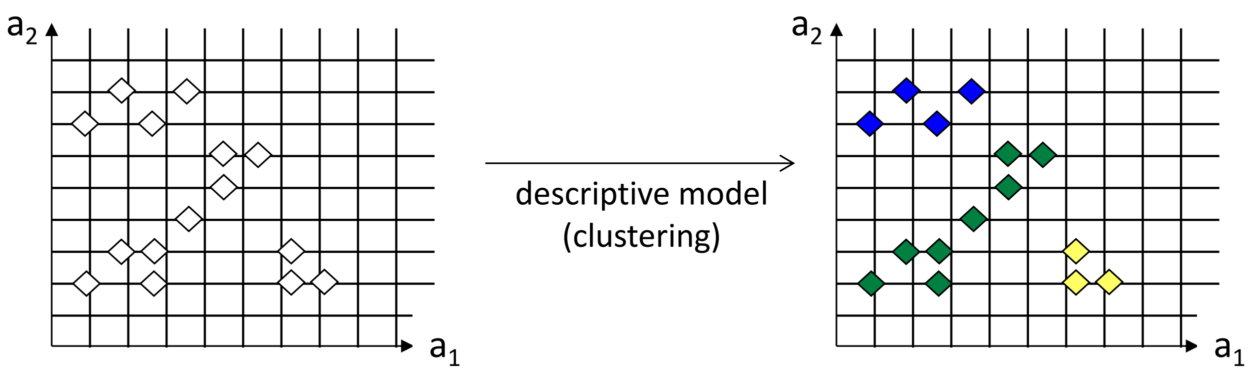
4. CLASSIFICATION

Clustering and Classification

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

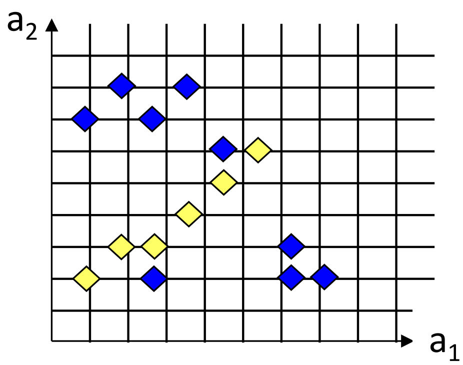


no class info

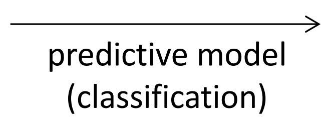
describe classes based on similarity of attribute values

