7. Supervised Learning: Logistic Regression

Logistic Regression

Example

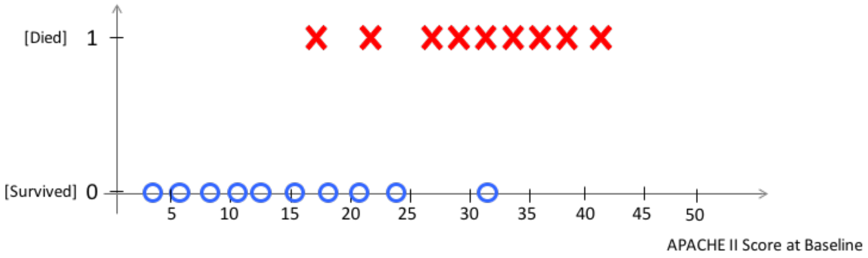
- Prediction of sepsis mortality based on features such as APACHE II score at baseline
- It is a supervised learning problem because one has access to input-output examples
- It is a classification problem because the output variable is discrete-valued
- Input variables also known as features
- Output variable also known as labels

Training set

Input Variable (APACHE II Score)	*Output Variable (Survived / Died)*
3	*Survived*
6	*Survived*
15	*Survived*
29	*Died*
38	*Died*

Training sample

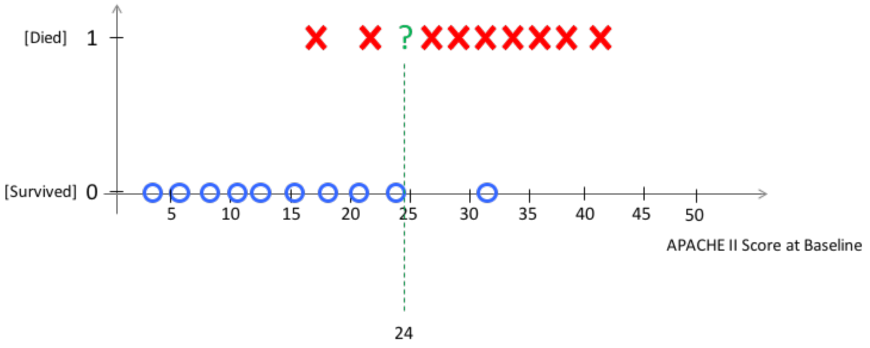
(x_i, y_i)



Testing set

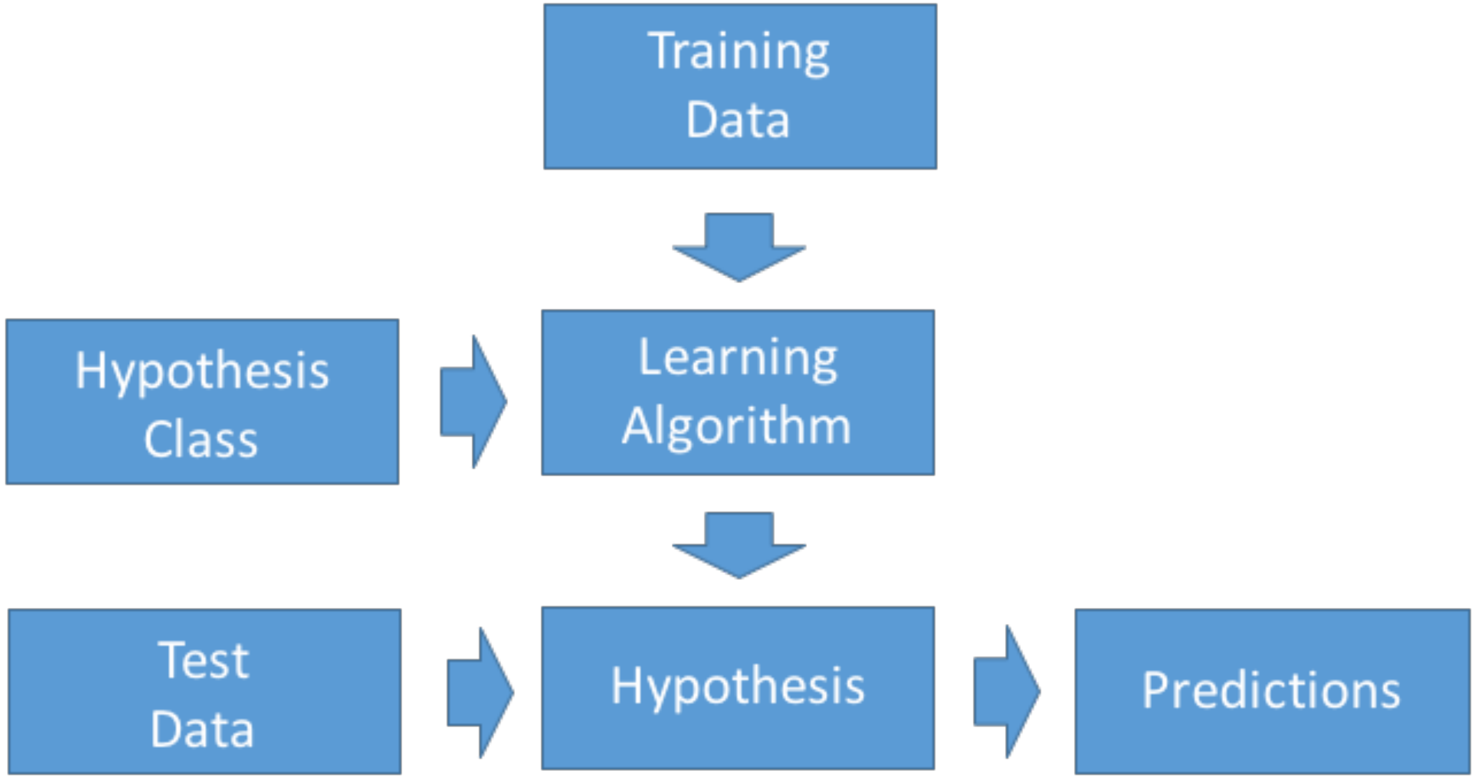
Input Variable (APACHE II Score)	*Output Variable (Survived / Died)*
24	*?*

