

# Naive Bayes and Decision Trees

Alipio Jorge (DCC-FCUP)

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# Classification

*The credit office of the bank now has to decide whether to give the loan or not to a specific client. Management feels that the current credit decision procedure is not efficient and that the bank can make more money and secure more good clients with a better process. The bank has an historical record of loans. Some were conceded and went well. Other were not conceded or had a bad outcome.*

- What is the business problem?
- The machine learning problem?
- What kind of **task** is it?

# Classification: types

- Decide if a new case belongs to a set of known classes
- a type of **supervised learning**
- **Binary classification**
  - Bank credit
  - Has cancer
  - This email is spam
  - Is the market going up or down tomorrow?
- **Multiclass**
  - Which disease does the patient have
  - Which folder for this email
  - What is the type of galaxy in this image

# Classification: process

- The Process (simplified CRISP)
  - Define problem
  - Prepare data
  - Build model (**classifier**) by applying a **learning algorithm**
  - Evaluate model
  - Deploy

# Classification: setup

- The data (most common setup)
  - **Examples** are pairs  $\langle x, y \rangle$ , also called **tuples**
    - $\langle x, y \rangle \in D$  where  $D$  is the **dataset**
    - $x_i$  is one row of of a  $n \times m$  table  $X$
    - The dimensions / columns of  $X$  are the **attributes**
    - $y_i$  is the **class** of  $x_i$
    - $y_i \in Y = \text{Classes} = \{C_1, C_2, \dots, C_k\}$
    - $y_i$  also called **labels**

# Classification: aim

- The **aim** of classification
  - **Given** a dataset  $D$  of pairs  $\langle x, y \rangle$
  - **Obtain**
    - a function  $\hat{f} : X \rightarrow \text{Classes}$
    - such that  $\hat{f}$  **approximates** an unknown function  $f(x)$  that assigns labels to objects

# Classification: the Bayesian view

- How can  $\hat{f}(x)$  be found?
- Suppose
  - we have a **new case**  $x$  to classify
- We want the class  $C_{max}$  that maximises  $P(C_j | x)$ 
  - so, *all* we have to do is **estimate**  $P(C_j | x)$  for each class
- How?
  - lots of different ways
- A simple and **principled** one?
  - **Naive Bayes**

# Naive Bayes

- Bayes theorem:

$$P(C_j | x) = \frac{P(x | C_j) \cdot P(C_j)}{P(x)}$$

- The class  $C_{max}$  that maximises this is the **maximum posteriori hypothesis**
- How is this calculated?
  - we assume that  $P(x)$  is **constant**
  - we estimate  $P(C_j) = \frac{|x_i \in C_j|}{|D|}$  from the data
  - and estimate  $P(x | C_j)$  – this is **trickier**



# The Naive Bayes trick

- In general estimating  $P(x \mid C_j)$  is **hard**
  - data is **sparse**
  - approximations can be **computationally expensive**
- The **trick** is to naïvely assume
  - the attributes are **class-conditional independent**

$$P(A_i \mid C, A_j) = P(A_i \mid C)$$

# The Naive Bayes trick

- This assumption is **not realistic**
  - but it is **good enough** to make the approach useful
- This assumption greatly **simplifies** the computation

$$P(x \mid C_j) = \prod_{i=1}^n P(x_i \mid C_j)$$

- Now, each  $P(x_i \mid C_j)$  is easy to estimate - Besides, it is **well founded** - driven from **first principles** - not **ad hoc**

# How Naive Bayes works

- Estimate the probabilities of  $P(x_{i,A}|C)$  from example  $i$  and attribute  $A$ 
  - $A$  is **categorical**:
    - the number of tuples of class  $C$  with value  $x_{i,A}$  in  $A$
    - divided by the size of class  $C$
  - $A$  is **continuous**:
    - assume a **Gaussian distribution**
    - estimate mean and standard deviation from sample of each  $A$  for each class

## Naive Bayes: example

- The `german_credit_data.csv` in kaggle (adapted from UCI)
- predict **Risk** (classes good and bad)

```
import pandas as pd
d=pd.read_csv('../Dados/german_credit_data.csv')
d[['Age', 'Sex', 'Risk']]
```

