Lecture notes

Knowledge Discovery in Databases

Summer Semester 2012

Lecture 4: Classification

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Tutorials: Erich Schubert

http://www.dbs.ifi.lmu.de/cms/Knowledge_Discovery_in_Databases_I_(KDD_I)

Sources

- Previous KDD I lectures on LMU (Johannes Aßfalg, Christian Böhm, Karsten Borgwardt, Martin Ester, Eshref Januzaj, Karin Kailing, Peer Kröger, Jörg Sander, Matthias Schubert, Arthur Zimek)
- Jiawei Han, Micheline Kamber and Jian Pei, *Data Mining: Concepts and Techniques, 3rd ed.,* Morgan Kaufmann, 2011.
- Margaret Dunham, Data Mining, *Introductory and Advanced Topics*, Prentice Hall, 2002.
- Tom Mitchel, *Machine Learning*, McGraw Hill, 1997.
- Wikipedia

Outline

- Introduction
- The classification process
- Classification (supervised) vs clustering (unsupervised)
- Decision trees
- Evaluation of classifiers
- Things you should know
- Homework/tutorial

Classification problem

Given:

- a dataset $D=\{t_1,t_2,\ldots,t_n\}$ and
- a set of classes $C=\{c_1,\ldots,c_k\}$

the classification problem is to define a mapping $f:D \rightarrow C$ where each t_i is assigned to one class c_j.

Classification

- predicts categorical (discrete, unordered) class labels
- Constructs a model (classifier) based on a training set
- Uses this model to predict the class label for new unknown-class instances

Prediction

- is similar, but may be viewed as having infinite number of classes
- more on prediction in next lectures

A simple classifier

ID	Alter	Autotyp	Risk
1	23	Familie	high
2	17	Sport	high
3	43	Sport	high
4	68	Familie	low
5	32	LKW	low

A simple classifier:

if Alter > 50 **then** Risk= low;

if Alter $\leq$ 50 **and** Autotyp=LKW **then** Risk=low;

if Alter $\leq$ 50 **and** Autotyp $\neq$ LKW **then** Risk = high.

Applications

- Credit approval
  - Classify bank loan applications as e.g. safe or risky.
- Fraud detection
  - e.g., in credit cards
- Churn prediction
  - E.g., in telecommunication companies
- Target marketing
  - Is the customer a potential buyer for a new computer?
- Medical diagnosis
- Character recognition
- …

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Classification techniques

- Typical approach:
  - Create specific model by evaluating training data (or using domain experts' knowledge).
    - Assess the quality of the model
  - Apply model developed to new data.
- Classes must be predefined!!!
- Many techniques
  - Decision trees
  - Naïve Bayes
  - kNN
  - Neural Networks
  - Support Vector Machines
  - ….

Classification technique (detailed)

- **Model construction:** describing a set of predetermined classes
  - The set of tuples used for model construction is training set
  - Each tuple/sample is assumed to belong to a predefined class, as determined by the class label attribute
  - The model is represented as classification rules, decision trees, or mathematical formulae
- **Model evaluation:** estimate accuracy of the model
  - The set of tuples used for model evaluation is test set
  - The class label of each tuple/sample in the test set is known in advance
  - The known label of test sample is compared with the classified result from the model
    - Accuracy rate is the percentage of test set samples that are correctly classified by the model
  - Test set is independent of training set, otherwise over-fitting will occur
- **Model usage:** for classifying future or unknown objects
  - If the accuracy is acceptable, use the model to classify data tuples whose class labels are not known

predefined class values

Class attribute: tenured={yes, no}

Training set

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

known class label attribute

Test set

NAME	RANK	YEARS	TENURED	PREDICTED
Maria	Assistant Prof	3	no	no
John	Associate Prof	7	yes	no
Franz	Professor	3	yes	yes

