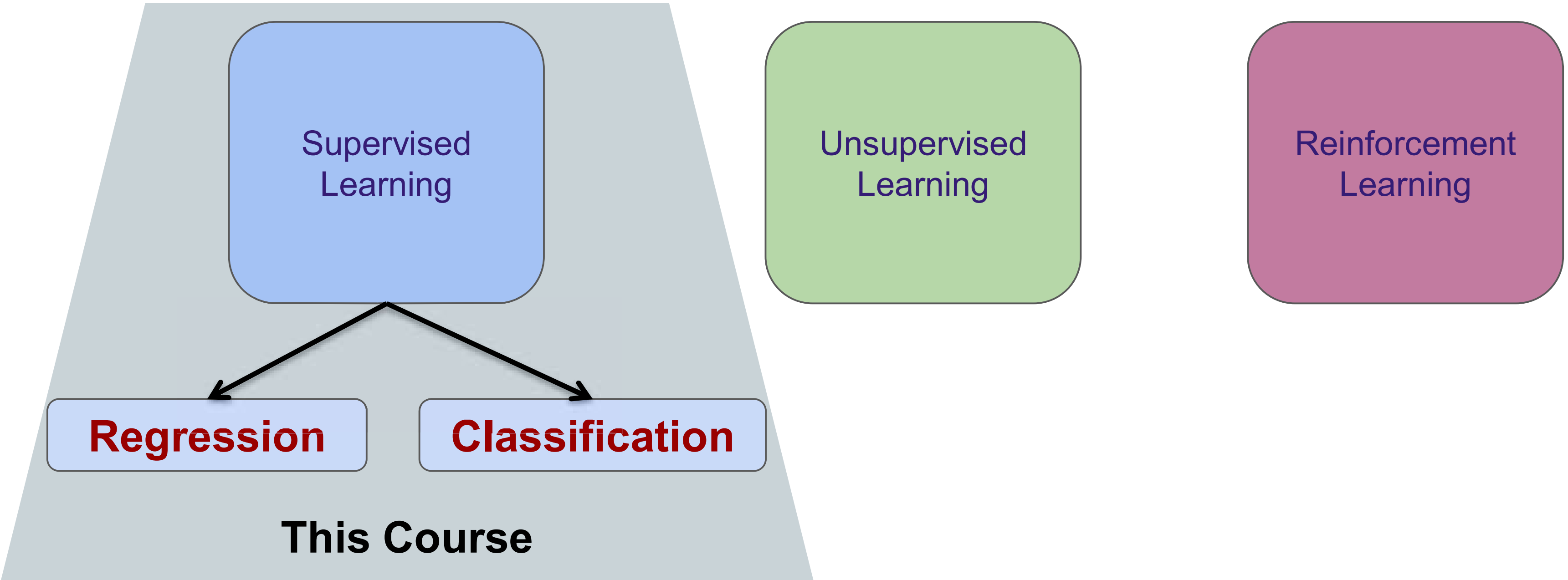
Course overview

1. Introduction to Classification
2. Linear Regression for Classification ?
3. Logistic Regression Model (Binary Classification)
    1. Logistic Regression Model
    2. Logistic Regression Cost function
4. Multi-Class Logistic Regression
5. Evaluating Classifiers
6. Cross Validation

Reminder of Machine Learning Types

- Machine learning tasks are typically classified into **three broad categories**

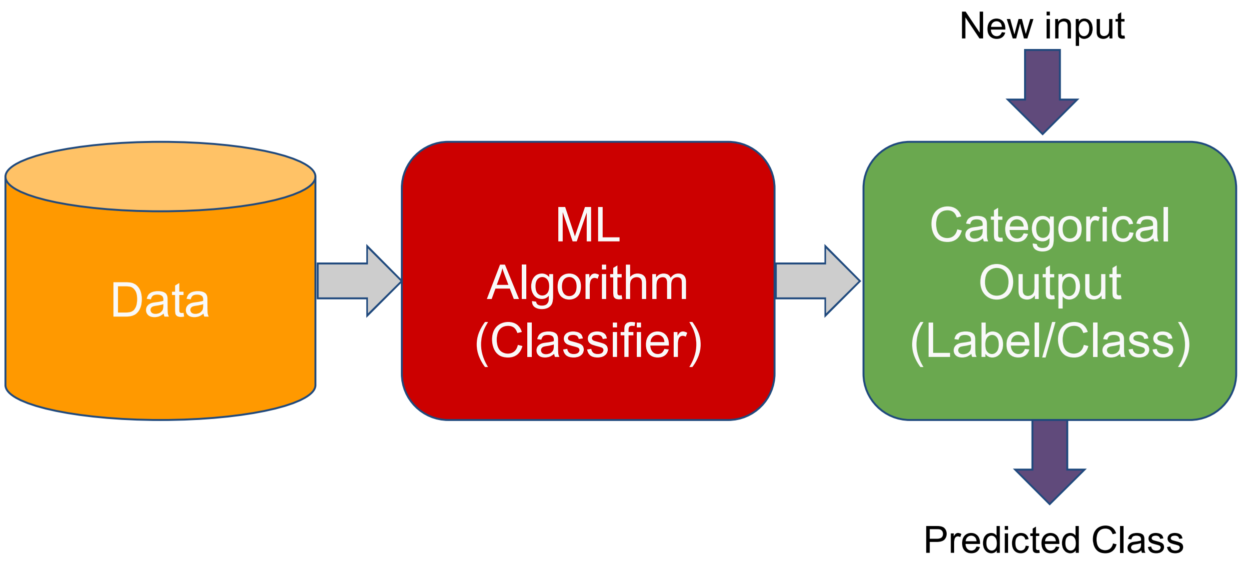


3.1
Introduction to Classification

Classification

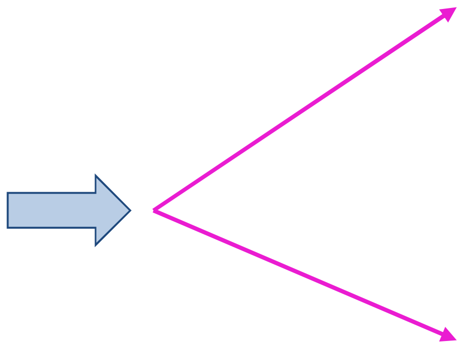
- **Goal:** Inputs are divided into two or more classes, and the ML algorithm must produce a model that assigns unseen inputs to one or more of these classes