	Age	Sex	Risk
0	67	male	good
1	22	female	bad
2	49	male	good
3	45	male	good
4	53	male	bad
5	35	male	good
6	53	male	good
7	35	male	good
8	61	male	good

## Naive Bayes: example

- $P(\text{Sex} = \text{male} \mid \text{Risk} = \text{good})$

```
freq_male_good=len(d[(d['Sex']=='male') & (d['Risk']=='good')])
freq_good=len(d[d['Risk']=='good'])
prob_male_good=freq_male_good/freq_good
prob_male_good
```

0.7128571428571429

## Naive Bayes: example

- $P(\text{Age} = 22 \mid \text{Risk} = \text{good})$

```
import numpy as np

mean_age_good=np.mean(d.loc[d['Risk']=='good',['Age']])
std_age_good=np.std(d.loc[d['Risk']=='good',['Age']])

from scipy.stats import norm

prob_22_good=norm.pdf((22-mean_age_good)/std_age_good)
prob_22_good

array([ 0.18248811])
```

## Naive Bayes: example

- $P(\text{Age} = 22 \mid \text{Risk} = \text{good}) \times P(\text{Sex} = \text{male} \mid \text{Risk} = \text{good})$ 
  - which is proportional to  $P(\text{Risk} = \text{good} \mid x)$

```
prob_male_good*prob_22_good
```

```
array([ 0.13008795])
```

- **Exercise:** write a python program that classifies any new case of this problem using Naive Bayes (without a predefined NB learner)

# Naive Bayes: implementations

- SciKitLearn
  - GaussianNB for continuous predictors
  - CategoricalNBfor categorical ones
  - and others...
- Mixed variables
  - MixedNB from mixed-naive-bayes library
    - not direct
  - other not so straight solutions
- One can always
  - Discretize continuous



# Does Naive Bayes have good results?

- **If assumptions hold** NB is **optimal in theory**
  - If we have **enough data** for good estimations
- **If not**
  - it can have **comparatively good results** in some domains
  - useful in **high dimensional** domains
  - there are methods that can **easily beat NB**

# Naive Bayes: further notes

- NB has little hyperparameters
- What if one of the probabilities is **zero**?
  - we can smooth probabilities using the correction of Laplace

$$P_{Laplace}(E) = \frac{E + \lambda}{N + k.\lambda}$$

- $\lambda$  typically is 1, and  $k$  is the number of values of  $E$ 
  - it is like always having one artificial observation per category
- A simple version of NB is easy to implement
  - see <https://towardsdatascience.com/introduction-to-na%C3%AFve-bayes-classifier-fa59e3e24aaf>

# Classification: Decision Trees

- **Where we are**

- We have seen how to approach **regression** problems using linear regression and the k-Nearest Neighbours (kNN) approach
- We have seen how to approach **classification** using kNN and naive Bayes

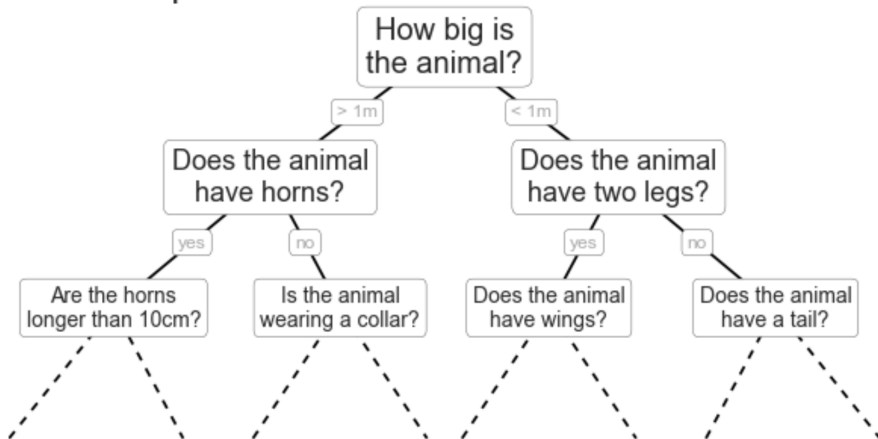
- **Next**

- we will study **Decision Trees**
  - versatile method
  - handles classification but can be adapted to regression
  - deals with different types of data
  - use a **search** procedure

