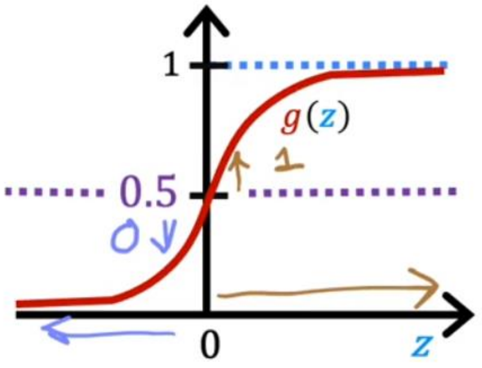
P(1)

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

Probability that y is 1,
given input $\vec{x}$, parameters $\vec{w}$,b

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

Decision Boundary



$f_{\vec{w},b}(\vec{x})$

$\boxed{z = \vec{w} \cdot \vec{x} + b}$

$\downarrow$

z

$\downarrow$

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

$$f_{\vec{w},b}(\vec{x}) = g(\underbrace{\vec{w} \cdot \vec{x} + b}_{z}) = \frac{1}{1 + e^{-(\vec{w} \cdot \vec{x} + b)}}$$

$$= P(y = 1 | x; \vec{w}, b) \quad 0.7 \quad 0.3$$

0 or 1? threshold

Is $f_{\vec{w},b}(\vec{x}) \geq 0.5$?

Yes: $\hat{y} = 1$ No: $\hat{y} = 0$

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

$$g(z) \geq 0.5$$

$$z \geq 0$$

$$\vec{w} \cdot \vec{x} + b \geq 0 \qquad \vec{w} \cdot \vec{x} + b < 0$$

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

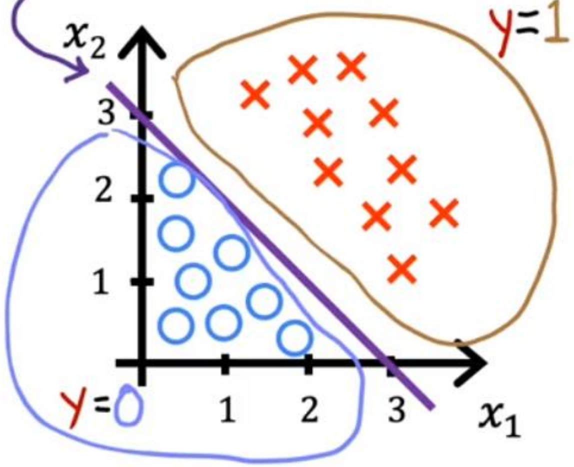
Decision Boundary

$$f_{\vec{w},b}(\vec{x}) = g(z) = g(\underbrace{w_1}_{1} x_1 + \underbrace{w_2}_{1} x_2 + \underbrace{b}_{-3})$$

Decision boundary $z = \vec{w} \cdot \vec{x} + b = 0$

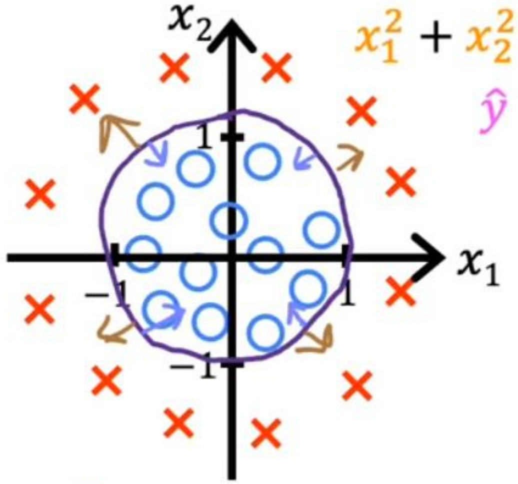
$$z = x_1 + x_2 - 3 = 0$$

$$x_1 + x_2 = 3$$



Decision Boundary

Non-linear decision boundaries



$x_1^2 + x_2^2 \geq 1$

$\hat{y} = 1$

$x_1^2 + x_2^2 < 1$

$\hat{y} = 0$

$$f_{\vec{w},b}(\vec{x}) = g(z) = g(\overbrace{\underset{1}{w_1} x_1^2 + \underset{1}{w_2} x_2^2 + \underset{-1}{b}}^{z})$$

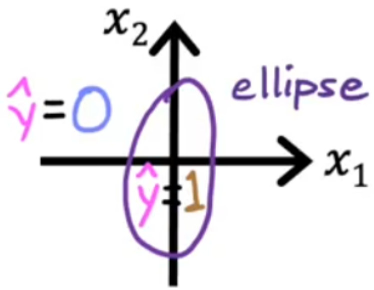
decision boundary

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

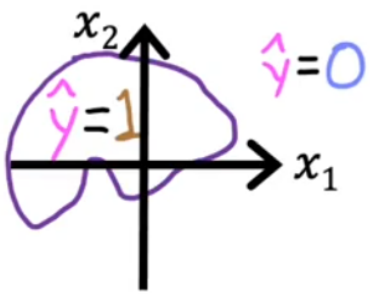
$$x_1^2 + x_2^2 = 1$$

Decision Boundary

Non-linear decision boundaries



$$f_{\vec{w},b}(\vec{x}) = g(z) = g(w_1x_1 + w_2x_2 + w_3x_1^2 + w_4x_1x_2 + w_5x_2^2 + w_6x_1^3 + \cdots + b)$$



2. Cost Function for Logistic Regression

Cost Function for Logistic Regression

Training set

	tumor size (cm) x_1	...	patient's age x_n	malignant? y
$i=1$	10		52	1
$\vdots$	2		73	0
	5		55	0
	12		49	1
$i=m$	...		...	...

