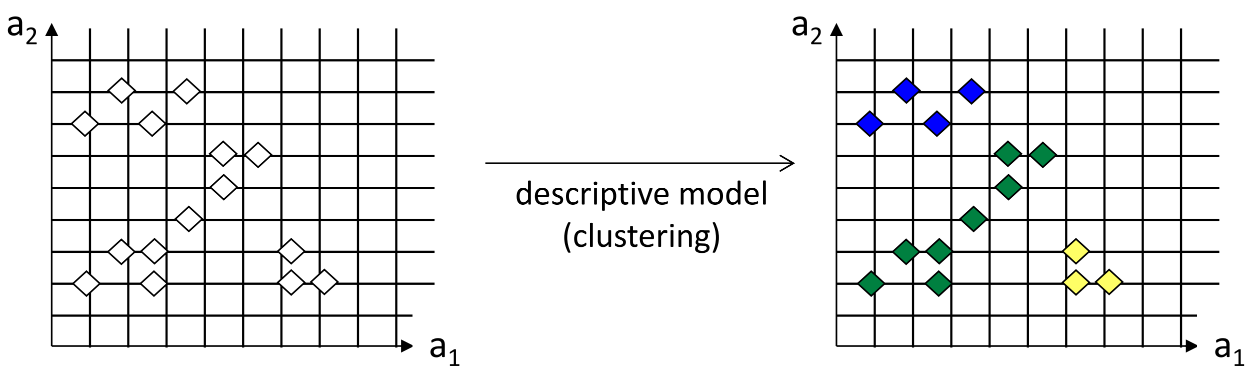
4. CLASSIFICATION

Clustering and Classification

Given a dataset of *objects* described by *attributes*, build a model that assigns objects to a *class (or label)*

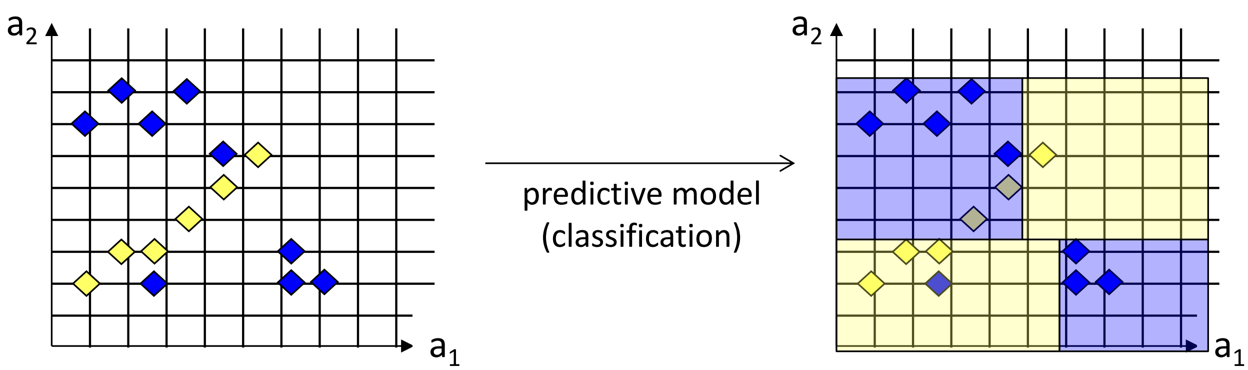


no class info

describe classes based on similarity of attribute values

Clustering and Classification

Given a dataset of *objects* described by *attributes*, build a model that assigns objects to a *class*



