UCK358E – INTR. TO ARTIFICIAL INTELLIGENCE

SPRING ‘23

LECTURE 4

LOGISTIC REGRESSION: CLASSIFICATION

Instructor: Asst. Prof. Barış Başpınar

Classification

Email: Spam / Not Spam?

Online Transactions: Fraudulent (Yes / No)?

Tumor: Malignant / Benign ?

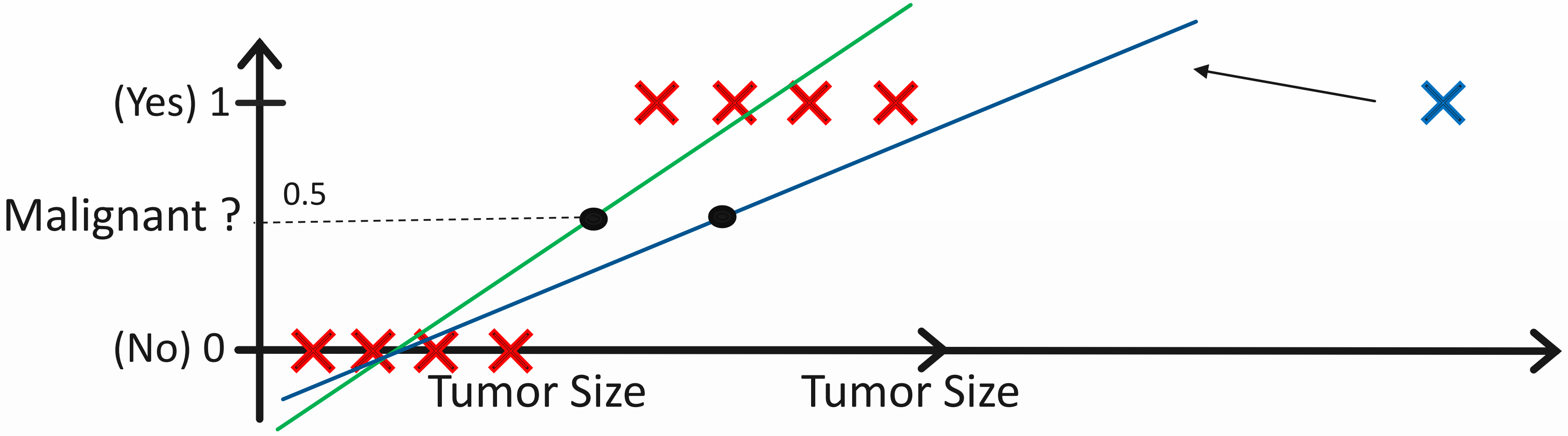
$y \in \{0, 1\}$

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

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

Binary classification

Classification



Applying linear regression into classification problem often isn't a good idea

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

Classification: y = 0 or 1

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

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

Hypothesis Representation

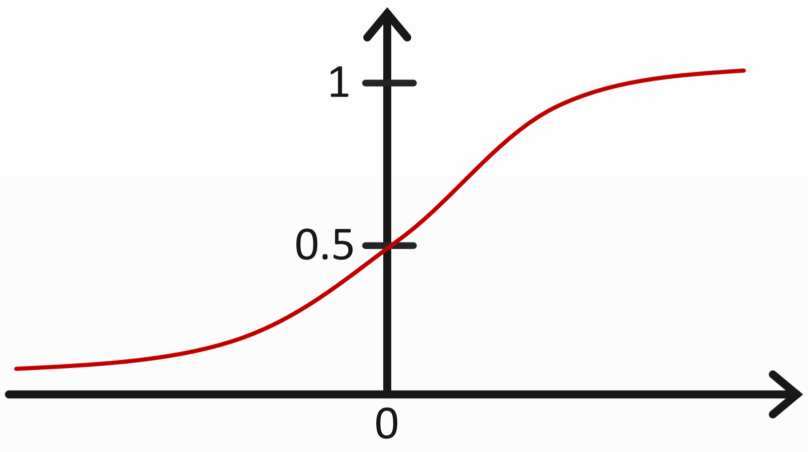
Logistic Regression Model

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

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

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

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