- An algorithm that implements classification is known as a **classifier**



Two-class(Binary) Classification

- **Emails type:** Output y has 2 categories



Spam

Not-spam

Input: x

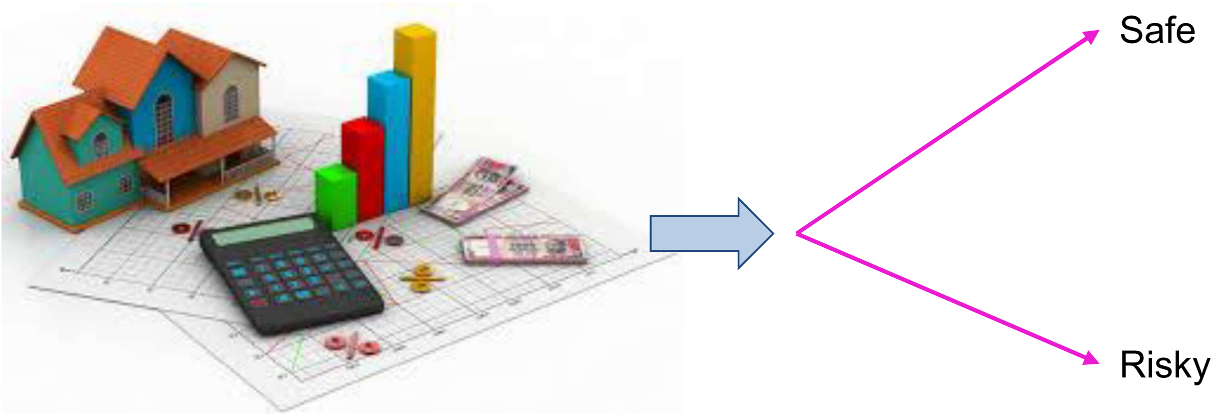
Mail sender, subjet, keywords, etc…

Output: y

Email type

Two-class(Binary) Classification

- **Loan demand:** Output y has 2 categories



Input: x

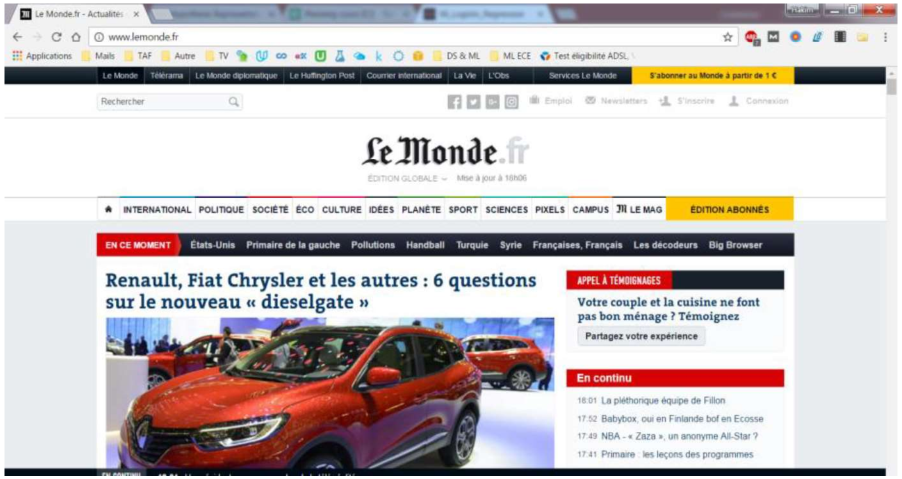
Client's characteristics
(age, Revenue, credit, etc..)

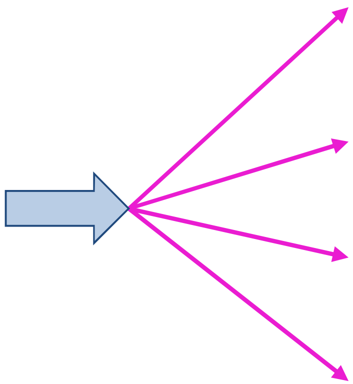
Output: y

Loan safety evaluation

Multi-class Classifier

- **News :** Output y has more than 2 categories





Sport

Education

Technology

Art

Input: x

Webpage: title, keywords, etc..

Output: y

News category

Multi-class Classifier

- **Weather:** Output y has more than 2 categories

Input: x

Altitude, region, date, etc…

Output: y

Weather status

Classification Algorithms

Linear Classifiers

Logistic Regression
Naive Bayes classifier
Linear discriminant

Support vector machines

Decision Trees

Random Forests

Boosting

Quadratic Classifiers

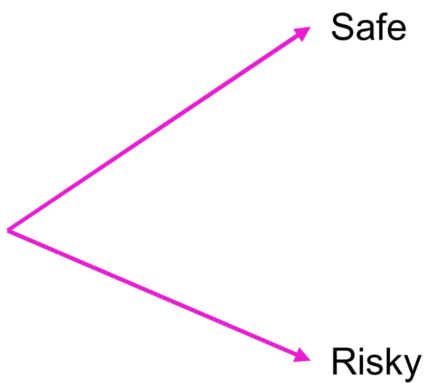
Neural Netwoks

K-nearest neighbor

Classification problem example

Can Linear Regression help ?

- Classification problem: Loan demand safety ?



Input: x
Client's characteristics
(age, Revenue, charges, etc..)

Output: y
Loan safety evaluation

Can Linear Regression help ?

- The classification problem is just like the regression problem
- Except that the **y values** to be predicted are discrete values.
  - Example: Loan demand evaluation: Safe or risky ?

Age	Revenue	Charges	...	Loan safety
20	1200	500	...	**0**
23	1700	450	...	**0**
25	1900	400	...	**0**
27	2000	450	...	**0**
40	2500	250	...	1
42	2750	200	...	1
45	2750	300	...	1
47	3000	100	...	1
x_1	x_2	x_3		y

?

Age	Loan safety
20	0
23	0
25	0
27	0
40	1
42	1
45	1
47	1
x	y

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

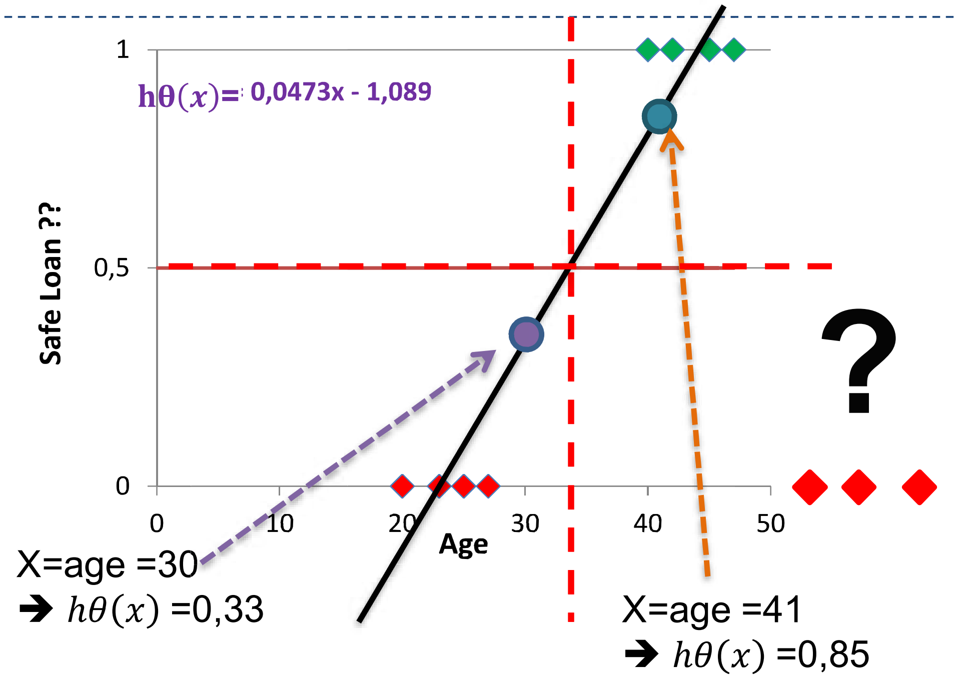
➔ y = 1: Positive Class **Safe**
➔ y = 0: Negative Class **Risky**

3.2
Linear Regression for classification ?

Can Linear Regression help ?