class info

predict classes based on known attribute values

Classification Problem

Input: set of objects with categorical/numerical attributes and one class label

Output: A model that returns the class label given the object attributes

- Model is a function represented as rules, decision trees, formulae

Classification belongs to *supervised* ML

- Objects have class information

Classification: General Approach

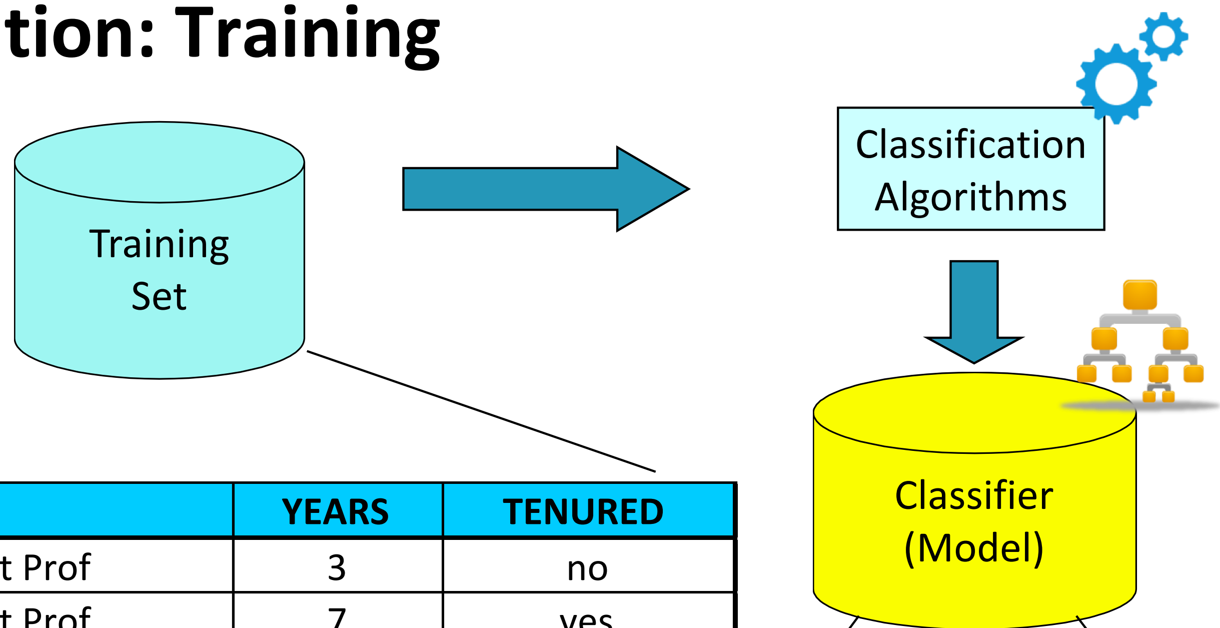
Model is learnt from a set of objects with known labels: **training set**

The quality of the model is evaluated by comparing the predicted class labels with those from a set of objects with known labels: **test set**

- Test set is independent of training set, otherwise over-fitting will occur

The model is applied to data with unknown labels: **prediction**

Classification: Training

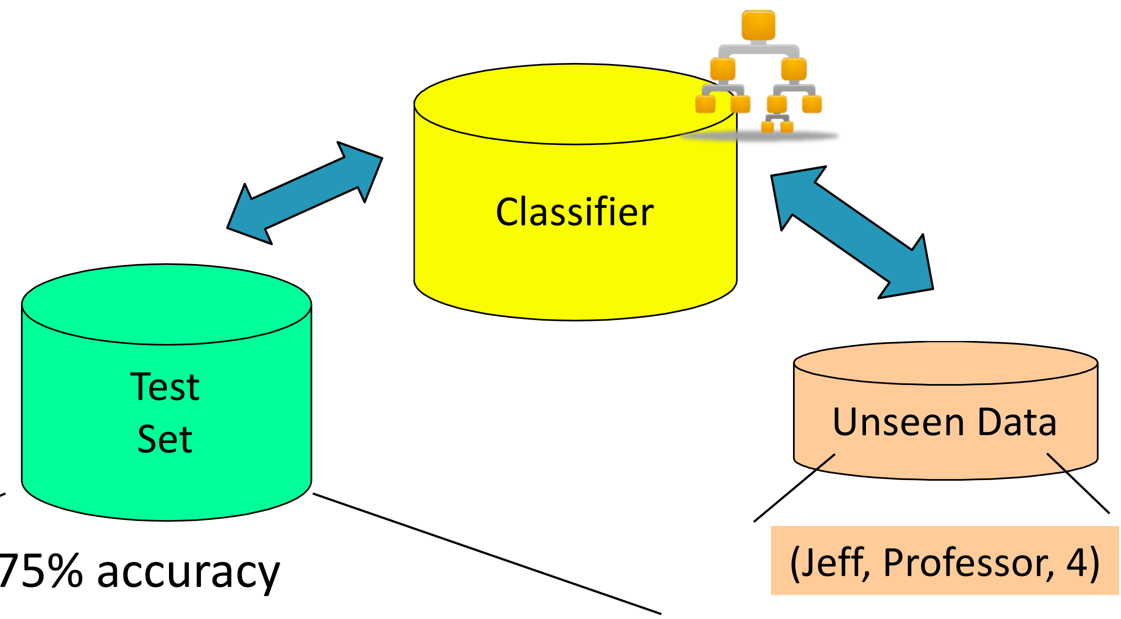


NAME	RANK	YEARS	TENURED
Mike	Assistant Prof	3	no
Mary	Assistant Prof	7	yes
Bill	Professor	2	yes
Jim	Associate Prof	7	yes
Dave	Assistant Prof	6	no
Anne	Associate Prof	3	no

Categorical attribute — Numerical attribute — Class label

IF rank = ‘professor’
OR years > 6
THEN tenured = ‘yes’

Classification: Model Test and Usage



NAME	RANK	YEARS	TENURED
Tom	Assistant Prof	2	no
Merlisa	Associate Prof	7	no
George	Professor	5	yes
Joseph	Assistant Prof	7	yes

Tenured?