known class label attribute

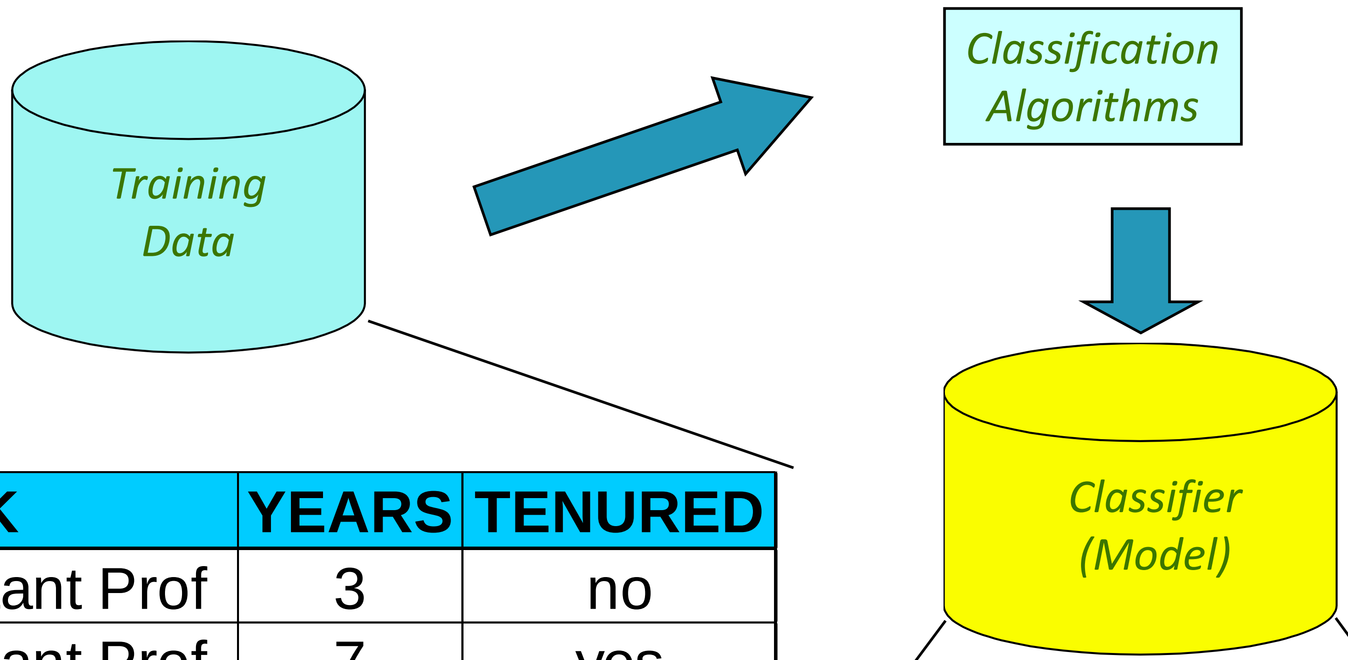
predicted class value by the model

NAME	RANK	YEARS	TENURED	PREDICTED
Jeff	Professor	4	?	yes
Patrick	Associate Prof	8	?	yes
Maria	Associate Prof	2	?	no

unknown class label attribute

predicted class value by the model

Model construction



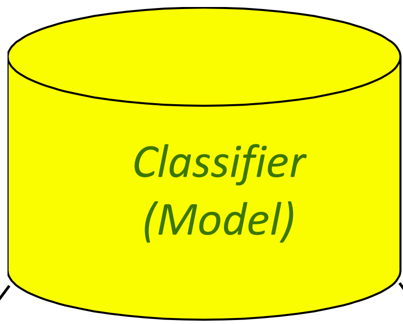
NAME	RANK	YEARS	TENURED
Mike	Assistant Prof	3	no
Mary	Assistant Prof	7	yes
Bill	Professor	2	yes
Jim	Associate Prof	7	yes
Dave	Assistant Prof	6	no
Anne	Associate Prof	3	no

Attributes *Class attribute*

IF rank = 'professor' OR years > 6
THEN tenured = 'yes'

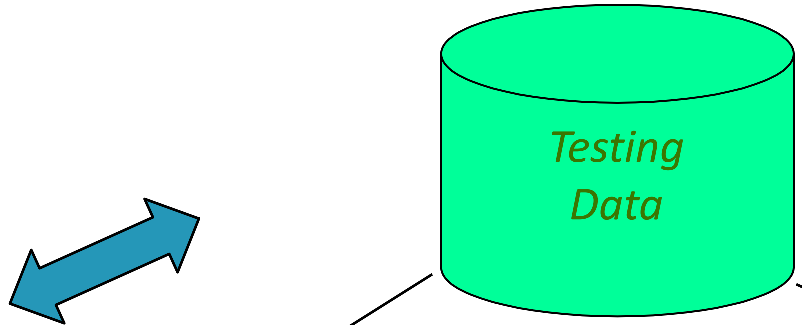
IF (rank!='professor') AND (years < 6)
THEN tenured = 'no'

Model evaluation



*IF rank = 'professor' OR years > 6
THEN tenured = 'yes'*

*IF (rank!='professor') AND (years < 6)
THEN tenured = 'no'*



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

Classifier quality
Is it acceptable?

Model usage for prediction

Training Data

Classification Algorithms

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

Classifier (Model)

IF (rank = 'professor') OR (years > 6) THEN tenured = 'yes'
IF (rank!='professor') AND (years < 6) THEN tenured = 'no'

Unseen Data

NAME	RANK	YEARS	TENURED
Jeff	Professor	4	?
Patrick	Assistant Profe	8	?
Maria	Assistant Profe	2	?

Tenured? → Yes

Tenured? → ?

Tenured? → ?

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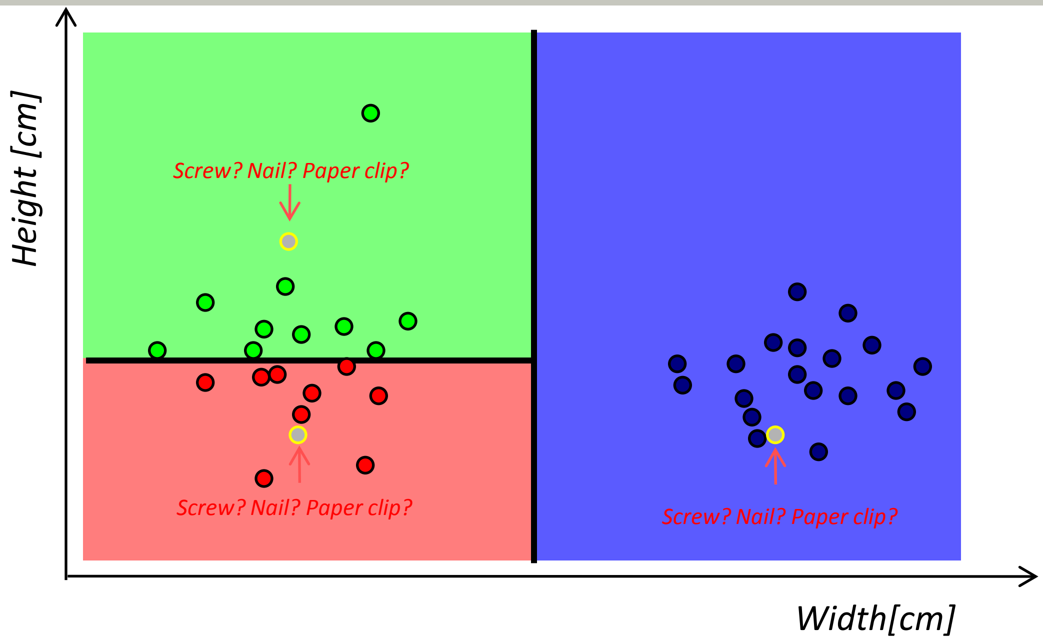
A supervised learning task