Testing Sample



Logistic Regression

Process

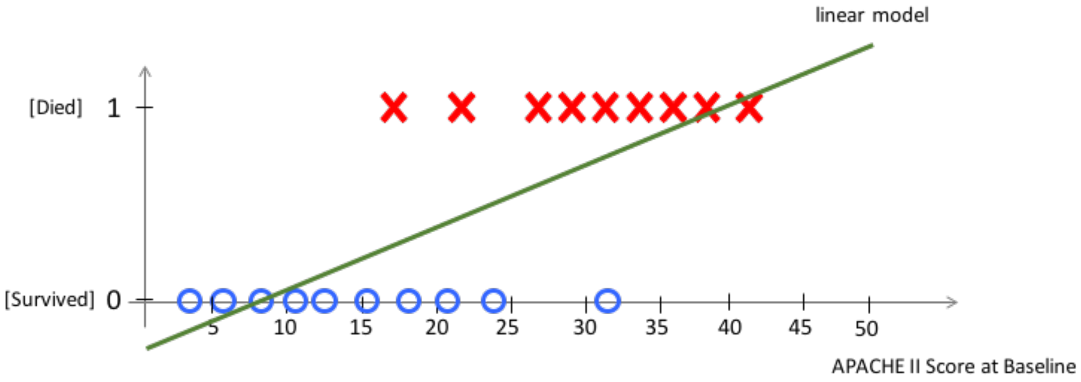


- One is given access to a **training data** – consisting of various **feature**-**label** pairs – and **testing data** – consisting of features points with unknown **label**.
- One is also given a **hypothesis** (or **model**) **class** containing a series of **hypotheses** (or **models**) that potentially explain the relationship between the **features** and **labels**.
- The **learning algorithm** selects a **hypothesis** (or **model**) from the **hypothesis** (or **model**) **class** that fits the **training data**.
- Such selected **hypothesis** can then be used on the **testing data** to determine the **label** associated with the new **features**.

Logistic Regression vs. Simple Linear Regression

Can we solve this classification problem using simple linear regression?

Example 1



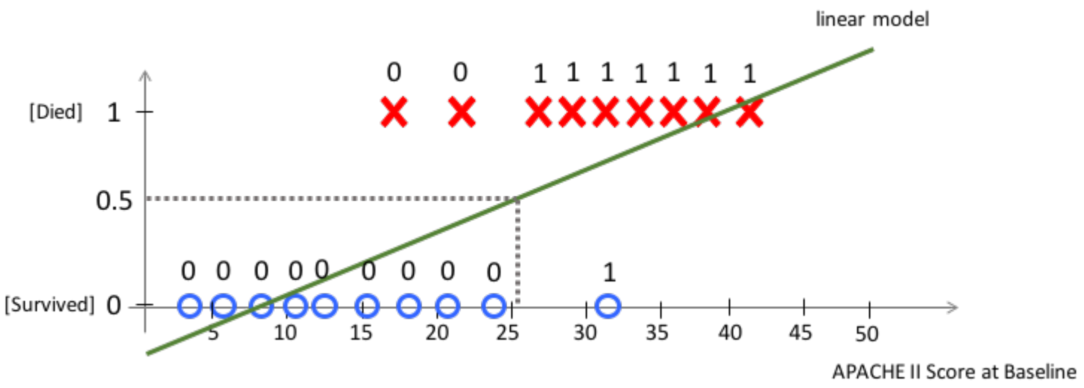
Classification Rule (Classification with Simple Linear Regression)

- If output of linear regressor is less than 0.5 declare SURVIVED
- If output of linear regressor is more than 0.5 declare DIED

Logistic Regression vs. Simple Linear Regression

Can we solve this classification problem using simple linear regression?

