



Machine Learning

# Logistic Regression

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# Classification

# Classification

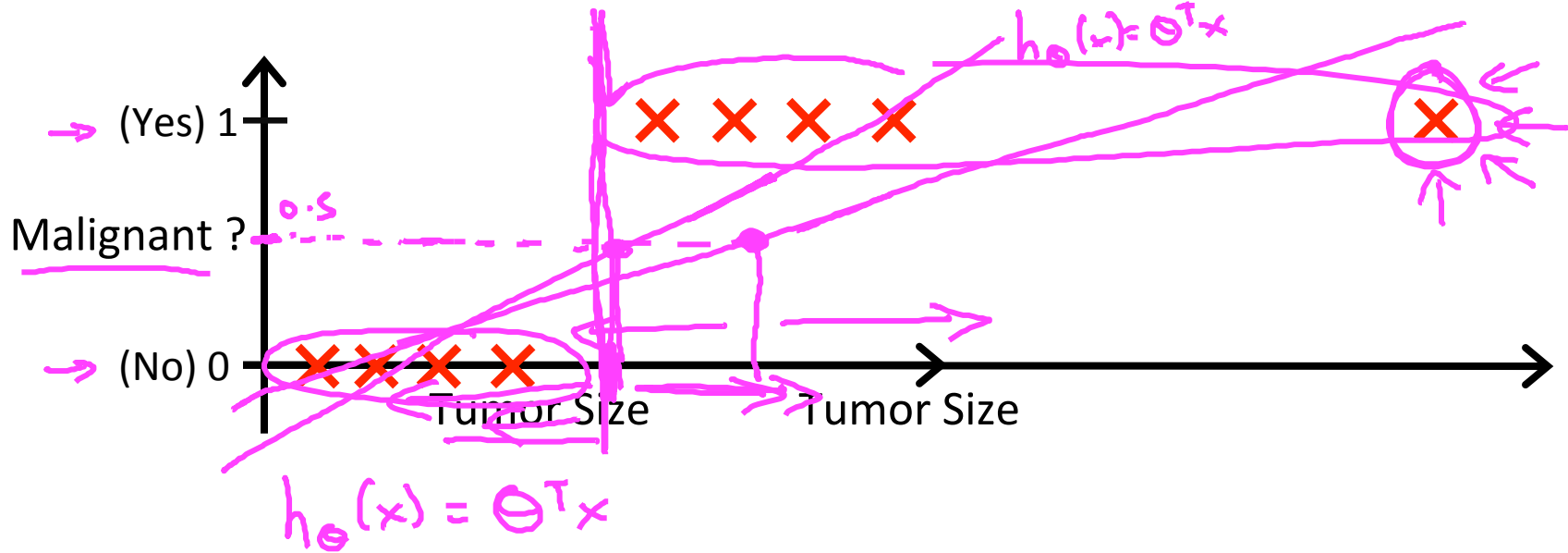
- Email: Spam / Not Spam?
- Online Transactions: Fraudulent (Yes / No)?
- Tumor: Malignant / Benign ?

→  $y \in \{0, 1\}$

0: "Negative Class" (e.g., benign tumor)

1: "Positive Class" (e.g., malignant tumor)

→  $y \in \{0, 1, 2, 3\}$



→ Threshold classifier output  $h_{\theta}(x)$  at 0.5:

→ If  $h_{\theta}(x) \geq 0.5$ , predict "y = 1"

If  $h_{\theta}(x) < 0.5$ , predict "y = 0"

Classification:

$$y = 0 \text{ or } 1$$

$h_{\theta}(x)$  can be  $> 1$  or  $< 0$

Logistic Regression:  $0 \leq h_{\theta}(x) \leq 1$

Classification



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# Logistic Regression

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## Hypothesis Representation

## Logistic Regression Model

Want  $0 \leq h_{\theta}(x) \leq 1$

$$h_{\theta}(x) = g(\theta^T x)$$

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

$\theta^T x$

Sigmoid function

Logistic function

$$h_{\theta}(x) = \frac{1}{1 + e^{-\theta^T x}}$$



Parameters  $\theta$ .