YES

Classification: Problem Formulation

Problem

Given a database D with n data items described by d categorical/numerical attributes and one categorical attribute (class label C)

Find

A function $f: X^d \rightarrow C$

rules
decision tree
formula

Such that

classifies *accurately* the items in the *training* set

generalises well for the (unknown) items in the *test* set

Characteristics of Classification Methods

Predictive accuracy

Speed and scalability

- Time to build the model
- Time to use the model
- In memory vs. on disk processing

Robustness

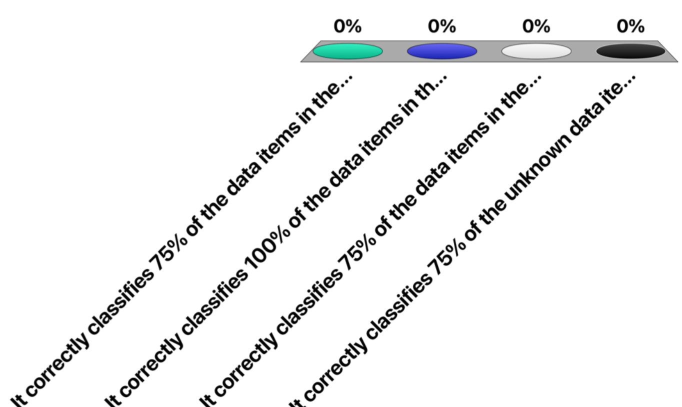
- Handling noise, outliers and missing values

Interpretability

- Understanding the model and its decisions (black box) vs. white box
- Compactness of the model

If a classifier has 75% accuracy, it means that ...

A. It correctly classifies 75% of the data items in the training set
B. It correctly classifies 100% of the data items in the training set but only 75% in the test set
C. It correctly classifies 75% of the data items in the test set
D. It correctly classifies 75% of the unknown data items

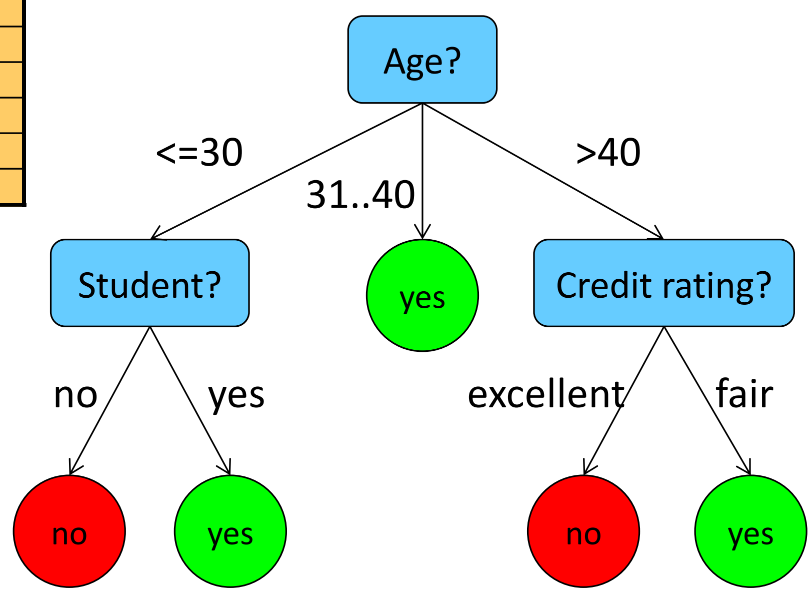


Decision Trees

age	income	student	credit_rating	buys_computer
<=30	high	no	fair	no
<=30	high	no	excellent	no
31…40	high	no	fair	yes
>40	medium	no	fair	yes
>40	low	yes	fair	yes
>40	low	yes	excellent	no
31…40	low	yes	excellent	yes
<=30	medium	no	fair	no
<=30	low	yes	fair	yes
>40	medium	yes	fair	yes
<=30	medium	yes	excellent	yes
31…40	medium	no	excellent	yes
31…40	high	yes	fair	yes
>40	medium	no	excellent	no

some columns are not used

– Nodes are tests on a single attribute
– Branches are attribute values
– Leaves are marked with class labels



Decision Tree Induction: Algorithm

Tree construction (top-down divide-and-conquer strategy)

- At the beginning, all training samples belong to the root
- Examples are partitioned recursively based on a selected “most discriminative” attribute
- Discriminative power determined based on information gain (ID3/C4.5)

Partitioning stops if

- All samples belong to the same class → assign the class label to the leaf
- There are no attributes left → majority voting to assign the class label to the leaf
- There are no samples left