- One method is to use linear regression

x	y
Age	Loan safety
20	0
23	0
25	0
27	0
40	1
42	1
45	1
47	1

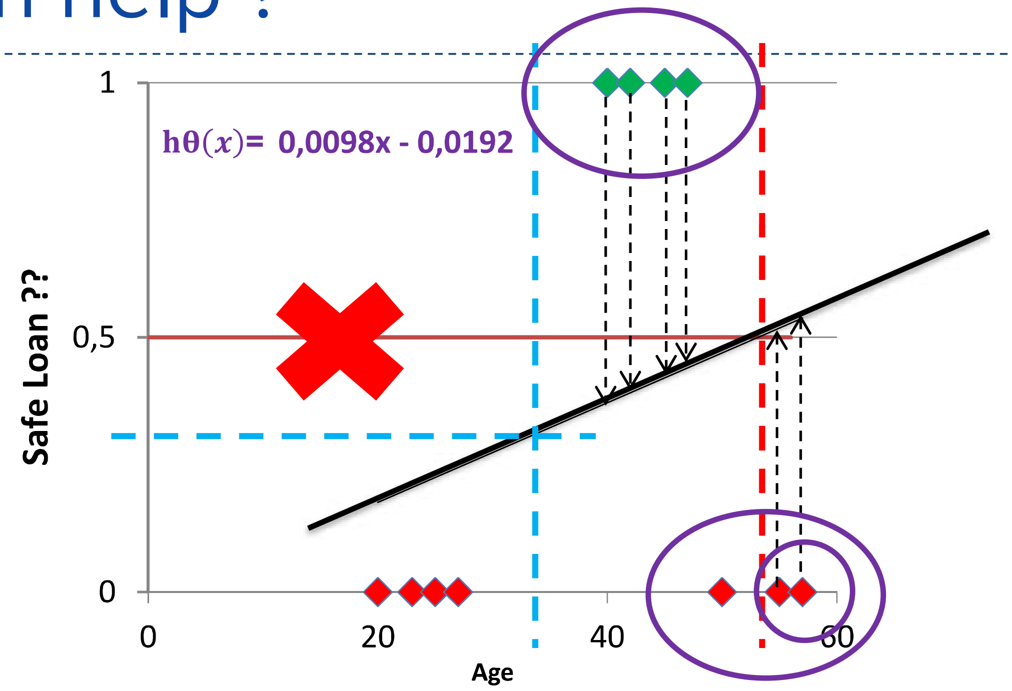


- Map all predictions greater than 0.5 as a 1 and all less than 0.5 as a 0
- Threshold classifier output $h\theta(x)$ at 0.5 :
  - if $h\theta(x) \geq 0{,}5$ ➔ predict: y="1"
  - if $h\theta(x) < 0{,}5$ ➔ predict: y="0"

Can Linear Regression help ?

- Linear Regression can sometimes be lucky ....but it is often not useful for classification problems

1st



- Another problem: is that classification need categorical values:
  - $y = 0 \text{ or } 1$
  - But with LR: $h_\theta(x)$ can be > 1 or < 0

2nd

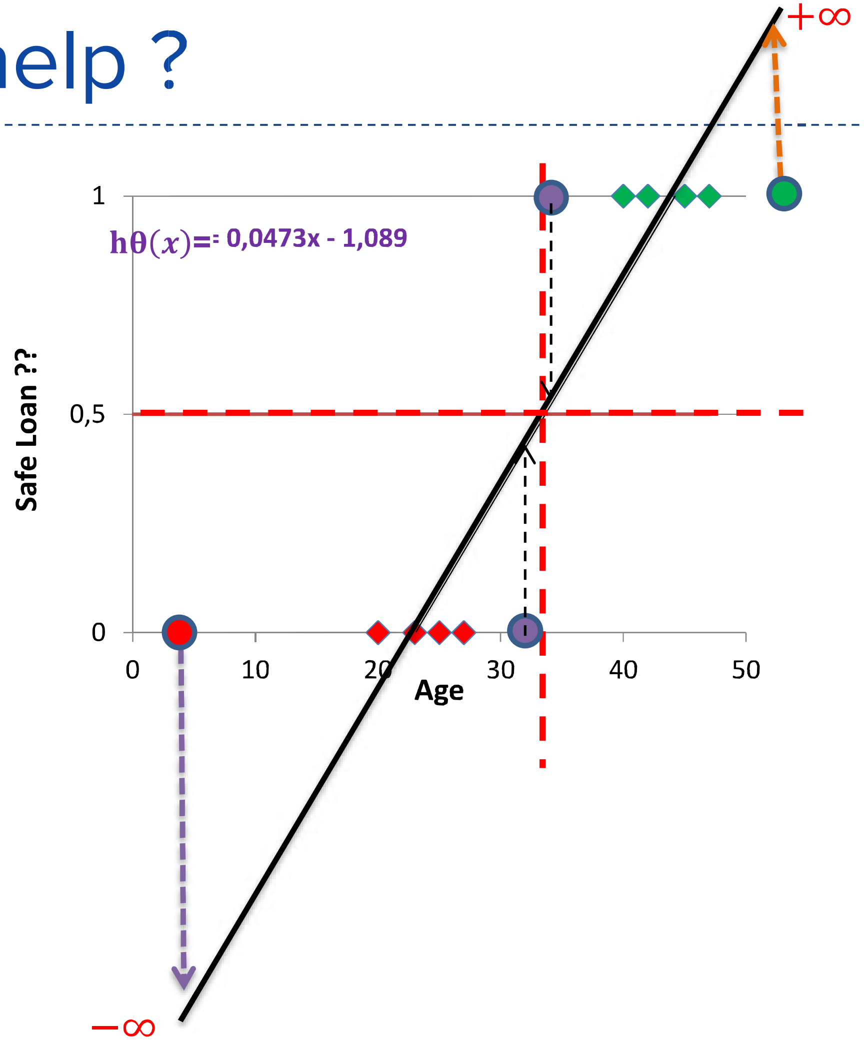
Can Linear Regression help ?

- How the model behaves with extreme points?
  - Certain predictions
- And with middle points ?
  - Not very certain

- **We need to know how confident our prediction is**

3rd

- Need for another Linear Classifier !!
  ➔ **Logistic Regression** $0 \leq h_\theta(x) \leq 1$

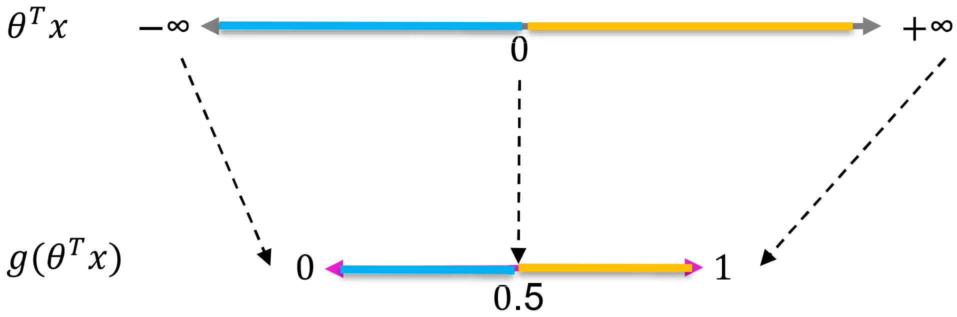


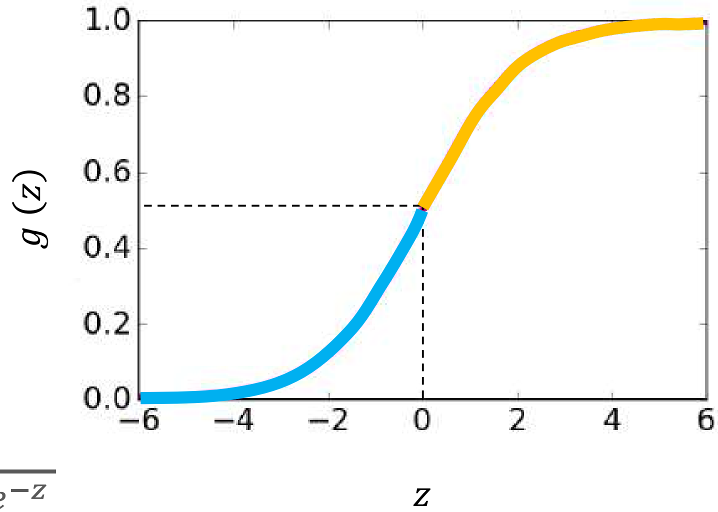
3.3
Logistic Regression

3.3.1 Logistic Regression intuition

Logistic Regression Model

- Change the form for our hypotheses $h_\theta(x) = \theta^T x$ to satisfy $0 \le h_\theta(x) \le 1$





