Decision Trees

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Decision trees: introduction

Objectives of a decision tree

- inference, learning, tree generation:
  - to achieve the best possible split, at leaf nodes, of the (training) samples of different classes
  - to build small tress
- use, exploitation:
  - to predict the class (classification)
  - to predict the value of a target variable (regression)

Decision trees: introduction

Strategy to build a decision tree from a training set X:

- progressive splitting of the training set into smaller and smaller subsets
- recursive splitting of X based on the value of attributes
- creating a labelled leaf, when all instances of a subset belong to the same class
- pruning: a branch with a mixed subset of distinct classes is labelled with the majority class (the resulting subtree is pruned)

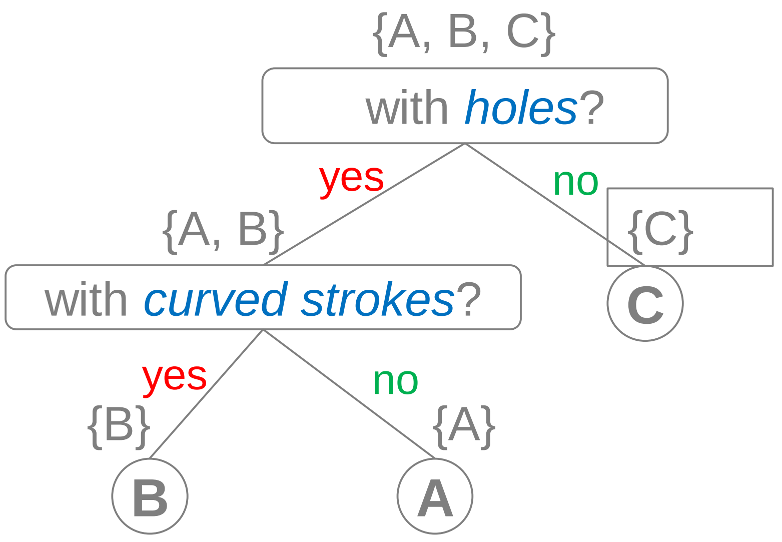
Decision trees: an example

You want to define a system to recognise 3 capital letters (e.g., Arial) based on the presence or absence of 2 features: *holes* and *curved strokes*

class	holes	curved strokes
A	yes	no
B	yes	yes
C	no	yes

comments:

- 3 classes: A, B, C
- 1 instance per class
- 2 discrete features



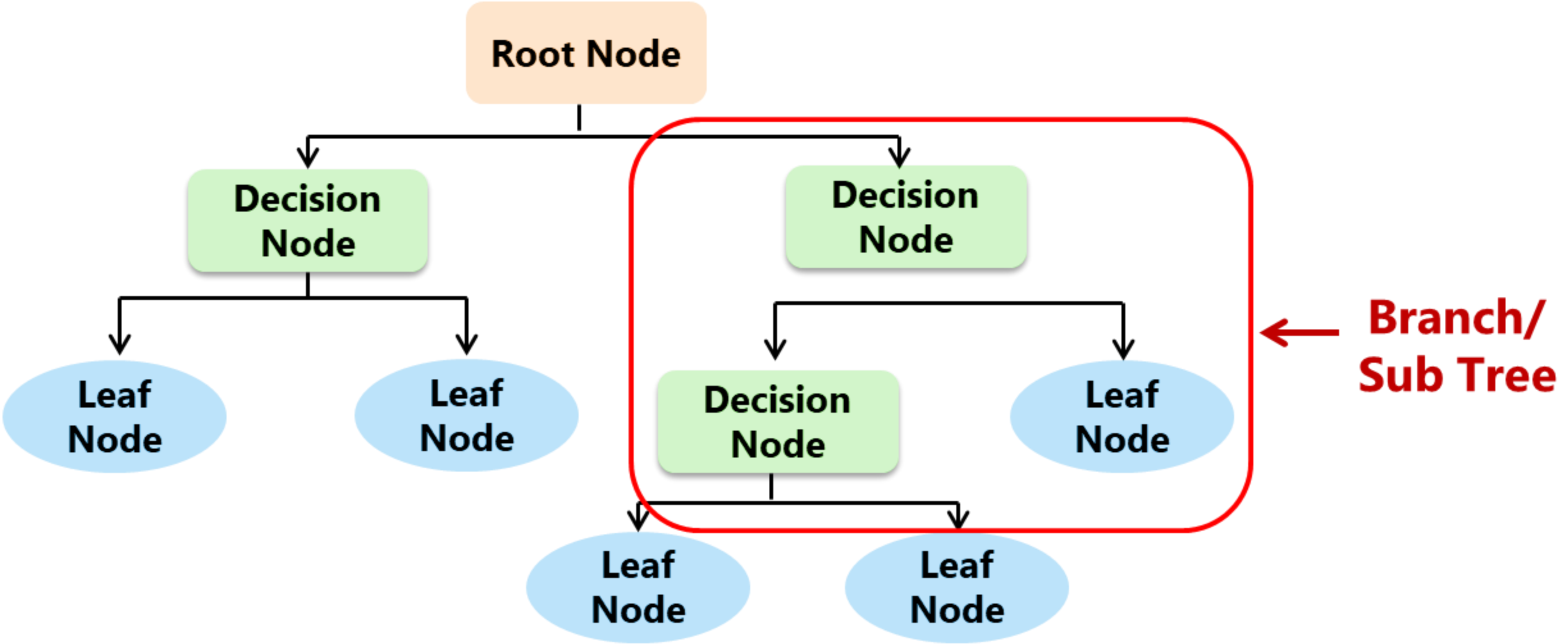
Decision trees: introduction

- prediction model (*non-parametric*); it does **not** learn a statistical model; **it learns an heuristic from known cases**

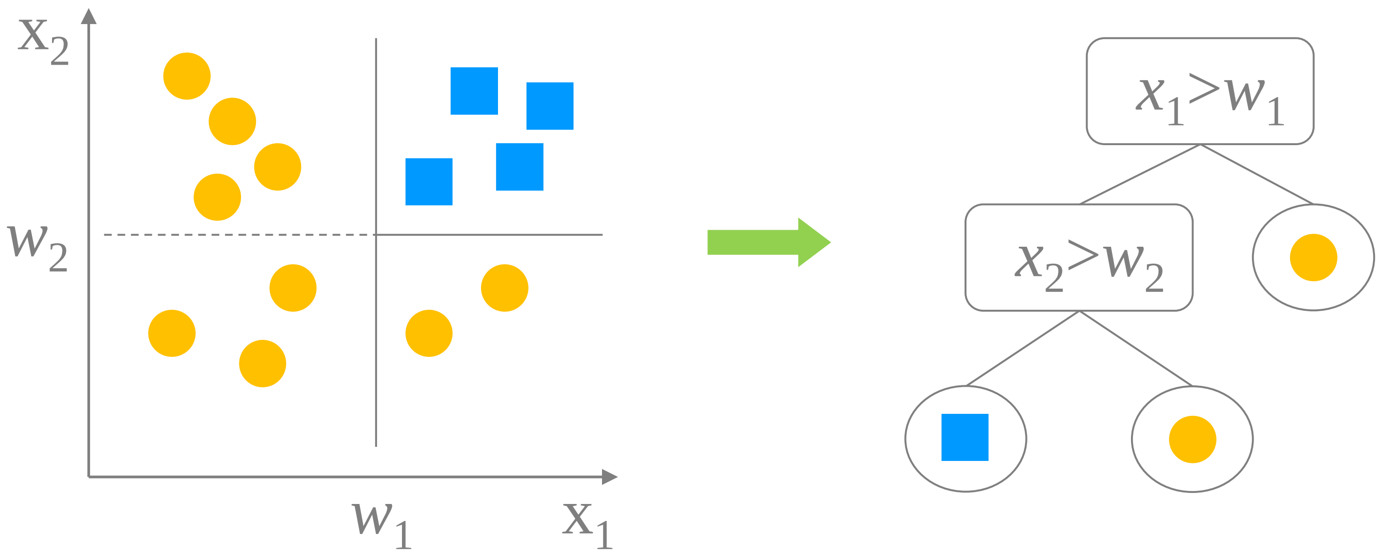
- tree structure with the following types of nodes:
  - **root node** is the top-most decision node and represents the entire set X that further gets divided according to the value of attributes
  - **internal decision node** $f_m(\mathrm{x})$ based on an attribute m; it produces as many branches as allowed by the splitting criterion adopted
  - **leaf node** (or **terminal node**), with output value (class, prediction); it groups instances, for example, of a single class