# Decision Trees

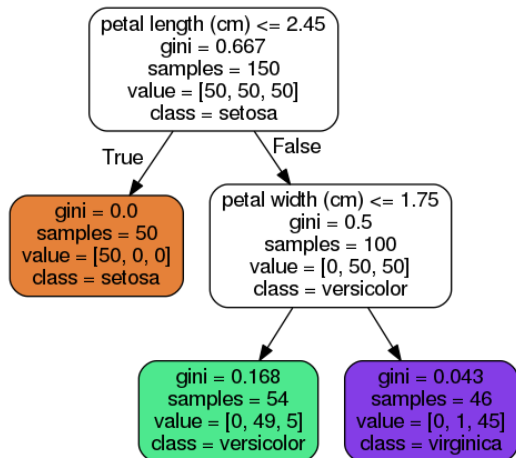
- The classification function  $\hat{f}$  can be implemented as a decision tree

## Example Decision Tree: Animal Classification

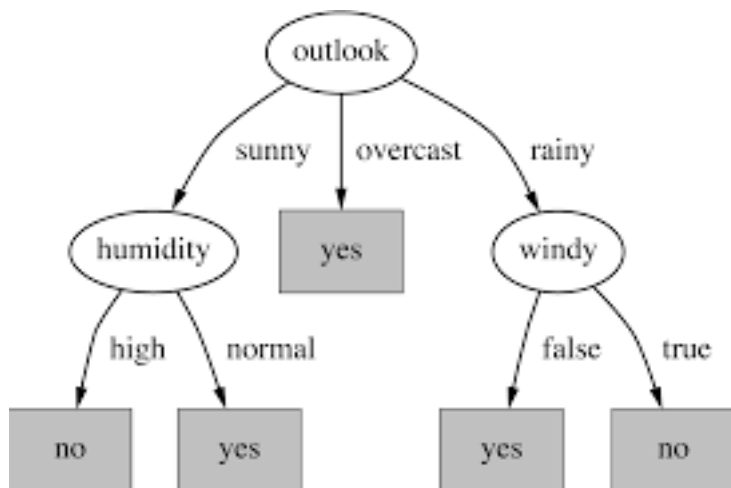


# Decision Trees

- We can obtain one for the iris classification problem



## Decision Trees: the golf example



# How are DT obtained?

- The **idea** is
  - start with all the examples
  - try to **divide** them in two or more groups where classes are as separated as possible
  - **repeat the process** recursively for each group
  - **until** all classes are separated in **small groups**
    - or the groups are too small
- This is called **TDIDT**: Top Down Induction of Decision Trees

## Let's try to do this with the golf data

```
golf=pd.read_csv('../Dados/golf_df.csv')  
golf
```

	Outlook	Temperature	Humidity	Windy	Play
0	sunny	hot	high	False	no
1	sunny	hot	high	True	no
2	overcast	hot	high	False	yes
3	rainy	mild	high	False	yes
4	rainy	cool	normal	False	yes
5	rainy	cool	normal	True	no
6	overcast	cool	normal	True	yes
7	sunny	mild	high	False	no
8	sunny	cool	normal	False	yes
9	rainy	mild	normal	False	yes
10	sunny	mild	normal	True	yes
11	overcast	mild	high	True	yes



# The golf data

- Looking at all the examples we have
  - 5 of class **no** and 9 of class **yes**
  - this is already a decision tree (with root only)
  - the majority class wins
- The separation of the classe is not very good, though

# The golf data

- Consider now splitting the group according to **Outlook**
  - Outlook has three values
    - **sunny**: (3 no, 2 yes)
    - **rainy**: (2, 3)
    - **overcast**: (0, 4)
  - this gives one **pure** group
    - better than before
    - if overcast we go play

# The golf data

- Is Outlook the best attribute for **splitting**?
  - we have to check with all the attributes
- for now, we will believe it is

# The golf data

- Now we try to refine each of the not pure **nodes of the tree**
  - Outlook=sunny
    - Humidity=normal: (0,2)
    - Humidity=high: (3,0)
  - Outlook=rainy
    - Windy=True: (2,0)
    - Windy=False: (0,3)
  - And we end up with a tree that completely separates the classes
    - all **leaves** are pure (one class only)