- Use the Sigmoid / Logistic Function : $g(z) = \dfrac{1}{1+e^{-z}}$

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

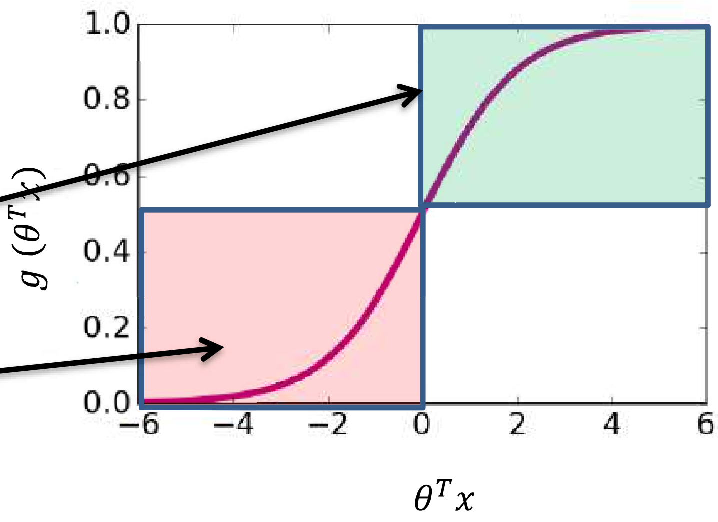
Interpretation of $h_\theta(x) = g\ (\theta^T x)$

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

- $h_\theta(x)$ = **estimated probability that y = 1** given the input x parameterized by θ
  - Example: $h_\theta(x)$= 0,8 ➔ The probability that the loan is safe (y=1) is equal to 80%

- $h_\theta(x) = \mathrm{P}(\mathrm{y} = 1 |\ \mathrm{x}; \theta) = 1 - P(\mathrm{y} = 0 |\ \mathrm{x}; \theta)$
- $\mathrm{P}(\mathrm{y} = 1 |\ \mathrm{x}; \theta) + P(\mathrm{y} = 0 |\ \mathrm{x}; \theta) = 1$

- Hypothesis:
  - ❑ $y = 1\ when\ g(\theta^T x) \geq 0{,}5$ ➔ $\theta^T x \geq 0$
  - ❑ $y = 0\ when\ g(\theta^T x) < 0{,}5$ ➔ $\theta^T x < 0$

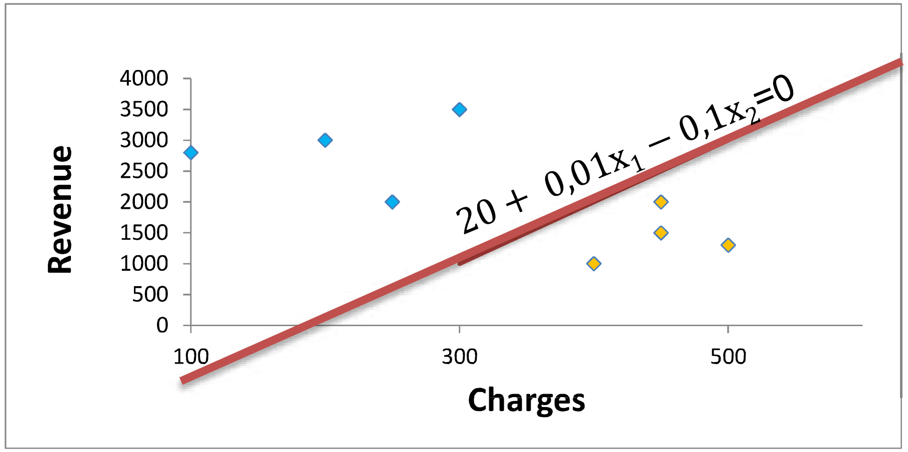


Decision Boundary

- Example: Loan demand evaluation model
  - Predict the loan safety class given the revenue and the charges values
  - $h_\theta(x) = g\,(\theta_0 + \theta_1 \mathrm{x}_1 + \theta_2 \mathrm{x}_2) = \mathrm{g}\,(20 + 0{,}01\ \#\mathrm{revenue} - 0{,}1\#\mathrm{charges})$

- Predict **1** : if $g(\theta^T x) \geq 0{,}5$ ➔ $\theta^T x \geq 0$
  - if $g\,(20 + 0{,}01\mathrm{x}_1 - 0{,}1\mathrm{x}_2) \geq 0.5$
  - $\Rightarrow 20 + 0{,}01\mathrm{x}_1 - 0{,}1\mathrm{x}_2 \geq 0$

- Predict **0** : if $g(\theta^T x) < 0{,}5$ ➔ $\theta^T x < 0$
  - if $g\,(20 + 0{,}01\mathrm{x}_1 - 0{,}1\mathrm{x}_2) < 0.5$
  - $\Rightarrow 20 + 0{,}01\mathrm{x}_1 - 0{,}1\mathrm{x}_2 < 0$



- $20 + 0{,}01\mathrm{x}_1 - 0{,}1\mathrm{x}_2$=0 is our decision boundary

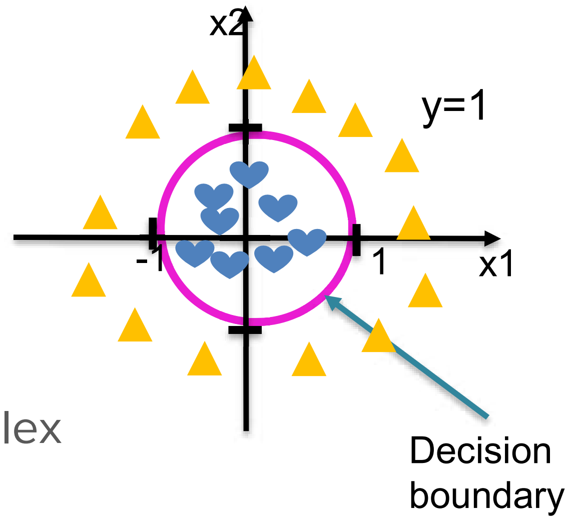
Decision Boundary

- Example: Loan demand evaluation model
- Predict the loan safety class given the revenue and the charges values
  - $h_\theta(x) = g\ (\theta_0 + \theta_1 \mathrm{x}_1 + \theta_2 \mathrm{x}_2) = \mathrm{g}\ (20 + 0{,}01\ \#\mathrm{revenue} - 0{,}1\#\mathrm{charges})$

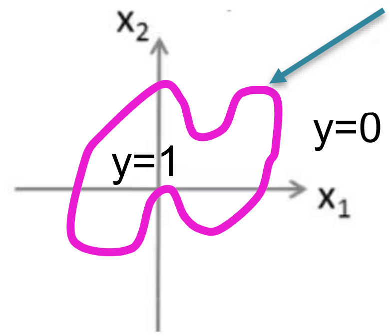
Charges	Revenue	$\theta^T x$	$g(\theta^T x)$	Safe loan ? (prediction)
500	1300	-17	4,14E-08	0
450	1500	-10	4,54E-05	0
400	1000	-10	4,54E-05	0
450	2000	-5	6,69E-03	0
250	2000	15	1,00E+00	1
200	3000	30	1,00E+00	1
300	3500	25	1,00E+00	1
100	2800	38	1,00E+00	1
450	2700	2	0,880797	1