- decision: for each new input instance x, $f_m(\mathrm{x})$ **guides** the analysis of x **from the root to a leaf** that provides the result **(class)**

Decision trees: types of nodes



Decision trees: learning (induction) of a decision tree



Data set

2 classes: ○, □

2 dimensions: x_1, x_2

Decision tree

rectangular nodes → decision *nodes*

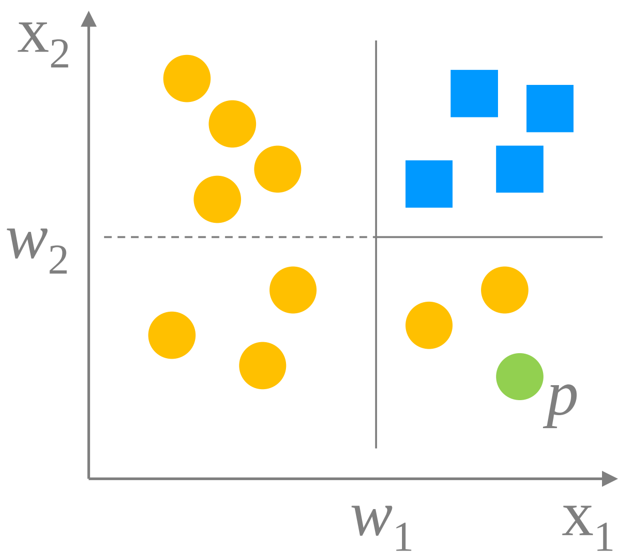
circular nodes → *leaf nodes*

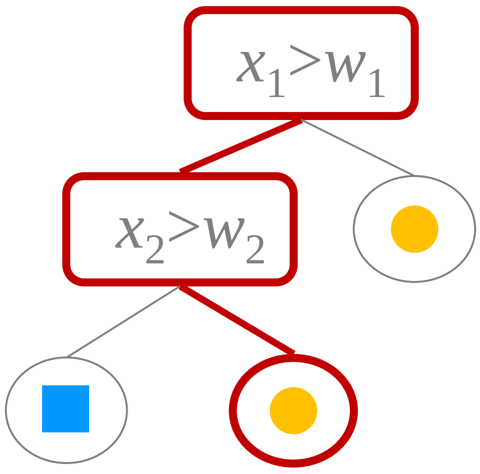
1st split: $x_1 > w_1$

2nd split: $x_2 > w_2$ (orthogonal to 1st)

Decision trees: classification

Given a point $p = (w_1+\delta, w_2-\delta)$, $\delta > 0$, the induced tree classifies p as belonging to class ○ (see coloured path): **it goes through the tree structure from the root node until reaching a leaf**





Decision trees: interpretability

- decision tree ≡ set of rules **IF-THEN-ELSE**
- for example, the previous tree is equivalent to:

IF $x_1 > w_1$ **THEN**

IF $x_2 > w_2$ **THEN**

class = □

ELSE

class = ○

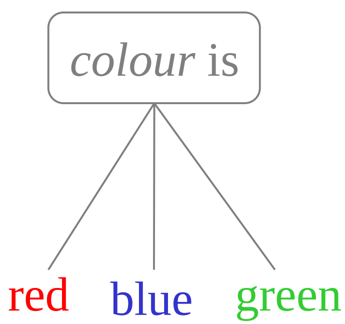
ELSE

class = ○

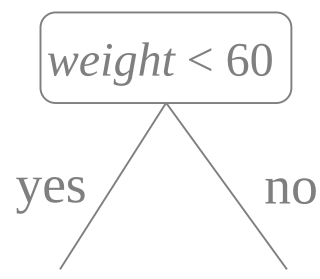
Univariate trees: introduction

the $f_m(x)$ of each internal node is defined in terms of a single dimension (attribute) x_i (*see previous example*)

if x_i is discrete, for example: x_i is an attribute *colour* …



if x_i is numeric (ordered), for example: x_i is an attribute *weight* ...