# The golf data

- From the tree we can obtain the **rules**
  - IF Outlook = overcast THEN Play=yes
  - IF Outlook = sunny AND Hum = normal THEN Play=yes
  - IF Outlook = sunny AND Hum = high THEN Play=no
  - IF Outlook = rainy AND Windy = True THEN Play=no
  - IF Outlook = rainy AND Windy = False THEN Play=yes
  - Each rule corresponds to a **branch** of the tree

# The golf data

- In the **real world**
  - leaves are not pure
  - datasets have continuous attributes as well
- However, Decision Trees
  - can be useful with real data
  - are human **readable**
  - can be combined in **ensembles** with success

# Top Down Induction of Decision Trees

- Selecting the best **split** for each node
- Given attribute  $A$  with values  $v_1, \dots, v_m$ 
  - Calculate **Information Gain** of  $A$
  - measure inspired in information theory

# TDIDT: selecting attributes

- How many bits do we need to represent the classes of the examples in a data set  $D$ ?
  - we have  $k$  classes
  - if they are uniformly distributed, *Entropy* is the highest
  - if all the cases are on one class, *Entropy* is **zero**

$$Entropy(D) = - \sum_{i=1}^k p_i \log_2(p_i)$$

- Suppose we have 4 classes
  - then we need **two bits** to transmit the label of each example
  - $-0.25 \times \log_2(0.25) = 0.5$
  - $0.5 \times 4 = 2$



## TDIDT: selecting attributes

- Now we **choose** the attribute that minimizes *Entropy*
- How do we measure it after a split?
  - we sum the entropies of each resulting group

$$Entropy_A(D) = \sum_{j=1}^m \frac{|D_j|}{|D|} \times Entropy(D_j)$$

## TDIDT: selecting attributes

- The best attribute is the one that maximizes the **Information Gain**

$$Gain(A) = Entropy(D) - Entropy_A(D)$$

# TDIDT: Gain Ratio and the Gini Index

- Information Gain **favours attributes** with many values
  - Dividing in more groups leads more easily to **pure groups**
  - the solution is to use the **Gain Ratio** instead
  - this ratio “discounts” the existence of many values
- Another measure of Attribute split quality
  - the **Gini Index**
  - can be used instead of the information gain

# Continuous attributes

- A categorical attribute has natural splits
  - Overcast=sunny, Overcast=rainy, Overcast=overcast
- What are the splits of a **continuous attribute** ?
  - Age<30, Age<44

Age	Risk
23	good
25	good
35	bad
43	bad
45	good
49	good

# Tree Pruning

- Trees can easily **overfit**
  - imagine a tree with one example in each leave
- It is often a good idea to **prune** the tree
  - cut some extremities of the branches
- **Prepruning**
  - stop growing the tree
  - if the **complexity** of the tree is too high
- **Post pruning**
  - grow the tree and then cut

# Other common parameters

- **Tree depth**
  - controls overfitting but is uninformed
- **Min Split:** Minimum number of cases to have a split
  - controls overfitting
  - we need enough cases for estimating entropy
- **Min Bucket:** Minimum number of cases in a node
  - controls overfitting
  - we need enough cases to decide for a class

# Decision tree induction complexity

- If we have  $N$  data points what is the **computational complexity** of computing a split for a regression problem?
  - $O(N)$
- And for multilevel trees?
  - tree has maximum depth  $d$  :  $O(N \cdot d)$
  - assuming the splits tend to be in the middle :  $O(N \cdot \log_2(N))$
  - in the case of unbalanced splits :  $O(N^2)$
- What is the computational complexity if we have  $p$  variables?
  - $O(p \cdot N \cdot \log_2(N))$
- But remember we have to **sort** the data

# Decision trees and search

- The best tree is **not found analytically**
- We **search** for the tree
  - We start with the root (first node)
  - We choose the best split
  - We commit to that choice
  - Until we find a satisfactory solution
- This is a **greedy search** procedure
  - we may find a **local optimum**
  - but it is **efficient**



# References

- Books
  - Han, Kamber & Pei, Data Mining Concepts and Techniques, Morgan Kaufman.
- Data
  - <https://www.kaggle.com/uciml/german-credit>
  - <https://www.kaggle.com/priy998/golf-play-dataset>
- Blog articles -<https://towardsdatascience.com/introduction-to-na%C3%AFve-bayes-classifier-fa59e3e24aaf>