## Interpretation of Hypothesis Output

$$h_{\theta}(x)$$

$h_{\theta}(x)$  = estimated probability that  $y = 1$  on input  $x$  ←

Example: If  $\underline{x} = \begin{bmatrix} x_0 \\ x_1 \end{bmatrix} = \begin{bmatrix} 1 \leftarrow \\ \text{tumorSize} \leftarrow \end{bmatrix}$

$h_{\theta}(x)$  = 0.7

$y = 1$

Tell patient that 70% chance of tumor being malignant

$$\underline{h_{\theta}(x)} = \underline{P(y=1|x;\theta)}$$

$y = 0 \text{ or } 1$

“probability that  $y = 1$ , given  $x$ ,  
parameterized by  $\theta$ ”

→  $P(y = 0|x;\theta) + P(y = 1|x;\theta) = 1$

→  $P(y = 0|x;\theta) = 1 - P(y = 1|x;\theta)$



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## Decision boundary



## Logistic regression

$$h_{\theta}(x) = g(\theta^T x)$$

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

Suppose predict “ $y = 1$ ” if  $h_{\theta}(x) \geq 0.5$

$$\theta^T x \geq 0$$

predict “ $y = 0$ ” if  $h_{\theta}(x) < 0.5$

$$\theta^T x < 0$$



$$g(z) \geq 0.5 \\ \text{when } z \geq 0 \\ h_{\theta}(x) = g(\theta^T x)$$

$$g(z) < 0.5 \\ \text{when } z < 0$$

# Decision Boundary



$$\theta = \begin{bmatrix} -3 \\ 1 \\ 1 \end{bmatrix} \leftarrow$$

$$h_{\theta}(x) = g(\underbrace{\theta_0}_{-3} + \underbrace{\theta_1}_{1}x_1 + \underbrace{\theta_2}_{1}x_2)$$

Decision boundary

Predict " $y = 1$ " if  $-3 + x_1 + x_2 \geq 0$

$\theta^T x$

$x_1, x_2$

$\rightarrow h_{\theta}(x) = 0.5$

$x_1 + x_2 = 3$

$\rightarrow$   $x_1 + x_2 \geq 3$

$\rightarrow x_1 + x_2 < 3$

$y = 0$

# Non-linear decision boundaries



$$h_{\theta}(x) = g(\theta_0 + \theta_1 x_1 + \theta_2 x_2 + \theta_3 x_1^2 + \theta_4 x_2^2)$$

$\begin{matrix} \text{---} \\ \text{---} \end{matrix}$      $\text{---} = 0$      $\text{---} = 0$   
 $\text{---}$      $\text{---}$      $\text{---}$

$$\theta = \begin{bmatrix} -1 \\ 0 \\ 0 \\ 1 \end{bmatrix}$$

Predict "y = 1" if  $-1 + x_1^2 + x_2^2 \geq 0$

$\boxed{x_1^2 + x_2^2 = 1}$      $\underbrace{-1 + x_1^2 + x_2^2 \geq 0}_{x_1^2 + x_2^2 \geq 1}$



$$h_{\theta}(x) = g(\theta_0 + \theta_1 x_1 + \theta_2 x_2 + \theta_3 \underline{x_1^2} + \theta_4 \underline{x_1^2 x_2} + \theta_5 \underline{x_1^2 x_2^2} + \theta_6 \underline{x_1^3 x_2} + \dots)$$



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## Cost function

Training  
set:

$$\{(x^{(1)}, y^{(1)}), (x^{(2)}, y^{(2)}), \dots, (x^{(m)}, y^{(m)})\}$$

m examples

$$x \in \begin{bmatrix} x_0 \\ x_1 \\ \dots \\ x_n \end{bmatrix}$$

$\mathbb{R}^{n+1}$

$$\underline{x_0 = 1}, \underline{y \in \{0, 1\}}$$

$$h_{\theta}(x) = \frac{1}{1 + e^{-\underline{\theta^T x}}}$$

How to choose parameters  $\theta$  ?

# Cost function

→ Linear regression:  
logistic

$$J(\theta) = \frac{1}{m} \sum_{i=1}^m \frac{1}{2} (h_{\theta}(x^{(i)}) - y^{(i)})^2$$

$$\text{cost}(h_{\theta}(x^{(i)}), y)$$

$$\text{Cost}(h_{\theta}(x), y) = \frac{1}{2} (h_{\theta}(x) - y)^2$$

$$\frac{1}{1 + e^{-\theta^T x}}$$



# Logistic regression cost function

$$\text{Cost}(\underline{h_\theta(x)}, y) = \begin{cases} \underline{-\log(h_\theta(x))} & \text{if } y = 1 \\ \underline{-\log(1 - h_\theta(x))} & \text{if } y = 0 \end{cases}$$



→ Cost = 0 if  $y = 1, h_\theta(x) = 1$   
But as  $h_\theta(x) \rightarrow 0$   
 $\text{Cost} \rightarrow \infty$

→ Captures intuition that if  $h_\theta(x) = 0$ ,  
(predict  $P(y = 1|x; \theta) = 0$ ), but  $y = 1$ ,  
we'll penalize learning algorithm by a very  
large cost.