binary partition of space

$L = \{\text{people} \mid weight < 60\}$

$R = \{\text{people} \mid weight \geq 60\}$

Univariate trees: tree learning algorithm

- tree induction ≡ tree learning
- algorithms of local search:
  - begin: root node with the whole set of instances
  - heuristic (recursive): to divide the set that arrives at a node m using the most discriminating attribute, that is, the one that generates more class homogeneous (i.e., **pure**) disjoint subsets
    - if the attribute is numeric, binary division; if the attribute is discrete, as many “children” (new nodes) as possible values
  - end: until get (labelled) **pure nodes**

Univariate trees: impurity of a node

objective: evaluate the degree of homogeneity of the set of instances X that reaches a node m

example: let $C = \{\omega_1 = \mathrm{A},\ \omega_2 = \mathrm{B}\}$ be the set of classes

- case 1: $\mathrm{X}^1 = \{(x_1, \mathrm{A}), (x_2, \mathrm{B}), (x_3, \mathrm{B}), (x_4, \mathrm{A}), (x_5, \mathrm{A}), (x_6, \mathrm{B})\}$
- case 2: $\mathrm{X}^2 = \{(x_1, \mathrm{A}), (x_2, \mathrm{B}), (x_3, \mathrm{A}), (x_4, \mathrm{A}), (x_5, \mathrm{A}), (x_6, \mathrm{A})\}$

observations:

- X^1 has 3 instances of each class (heterogeneous)
- X^2 has 5 instances of A and 1 of B (almost homogeneous)
- intuition: X^1 is **more impure** than X^2 or X^2 is **more pure** than X^1

Univariate trees: an impurity measure

impurity measure of a node *m*; given:

- N_m, the number of instances that reach m
- $N_{i,m}$, the number of instances in m that belong to class ω_i
- $P_{i,m} = N_{i,m}/N_m$, the probability of class ω_i in m
- I_m, **entropy**, a measure of impurity (c classes):

$$I_m = -\sum_{i=1}^{c} P_{i,m} \cdot \log_2 P_{i,m}$$

(Note: $0 \cdot \log 0 = 0$)

Univariate trees: how to apply the measure

… it continues from previous example: suppose we can choose whether node m is reached by X^1 or X^2

- in both cases $N_m = 6$
- in X^1: $N_{1,m} = 3$, $N_{2,m} = 3 \Rightarrow p_{1,m} = 0.50$, $p_{2,m} = 0.50$
- in X^2: $N_{1,m} = 5$, $N_{2,m} = 1 \Rightarrow p_{1,m} = 0.83$, $p_{2,m} = 0.17$

evaluation of entropy (impurity measure):

- in X^1, $I_m = -(0.5\ log_2 0.5 + 0.5\ log_2 0.5) = 1$ (+ *impure*)
- in X^2, $I_m = -(0.83\ log_2 0.83 + 0.17\ log_2 0.17) = 0.66$ (+ *pure*)

if one could choose … it would be better X^2 to reach *m* because its entropy is lower (i.e. higher purity)

Univariate trees: generalization to 2 classes

context: impurity value at node m for 2 classes

- $N_m = N_{1,m} + N_{2,m} \Rightarrow$
  $p_{1,m} + p_{2,m} = 1 \Rightarrow$
  $p_{2,m} = 1 - p_{1,m}$
- I_m, entropy for c = 2 classes
  (let it be $p \equiv p_{1,m}$):

$$\boxed{I_m = -p\log_2(p) - (1-p)\log_2(1-p)}$$

Univariate tree: pure node (impurity 0)

a node m is pure if all instances reaching m are of the same class, that is, **if $N_{1,m} = 0$ or $N_{2,m} = 0$**; suppose $N_{1,m} = 0$, then

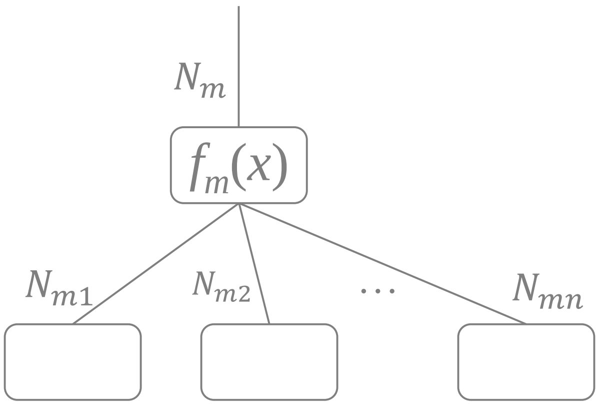
$$N_{1,m} = 0 \;\Rightarrow\; p_{1,m} = 0,\;\; p_{2,m} = 1 \Rightarrow I_m = 0$$