Sigmoid function
Logistic function

Interpretation of Hypothesis Output

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

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

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

Tell patient that 70% chance of tumor being malignant

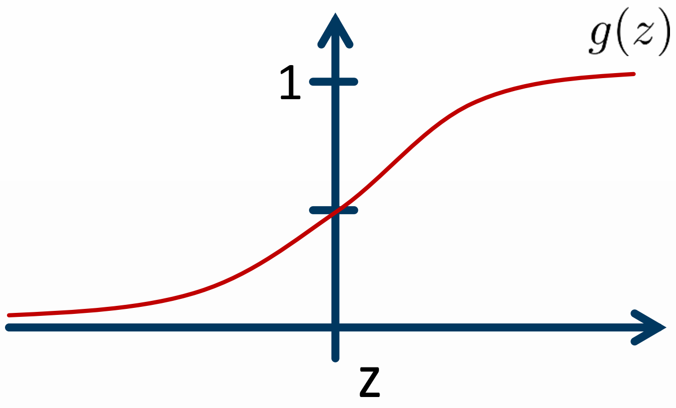
"probability that y = 1, given x, parameterized by θ"

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

Logistic regression

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

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



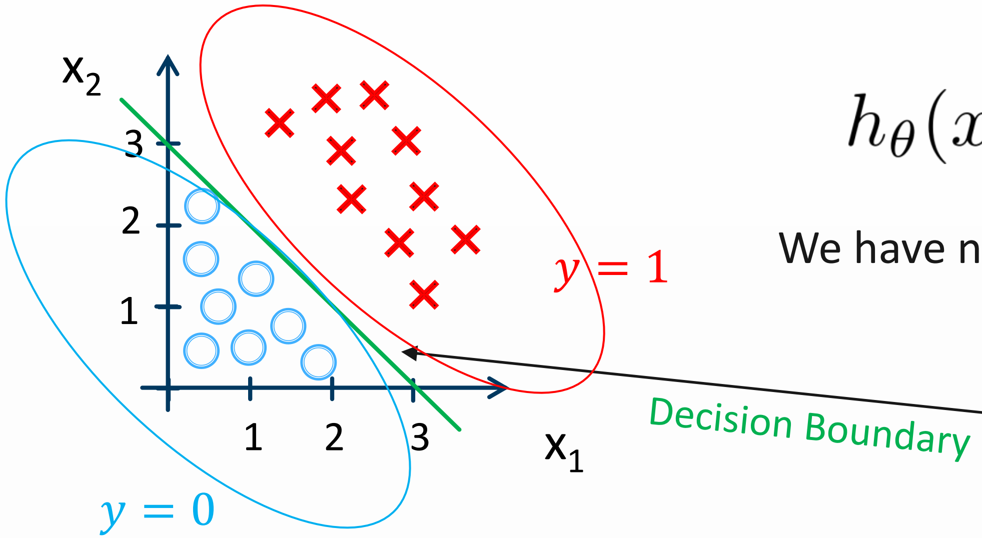
Suppose predict "$y = 1$" if $h_\theta(x) \geq 0.5$

$$g(z) \geq 0.5 \quad \rightarrow \quad z \geq 0 \quad \rightarrow \quad \theta^T x \geq 0$$

predict "$y = 0$" if $h_\theta(x) < 0.5$

$$g(z) < 0.5 \quad \rightarrow \quad z < 0 \quad \rightarrow \quad \theta^T x < 0$$

Decision Boundary



$$h_\theta(x) = g(\theta_0 + \theta_1 x_1 + \theta_2 x_2)$$

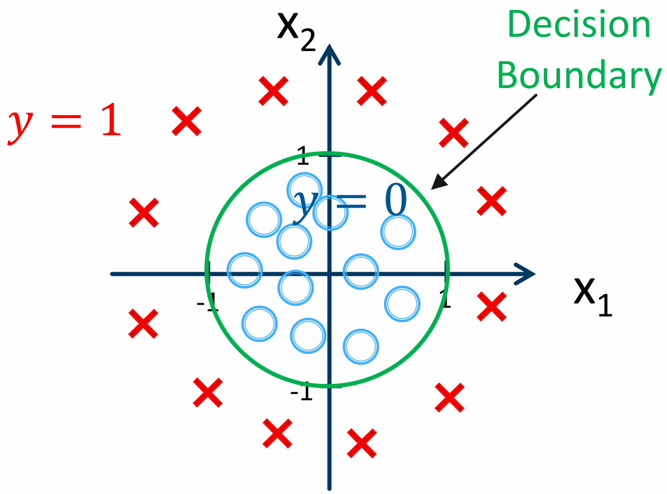
We have not talked how to choose θ yet. Assume that:

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

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

$\boxed{x_1 + x_2 = 3}$ → $h_\theta(x) = 0.5$ → $y = 1$

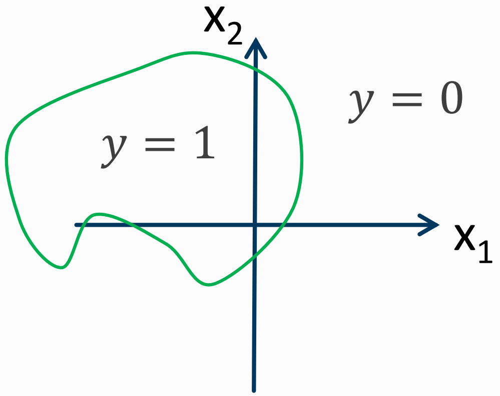
Non-linear Decision Boundary



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

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

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



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

Cost Function

Training set: $\{(x^{(1)}, y^{(1)}), (x^{(2)}, y^{(2)}), \cdots, (x^{(m)}, y^{(m)})\}$

m examples $\qquad x \in \begin{bmatrix} x_0 \\ x_1 \\ \dots \\ x_n \end{bmatrix} \qquad x_0 = 1, y \in \{0, 1\}$

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

How to choose parameters θ ?

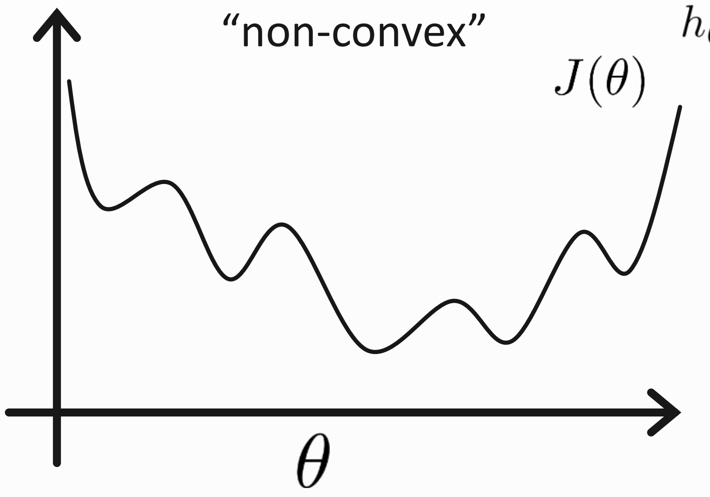
Cost Function

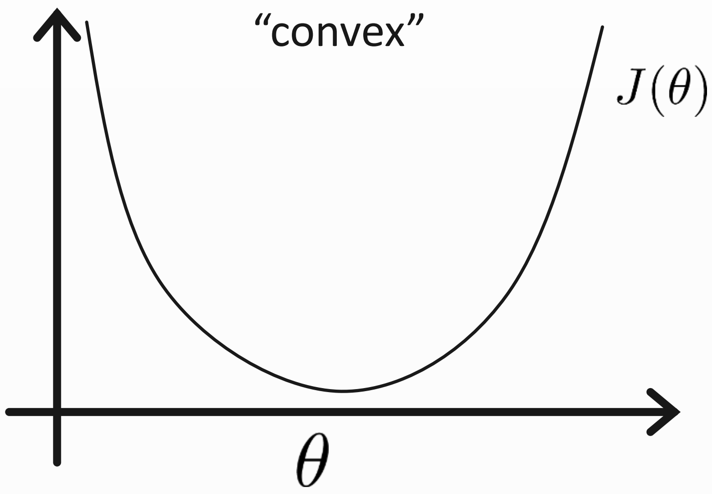
Linear regression: $J(\theta) = \frac{1}{m}\sum_{i=1}^{m} \frac{1}{2}\left(h_\theta(x^{(i)}) - y^{(i)}\right)^2$

$$\mathrm{Cost}(h_\theta(x^{(i)}), y^{(i)}) = \frac{1}{2}\left(h_\theta(x^{(i)}) - y^{(i)}\right)^2$$