$i = 1, \ldots, m$ ← training examples

$j = 1, \ldots, n$ ← features

target y is 0 or 1

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

How to choose $\vec{w} = [w_1 \quad w_2 \quad \cdots \quad w_n]$ and b?

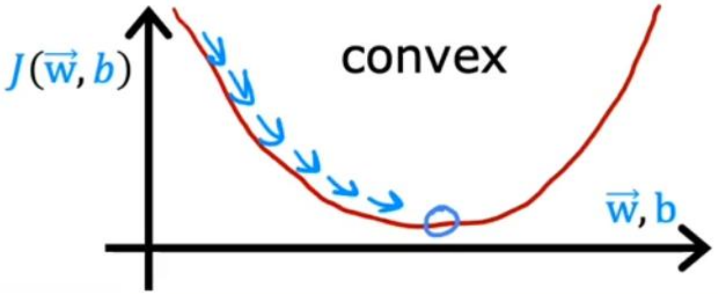
Cost Function for Logistic Regression

Squared error cost

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

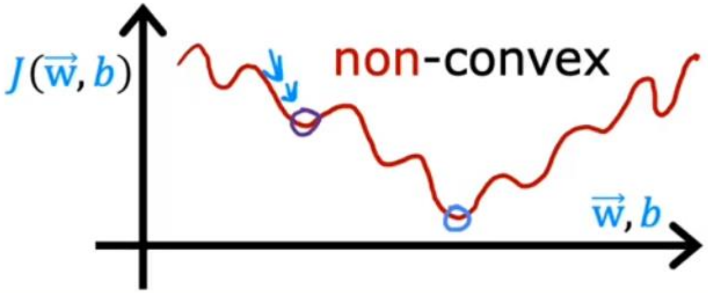
linear regression

$$f_{\vec{w},b}(\vec{x}) = \vec{w}\cdot\vec{x} + b$$



logistic regression

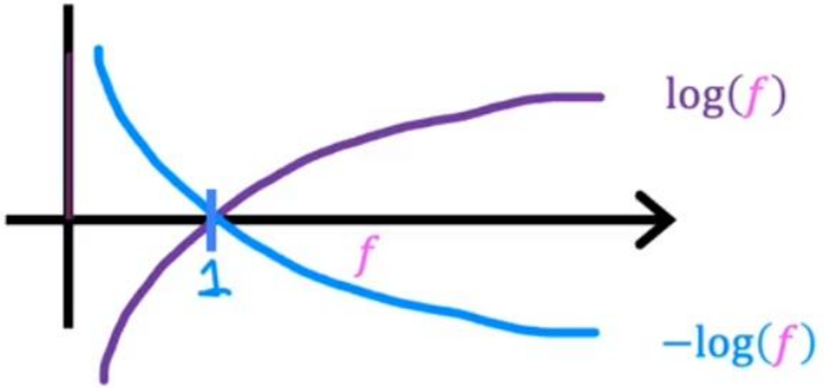
$$f_{\vec{w},b}(\vec{x}) = \frac{1}{1 + e^{-(\vec{w}\cdot\vec{x}+b)}}$$



Cost Function for Logistic Regression

Logistic loss function

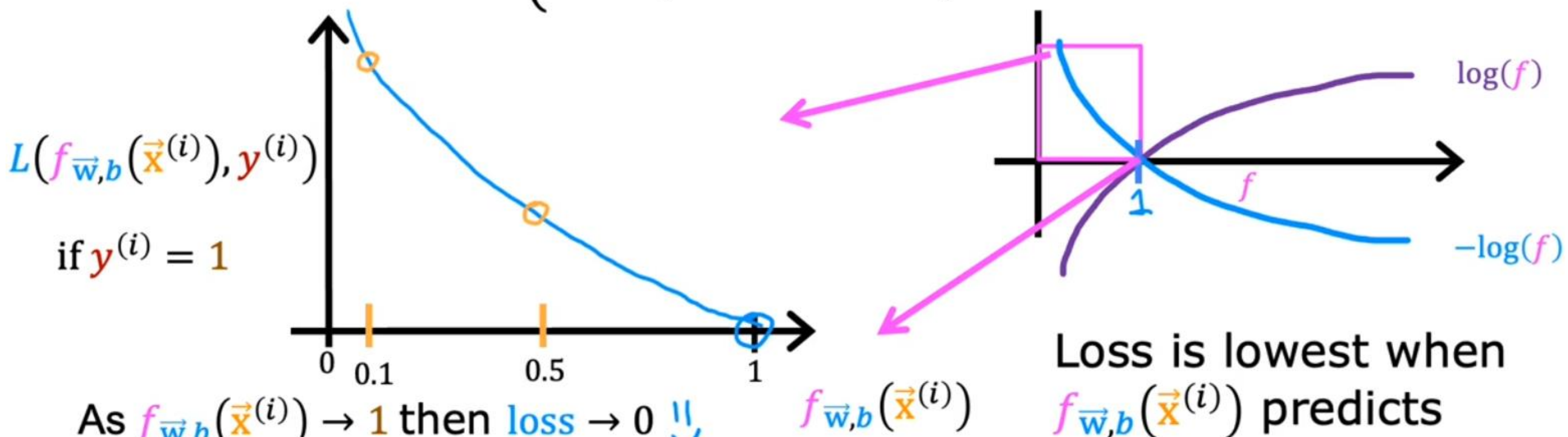
$$L\left(f_{\vec{\mathrm{w}},b}\left(\vec{\mathrm{x}}^{(i)}\right), y^{(i)}\right) = \begin{cases} -\log\left(f_{\vec{\mathrm{w}},b}\left(\vec{\mathrm{x}}^{(i)}\right)\right) & \text{if } y^{(i)} = 1 \\ -\log\left(1 - f_{\vec{\mathrm{w}},b}\left(\vec{\mathrm{x}}^{(i)}\right)\right) & \text{if } y^{(i)}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