Example 1



Classification Rule (Classification with Simple Linear Regression)

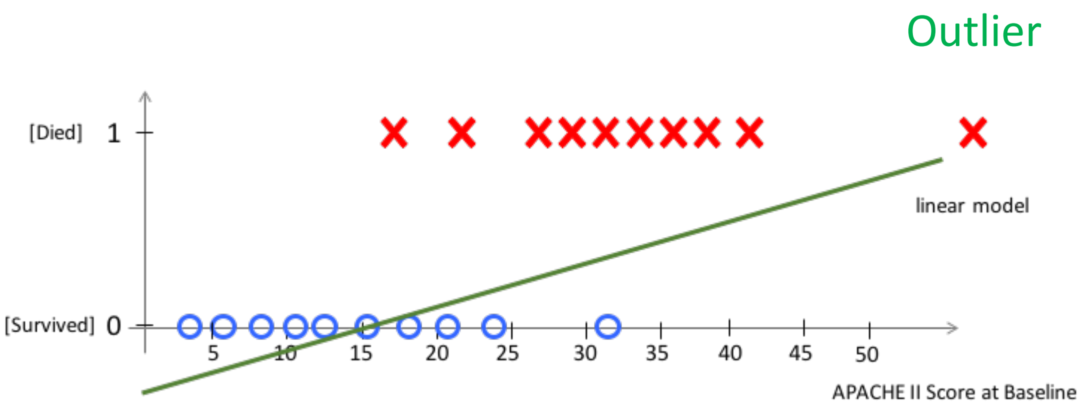
- If output of linear regressor is less than 0.5 declare SURVIVED
- If output of linear regressor is more than 0.5 declare DIED

Classification performance is relatively good!

Logistic Regression vs. Simple Linear Regression

Can we solve this classification problem using simple linear regression?

Example 2



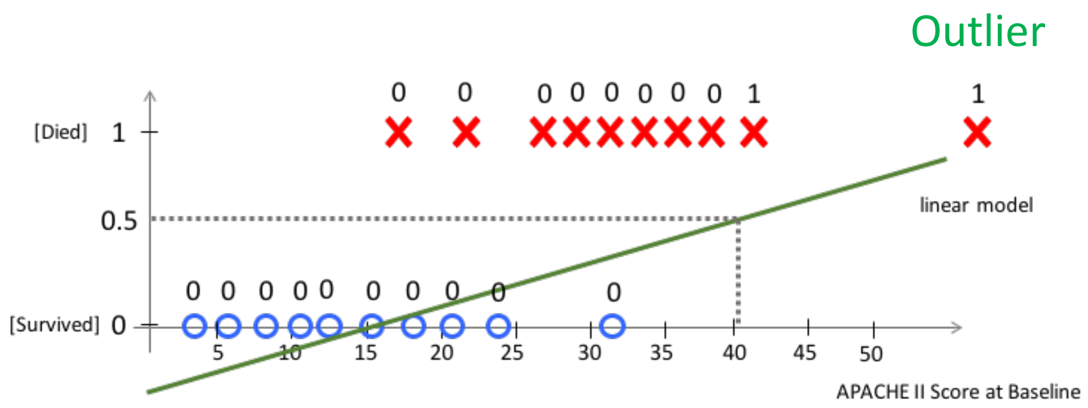
Classification Rule (Classification with Simple Linear Regression)

- If output of linear regressor is less than 0.5 declare SURVIVED
- If output of linear regressor is more than 0.5 declare DIED

Logistic Regression vs. Simple Linear Regression

Can we solve this classification problem using simple linear regression?

Example 2



Classification Rule (Classification with Simple Linear Regression)

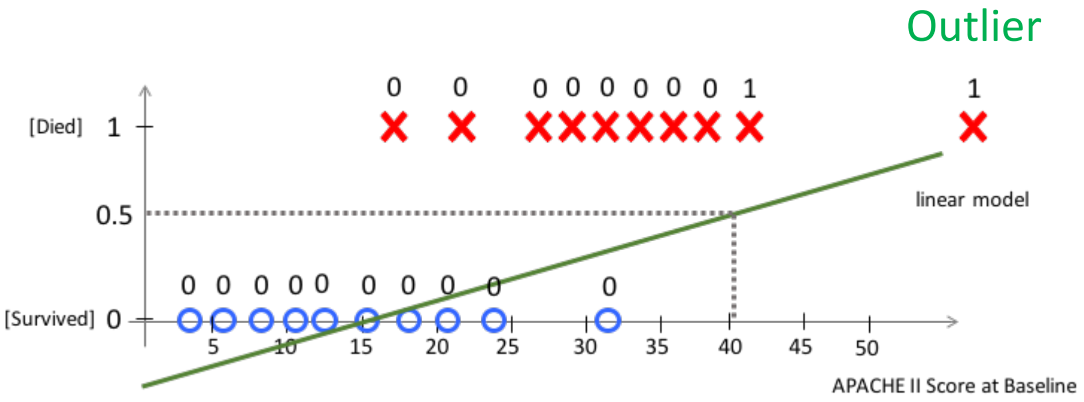
- If output of linear regressor is less than 0.5 declare SURVIVED
- If output of linear regressor is more than 0.5 declare DIED

Classification performance is very poor!