- Classification is a supervised learning task
  - Supervision: The training data (observations, measurements, etc.) are accompanied by *labels* indicating the *class* of the observations
  - New data is classified based on the training set

- Clustering is an unsupervised learning task
  - The class labels of training data is unknown
  - Given a set of measurements, observations, etc., the goal is to group the data into groups of similar data (clusters)

Supervised learning example



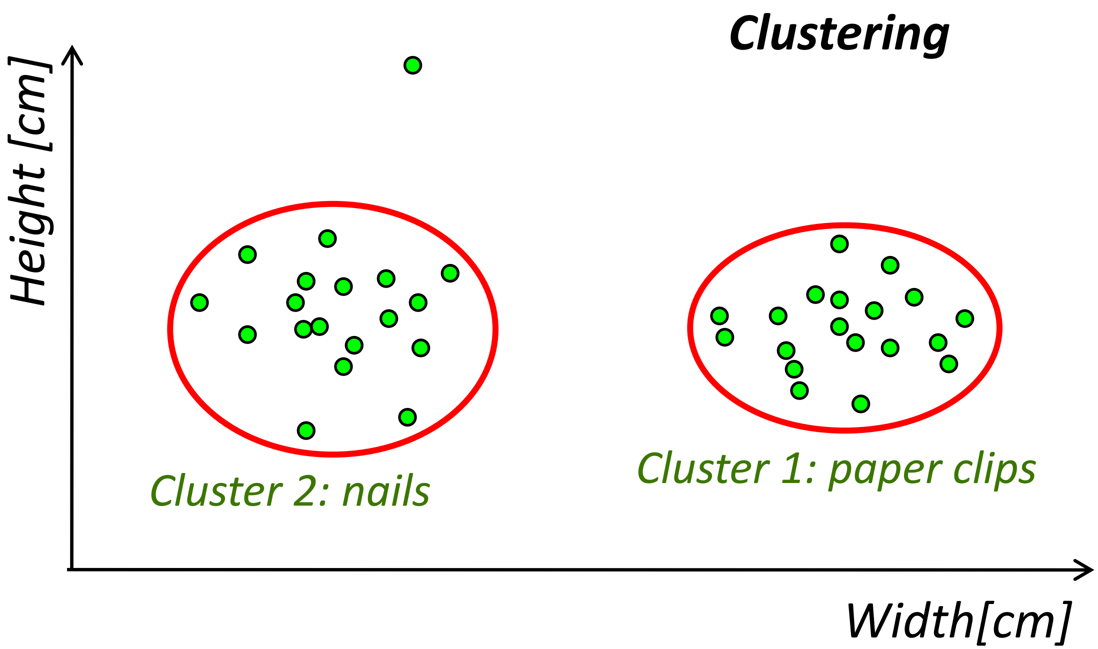
Classification model

- *Screw* 
- *Nails* 
- *Paper clips* 

- *New object (unknown class)*

Question:
What is the class of a new object???
Is it a screw, a nail or a paper clip?

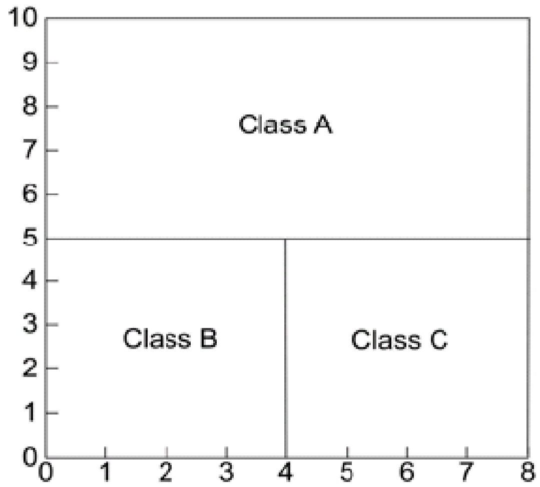
Unsupervised learning example

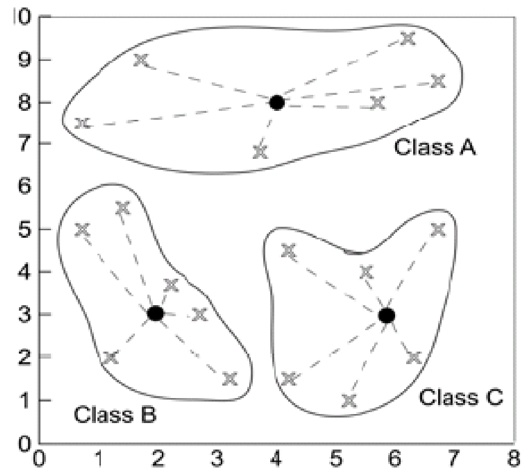


Question:
Is there any structure in data (based on their characteristics, i.e., width, height)?