Cost Function for Logistic Regression

Logistic loss function

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



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

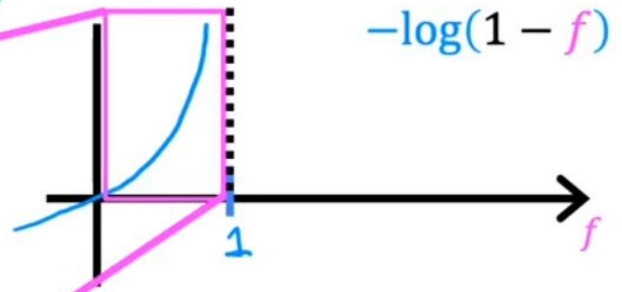
As $f_{\vec{\mathrm{w}},b}\left(\vec{\mathrm{x}}^{(i)}\right) \to 0$ then loss $\to \infty$

Loss is lowest when $f_{\vec{\mathrm{w}},b}\left(\vec{\mathrm{x}}^{(i)}\right)$ predicts close to true label $y^{(i)}$.

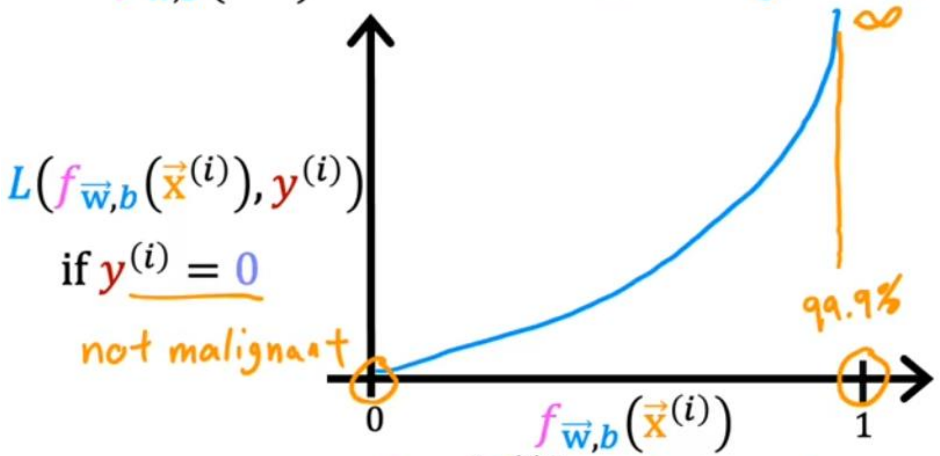
Cost Function for Logistic Regression

Logistic loss function

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



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



As $f_{\vec{\mathrm{w}},b}\left(\vec{\mathrm{x}}^{(i)}\right) \to 1$ then loss $\to \infty$

The further prediction $f_{\vec{\mathrm{w}},b}\left(\vec{\mathrm{x}}^{(i)}\right)$ is from target $y^{(i)}$, the higher the loss.

Cost Function for Logistic Regression

Cost

$$\overset{\text{cost}}{J(\vec{w}, b)} = \frac{1}{m}\sum_{i=1}^{m} L\Big(\underbrace{f_{\vec{w},b}(\vec{x}^{(i)}), y^{(i)}}_{\text{loss}}\Big)$$

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

convex
↳ can reach a global minimum

find w, b that minimize cost J

Cost Function for Logistic Regression

Simplified loss function

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

$$\boxed{L\left(f_{\vec{w},b}\left(\vec{x}^{(i)}\right), y^{(i)}\right) = -y^{(i)}\log\left(f_{\vec{w},b}\left(\vec{x}^{(i)}\right)\right) - \left(1 - y^{(i)}\right)\log\left(1 - f_{\vec{w},b}\left(\vec{x}^{(i)}\right)\right)}$$