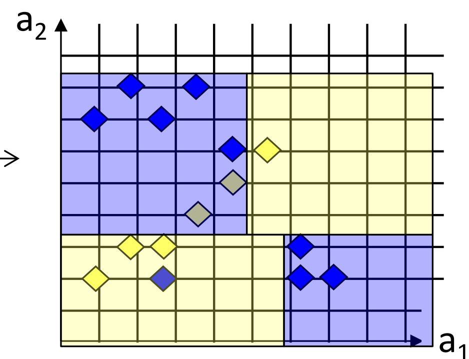
Clustering and Classification

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

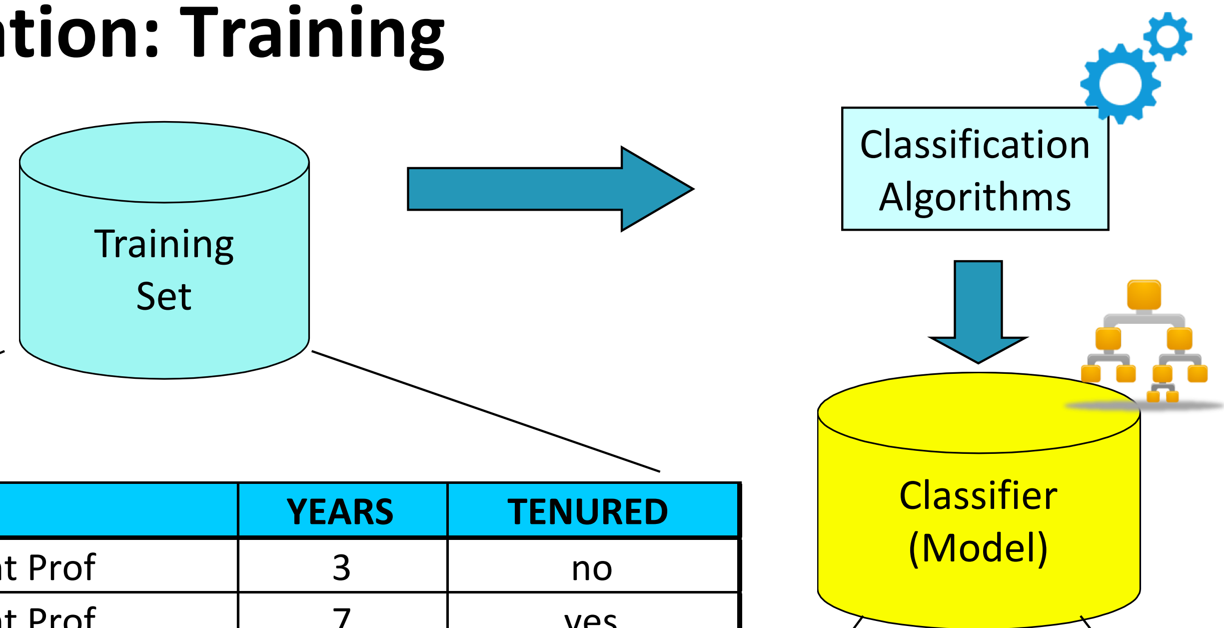
Model is learnt from a set of objects with known labels: **training set**