Classification techniques

- Statistical methods
  - Bayesian classifiers etc
- Partitioning methods
  - Decision trees etc
- Similarity based methods
  - K-Nearest Neighbors etc





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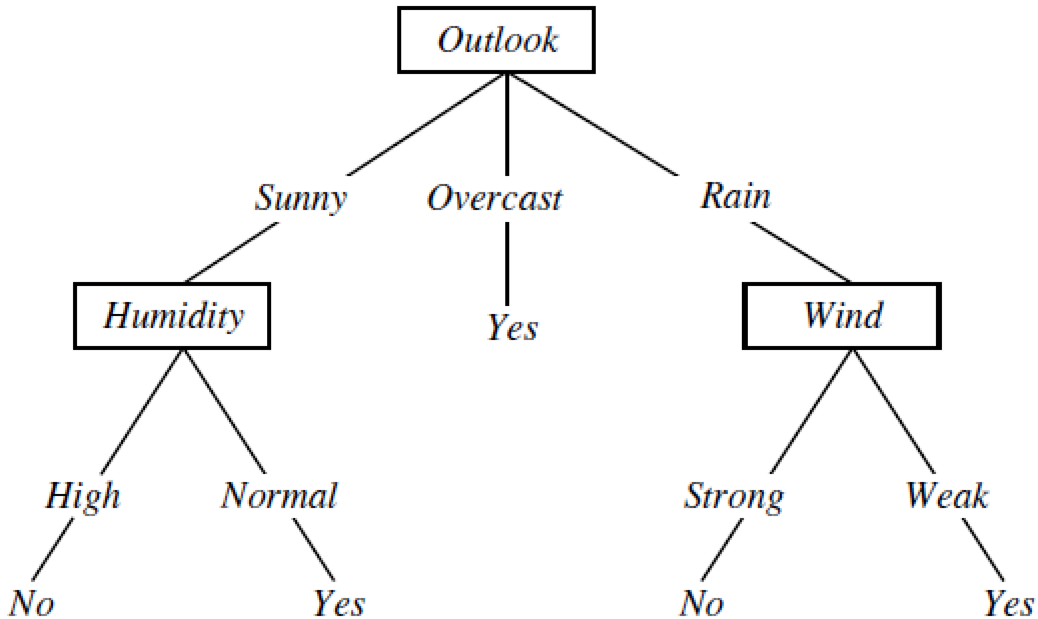
Decision trees (DTs)

- One of the most popular classification methods
- DTs are included in many commercial systems nowadays
- Easy to interpret, human readable, intuitive
- Simple and fast methods
- Partition based method: Partitions the space into rectangular regions
- Many algorithms have been proposed
  - ID3 (Quinlan 1986), C4.5 (Quinlan 1993), CART (Breiman et al 1984)….

Decision tree for the “play tennis” problem



Training set

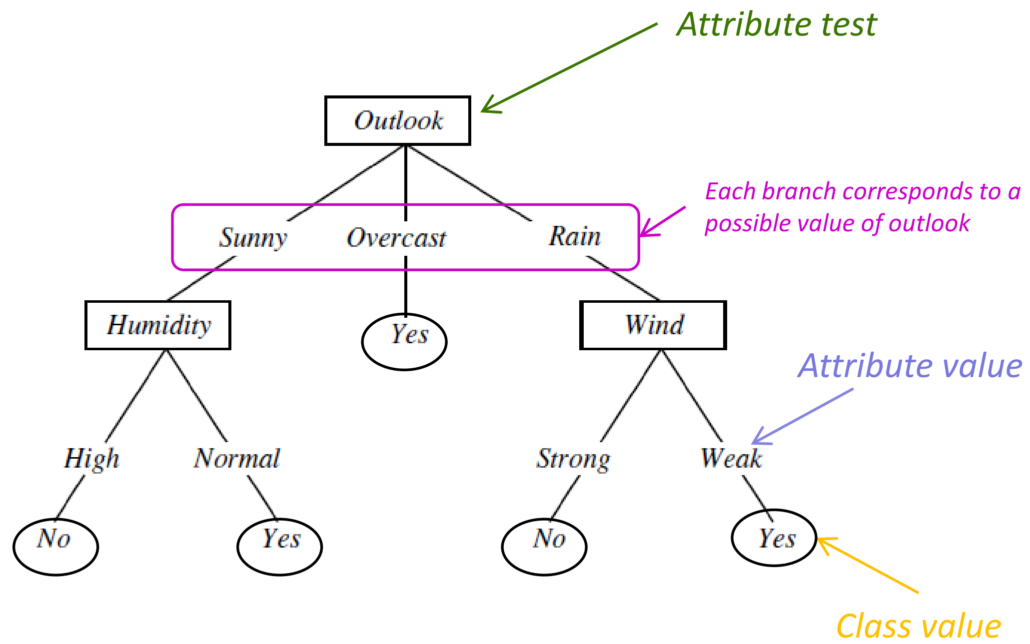
Day	Outlook	Temperature	Humidity	Wind	PlayTennis
D1	Sunny	Hot	High	Weak	No
D2	Sunny	Hot	High	Strong	No
D3	Overcast	Hot	High	Weak	Yes
D4	Rain	Mild	High	Weak	Yes
D5	Rain	Cool	Normal	Weak	Yes
D6	Rain	Cool	Normal	Strong	No
D7	Overcast	Cool	Normal	Strong	Yes
D8	Sunny	Mild	High	Weak	No
D9	Sunny	Cool	Normal	Weak	Yes
D10	Rain	Mild	Normal	Weak	Yes
D11	Sunny	Mild	Normal	Strong	Yes
D12	Overcast	Mild	High	Strong	Yes
D13	Overcast	Hot	Normal	Weak	Yes
D14	Rain	Mild	High	Strong	No