Cost Function for Logistic Regression

Simplified cost function

loss

$$L\left(f_{\vec{w},b}\left(\vec{x}^{(i)}\right), y^{(i)}\right) = -y^{(i)}\log\left(f_{\vec{w},b}\left(\vec{x}^{(i)}\right)\right) - \left(1 - y^{(i)}\right)\log\left(1 - f_{\vec{w},b}\left(\vec{x}^{(i)}\right)\right)$$

cost

$$J(\vec{w}, b) = \frac{1}{m}\sum_{i=1}^{m}\left[L\left(f_{\vec{w},b}\left(\vec{x}^{(i)}\right), y^{(i)}\right)\right]$$

$$= -\frac{1}{m}\sum_{i=1}^{m}\left[y^{(i)}\log\left(f_{\vec{w},b}\left(\vec{x}^{(i)}\right)\right) + \left(1 - y^{(i)}\right)\log\left(1 - f_{\vec{w},b}\left(\vec{x}^{(i)}\right)\right)\right]$$

3. Gradient Descent for Logistic Regression

Gradient Descent for Logistic Regression

Training logistic regression

Find $\vec{w}, b$

Given new $\vec{x}$, output $f_{\vec{w},b}(\vec{x}) = \frac{1}{1+e^{-(\vec{w}\cdot\vec{x}+b)}}$

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

Gradient Descent for Logistic Regression

Gradient descent

cost

$$J(\vec{w}, b) = -\frac{1}{m}\sum_{i=1}^{m}\left[y^{(i)}\log\left(f_{\vec{w},b}(\vec{x}^{(i)})\right) + (1-y^{(i)})\log\left(1-f_{\vec{w},b}(\vec{x}^{(i)})\right)\right]$$

repeat {

$j=1 \ldots n$

$$w_j = w_j - \alpha \frac{\partial}{\partial w_j} J(\vec{w}, b)$$

$$\frac{\partial}{\partial w_j} J(\vec{w}, b) = \frac{1}{m}\sum_{i=1}^{m}\left(f_{\vec{w},b}(\vec{x}^{(i)}) - y^{(i)}\right)x_j^{(i)}$$

$$b = b - \alpha \frac{\partial}{\partial b} J(\vec{w}, b)$$

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

} simultaneous updates

Gradient Descent for Logistic Regression

Gradient descent for logistic regression

repeat {

looks like linear regression!

$$w_j = w_j - \alpha \left[\frac{1}{m} \sum_{i=1}^{m} \left(f_{\vec{w},b}(\vec{x}^{(i)}) - y^{(i)} \right) x_j^{(i)} \right]$$

$$b = b - \alpha \left[\frac{1}{m} \sum_{i=1}^{m} \left(f_{\vec{w},b}(\vec{x}^{(i)}) - y^{(i)} \right) \right]$$

} simultaneous updates

Same concepts:

- Monitor gradient descent (learning curve)
- Vectorized implementation
- Feature scaling

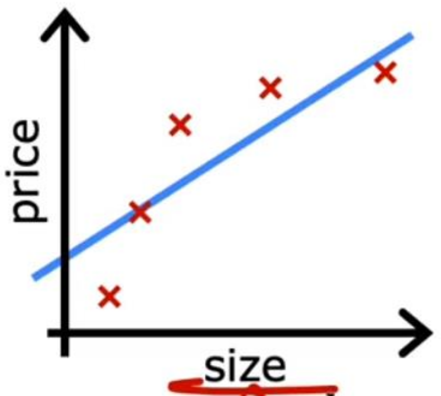
Linear regression $f_{\vec{w},b}(\vec{x}) = \vec{w} \cdot \vec{x} + b$

Logistic regression $f_{\vec{w},b}(\vec{x}) = \dfrac{1}{1 + e^{-(\vec{w} \cdot \vec{x} + b)}}$