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

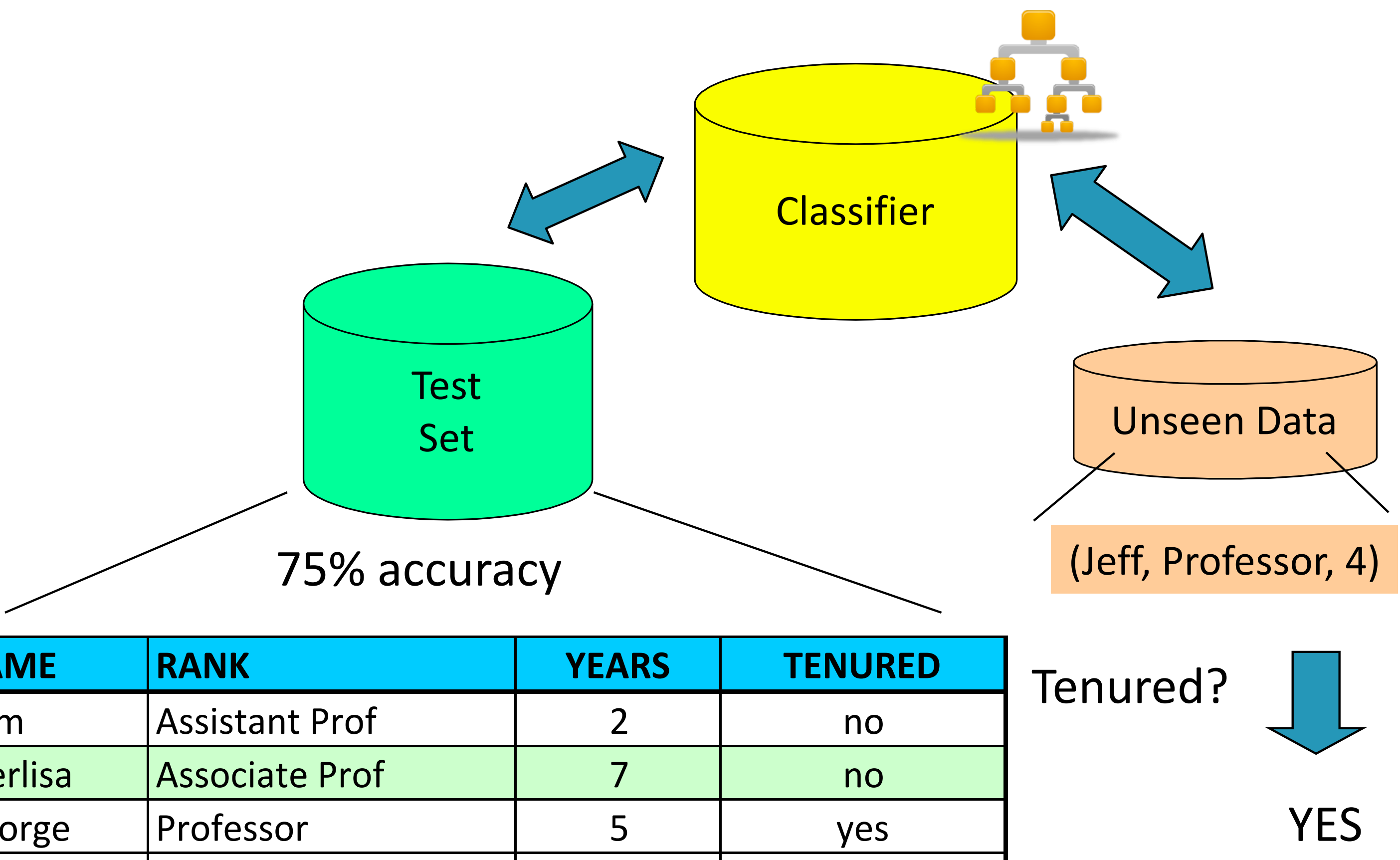


NAME	RANK	YEARS	TENURED
Mike	Assistant Prof	3	no
Mary	Assistant Prof	7	yes
Bill	Professor	2	yes
Jim	Associate Prof	7	yes
Dave	Assistant Prof	6	no
Anne	Associate Prof	3	no

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

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

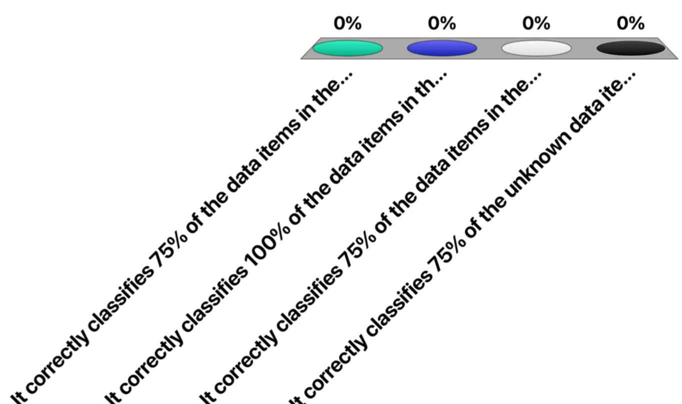
- Handling noise, outliers and missing values

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 ...