Representation

- Representation
  - Each *internal node* specifies a test of some attribute of the instance
  - Each *branch* descending from a node corresponds to one of the possible values for this attribute
  - Each *leaf node* assigns a class label
- Decision trees classify instances by sorting them down the tree from the root to some leaf node, which provides the classification of the instance

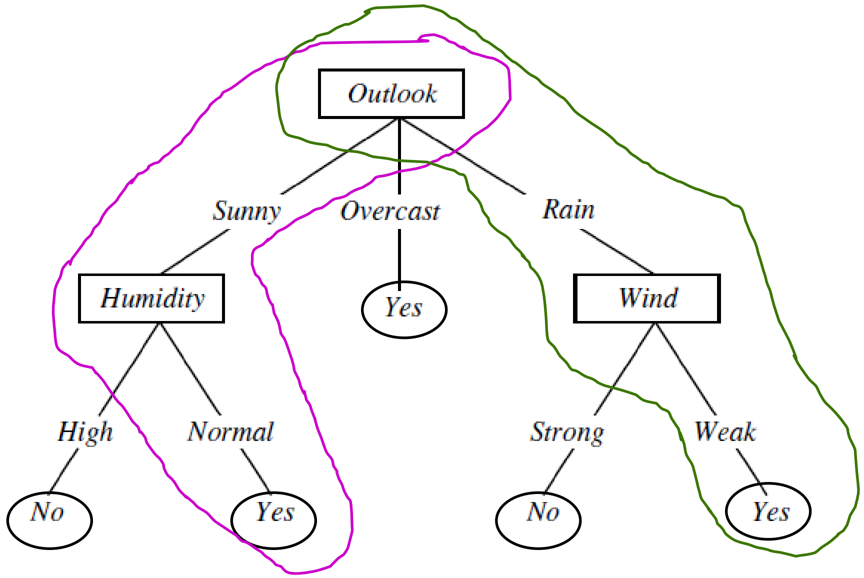
Training set

Day	Outlook	Temperature	Humidity	Wind	PlayTennis
D1	Sunny	Hot	High	Weak	No
D2	Sunny	Hot	High	Strong	No
D3	Overcast	Hot	High	Weak	Yes
D4	Rain	Mild	High	Weak	Yes
D5	Rain	Cool	Normal	Weak	Yes
D6	Rain	Cool	Normal	Strong	No
D7	Overcast	Cool	Normal	Strong	Yes
D8	Sunny	Mild	High	Weak	No
D9	Sunny	Cool	Normal	Weak	Yes
D10	Rain	Mild	Normal	Weak	Yes
D11	Sunny	Mild	Normal	Strong	Yes
D12	Overcast	Mild	High	Strong	Yes
D13	Overcast	Hot	Normal	Weak	Yes
D14	Rain	Mild	High	Strong	No



Representation cont'

- Decision trees represent a disjunction of conjunctions of constraints on the attribute values of the instances
- Each path from the root to a leaf node, corresponds to a conjunction of attribute tests
- The whole tree corresponds to a disjunction of these conjunctions
- We can "translate" each path into IF-THEN rules (human readable)



IF ((Outlook = Sunny) ^ (Humidity = Normal)),
THEN (Play tennis=Yes)

IF ((Outlook = Rain) ^ (Wind = Weak)),
THEN (Play tennis=Yes)

The basic decision tree learning algorithm

Basic algorithm (ID3, Quinlan 1986)

- Tree is constructed in a top-down recursive divide-and-conquer manner
- At start, all the training examples are at the root node
- The question is “which attribute should be tested at the root?”
  - Attributes are evaluated using some statistical measure, which determines how well each attribute alone classifies the training examples
  - The best attribute is selected and used as the test attribute at the root
- For each possible value of the test attribute, a descendant of the root node is created and the instances are mapped to the appropriate descendant node.
- The procedure is repeated for each descendant node, so instances are partitioned recursively.

When do we stop partitioning?

- All samples for a given node belong to the same class
- There are no remaining attributes for further partitioning – *majority voting* is employed for classifying the leaf

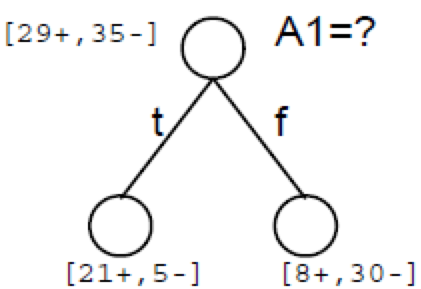
Algorithm cont'

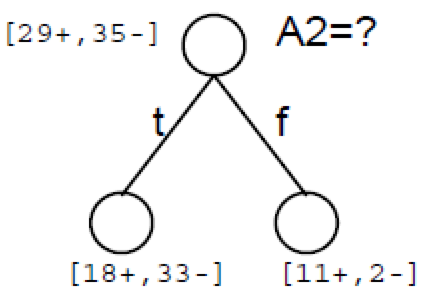
- Pseudocode

Main loop:

1. $A \leftarrow$ the "best" decision attribute for next *node*
2. Assign A as decision attribute for *node*
3. For each value of A, create new descendant of *node*
4. Sort training examples to leaf nodes
5. If training examples perfectly classified, Then STOP, Else iterate over new leaf nodes

- But, …. which attribute is the best?