4. The Problem of Overfitting

Overfitting

Regression example

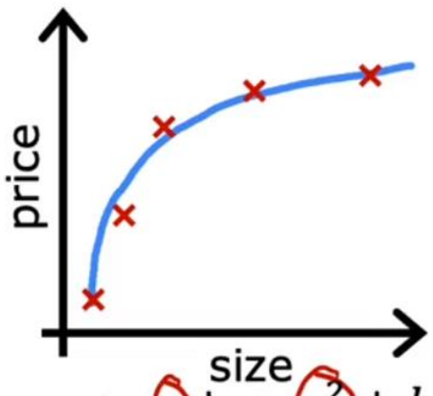


$w_1 x + b$

underfit

- Does not fit the training set well

high bias

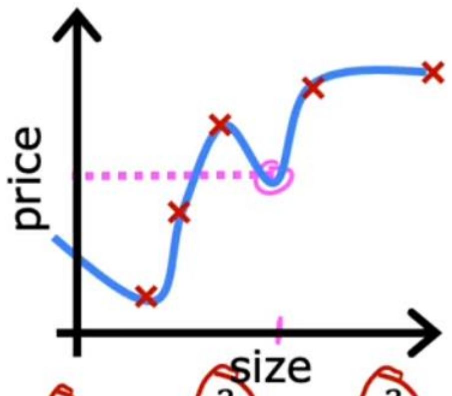


$w_1 x + w_2 x^2 + b$

just right

- Fits training set pretty well

generalization



$w_1 x + w_2 x^2 + w_3 x^3 + w_4 x^4 + b$

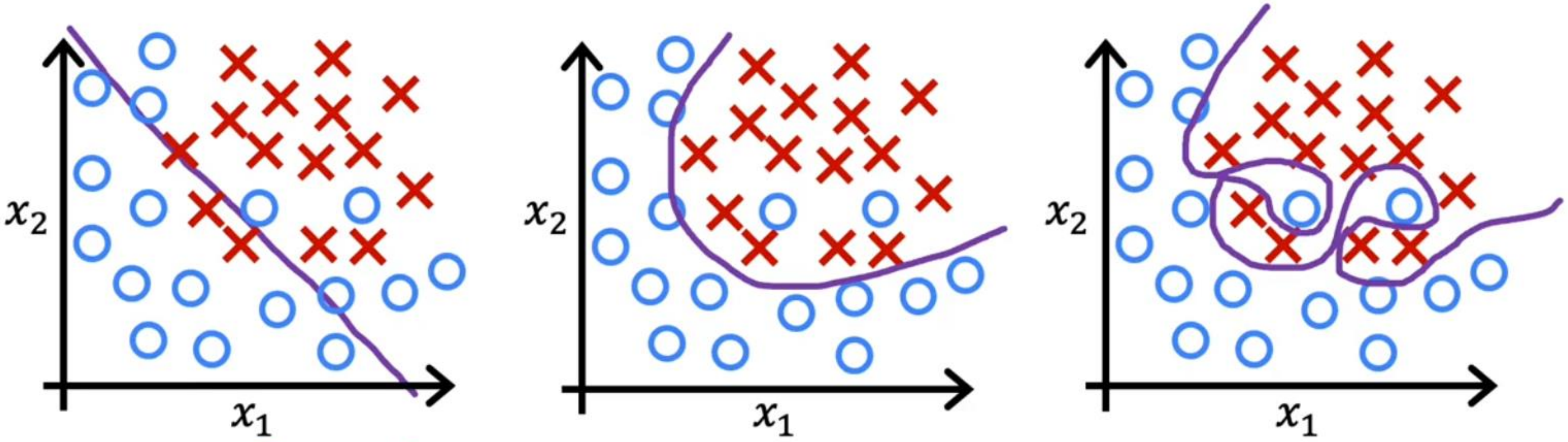
overfit

- Fits the training set extremely well

high variance

Overfitting

Classification



$$z = w_1 x_1 + w_2 x_2 + b$$
$$f_{\vec{\mathrm{w}},b}(\vec{\mathrm{x}}) = g(z)$$
g is the sigmoid function

underfit   high bias

$$z = w_1x_1 + w_2x_2$$
$$+w_3x_1^2 + w_4x_2^2$$
$$+w_5x_1x_2 + b$$

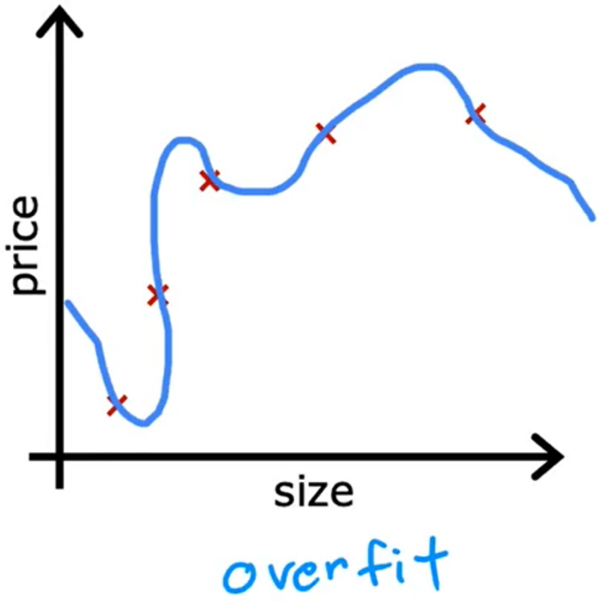
just right

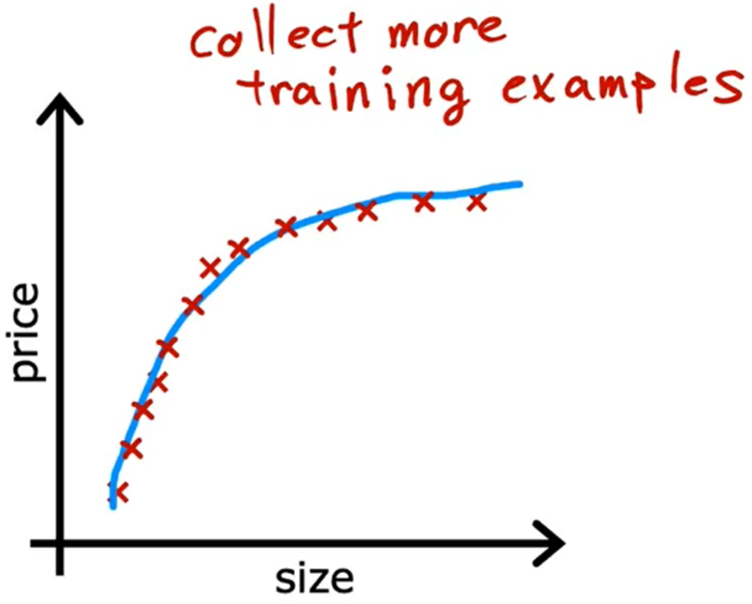
$$z = w_1x_1 + w_2x_2$$
$$+w_3x_1^2x_2 + w_4x_1^2x_2^2$$
$$+w_5x_1^2x_2^3 + w_6x_1^3x_2$$
$$+ \cdots + b$$