Example: Decision Tree Induction

age	income	student	credit_rating	buys_computer
<=30	high	no	fair	no
<=30	high	no	excellent	no
31…40	high	no	fair	yes
>40	medium	no	fair	yes
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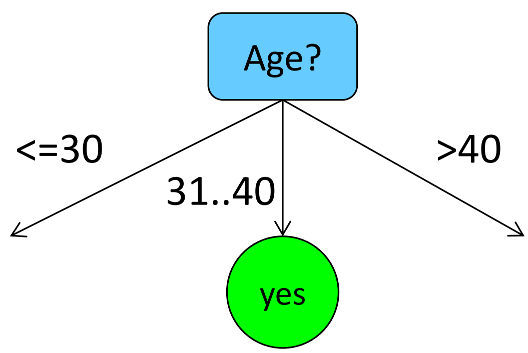

buys_computer is always yes if
31 < age < 40

Example: Decision Tree Induction

age	income	student	credit_rating	buys_computer
<=30	high	no	fair	no
<=30	high	no	excellent	no
31..40	high	no	fair	yes
>40	medium	no	fair	yes
>40	low	yes	fair	yes
>40	low	yes	excellent	no
31..40	low	yes	excellent	yes
<=30	medium	no	fair	no
<=30	low	yes	fair	yes
>40	medium	yes	fair	yes
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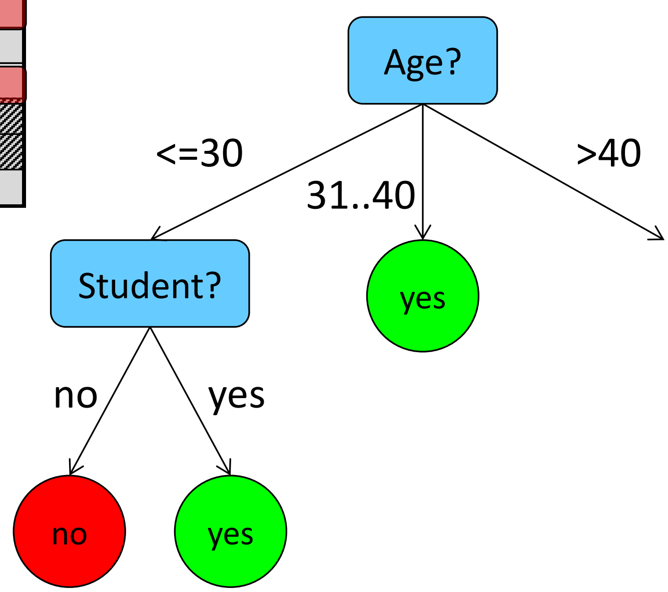

Example: Decision Tree Induction

age	income	student	credit_rating	buys_computer
<=30	high	no	fair	no
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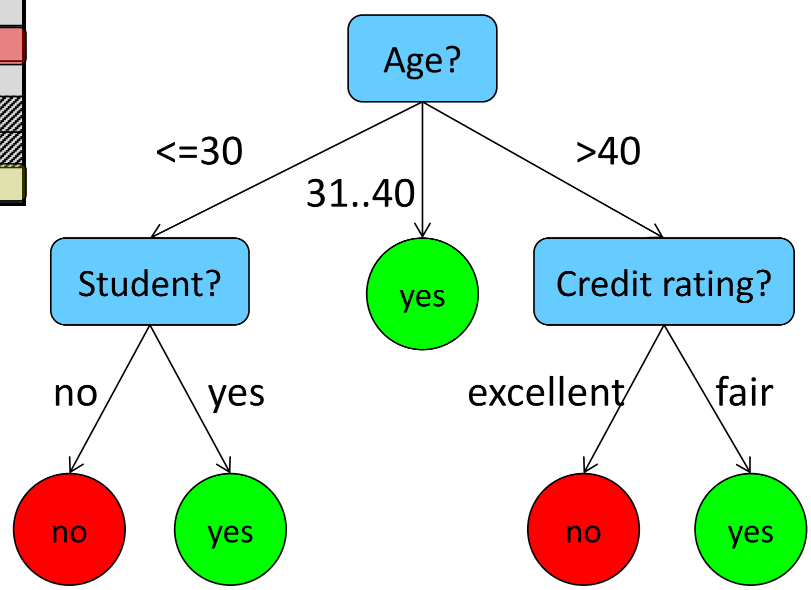

Attribute Selection

At a given branch in the tree, the set of samples S to be classified has P positive and N negative instances

The entropy of the set S is $\boxed{\text{Entropy of set is the entropy of the label}}$

$$H(P, N) = -\frac{P}{P+N}\log_2\frac{P}{P+N} - \frac{N}{P+N}\log_2\frac{N}{P+N}$$