- The goal is to select the attribute that is most *useful* for classifying examples.
- By useful we mean that the resulting partitioning is as *pure* as possible
- A partition is *pure* if all its instances belong to the same class.

Attribute selection measure: Information gain

- Used in ID3
- It uses entropy, a measure of pureness of the data
- The information gain Gain(S,A) of an attribute A relative to a collection of examples S measures the gain reduction in S due to splitting on A:

$$Gain(S,A) = \boxed{Entropy(S)} - \boxed{\sum_{v \in Values(A)} \frac{|S_v|}{|S|} Entropy(S_v)}$$

Before splitting

After splitting on A

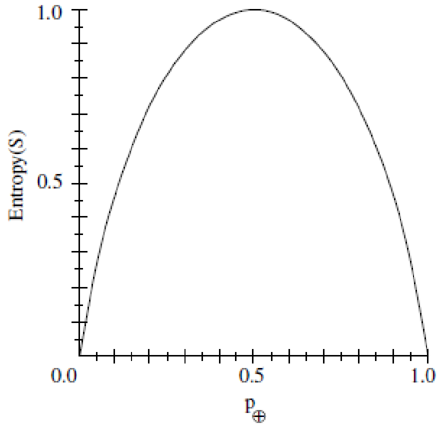
- Gain measures the expected reduction in entropy due to splitting on A

- The attribute with the higher entropy reduction is chosen

Entropy

- Let S be a collection of positive and negative examples for a binary classification problem, C={+, -}.
- p_+: the percentage of positive examples in S
- p_-: the percentage of negative examples in S
- Entropy measures the impurity of S:

$$Entropy(S) = -p_+ \log_2(p_+) - p_- \log_2(p_-)$$



- Examples :
  - Let S: [9+,5-] $Entropy(S) = -\frac{9}{14}\log_2(\frac{9}{14}) - \frac{5}{14}\log_2(\frac{5}{14}) = 0.940$
  - Let S: [7+,7-] $Entropy(S) = -\frac{7}{14}\log_2(\frac{7}{14}) - \frac{7}{14}\log_2(\frac{7}{14}) = 1$
  - Let S: [14+,0-] $Entropy(S) = -\frac{14}{14}\log_2(\frac{14}{14}) - \frac{0}{14}\log_2(\frac{0}{14}) = 0$

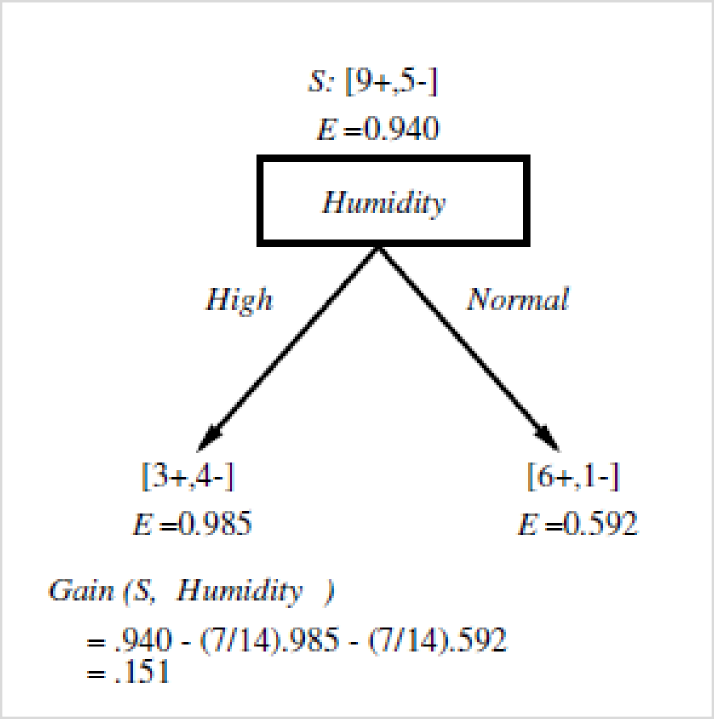
in the general case (k-classification problem)

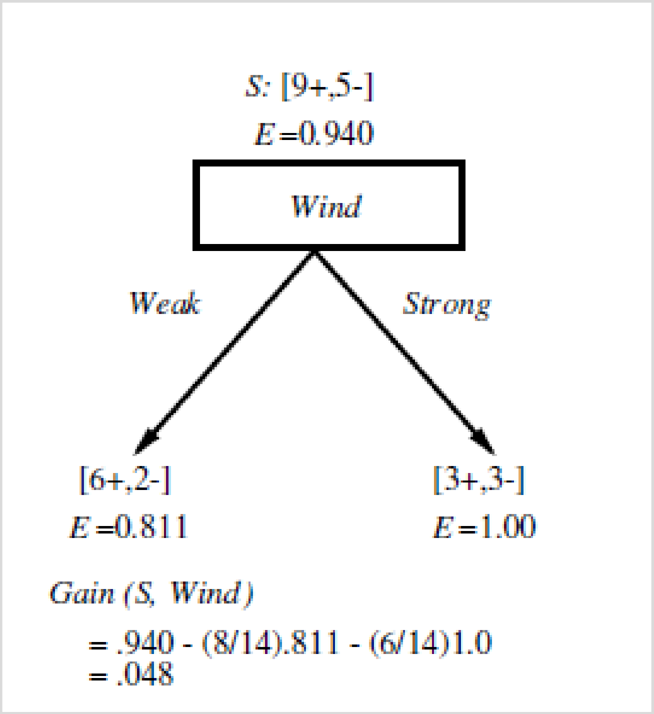
$$Entropy(S) = \sum_{i=1}^{k} - p_i \log_2(p_i)$$