Non-linear decision boundaries

- Example: $h_\theta(x) = g\,(\theta_0 + \theta_1 x_1 + \theta_2 x_2 + \theta_3 x_1{}^2 + \theta_4 x_2{}^2)$
  - $\theta = [-1, 0, 0, 1, 1]$
  - Predict 1 if $-1 + x_1{}^2 + x_2{}^2 \geq 0 \Rightarrow x_1{}^2 + x_2{}^2 \geq 1$
  - Predict 0 if $-1 + x_1{}^2 + x_2{}^2 < 0 \Rightarrow x_1{}^2 + x_2{}^2 < 1$



- As with polynomial regression, we can have more complex decision boundaries by adding higher polynomial terms
- $h_\theta(x) = g\,(\theta_0 + \theta_1 x_1 + \theta_2 x_2 + \theta_3 x_1{}^2 + \theta_4 x_2{}^2 + \theta_5 x_1{}^3 + \theta_6 x_2{}^3)$



3.3.2
Cost Function (1)

Cost Fuction 1: Intuition

- Quality Metric

Real Data

Charges	Revenue	$\theta^T x$	Safe loan ?
100	2800	38	**1**

Charges	Revenue	$\theta^T x$	Safe loan ?
450	1500	-10	**0**

Predictions ?

A good model must predict: 1

A good model must predict: 0

Pick θ to maximize:
$P(y = 1 | x; \theta)$

That is
$P(y = 1 | x1 = 100, x2 = 2800; \theta)$

Pick θ to maximize:
$P(y = 0 | x; \theta)$

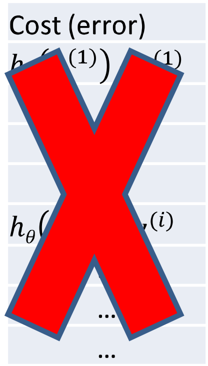
That is
$P(y = 0 | x1 = 450, x2 = 1500; \theta)$

Cost Fuction 1: Intuition

- Cost function for Linear regression

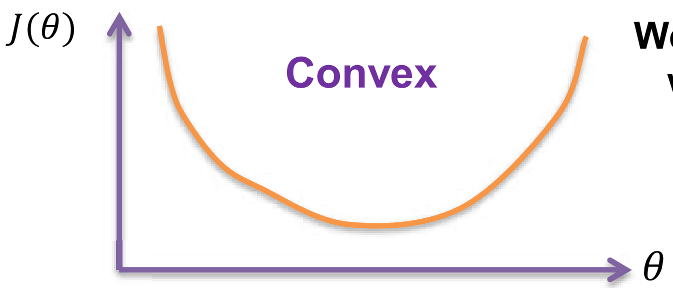
$$J(\theta_0, \theta_1, \ldots, \theta_n) = \frac{1}{2m}\sum_{i=1}^{m}(h_\theta(x^{(i)}) - y^{(i)})^2$$

Charges	Revenue	$\theta^T x$	y =Safe loan (real)	predicion
500	1300	-17	0	0
450	1500	-10	0	0
400	1000	-10	0	0
450	2000	-5	0	1
250	2000	15	1	1
200	3000	30	1	1
300	3500	25	1	0
100	2800	38	1	1

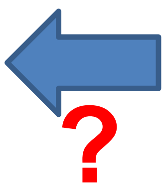


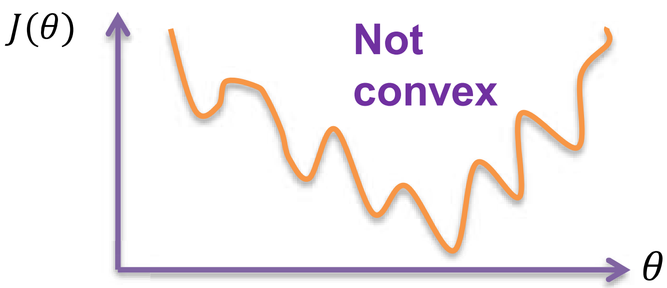
$$\frac{1}{1 + e^{-\theta^T x}}$$

Not linear



We need a cost fucntion with a convex shape





Cost Fuction 1: Intuition

- Cost function for Logistic regression model

Charges	Revenue	$\theta^T x$	y =Safe loan (real)	predicion	Cost (error)	
500	1300	-17	0	0	$\text{Cost}(h_\theta(x^{(1)}), y^{(1)})$	Cost= 0
450	1500	-10	0	0	...	Cost= 0
400	1000	-10	0	0	...	
450	2000	-5	0	1	...	**Impose high penalties (costs)**
250	2000	15	1	1	$\text{Cost}(h_\theta(x^{(i)}), y^{(i)})$	
200	3000	30	1	1	...	
300	3500	25	1	0	...	
100	2800	38	1	1	...	Cost= 0

Cost Fuction 1: Intuition (for one data point)

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

Predicted value Real value

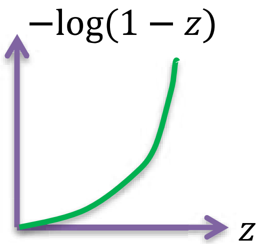
- $\boxed{\textbf{If } y = 0 : \mathrm{Cost}(h_\theta(x), y) = -(1-y) * \log(1-h_\theta(x))}$ $\boxed{\textbf{If } y = 1 : \mathrm{Cost}(h_\theta(x), y) = -(y) * \log(h_\theta(x))}$

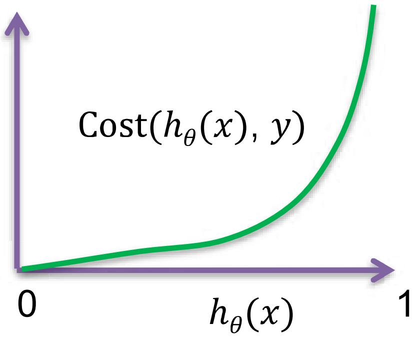
$h_\theta(x) = 0 \Rightarrow \mathrm{Cost}(h_\theta(x), y) = 0$

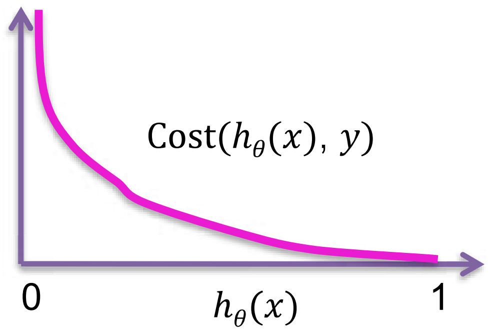
$h_\theta(x) = 1 \Rightarrow \mathrm{Cost}(h_\theta(x), y) = \infty$ High penalty

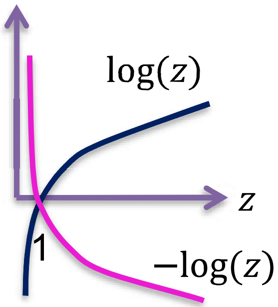
$h_\theta(x) = 1 \Rightarrow \mathrm{Cost}(h_\theta(x), y) = 0$

$h_\theta(x) = 0 \Rightarrow \mathrm{Cost}(h_\theta(x), y) = \infty$ High penalty