Note

- If P=0 or N=0 H(P, N) = 0 → no uncertainty
- If P=N H(P, N) = 1 → maximal uncertainty

Entropy always computed wrt label

Attribute Selection: Example

age	income	student	credit_rating	buys_computer
<=30	high	no	fair	no
<=30	high	no	excellent	no
31…40	high	no	fair	yes
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<=30	medium	yes	excellent	yes
31…40	medium	no	excellent	yes
31…40	high	yes	fair	yes
>40	medium	no	excellent	no

$H_S = H(9, 5) = 0.94$

Entropy of set = entropy of label (buys_computer)

Age [<=30] $H(2, 3) = 0.97$
Age [31...40] $H(4, 0) = 0$
Age [>40] $H(3, 2) = 0.97$

Income [high] $H(2, 2) = 1$
Income [med] $H(4, 2) = 0.92$
Income [low] $H(3, 1) = 0.81$

Student [yes] $H(6, 1) = 0.59$
Student [no] $H(3, 4) = 0.98$

Rating [fair] $H(6, 2) = 0.81$
Rating [exc] $H(3, 3) = 1$

Entropies are all computed wrt label

Attribute Selection: Example

age	income	student	credit_rating	buys_computer
<=30	high	no	fair	no
<=30	high	no	excellent	no
31…40	high	no	fair	yes
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31…40	medium	no	excellent	yes
31…40	high	yes	fair	yes
>40	medium	no	excellent	no

$H_S = H(9, 5) = 0.94$

$$\boxed{\begin{aligned} H_{Age} &= p([<=30]) \cdot H(2, 3) + p([31...40]) \cdot H(4, 0) + p([>40]) \cdot H(3, 2) = \\ &= 5/14 \cdot 0.97 + 4/14 \cdot 0 + 5/14 \cdot 0.97 = 0.69 \end{aligned}}$$

$$\begin{aligned} H_{Income} &= p([high]) \cdot H(2, 2) + p([med]) \cdot H(4, 2) + p([low]) \cdot H(3, 1) = \\ &= 4/14 \cdot 1 + 6/14 \cdot 0.92 + 4/14 \cdot 0.81 = 0.91 \end{aligned}$$

$$H_{Student} = p([yes]) \cdot H(6, 1) + p([no]) \cdot H(3, 4) = 7/14 \cdot 0.59 + 7/14 \cdot 0.98 = 0.78$$

$$H_{Rating} = p([fair]) \cdot H(6, 2) + p([exc]) \cdot H(3, 3) = 8/14 \cdot 0.81 + 6/14 \cdot 1 = 0.89$$

conditional entropy =
probability of being in that subgroup x entropy of subgroup

we split using the attribute with the smallest uncertainty.

conditional entropy =
probability of being in that subgroup x entropy of subgroup

Attribute Selection: Information Gain

Attribute A partitions S into S_1, S_2, ... S_v

Entropy of attribute A is

$$H(A) = \sum_{i=1}^{v} \frac{P_i + N_i}{P + N} H(P_i, N_i)$$

The information gain obtained by splitting S using A is

$$Gain(A) = H(P, N) - H(A)$$

H(P,N) = total / true uncertainty
H(A) = uncertainty of category

Gain(Age) = 0.94 – 0.69 = 0.25 ← split on age

Gain(Income) = 0.94 – 0.91 = 0.03

Gain(Student) = 0.94 – 0.78 = 0.16

Gain(Rating) = 0.94 – 0.89 = 0.05

if H(A) = H(P,N), then gain = 0

if the uncertainty of the attribute is equal to the uncertainty of S, then gain is 0

the attribute has no impact on classification

Information Gain = Entropy of set before splitting - Entropy of set we split at

- Entropy of set before splitting is a "constant"
- We wanna reduce uncertainty so we choose the splitting attribute that has the lowest entropy

Given the distribution of positive and negative samples for attributes A_1 and A_2, which is the best attribute for splitting?

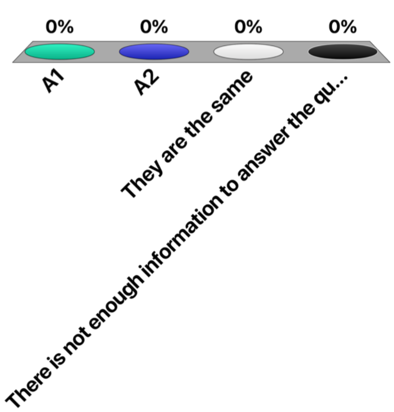
A_1	P	N
a	2	2
b	4	0
A_2	**P**	**N**
x	3	1
y	3	1