Logistic regression's hypothesis

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



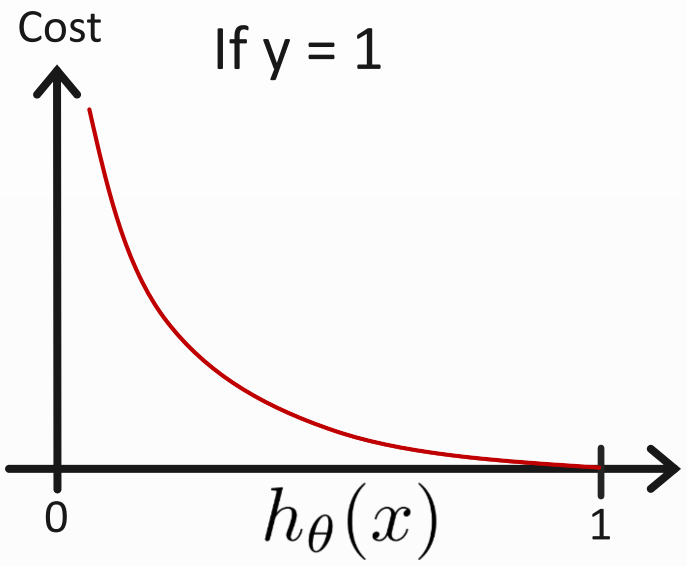


Define a different cost function that is convex in which the gradient descent can converge to the global minimum

Cost Function

Logistic regression cost function

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



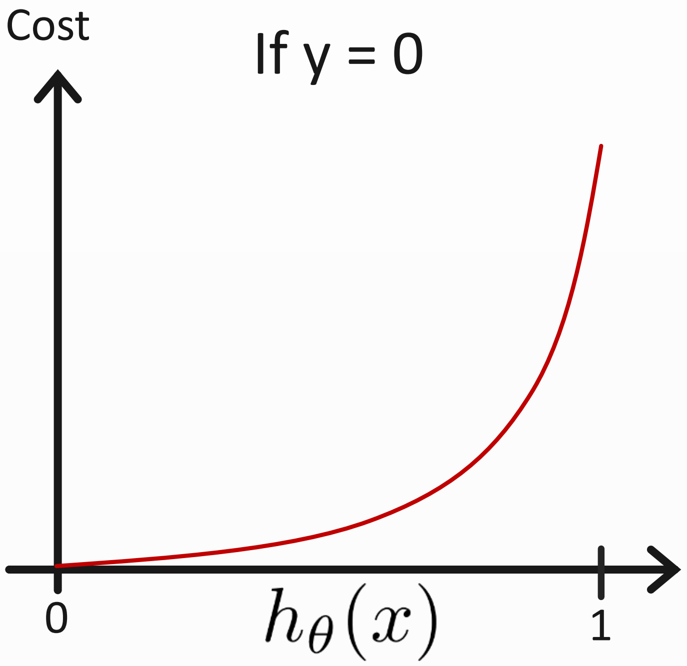
$\text{Cost} = 0$ if $y = 1, h_\theta(x) = 1$
But as $h_\theta(x) \to 0$
$Cost \to \infty$

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.

Cost Function

Logistic regression cost function

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



Cost Function and Gradient Descent

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

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

Note: $y = 0$ or 1 always

Compact way to present this cost function:

$$\mathrm{Cost}(h_\theta(x), y) = -y\log(h_\theta(x)) - (1-y)\log(1 - h_\theta(x))$$

"convex"

This cost function can also be derived from statistics using the principle of Maximum Likelihood Estimation

Cost Function and Gradient Descent

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

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

To fit parameters θ:

$$\min_\theta J(\theta)$$

To make a prediction given new x:

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

Cost Function and Gradient Descent

Gradient Descent

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

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

Repeat $\{$

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

(simultaneously update all θ_j)

$\}$

Cost Function and Gradient Descent

Gradient Descent

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

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

Repeat $\{$

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

(simultaneously update all θ_j)

$\}$

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

Algorithm looks identical to linear regression!
But the definition of the hypothesis has changed.