overfit

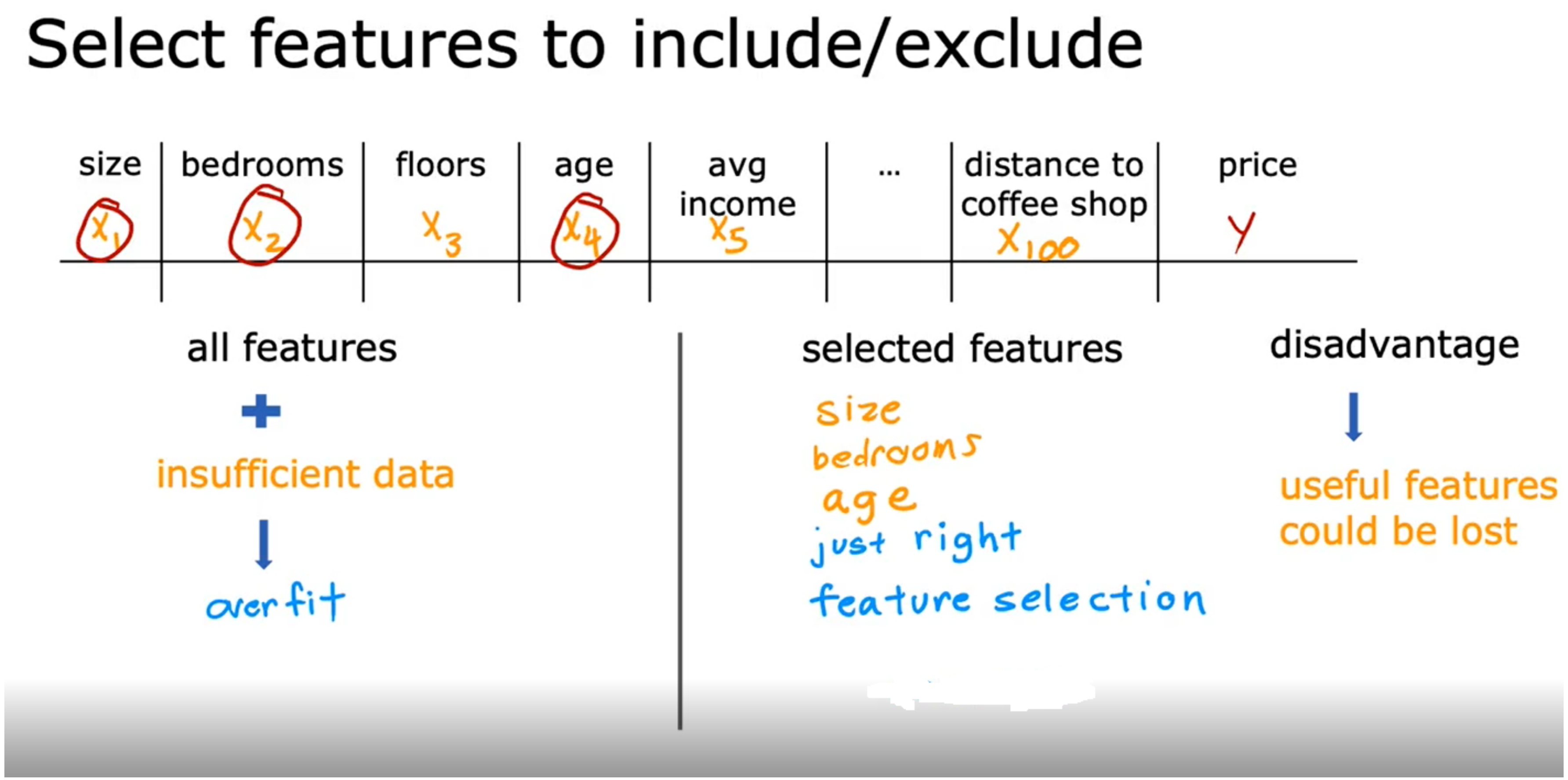
Addressing Overfitting

Collect more training examples





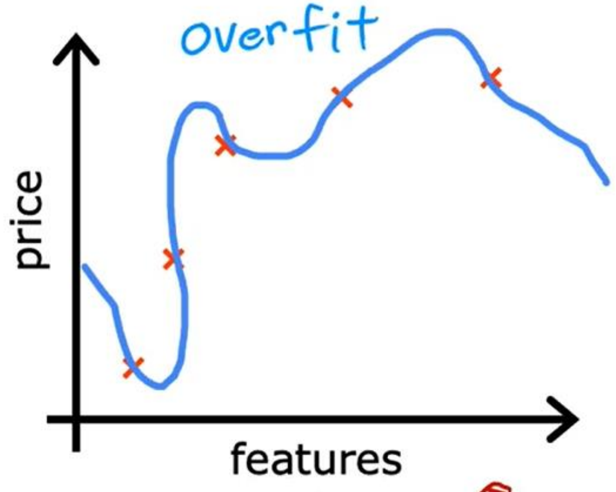
Addressing Overfitting

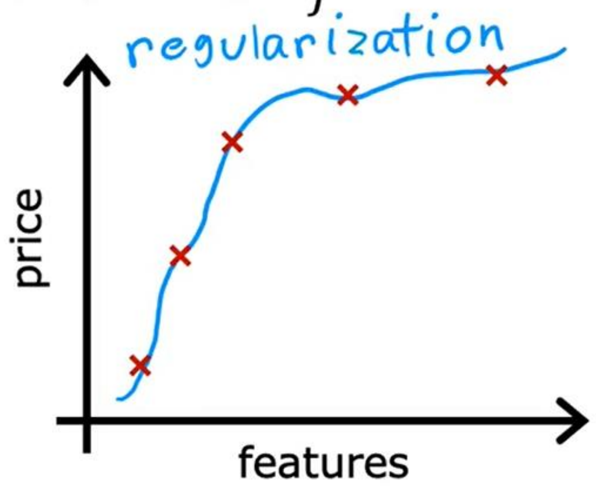


Addressing Overfitting

Regularization

Reduce the size of parameters w_j





$$f(x) = 28x - 385x^2 + 39x^3 - \underbrace{\cancel{174}x^4}_{0} + 100$$

large values for w_j

eliminate feature

$$f(x) = 13x - 0.23x^2 + \underbrace{0.000014}x^3 - \underbrace{0.0001}\,x^4 + 10$$

small values for w_j

Addressing Overfitting

Addressing overfitting

Options

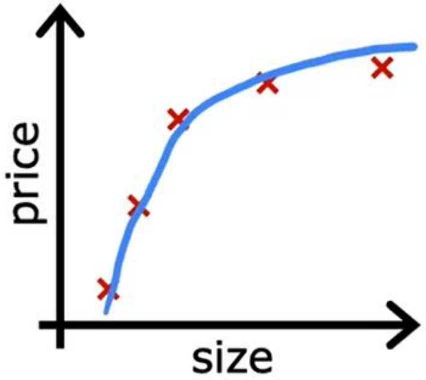
1. Collect more data

2. Select features
   – Feature selection

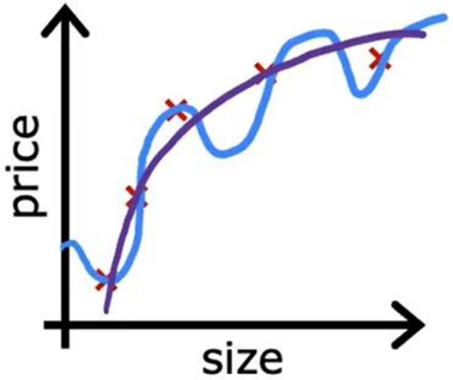
3. Reduce size of parameters
   – “Regularization”

Cost Function with Regularization

Intuition



$w_1x + w_2x^2 + b$



$w_1x + w_2x^2 + \cancel{\underbrace{w_3}_{\approx 0}x^3} + \cancel{\underbrace{w_4}_{\approx 0}x^4} + b$

make w_3, w_4 really small (≈ 0)

$$\min_{\vec{w},b} \frac{1}{2m}\sum_{i=1}^{m}\left(f_{\vec{w},b}(\vec{x}^{(i)}) - y^{(i)}\right)^2 + \cancel{1000\underbrace{w_3^2}_{0.001}} + \cancel{1000\underbrace{w_4^2}_{0.002}}$$

Cost Function with Regularization

Regularization