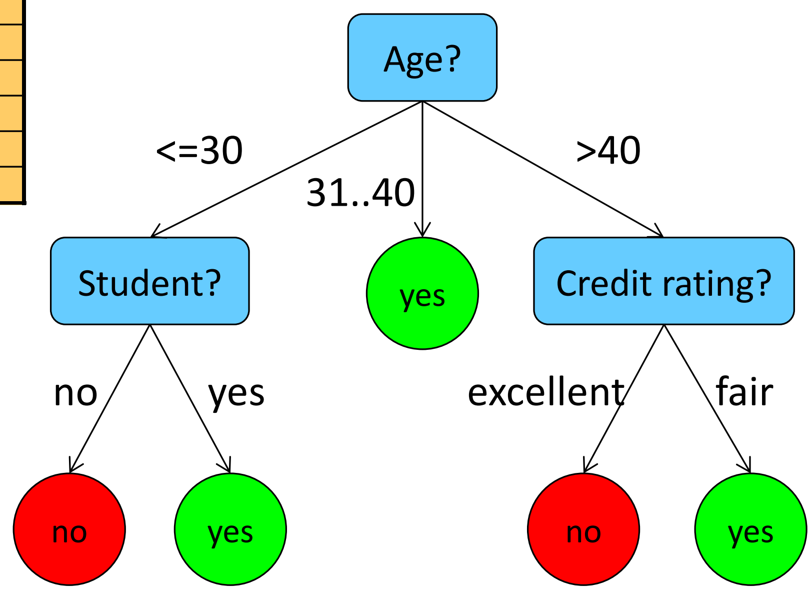
A. It correctly classifies 75% of the data items in the training set
B. It correctly classifies 100% of the data items in the training set but only 75% in the test set
C. It correctly classifies 75% of the data items in the test set
D. It correctly classifies 75% of the unknown data items



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

- 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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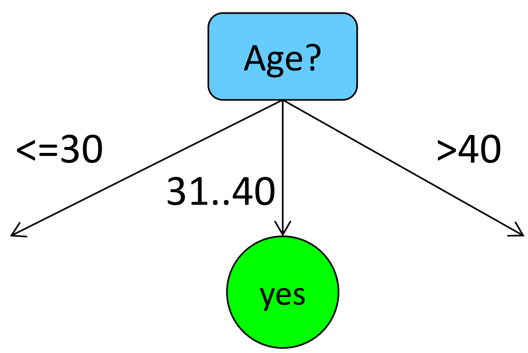

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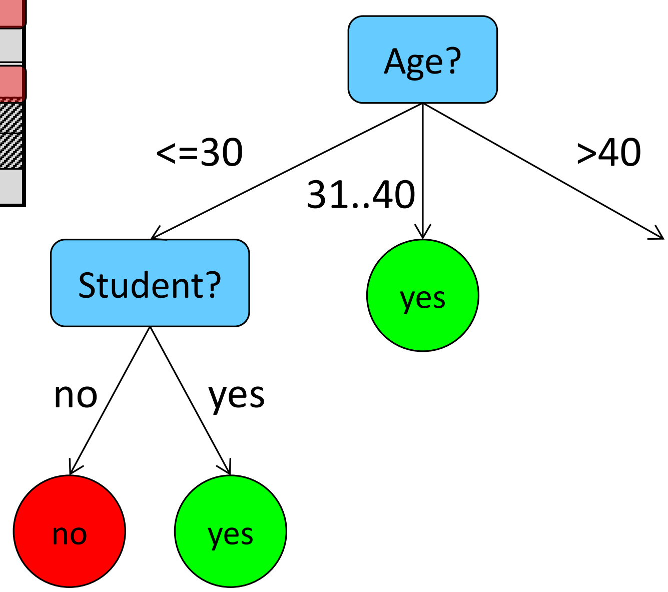

Example: Decision Tree Induction

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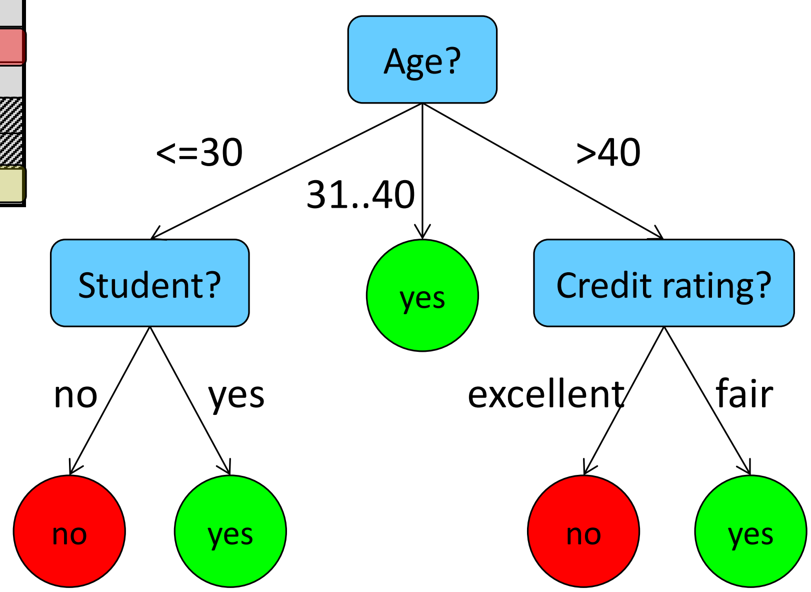