Advanced Optimization

Given θ, we have code that can compute

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

Optimization algorithms:

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

Advantages:

- No need to manually pick α
- Often faster than gradient descent

Disadvantages:

- More complex

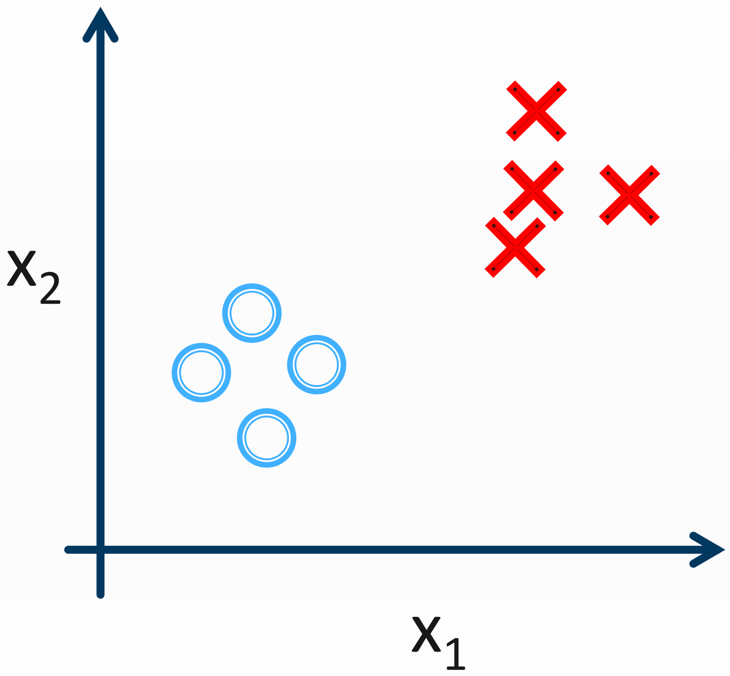
Multi-class Classification

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

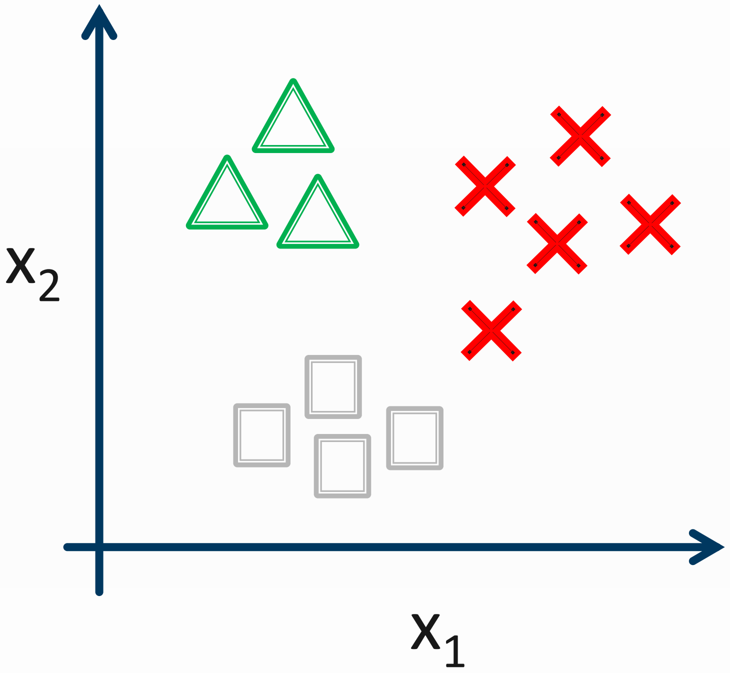
Medical diagrams: Not ill, Cold, Flu

Weather: Sunny, Cloudy, Rain, Snow

Binary classification:

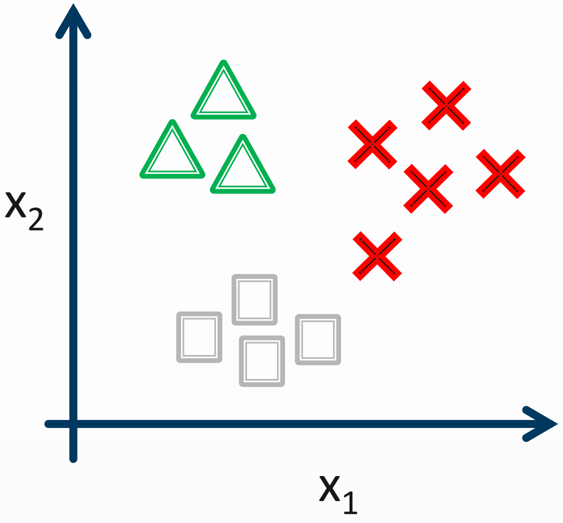


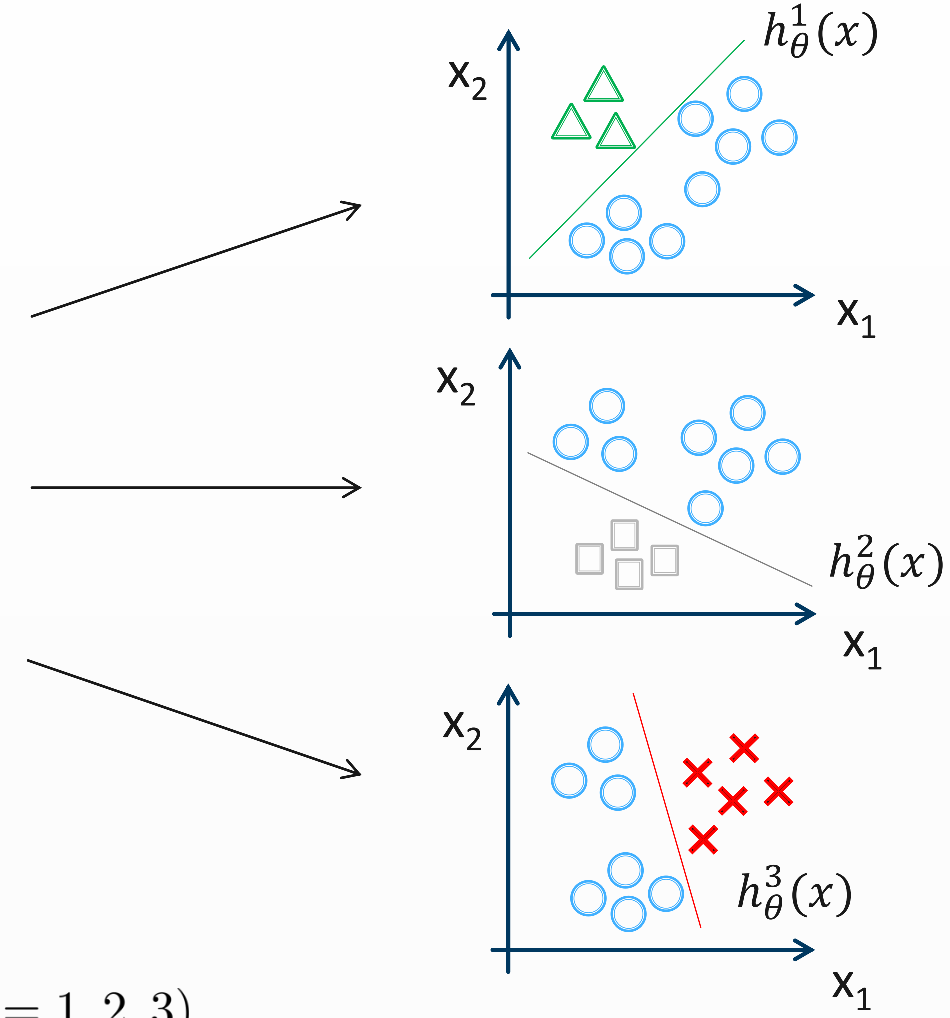
Multi-class classification:



Multi-class Classification

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





Class 1:

Class 2:

Class 3:

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

Multi-class Classification

One-vs-all

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

On a new input x, to make a prediction, pick the class i that maximizes

$$\max_i h_\theta^{(i)}(x)$$

Logistic Regression Tips

- **Binary Output Variable**: This might be obvious as we have already mentioned it, but logistic regression is intended for binary (two-class) classification problems. It will predict the probability of an instance belonging to the default class, which can be snapped into a 0 or 1 classification.

- **Remove Noise**: Logistic regression assumes no error in the output variable (y), consider removing outliers and possibly misclassified instances from your training data.

- **Gaussian Distribution**: Logistic regression is a linear algorithm (with a non-linear transform on output). It does assume a linear relationship between the input variables with the output. Data transforms of your input variables that better expose this linear relationship can result in a more accurate model. For example, you can use log, root, Box-Cox and other univariate transforms to better expose this relationship.

- **Remove Correlated Inputs**: Like linear regression, the model can overfit if you have multiple highly-correlated inputs. Consider calculating the pairwise correlations between all inputs and removing highly correlated inputs.

- **Fail to Converge**: It is possible for the expected likelihood estimation process that learns the coefficients to fail to converge. This can happen if there are many highly correlated inputs in your data or the data is very sparse (e.g. lots of zeros in your input data).

References

- A. Ng. Machine Learning, Lecture Notes.
- I. Goodfellow, Y. Bengio and A. Courville, “Deep Learning”, 2016.