- Entropy = 0, when all members belong to the same class
- Entropy = 1, when there is an equal number of positive and negative examples

Information Gain example 1

Which attribute to choose next???





Information Gain example 2

Training set

Day	Outlook	Temperature	Humidity	Wind	PlayTennis
D1	Sunny	Hot	High	Weak	No
D2	Sunny	Hot	High	Strong	No
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D4	Rain	Mild	High	Weak	Yes
D5	Rain	Cool	Normal	Weak	Yes
D6	Rain	Cool	Normal	Strong	No
D7	Overcast	Cool	Normal	Strong	Yes
D8	Sunny	Mild	High	Weak	No
D9	Sunny	Cool	Normal	Weak	Yes
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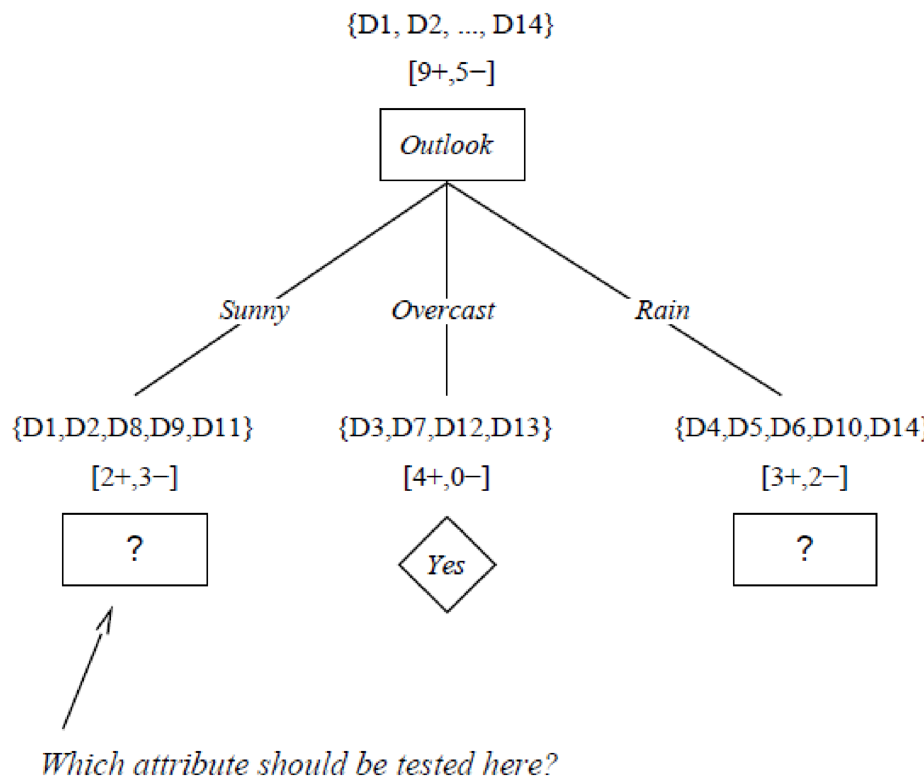


$S_{sunny} = \{D1, D2, D8, D9, D11\}$

$Gain\ (S_{sunny}, Humidity) = .970 - (3/5)\ 0.0 - (2/5)\ 0.0 = .970$

$Gain\ (S_{sunny}, Temperature) = .970 - (2/5)\ 0.0 - (2/5)\ 1.0 - (1/5)\ 0.0 = .570$

$Gain\ (S_{sunny}, Wind) = .970 - (2/5)\ 1.0 - (3/5)\ .918 = .019$

Attribute selection measure: Gain ratio

- Information gain is biased towards attributes with a large number of values
  - Consider the attribute ID (unique identifier)
- C4.5 (a successor of ID3) uses gain ratio to overcome the problem, which normalizes the gain

•High split info: partitions have more or less the same size (uniform)
• Low split info: few partitions hold most of the tuples (peaks)

$$\mathrm{GainRatio}(S,A) = \frac{\mathrm{Gain}(S,A)}{\mathrm{SplitInformation}(S,A)}$$

Measures the information w.r.t. classification

Measures the information generated by splitting S into |Values(A)| partitions

$$SplitInformation(S,A) = -\sum_{v \in Values(A)} \frac{|S_v|}{|S|} \times \log_2\left(\frac{|S_v|}{|S|}\right)$$