# Logistic regression cost function

$$\text{Cost}(h_{\theta}(x), y) = \begin{cases} -\log(h_{\theta}(x)) & \text{if } y = 1 \\ -\log(1 - h_{\theta}(x)) & \text{if } y = 0 \end{cases}$$







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Simplified cost function  
and gradient descent

## Logistic regression cost function

$$\rightarrow J(\theta) = \frac{1}{m} \sum_{i=1}^m \text{Cost}(h_{\theta}(x^{(i)}), y^{(i)})$$

$$\rightarrow \text{Cost}(h_{\theta}(x), y) = \begin{cases} -\log(h_{\theta}(x)) & \text{if } y = 1 \\ -\log(1 - h_{\theta}(x)) & \text{if } y = 0 \end{cases}$$

Note:  $y = 0$  or  $1$  always

$$\rightarrow \text{Cost}(h_{\theta}(x), y) = -\underbrace{y \log(h_{\theta}(x)))}_{=0} - \underbrace{(1-y) \log(1-h_{\theta}(x)))}_{=1}$$

If  $y=1$ :  $\text{Cost}(h_{\theta}(x), y) = -\log h_{\theta}(x) \leftarrow$

If  $y=0$ :  $\text{Cost}(h_{\theta}(x), y) = \underline{-\log(1-h_{\theta}(x))}$

## Logistic regression cost function

$$J(\theta) = \frac{1}{m} \sum_{i=1}^m \text{Cost}(h_{\theta}(x^{(i)}), y^{(i)})$$
$$= -\frac{1}{m} \left[ \sum_{i=1}^m y^{(i)} \log h_{\theta}(x^{(i)}) + (1 - y^{(i)}) \log (1 - h_{\theta}(x^{(i)})) \right]$$

To fit parameters  $\theta$  :

$$\min_{\theta} J(\theta)$$

Get  $\underline{\theta}$

To make a prediction given new  $\underline{x}$ :

$$\text{Output } \underline{h_{\theta}(x)} = \frac{1}{1 + e^{-\theta^T x}}$$

$$\underline{p(y=1 | x; \theta)}$$

# Gradient Descent

$$\rightarrow J(\theta) = -\frac{1}{m} \left[ \sum_{i=1}^m y^{(i)} \log h_{\theta}(x^{(i)}) + (1 - y^{(i)}) \log (1 - h_{\theta}(x^{(i)})) \right]$$

Want  $\min_{\theta} J(\theta)$ :

Repeat {

$$\theta_j := \theta_j - \alpha \frac{\partial}{\partial \theta_j} J(\theta)$$

}

(simultaneously update all  $\theta_j$ )

$$\frac{\partial}{\partial \theta_j} J(\theta) = \frac{1}{m} \sum_{i=1}^m (h_{\theta}(x^{(i)}) - y^{(i)}) x_j^{(i)}$$

# Gradient Descent

$$J(\theta) = -\frac{1}{m} \left[ \sum_{i=1}^m y^{(i)} \log h_{\theta}(x^{(i)}) + (1 - y^{(i)}) \log (1 - h_{\theta}(x^{(i)})) \right]$$

Want  $\min_{\theta} J(\theta)$ :

Repeat {

→  $\theta_j := \theta_j - \alpha \sum_{i=1}^m (h_{\theta}(x^{(i)}) - y^{(i)}) x_j^{(i)}$

}

(simultaneously update all  $\theta_j$ )

$\Theta = \begin{bmatrix} \theta_0 \\ \theta_1 \\ \theta_2 \\ \vdots \\ \theta_n \end{bmatrix}$  for  $i=0$  to  $n$

$h_{\theta}(x) = \Theta^T x$

$h_{\theta}(x) = \frac{1}{1 + e^{-\Theta^T x}}$

Algorithm looks identical to linear regression!



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# Logistic Regression

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# Advanced optimization

# Optimization algorithm

Cost function  $J(\theta)$ . Want  $\min_{\theta}$   $J(\theta)$ .