Attribute Selection

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

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

Note

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

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
>40	medium	no	fair	yes
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31…40	medium	no	excellent	yes
31…40	high	yes	fair	yes
>40	medium	no	excellent	no

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

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

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
>40	medium	no	fair	yes
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31…40	medium	no	excellent	yes
31…40	high	yes	fair	yes
>40	medium	no	excellent	no

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

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

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

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

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

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

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

$\boxed{\text{Gain(Age)} = 0.94 - 0.69 = 0.25}$ ← split on age

Gain(Income) = 0.94 – 0.91 = 0.03

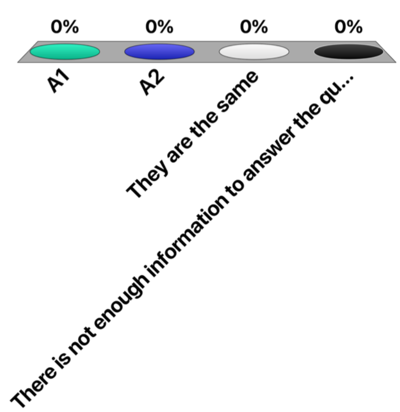
Gain(Student) = 0.94 – 0.78 = 0.16

Gain(Rating) = 0.94 – 0.89 = 0.05

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

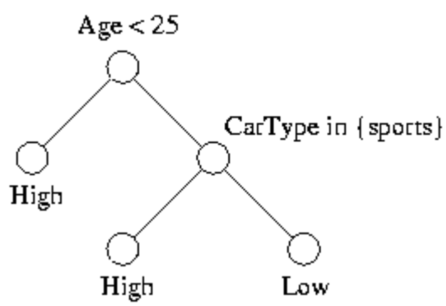
– For continuous attributes A a split is defined by val(A) < X

– 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

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

Example

Attribute List

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

Position of cursor in scan

← position 0

← position 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(P, N) = H(4, 2) =0.918

H(A) = 0 + ½ H(1, 2) =0.459

Gain = H(P, N) – H(A) = 0.459

Attribute List

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

⇒

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

Example

Attribute lists for node 0

L: rows with Tid 1, 5, 0
R: rows with Tid 4, 2, 3

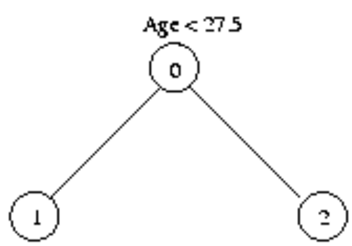
Age	Class	Tid
17	High	1
20	High	5
23	High	0
32	Low	4
43	High	2
68	Low	3

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



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

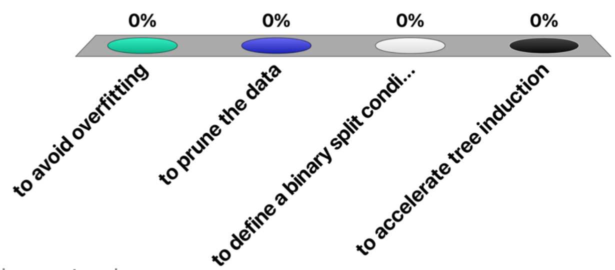
Attribute lists for node 2

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, …

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

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?