Cost Fuction 1: Intuition (for all data points)

- For one data point: $\mathrm{Cost}(h_\theta(x), y) = -(y) * \log(h_\theta(x)) - (1-y) * \log(1 - h_\theta(x))$

- For all data points: $J(\boldsymbol{\theta}) = \sum_{i=1}^{m} \mathrm{Cost}(h_\theta(x), y)$

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

- To find the optimal values of $\boldsymbol{\theta}$: $\min_{\theta} J(\boldsymbol{\theta})$

- Gradien descent:
  - Initiate with a random set of values for θ
  - At each iteration: update the values of $\boldsymbol{\theta}$
  - For each feature x_j ,$\theta_j = \theta_j - \alpha \sum_{i=1}^{m} (h_\theta\left(x^{(i)}\right) - y^{(i)}).x_j^{(i)}$

3.3.2
Cost Function (2)

Cost Fuction 2: Maximum-Likelihood

- Quality Metric

Real Data

Charges	Revenue	$\theta^T x$	Safe loan ?
100	2800	38	**1**

Charges	Revenue	$\theta^T x$	Safe loan ?
450	1500	-10	**0**

Predictions ?

A good model must predict: 1

A good model must predict: 0

Pick θ to maximize:
$$P(y = 1 |\, x; \theta)$$

That is
$$P\left(y = 1 \,\middle|\, x1 = 100, x2 = 2800;\ \theta\right)$$

Pick θ to maximize:
$$P(y = 0 |\, x; \theta)$$

That is
$$P\left(y = 0 \,\middle|\, x1 = 450, x2 = 1500;\ \theta\right)$$

Cost Fuction 2: Maximum-Likelihood

- Quality Metric: Maximizing likelihood, i.e the probability of good predictions

Charges	Revenue	$\theta^T x$	y =Safe loan	Choose θ to maximize
500	1300	-17	0	$\mathrm{P}(\mathrm{y}=0 \mid \mathrm{x}; \theta)$
450	1500	-10	0	$\mathrm{P}(\mathrm{y}=0 \mid \mathrm{x}; \theta)$
400	1000	-10	0	$\mathrm{P}(\mathrm{y}=0 \mid \mathrm{x}; \theta)$
450	2000	-5	0	$\mathrm{P}(\mathrm{y}=0 \mid \mathrm{x}; \theta)$
250	2000	15	1	$\mathrm{P}(\mathrm{y}=1 \mid \mathrm{x}; \theta)$
200	3000	30	1	$\mathrm{P}(\mathrm{y}=1 \mid \mathrm{x}; \theta)$
300	3500	25	1	$\mathrm{P}(\mathrm{y}=1 \mid \mathrm{x}; \theta)$
100	2800	38	1	$\mathrm{P}(\mathrm{y}=1 \mid \mathrm{x}; \theta)$

- Maximize function over all possible $\theta_0, \theta_1, \theta_2$:

$$\max_{\theta_0,\theta_1,\theta_2} \prod_{i=0}^{m} \mathrm{P}(\mathrm{y}_i \mid \mathrm{x}; \theta)$$

3.4
Multiclass classification

Multi-class Classification: Example

- **Image labelling**

dog 0.997… | pet 0.992… | canine 0.991…
mammal 0.990… | cute 0.990…
puppy 0.989… | animal 0.989…
grass 0.988… | breed 0.965…
purebred 0.959… | adorable 0.956…
pedigree 0.956… | little 0.955…

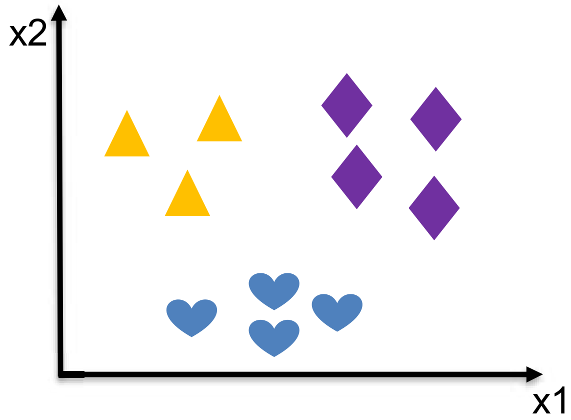
Input: x
Image pixels

Output: y
Object in image

Multi-class Classification: Formulation

- C possible classes: y can be 1, 2,..., C
- m data points

Data point	x_1	x_2	y
$x^{(1)}, y^{(1)}$	1	4	$\blacktriangle$
$x^{(2)}, y^{(2)}$	3	1	$\heartsuit$
$x^{(3)}, y^{(3)}$	3	3	$\blacklozenge$
$x^{(4)}, y^{(4)}$	4	4	$\blacklozenge$
………..			



Learn:

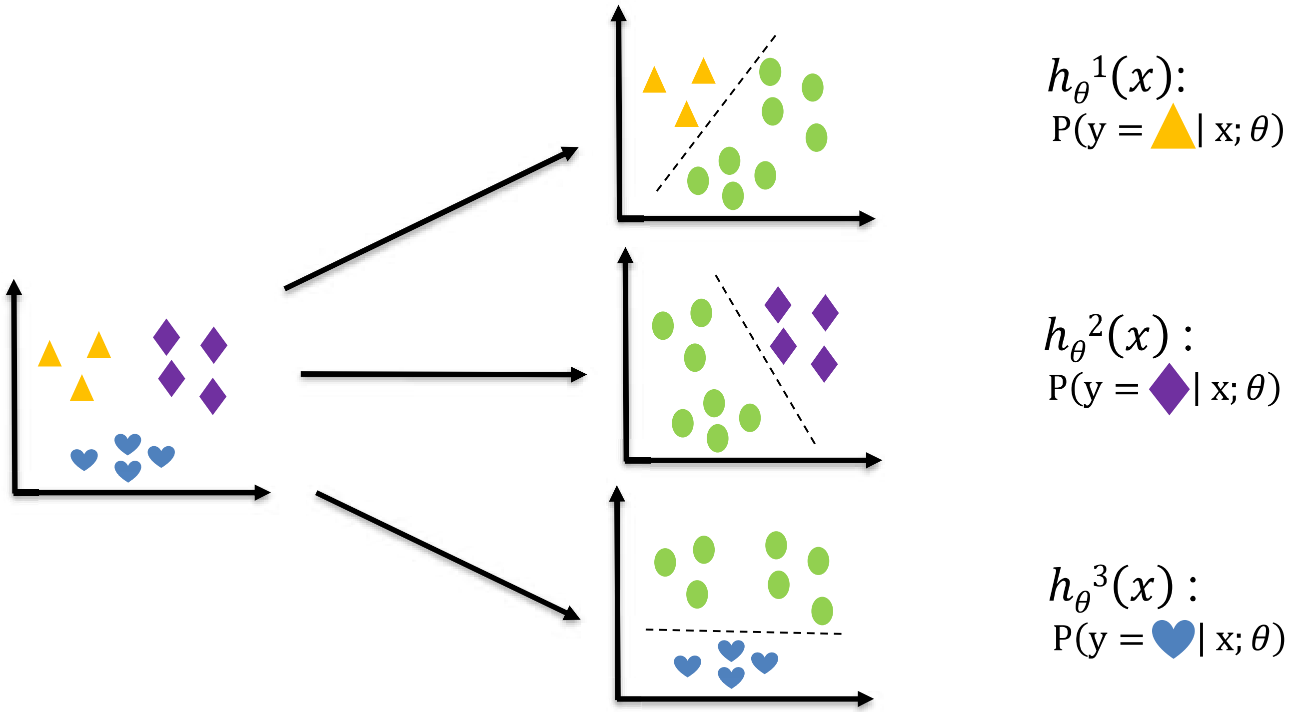
$P(y = \blacktriangle \mid x; \theta)$

$P(y = \heartsuit \mid x; \theta)$

$P(y = \blacklozenge \mid x; \theta)$

Multi-class Classification: One-vs-all (one-vs-rest)