small values $w_1, w_2, \cdots, w_n, b$

simpler model $w_3 \approx 0$

less likely to overfit $w_4 \approx 0$

size	bedrooms	floors	age	avg income	...	distance to coffee shop	price
x_1	x_2	x_3	x_4	x_5		x_{100}	y

$n = 100$

$w_1, w_1, w_2, \cdots, w_{100}, b$

n features

$$J(\vec{w}, b) = \frac{1}{2m}\left[\sum_{i=1}^{m}\left(f_{\vec{w},b}\left(\vec{x}^{(i)}\right) - y^{(i)}\right)^2 + \underbrace{\frac{\lambda}{2m}\sum_{j=1}^{n} w_j^2}_{\text{regularization term}} + \frac{\lambda}{2m} b^2\right]$$

"lambda"

regularization parameter

$\lambda > 0$

can include or exclude b

Cost Function with Regularization

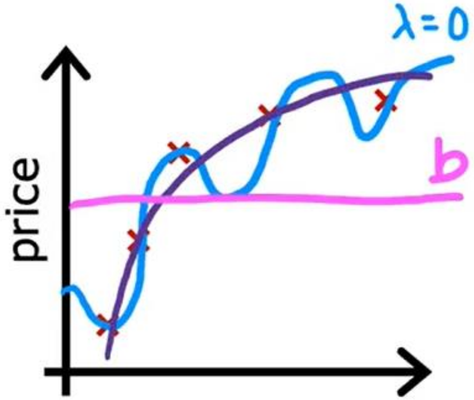
Regularization

$$\min_{\vec{w},b} J(\vec{w},b) = \min_{\vec{w},b} \left[\overbrace{\frac{1}{2m}\sum_{i=1}^{m}\left(f_{\vec{w},b}(\vec{x}^{(i)}) - y^{(i)}\right)^2}^{\text{mean squared error}} + \overbrace{\frac{\lambda}{2m}\sum_{j=1}^{n} w_j^2}^{\text{regularization term}} \right]$$

fit data

Keep w_j small

λ balances both goals



choose $\lambda = 10^{10}$

$$f_{\vec{w},b}(\vec{x}) = \underset{\approx 0}{\cancel{w_1 x}} + \underset{\approx 0}{\cancel{w_2 x^2}} + \underset{\approx 0}{\cancel{w_3 x^3}} + \underset{\approx 0}{\cancel{w_4 x^4}} + b$$