Logistic Regression vs. Simple Linear Regression

Can we solve this classification problem using simple linear regression?

Example 2



Classification Rule (Classification with Simple Linear Regression)

- If output of linear regressor is less than 0.5 declare SURVIVED
- If output of linear regressor is more than 0.5 declare DIED

Classification

The output should be 0 or 1

Linear Regression

The output can be less than 0
and can be greater than 1 .

Logistic Regression

The output is between 0 and 1

Logistic Regression: Model

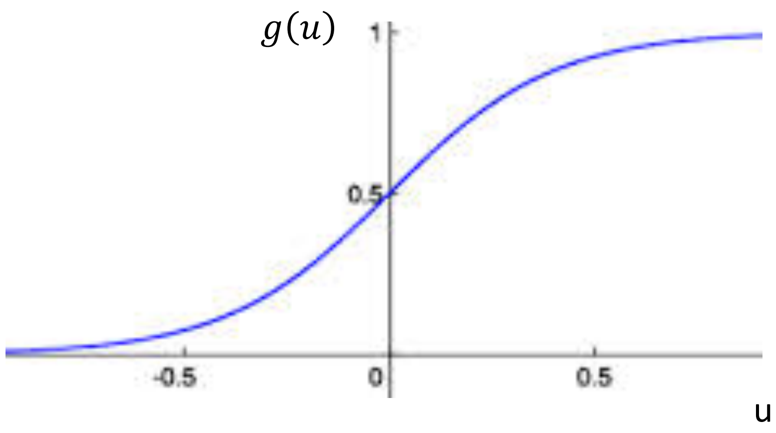
Model

The hypothesis is such that:

$$\boxed{h_{\boldsymbol{\theta}}(\boldsymbol{x}) = \mathrm{g}(\boldsymbol{\theta}^t \boldsymbol{x}) = \frac{1}{1 + e^{-\boldsymbol{\theta}^t \boldsymbol{x}}}}$$

where $\boldsymbol{\theta} = (\theta_0, \theta_1, \dots, \theta_m)^t$ is the param. vector
and $\boldsymbol{x} = (1, x_1, \dots, x_m)^t$ is the feature vector

Logistic or Sigmoid Function



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

Interpretation

$$\Pr(\hat{y} = 1 | \boldsymbol{x}; \boldsymbol{\theta}) = h_{\boldsymbol{\theta}}(\boldsymbol{x}) \implies \Pr(\hat{y} = 0 | \boldsymbol{x}; \boldsymbol{\theta}) = 1 - h_{\boldsymbol{\theta}}(\boldsymbol{x})$$

$$\Pr(\hat{y} = 1 | \boldsymbol{x}; \boldsymbol{\theta}) = 0.7 \implies \text{A patient has a 70\% chance of a tumor being malignant}$$

Logistic Regression: Decision Regions

Classifier

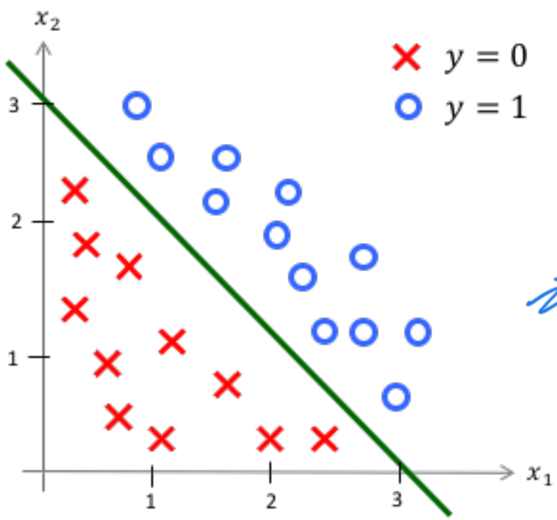
$$\hat{y} = 1 \quad \Leftarrow \quad \Pr(\hat{y} = 1 | \boldsymbol{x}; \boldsymbol{\theta}) \geq 0.5$$

$$\hat{y} = 0 \quad \Leftarrow \quad \Pr(\hat{y} = 1 | \boldsymbol{x}; \boldsymbol{\theta}) < 0.5$$

$$\hat{y} = 1 \quad \Leftarrow \quad \boldsymbol{\theta}^t \boldsymbol{x} \geq 0$$