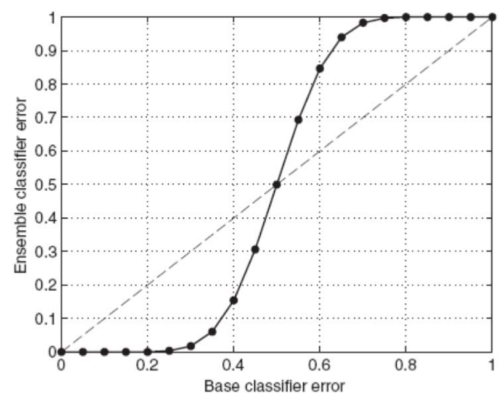
Assume there are 25 base classifiers

– Each classifier has error rate = 0.35

– Assume classifiers are independent

Probability that the ensemble classifier makes a wrong prediction

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



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

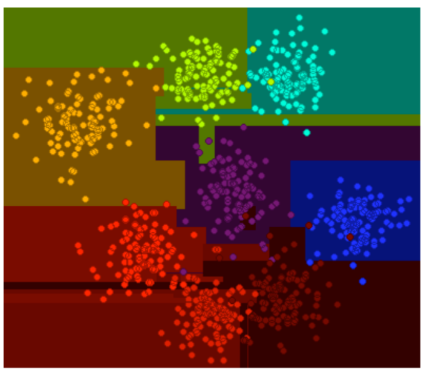
Random Forests: Algorithm

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

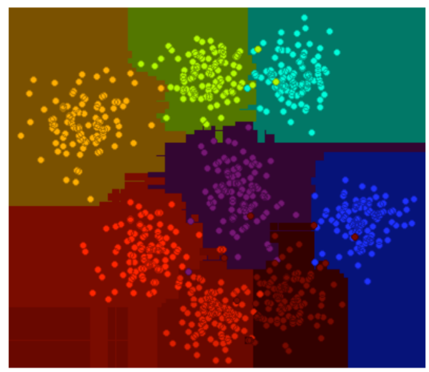
Typical parameters

- m ≈ sqrt(p), or smaller
- K ≈ 500

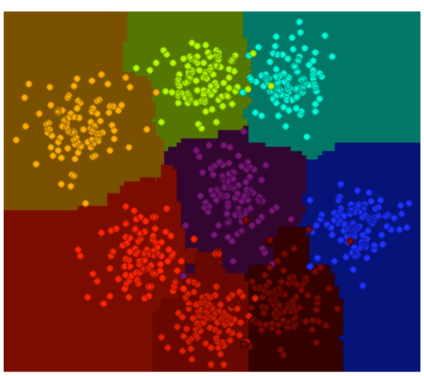
Illustration of Random Forests



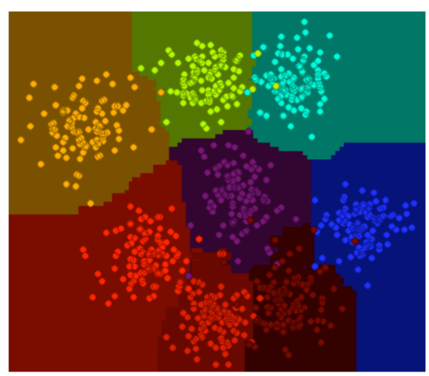
1 rCART



10 rCARTs



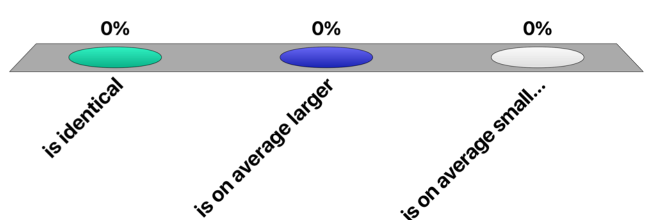
100 rCARTs



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



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.