Given  $\theta$ , we have code that can compute

$\rightarrow - J(\theta)$   
 $\rightarrow - \frac{\partial}{\partial \theta_j} J(\theta)$  (for  $j = 0, 1, \dots, n$ )

Gradient descent:

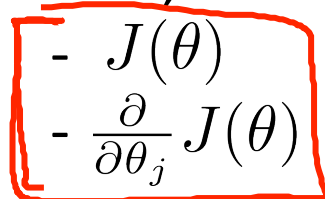
Repeat {

$\rightarrow \theta_j := \theta_j - \alpha \frac{\partial}{\partial \theta_j} J(\theta)$

}



# Optimization algorithm

Given  $\theta$ , we have code that can compute


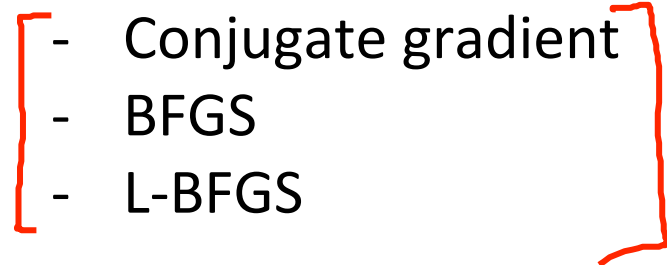


- $J(\theta)$
- $\frac{\partial}{\partial \theta_j} J(\theta)$


(for  $j = 0, 1, \dots, n$ )



Optimization algorithms:

- 
- Gradient descent
  - Conjugate gradient
  - BFGS
  - L-BFGS
- 

Advantages:

- No need to manually pick  $\alpha$
  - Often faster than gradient descent.
- 

Disadvantages:

- More complex 



Example:

$\min_{\theta} J(\theta)$

$$\theta = \begin{bmatrix} \theta_1 \\ \theta_2 \end{bmatrix}$$

$\theta_1 = 5, \theta_2 = 5.$

$$J(\theta) = (\theta_1 - 5)^2 + (\theta_2 - 5)^2$$

$$\frac{\partial}{\partial \theta_1} J(\theta) = 2(\theta_1 - 5)$$

$$\frac{\partial}{\partial \theta_2} J(\theta) = 2(\theta_2 - 5)$$

```
function [jVal, gradient]
    = costFunction(theta)
    jVal = (theta(1)-5)^2 + ...
          (theta(2)-5)^2;
    gradient = zeros(2,1);
    gradient(1) = 2*(theta(1)-5);
    gradient(2) = 2*(theta(2)-5);
```

```
options = optimset('GradObj', 'on', 'MaxIter', '100');
```

```
initialTheta = zeros(2,1);
```

```
[optTheta, functionVal, exitFlag] ...
    = fminunc(@costFunction, initialTheta, options);
```

↑

↑

$\theta \in \mathbb{R}^d$   $d \geq 2$ .

$$\underline{\text{theta}} = \begin{bmatrix} \theta_0 \\ \theta_1 \\ \vdots \\ \theta_n \end{bmatrix}$$

Handwritten annotations:

- $\theta_0$  is labeled  $\text{theta}(1)$  with an arrow pointing to it.
- $\theta_1$  is labeled  $\text{theta}(2)$  with an arrow pointing to it.
- $\theta_n$  is labeled  $\text{theta}(n+1)$  with an arrow pointing to it.

```
function [jVal gradient] = costFunction(theta)
```

```
    jVal = [code to compute  $J(\theta)$ ];
```

```
    gradient(1) = [code to compute  $\frac{\partial}{\partial \theta_0} J(\theta)$ ];
```

```
    gradient(2) = [code to compute  $\frac{\partial}{\partial \theta_1} J(\theta)$ ];
```

```
    :
```

```
    gradient(n+1) = [code to compute  $\frac{\partial}{\partial \theta_n} J(\theta)$ ] ;
```



Machine Learning

# Logistic Regression

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Multi-class classification:  
One-vs-all

# Multiclass classification

Email foldering/tagging: Work, Friends, Family, Hobby

$y=1$   $y=2$   $y=3$   $y=4$

Medical diagrams: Not ill, Cold, Flu

$y=1$  2 3

Weather: Sunny, Cloudy, Rain, Snow

$y=1$  2 3 4  $\leftarrow$



Binary classification:



Multi-class classification:





## One-vs-all (one-vs-rest):



Class 1:  

Class 2:  

Class 3:  

$$h_{\theta}^{(i)}(x) = P(y = i | x; \theta) \quad (i = 1, 2, 3)$$



# One-vs-all

Train a logistic regression classifier  $\underline{h_{\theta}^{(i)}(x)}$  for each class  $\underline{i}$  to predict the probability that  $\underline{y = i}$ .

On a new input  $\underline{x}$ , to make a prediction, pick the class  $i$  that maximizes

$$\max_{\underline{i}} \underline{h_{\theta}^{(i)}(x)}$$