$$\hat{y} = 0 \quad \Leftarrow \quad \boldsymbol{\theta}^t \boldsymbol{x} < 0$$

Linear Classifiers



$\Rightarrow \theta^t x = 0$

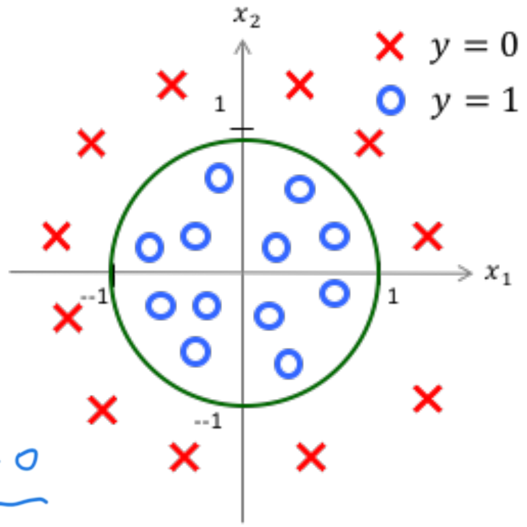
$\begin{pmatrix} -3 \\ 1 \\ 1 \end{pmatrix} (x_1 \;\; x_2 \;\; x_3) = 0$

$-3 + x_1 + x_2 = 0$

Linear

The hypothesis is $h_{\boldsymbol{\theta}}(x) = g(\theta_0 + \theta_1 x_1 + \theta_2 x_2)$ with $\theta = (-3,1,1)^t$.

Nonlinear Classifiers



The hypothesis is $h_{\boldsymbol{\theta}}(x) = g(\theta_0 + \theta_1 x_1 + \theta_2 x_2 + \theta_3 x_1^2 + \theta_4 x_2^2)$ with $\theta = (-1,0,0,1,1)^t$.

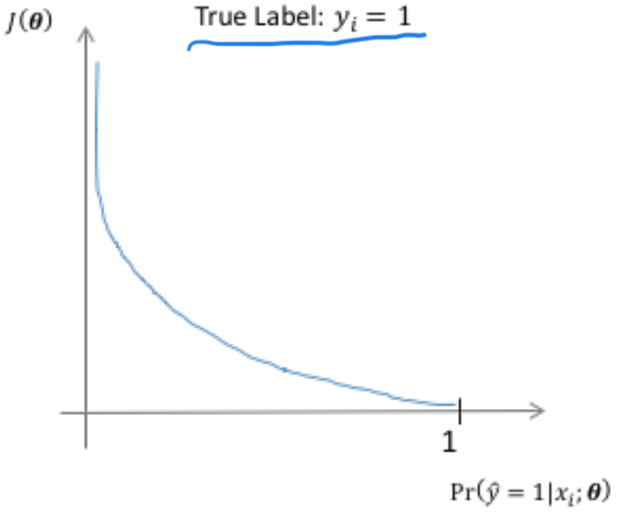
Logistic Regression: Cost Function

How does the learning algorithm select the linear hypothesis / model? We need a cost function... log

Cost Function

$$J(\boldsymbol{\theta}) = -\frac{1}{n}\sum_{i=1}^{n} \mathrm{y_i} \cdot \log_2\left(\Pr(\hat{y} = 1|x_i; \boldsymbol{\theta})\right) + (1 - y_i) \cdot \log_2\left(1 - \Pr(\hat{y} = 1|x_i; \boldsymbol{\theta})\right)$$

Why this cost function?



$y^{(i)} = 1 \wedge \Pr\left(\hat{y} = 1|x^{(i)}; \boldsymbol{\theta}\right) \approx 1 \Longrightarrow$ cost is small

$y^{(i)} = 1 \wedge \Pr\left(\hat{y} = 1|x^{(i)}; \boldsymbol{\theta}\right) \approx 0 \Longrightarrow$ cost is large

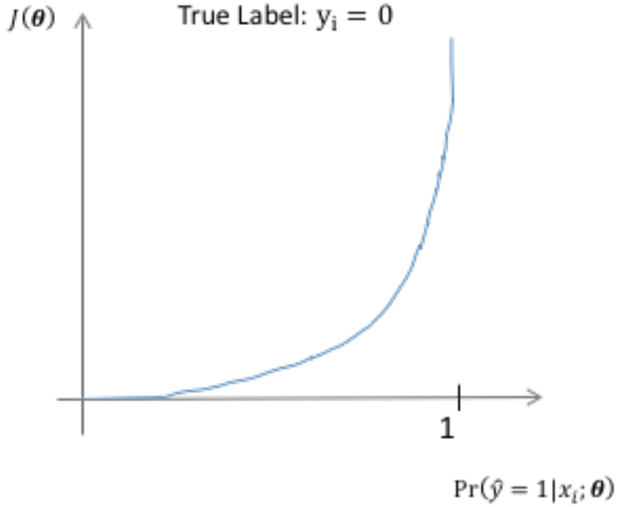
Logistic Regression: Cost Function

How does the learning algorithm select the linear hypothesis / model? We need a cost function…

Cost Function

$$J(\boldsymbol{\theta}) = -\frac{1}{n}\sum_{i=1}^{n} \mathrm{y_i} \cdot \log_2\big(\Pr(\hat{y} = 1|x_i;\boldsymbol{\theta})\big) + (1 - y_i) \cdot \log_2\big(1 - \Pr(\hat{y} = 1|x_i;\boldsymbol{\theta})\big)$$

Why this cost function?