- Transform the original classification model to C 2-class models



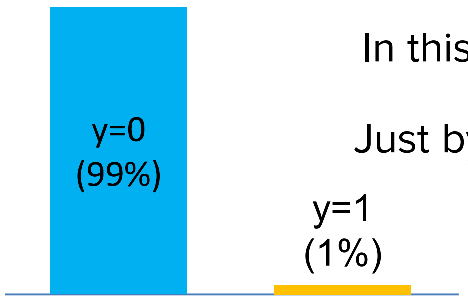
- On a new input, to make a prediction, pick the class that maximizes: $max_i \; h_\theta{}^i(x)$

3.5
Evaluating classifiers

Evaluating classifiers: Accuracy

- Accuracy = $\frac{number\ of\ data\ points\ classified\ correctly}{all\ data\ points}$

- is 99% accuracy good?
  - Can be excellent, good, mediocre, poor, terrible
  - It depends on the proportion of the classes in your dataset.



In this example, 99% od the data is labeled as the negative class.

Just by predicting everything to y = 0, we can have an accuracy of 99%

- Accuracy is not ideal for skewed (imbalanced) classes !!

Evaluating classifiers: Confusion matrix

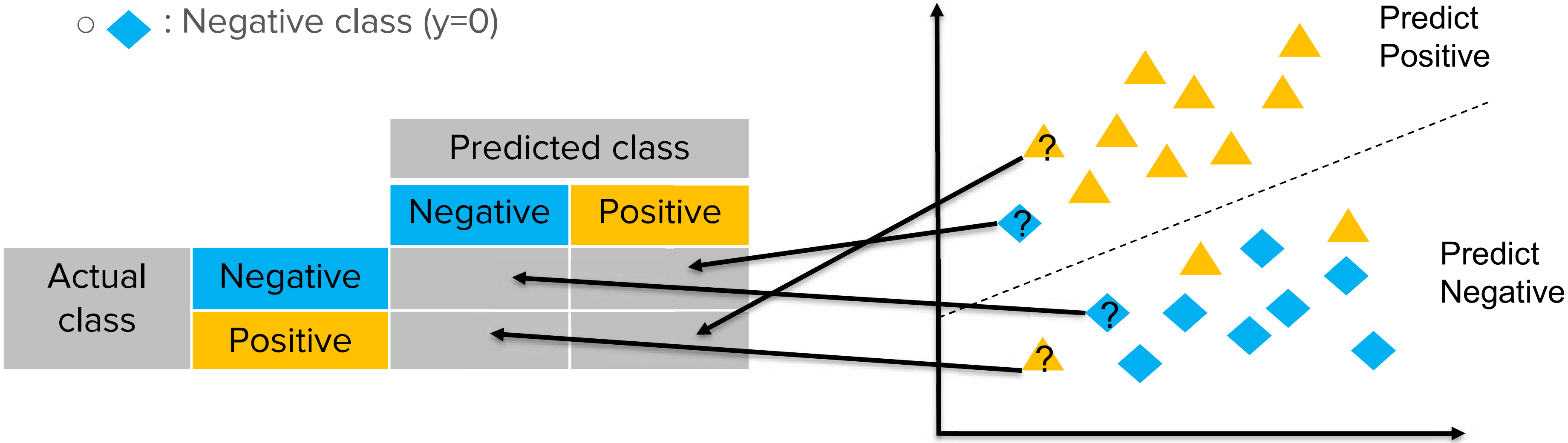
- In many cases in real life problems, you care more about well predicting one class than the others:
  - Cancer detection: care more about cancer gets detected. You can tolerate occasionally false detections but not overlooking real cancers.

Y = 0 (no cancer)	You can tolerate having errors when predicting this class: predict patient has cancer when it's not the case
Y = 1 (cancer)	You can not tolerate having errors when predicting this class: predict patient has no cancer when it's the case

- There is a need for a performance metric that can favor one type of an error than an other.

Evaluating classifiers: Confusion matrix

- We have two classes:
  - : positive class (y = 1)
  - : Negative class (y=0)

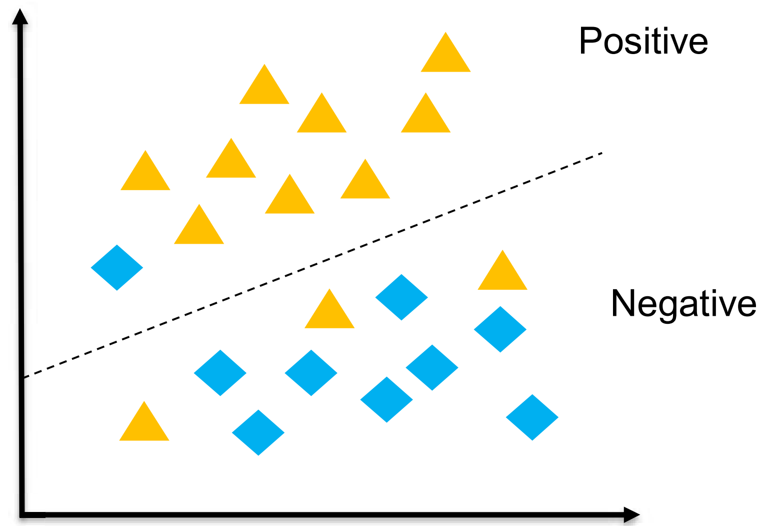


- Match each data point to the appropriate cell

Evaluating classifiers: Confusion matrix

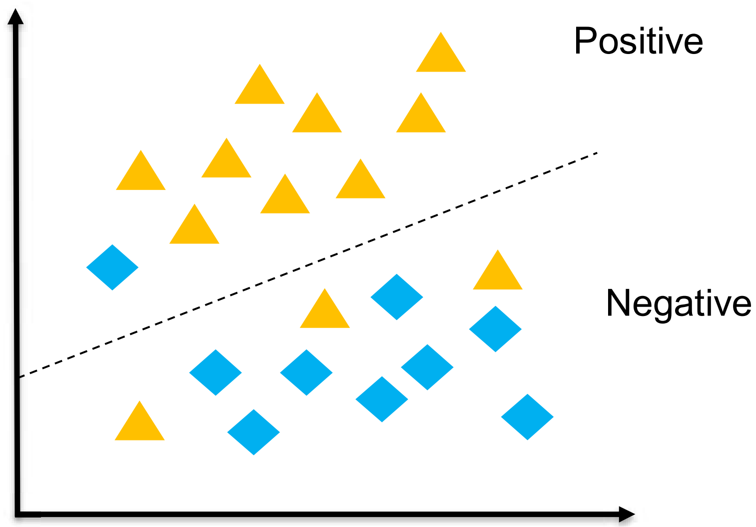
- Fill the cells with the corresponding numbers
  - : positive class (y = 1)
  - : Negative class (y=0)

		Predicted class	
		Negative	Positive
Actual class	Negative	?	?
	Positive	?	?