a node m is pure $\Leftrightarrow$ $I_m = 0$ (impurity 0)

a pure node becomes a leaf that is assigned the class label of its instances

Univariate trees: impurity of a split

- K classes or categories
- x is the attribute chosen to split an impure node



$$\sum_{j=1}^{n} N_{m,j} = N_m$$

$N_{m,j}^{i}$ instances of the $N_{m,j}$ belong to ω_i such that $\sum_{i=1}^{K} N_{m,j}^{i} = N_{m,j}$

$p_{m,j}^{i} = \frac{N_{m,j}^{i}}{N_{m,j}}$ is the probability of ω_i in the branch j

Impurity of a split:

$$I_m^* = -\sum_{j=1}^{n} \frac{N_{m,j}}{N_m} \left(\sum_{i=1}^{K} p_{m,j}^{i} \log_2 p_{m,j}^{i} \right)$$

Univariate trees: choice of the attribute; local optimization

Local optimization:

in each node (not pure) in which it is intended to continue splitting the training set, the most discriminating attribute will be chosen, that is, the one that produces a split that is:

- the least impure ≡
- the most homogeneous ≡
- with the greatest class separation

Univariate trees: general tree induction algorithm

generate_tree (T_{tra}, α): m

if entropy $I_m(T_{tra}) \le \alpha$:

$m \leftarrow$ class label of the most represented class in T_{tra}

else

a = the_most_discriminating_attribute (T_{tra})

$m \leftarrow a$

for each branch a_i of a:

$tra_i = \{x \in T_{tra} \mid x$ satisfies the condition of $a_i\}$

h = generate_tree (tra_i, α)

add_child (m, h)

return m

Univariate trees: function "the most discriminating attribute"

the_most_discriminating_attribute (*tra*): a

$mín\_entr \leftarrow$ MAX

for each attribute x_i:

if x_i is discrete:

divide *tra* into $tra_1, \ldots, tra_N$ based on the values of x_i

e $\leftarrow I^*_m(tra_1, tra_2, \ldots, tra_N)$

if $e < mín\_entr$: $mín\_entr \leftarrow e$; $a \leftarrow x_i$

else // x_i is numeric

for each possible binary division (tra_1, tra_2):

e $\leftarrow I^*_m(tra_1, tra_2)$

if $e < mín\_entr$: $mín\_entr \leftarrow e$; $a \leftarrow x_i$

return a

Pruning: introduction

Context

- it is common to find high overlapping or outliers
- to generate a “pure” tree trying to learn from:
  - outliers
  - small sample size (small number of instances)
  - overlapping

  reduces the generalization of the model (overfitting)

Alternative

- pre-pruning: do not split nodes with few instances while growing the tree
- post-pruning: after building the tree to its depth, remove unnecessary subtrees

Pruning: pre-pruning

Idea

- let m be a node and N_m the number of samples (instances)
- stop splitting the training set

  if m is pure (*"natural end"*) or if $N_m < \theta$ (pruning)
- label m with the majority class among the N_m instances

Pruning: post-pruning

Idea**:** to generate 3 independent (and disjoint) sets for training, pruning, and test

- training: generate the complete tree, with all its pure leaves, using the training set
- pruning (it is part of the learning stage):
  - replace each subtree by a leaf node with the label of the majority instances covered by that subtree
  - prune the subtree if the "surrogate" leaf node does not worsen its performance with the pruning set
- evaluation: obtain a performance measure of the final (pruned) tree by classifying the test set

Pruning: summary

Experiments show that:

- post-pruning produces more accurate trees (both classification and regression) than pre-pruning
- pre-pruning is much faster than post-pruning

Decision trees: advantages

- Comprehensive: it is good for interpreting data in a highly visual way
- Simplicity: it is one of the simplest algorithms since it has no complex formulas or data structures

Decision trees: disadvantages

- It is computationally expensive. At each node, the candidate split must be sorted before determining the best
- It is sometimes unstable as small variations in data might lead to the formation of a new tree