$y^{(i)} = 0 \wedge \Pr\big(\hat{y} = 1|x^{(i)};\boldsymbol{\theta}\big) \approx 1 \implies$ cost is large

$y^{(i)} = 0 \wedge \Pr\big(\hat{y} = 1|x^{(i)};\boldsymbol{\theta}\big) \approx 0 \implies$ cost is small

Logistic Regression: Learning Algorithm

Learning Algorithm

We should select the logistic regression model parameters that minimize the cost function as follows:

$$\boldsymbol{\theta}^* = \underset{\boldsymbol{\theta}}{\operatorname{argmin}}\, J(\boldsymbol{\theta})$$

New Predictions

The new predictions are then given by:

$$Pr(\hat{y} = 1|\boldsymbol{x}; \boldsymbol{\theta}^*) = \mathrm{g}(\boldsymbol{\theta}^{*t}\boldsymbol{x}) = \frac{1}{1 + e^{-\boldsymbol{\theta}^{*t}\boldsymbol{x}}}$$

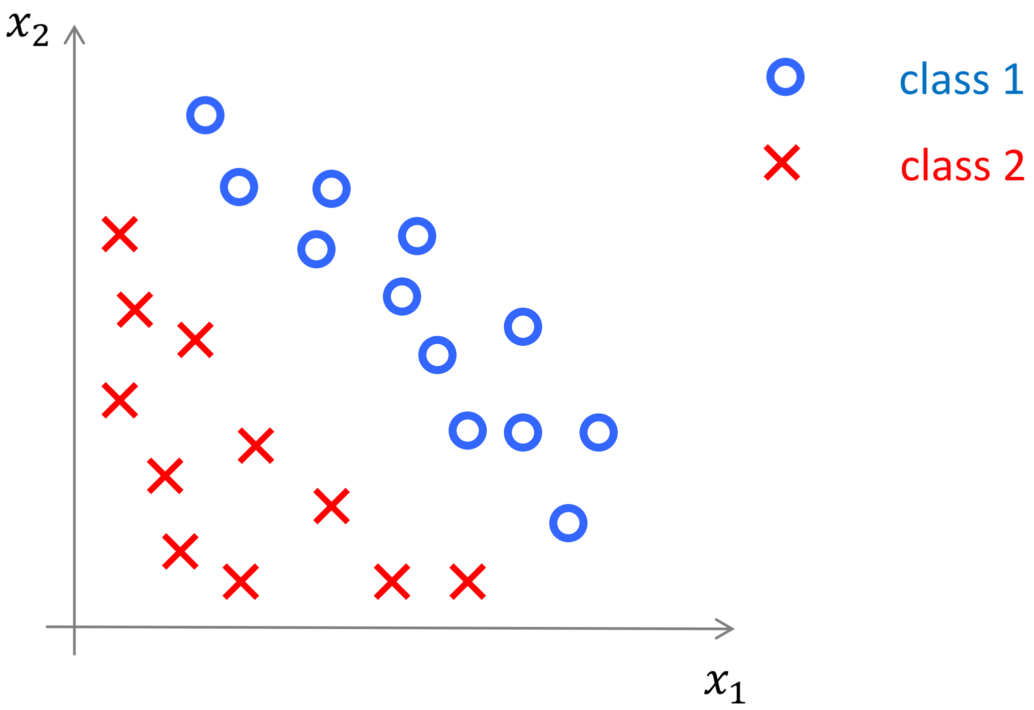
There is no closed-form solution for the optimal parameters