A. A1

B. A2

C. They are the same

D. There is not enough information to answer the question



Pruning

The construction phase does not filter out noise → **overfitting**

Pruning strategies

- Stop partitioning a node when large majority of samples is positive or negative, i.e., N/(N+P) or P/(N+P) > 1 - ε
- Build the full tree, then replace nodes with leaves labelled with the majority class, if classification accuracy does not change
- Apply Minimum Description Length (MDL) principle

Minimum Description Length Pruning

Let M_1, M_2, ..., M_n be a list of candidate models (i.e., trees). The best model is the one that minimizes

$$L(M) + L(D|M)$$

where

- $L(M)$ is the length in bits of the description of the model (#nodes, #leaves, #arcs ...)
- $L(D|M)$ is the is the length in bits of the description of the data when encoded with the model (#misclassifications)

Extracting Classification Rules from Trees

Represent the knowledge in the form of IF-THEN rules

- One rule is created for each path from the root to a leaf
- Each attribute-value pair along a path forms a conjunction
- The leaf node holds the class prediction

Rules are easier for humans to understand

Example

IF *age* = "<=30" AND *student* = "*no*" THEN *buys_computer* = "*no*"
IF *age* = "<=30" AND *student* = "*yes*" THEN *buys_computer* = "*yes*"
IF *age* = "31…40" THEN *buys_computer* = "*yes*"
IF *age* = ">40" AND *credit_rating* = "*excellent*" THEN *buys_computer* = "*yes*"
IF *age* = ">40" AND *credit_rating* = "*fair*" THEN *buys_computer* = "*no*"

Decision Trees: Continuous Attributes

With continuous attributes we can not have a separate branch for each value

– use **binary decision trees**

Binary decision trees

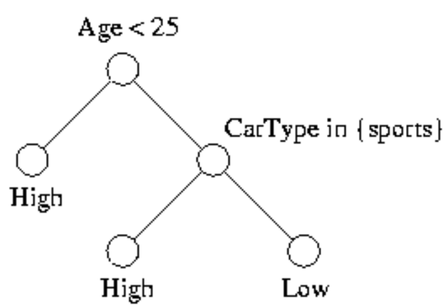
– For continuous attributes A a split is defined by val(A) < X

– For categorical attributes A a split is defined by a subset X $\subseteq$ domain(A)

Example: Binary Decision Tree

rid	Age	Car Type	Risk
0	23	family	High
1	17	sports	High
2	43	sports	High
3	68	family	Low
4	32	truck	Low
5	20	family	High

(a) Training Set



(b) Decision Tree

Splitting Continuous Attributes

Approach

- Sort the data according to attribute value
- Determine the value of X which maximizes information gain by scanning through the data items

X is the continuous attribute (eg age)

Only if the class label changes, a relevant decision point exists

0	**1**	**2**	**4**	**6**	**7**	**8**	**10**
P	P	P	N	N	N	P	P

Possible split points

Top Row Example: Age, we split at 25 because all labels are high

Here, we need to decide whether to split using age or car type.
- For each attribute, we find the interval that maximizes information gain
- We pick the attribute that results in the highest information gain

We actually should also compute between (32,43) and (43,58)

H(A) = H(P,N)

Example

0.5H(3,0) + 0.5H(1,2)

Attribute List

Age	Class	tid	Position of cursor in scan
			position 0
17	High	1	
20	High	5	
23	High	0	
			position 3
32	Low	4	
43	High	2	
68	Low	3	
			position 6

cursor position 0:

	H	L
C_{below}	0	0
C_{above}	4	2

cursor position 3:

	H	L
C_{below}	3	0
C_{above}	1	2

cursor position 6:

	H	L
C_{below}	4	2
C_{above}	0	0

H(A) = H(P,N)

H(P, N) = H(4, 2) =0.918

H(A) = 0 + ½ H(1, 2) =0.459

Gain = H(P, N) – H(A) = 0.459

split using age because higher information gain

Attribute List

Car Type	Class	tid
family	High	0
sports	High	1
sports	High	2
family	Low	3
truck	Low	4
family	High	5

$\Rightarrow$

Count Matrix

	H	L
family	2	1
sports	2	0
truck	0	1

splitting to {sports} and {family, truck}

H(A) = 0 + 2/3 H(2, 2) =0.666

Gain = H(P, N) – H(A) = 0.251

Scalability of Continuous Attribute Splits

Naive implementation

- At each step the data set is split in subsets that are associated with a tree node

Problem

- For evaluating which attribute to split, data needs to be sorted according to these attributes
- Becomes dominating cost

Scalability of Continuous Attribute Splits

Idea: Presorting of data and maintaining order throughout tree construction

- Requires separate sorted attribute tables for each attribute

Updating attribute tables

- Attribute used for split: splitting attribute table straightforward
- Other attributes
  - Build Hash Table associating tuple identifiers (TIDs) of data items with partitions
  - Select data from other attribute tables by scanning and probing the hash table