Evaluating classifiers: Confusion matrix

		Predicted class	
		Negative	Positive
Actual class	Negative	True Negative	False Positive
	Positive	False Negative	True Positive



- Sklearn: http://scikit-learn.org/stable/modules/generated/sklearn.metrics.confusion_matrix.html

Evaluating classifiers: Precision - Recall

		Predicted class	
		Negative	Positive
Actual class	Negative	True Negative	False Positive
	Positive	False Negative	True Positive

- Precision for the positive class answers the following question:
- Out of all the examples the classifier labeled as positive, what fraction were correct?

- Precision = $\frac{True\ positive}{True\ positive + False\ positive} = \frac{9}{9+1} = 90\%$

Evaluating classifiers: Precision - Recall

		Predicted class	
		Negative	Positive
Actual class	Negative	True Negative	False Positive
	Positive	False Negative	True Positive

- Recall for the positive class answers the following question :
- Out of all the positive examples there were, what fraction did the classifier pick up?

- Recall = $\frac{True\ positive}{True\ positive + False\ negative} = \frac{9}{9+3} = 75\%$

Evaluating classifiers: F1 score

- Given the nature of the problem, you can optimize the model to get a better precision or a better recall.

- It is possible to optimize both by combining precision and recall into a single value, called **F1 score**.

- $F1\ score = 2 * \frac{precsion\ *recall}{precision + recall} = 81.81\%$

- Best value at 1, worse at 0.

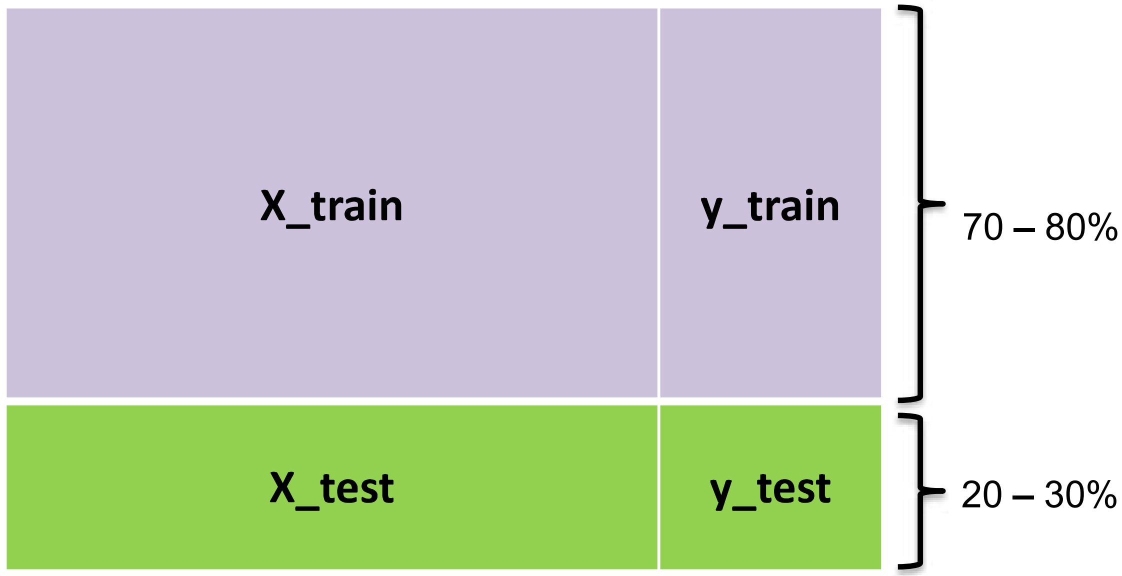
3.6
K-fold
cross-validation

Cross-Validation: Why ?

- **Data = Training set + Testing set**

One-round Cross Validation

We need to derive the most accurate estimate of model prediction performance !!!

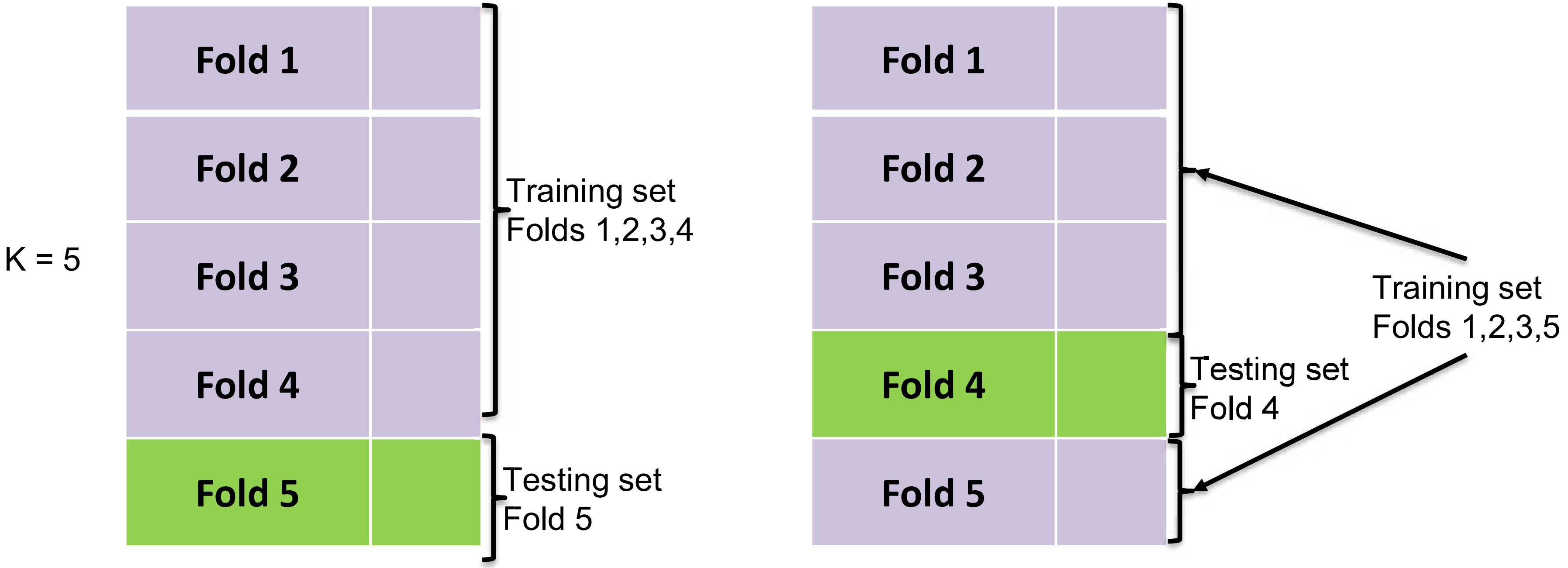


Gives an insight on how the model will generalize to an independent dataset

- Each data point is used only once for training or for testing
- Variability may arise !!
- Moreover: Sometimes we do not have enough data available to make reliable partitions

Cross Validation example: K-fold

- Partition the dataset into **K** folds (bins) of equal size.



- for each k = 1, 2, . . . K, fit the model to the other K − 1 parts and compute its error in predicting the k^{th} part.

Cross Validation example: K-fold

- Run **K** separate learning experiments.
  - Pick testing set
  - Train
  - Test on testing test and compute performance
    - Example: Linear Regression : R^2 , Logistic Regression: Accuracy

- Average the performance from those **K** experiments

- Typically, K=5 or 10

- K-Fold is more robust for parameter tuning (choose the regularization parameter, the learning rate, ..)

More about Cross-Validation

- Multiple rounds of cross-validation are performed using different partitions, and the validation results are averaged over the rounds

- Common Types of Cross-Validation:
  - Non-exhaustive cross-validation
    - *k*-fold cross-validation
    - 2-fold cross-validation

  - Exhaustive cross-validation
    - Leave-p-out cross-validation
    - Leave-one-out cross-validation

Thank you for your attention