⇩

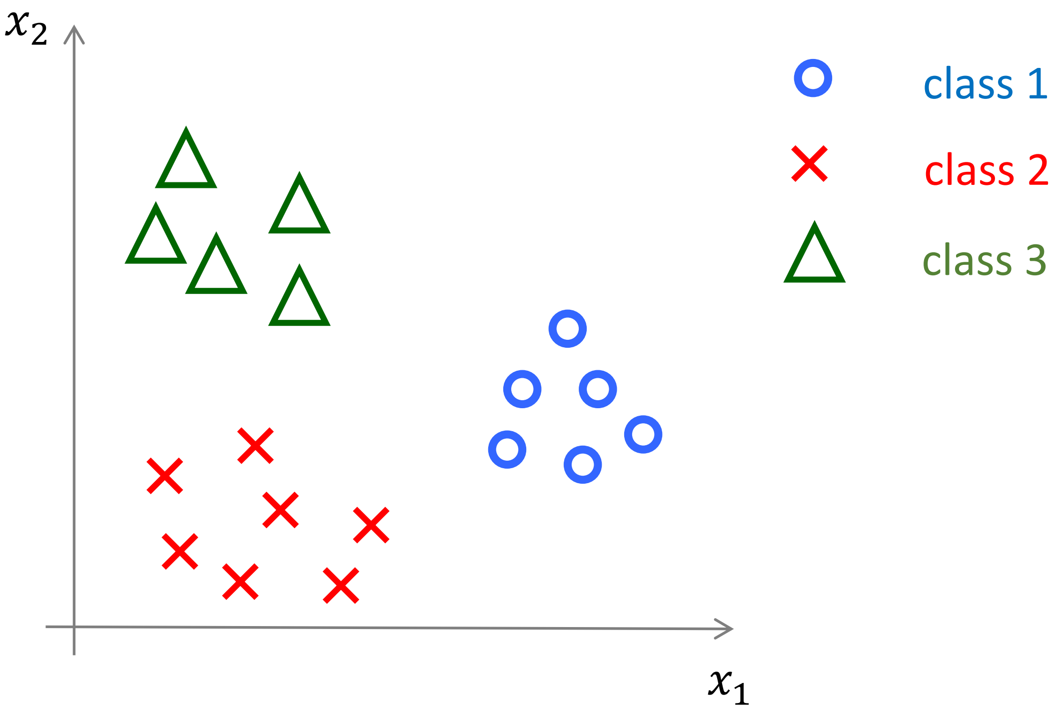
Gradient descent algorithm

Multiclass Classification

Binary Classification Problem



Multiclass Classification Problem



Multiclass Classification: One-vs-All

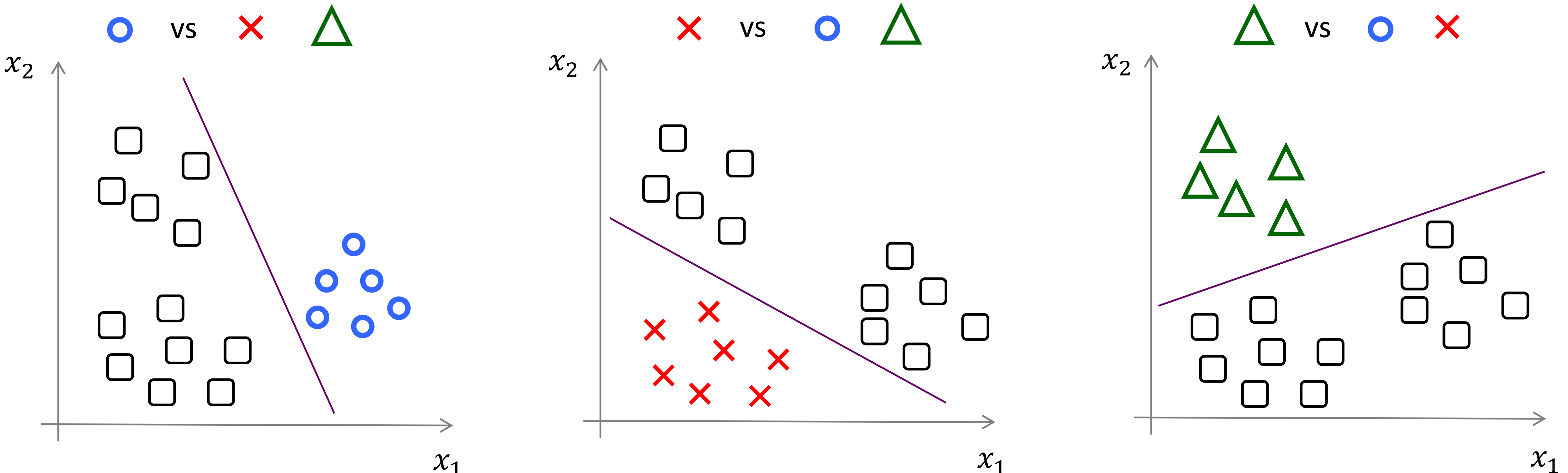
Procedure

(1) Convert a *M*-class classification problem onto *M* binary classification problems.

(2) Learn a binary classifier – e.g. a logistic regressor – for each binary classification problem delivering a confidence score.

(3) Apply the *M* binary classifiers on new data to obtain *M* confidence scores.

(4) Report the class with the highest confidence score.