- scan table to see if it belongs to L node
- get its hash value
- index from car type table

Example

Attribute lists for node 0

L: Tid 1, 5, 0 (Age 17, 20, 23)
R: Tid 4, 2, 3 (Age 32, 43, 68)

Age	Class	Tid
17	High	1
20	High	5
23	High	0
32	Low	4
43	High	2
68	Low	3

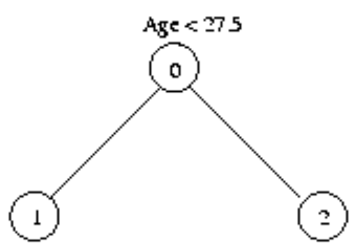
Car Type	Class	Tid
family	High	0
sports	High	1
sports	High	2
family	Low	3
truck	Low	4
family	High	5

probe →

hash table

0	L
1	L
2	R
3	R
4	R
5	L

age hash table



Attribute lists for node 1

Age	Class	Tid
17	High	1
20	High	5
23	High	0

Car Type	Class	Tid
family	High	0
sports	High	1
family	High	5

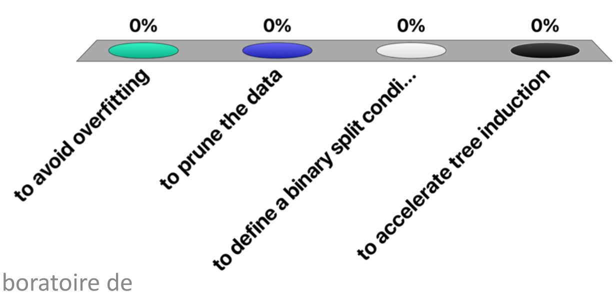
Attribute lists for node 2

Age	Class	Tid
32	Low	4
43	High	2
68	Low	3

Car Type	Class	Tid
sports	High	2
family	Low	3
truck	Low	4

When splitting a continuous attribute, its values need to be sorted …

A. to avoid overfitting
B. to prune the data
C. to define a binary split condition
D. to accelerate tree induction



Characteristics of Decision Tree Induction

Strengths

- Automatic feature selection
- Minimal data preparation
- Non-linear model
- Easy to interpret and explain

Weaknesses

- Sensitive to small perturbation in the data
- Tend to overfit
- Have to be re-trained from scratch with new data

Decision Tree Induction: Properties

Model: flow-chart like tree structure

Score function: classification accuracy

Optimisation: top-down tree construction + pruning

Data Management: avoiding sorting during splits

Classification Algorithms

Decision tree induction is a (well-known) example of a classification algorithm

Alternatives

- Basic methods: Naïve Bayes, kNN, logistic regression, ..
- Ensemble methods: random forest, gradient boosting, …
- Support vector machines
- Neural networks: CNN, rNN, LSTM, …

After a weak learner is added, the data are reweighted: examples that are misclassified gain weight and examples that are classified correctly lose weight. Thus, future weak learners focus more on the examples that previous weak learners misclassified.

Ensemble Methods

Idea

- Take a collection of simple or **weak** learners
- Combine their results to make a single, **strong** learner

Types

- **Bagging:** train learners in parallel on different samples of the data, then combine outputs through voting or averaging

  sampling with replacement
- **Stacking:** combine model outputs using a second-stage learner like linear regression
- **Boosting:** train learners on the filtered output of other learners

  - give higher weight to points that have been wrongly sampled

Random Forests

Learn K different decision trees from independent samples of the data (bagging)

- vote between different learners, so models should not be too similar

Aggregate output: majority vote

Why do Ensemble Methods Work?

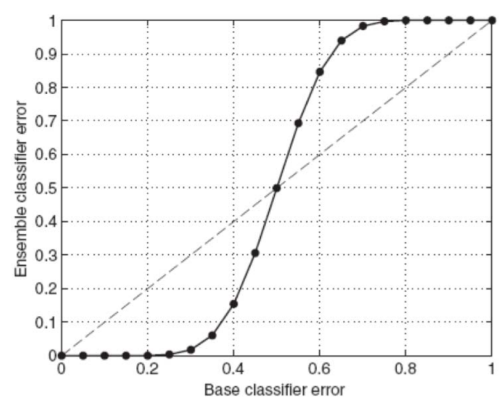
Assume there are 25 base classifiers

– Each classifier has error rate = 0.35

– Assume classifiers are independent

Probability that the ensemble classifier makes a wrong prediction

$$P(\text{wrong prediction}) = \sum_{\boxed{i=13}}^{25} \binom{25}{i} \varepsilon^i (1-\varepsilon)^{25-i} = 0.06$$