$f(x) = b$

Choose λ

Linear Regression with Regularization

Regularized linear regression

$$\min_{\vec{w},b} J(\vec{w},b) = \min_{\vec{w},b}\left[\frac{1}{2m}\sum_{i=1}^{m}\left(f_{\vec{w},b}(\vec{x}^{(i)}) - y^{(i)}\right)^2 + \frac{\lambda}{2m}\sum_{j=1}^{n} w_j^2\right]$$

Gradient descent

repeat {

$$w_j = w_j - \alpha \frac{\partial}{\partial w_j} J(\vec{w},b) \qquad = \frac{1}{m}\sum_{i=1}^{m}\left(f_{\vec{w},b}(\vec{x}^{(i)}) - y^{(i)}\right) x_j^{(i)} + \frac{\lambda}{m} w_j$$

$j = 1, \ldots, n$

$$b = b - \alpha \frac{\partial}{\partial b} J(\vec{w},b) \qquad = \frac{1}{m}\sum_{i=1}^{m}\left(f_{\vec{w},b}(\vec{x}^{(i)}) - y^{(i)}\right)$$

} simultaneous update

don't have to regularize b

Linear Regression with Regularization

Implementing gradient descent

repeat {

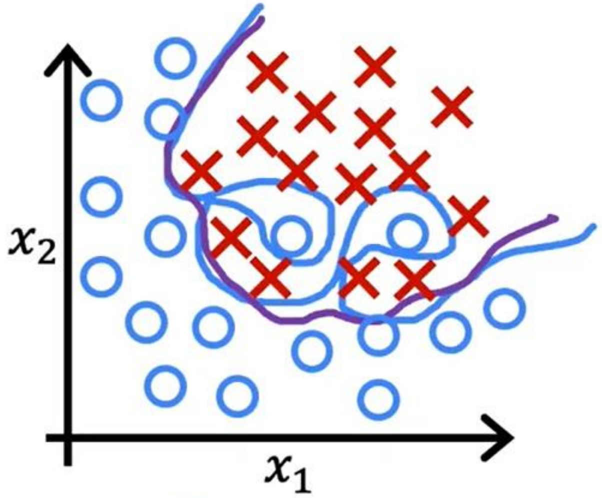
$$w_j = w_j - \alpha \left[\frac{1}{m} \sum_{i=1}^{m} \left[\left(f_{\vec{\mathrm{w}},b}\left(\vec{\mathrm{x}}^{(i)}\right) - y^{(i)} \right) x_j^{(i)} \right] + \frac{\lambda}{m} w_j \right]$$

$$b = b - \alpha \frac{1}{m} \sum_{i=1}^{m} \left(f_{\vec{\mathrm{w}},b}\left(\vec{\mathrm{x}}^{(i)}\right) - y^{(i)} \right)$$

} simultaneous update

Logistic Regression with Regularization

Regularized logistic regression



$$z = w_1x_1 + w_2x_2 + w_3x_1^2x_2 + w_4x_1^2x_2^2 + w_5x_1^2x_2^3 + \cdots + b$$

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

Cost function

$$J(\vec{w},b) = -\frac{1}{m}\sum_{i=1}^{m}\left[y^{(i)}\log\left(f_{\vec{w},b}(\vec{x}^{(i)})\right) + (1-y^{(i)})\log\left(1-f_{\vec{w},b}(\vec{x}^{(i)})\right)\right] + \frac{\lambda}{2m}\sum_{j=1}^{n} w_j^2$$

$$\min_{\vec{w},b} J(\vec{w},b) \rightarrow w_j \downarrow$$

Logistic Regression with Regularization

Regularized logistic regression

$$J(\vec{\mathrm{w}},b) = -\frac{1}{m}\sum_{i=1}^{m}\left[y^{(i)}\log\left(f_{\vec{\mathrm{w}},b}(\vec{\mathrm{x}}^{(i)})\right) + (1-y^{(i)})\log\left(1-f_{\vec{\mathrm{w}},b}(\vec{\mathrm{x}}^{(i)})\right)\right] + \frac{\lambda}{2m}\sum_{j=1}^{n} w_j^2$$

$\min_{\vec{\mathrm{w}},b}$

Gradient descent

Looks same as for linear regression!

repeat {

$$w_j = w_j - \alpha \frac{\partial}{\partial w_j} J(\vec{\mathrm{w}},b) \qquad = \frac{1}{m}\sum_{i=1}^{m}\left[\left(f_{\vec{\mathrm{w}},b}(\vec{\mathrm{x}}^{(i)}) - y^{(i)}\right)x_j^{(i)}\right] + \frac{\lambda}{m} w_j$$

$j = 1 \ldots n$

logistic regression

$$b = b - \alpha \frac{\partial}{\partial b} J(\vec{\mathrm{w}},b) \qquad = \frac{1}{m}\sum_{i=1}^{m}\left(f_{\vec{\mathrm{w}},b}(\vec{\mathrm{x}}^{(i)}) - y^{(i)}\right)$$

}

don't have to regularize