Multiclass Classification: One-vs-One

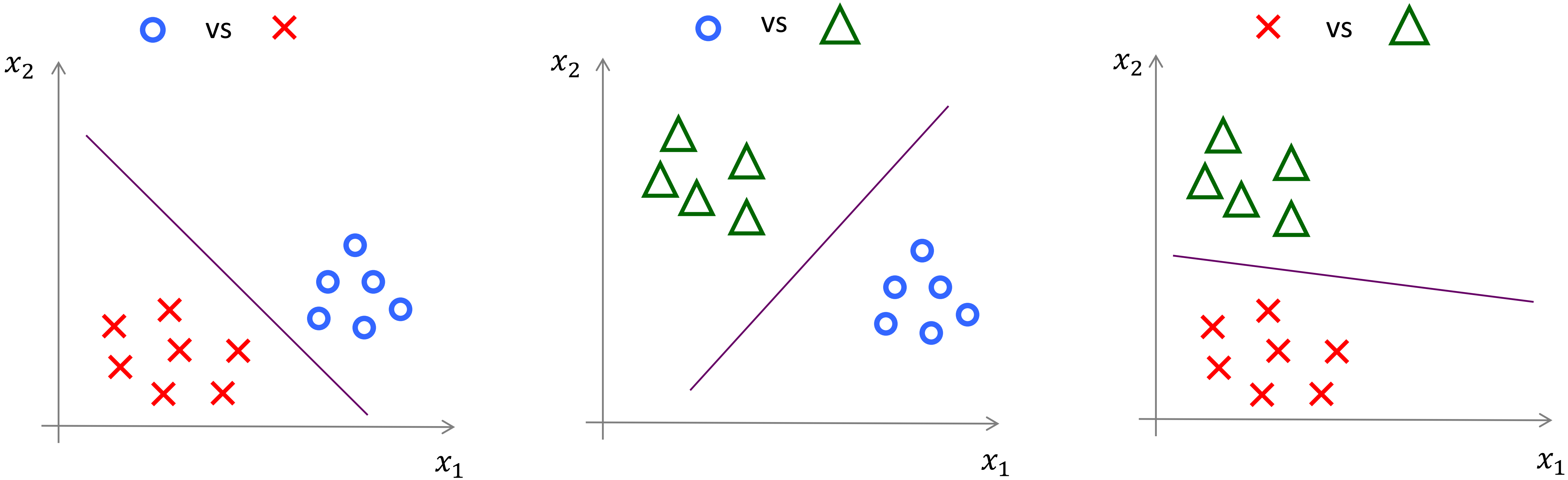
Procedure

(1) Convert a M-class problem onto $(M-1)M/2$ binary classification problems.

(2) Learn a binary classifier – e.g. a logistic regressor – for each binary classification problem delivering a confidence score.

(3) Apply the M binary classifiers on new data to obtain M confidence scores.

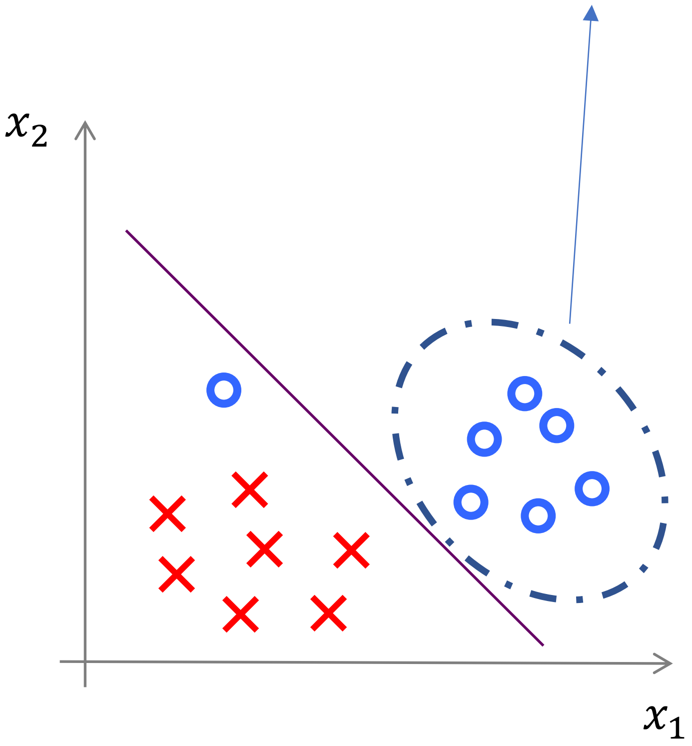
(4) Report the class that has been “voted” the highest by the different classifiers.



Precision vs Recall

$$\text{Precision} = \frac{\text{true positive}}{\text{No. of predicted positive}}$$

$$\text{Recall} = \frac{\text{true positive}}{\text{No. of actual positive}}$$



- We want to predict y=1 only in very confident sets

Predict 1 if $h(x) \geq \cancel{0.5}$ 0.7
Predict 1 if $h(x) < \cancel{0.5}$ 0.7

High-precision and low recall classifier

- We want to predict y=1 avoiding false negative

Predict 1 if $h(x) \geq \cancel{0.5}$ 0.3
Predict 1 if $h(x) < \cancel{0.5}$ 0.3

Low-precision and high recall classifier

Confusion Matrix

True Positive

Actual Values

Predicted Values	Positive (1)	Negative (0)
Positive (1)	TP	FP
Negative (0)	FN	TN