Tan, Steinbach, Kumar

Sampling Strategies

Two sampling strategies

Sampling data

- select a subset of the data → Each tree is trained on different data

Sampling attributes

- select a subset of attributes → corresponding nodes in different trees (usually) don't use the same feature to split

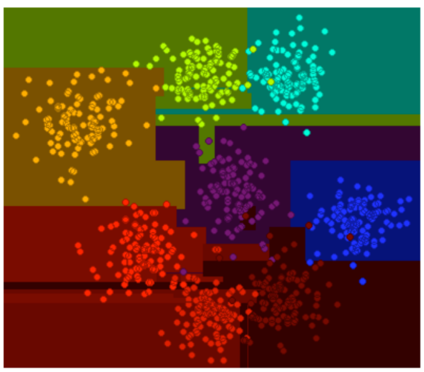
Random Forests: Algorithm

1. Draw K bootstrap **samples of size N** from original dataset, with replacement (bootstrapping) $\boxed{\text{all attributes taken}}$
2. While constructing the decision tree, select a random set of **m attributes** out of the p attributes available to infer split (feature bagging) $\boxed{\text{some attributes taken}}$

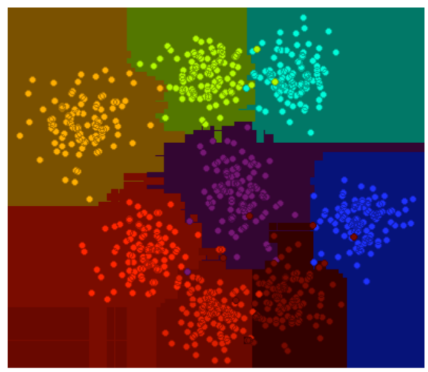
Typical parameters

- m ≈ sqrt(p), or smaller
- K ≈ 500

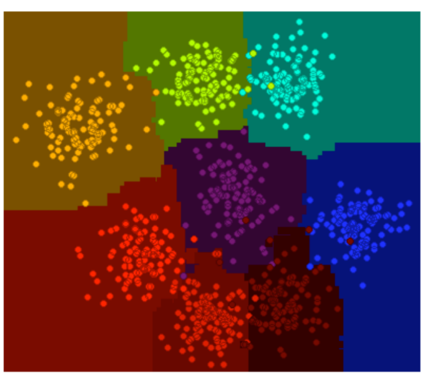
Illustration of Random Forests



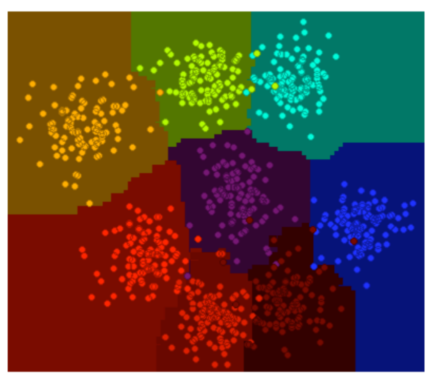
1 rCART



10 rCARTs



100 rCARTs

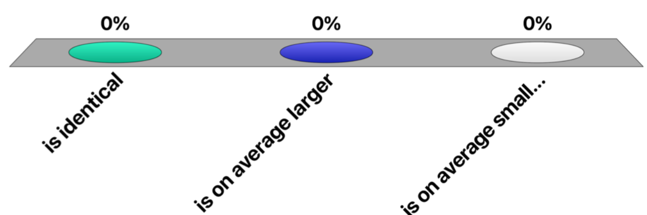


500 rCARTs

The computational cost for constructing a RF with K as compared to constructing K decision trees on the same data

A. is identical
B. is on average larger
C. is on average smaller

we use lesser attributes. lesser branches



Characteristics of Random Forests

Strengths

– Ensembles can model extremely complex decision boundaries without overfitting
– Probably the most popular classifier for **dense data** (<= a few thousand features)
– Easy to implement (train a lot of trees)
– Parallelizes easily, good match for MapReduce

Characteristics of Random Forests

Weaknesses

- Deep Neural Networks generally do better
- Needs many passes over the data – at least the max depth of the trees
- Relatively easy to overfit – hard to balance accuracy/fit tradeoff

References

Textbook

– Jiawei Han, Data Mining: concepts and techniques, Morgan Kaufman, 2000, ISBN 1-55860-489-8

References

– Leo Breiman (2001) “Random Forests” Machine Learning, 45, 5-32.

– Shafer, John, Rakesh Agrawal, and Manish Mehta. "SPRINT: A scalable parallel classifier for data mining." *Proc. 1996 Int. Conf. Very Large Data Bases*. 1996.