- Example:
  - Humidity={High, Low}
  - Wind={Weak, Strong}
  - Outlook = {Sunny, Overcast, Rain}

$$SplitInformation(S,Humidity) = -\frac{7}{14} \times \log_2\left(\frac{7}{14}\right) - \frac{7}{14} \times \log_2\left(\frac{7}{14}\right) = 1$$

$$SplitInformation(S,Wind) = -\frac{8}{14} \times \log_2\left(\frac{8}{14}\right) - \frac{6}{14} \times \log_2\left(\frac{6}{14}\right) = 0.9852$$

$$SplitInformation(S,Outlook) = -\frac{5}{14} \times \log_2\left(\frac{5}{14}\right) - \frac{4}{14} \times \log_2\left(\frac{4}{14}\right) - \frac{5}{14} \times \log_2\left(\frac{5}{14}\right) = 1.5774$$

- The attribute with the maximum gain ratio is selected as the splitting attribute

Attribute selection measure: Gini Index (CART)

- Let a dataset S containing examples from k classes. Let p_j be the probability of class j in S. The Gini Index of S is given by:

$$Gini(S) = 1 - \sum_{j=1}^{k} p_j^2$$

- Gini index considers a binary split for each attribute
- If S is split based on attribute A into two subsets S_1 and S_2:

$$Gini(S, A) = \frac{|S_1|}{|S|} Gini(S_1) + \frac{|S_2|}{|S|} Gini(S_2)$$

- Reduction in impurity:

$$\Delta Gini(S, A) = Gini(S) - Gini(S, A)$$

- The attribute A that provides the smallest $Gini(S,A)$ (or the largest reduction in impurity) is chosen to split the node
- How to find the binary splits?
  - For discrete-valued attributes, we consider all possible subsets that can be formed by values of A
  - For numerical attributes, we find the split points (slides 41-42)

Gini index example

Let S has 9 tuples in buys_computer = "yes" and 5 in "no"

$$gini(S) = 1 - \left(\frac{9}{14}\right)^2 - \left(\frac{5}{14}\right)^2 = 0.459$$

Suppose the attribute income partitions S into 10 in S_1: {low, medium} and 4 in S_2

$$\begin{aligned} gini_{income \in \{low, medium\}}(D) &= \left(\frac{10}{14}\right) Gini(D_1) + \left(\frac{4}{14}\right) Gini(D_1) \\ &= \frac{10}{14}(1 - (\frac{6}{10})^2 - (\frac{4}{10})^2) + \frac{4}{14}(1 - (\frac{1}{4})^2 - (\frac{3}{4})^2) \\ &= 0.450 \\ &= Gini_{income \in \{high\}}(D) \end{aligned}$$

The Gini Index measures of the remaining partitions for the income attribute:

$$Gini_{\{low, high\} and \{medium\}}(D) = 0.315$$

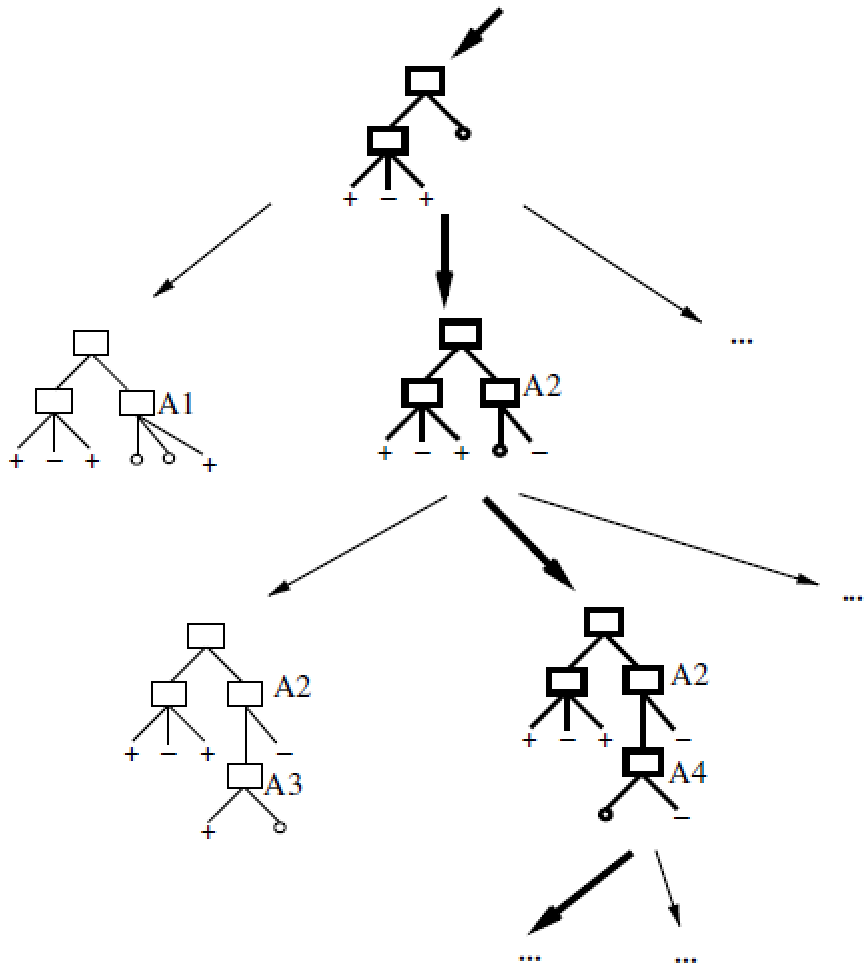
$$Gini_{\{medium, high\} and \{low\}}(D) = 0.300$$

So, the best binary split for income is on {medium, high} and {low}

Comparing Attribute Selection Measures

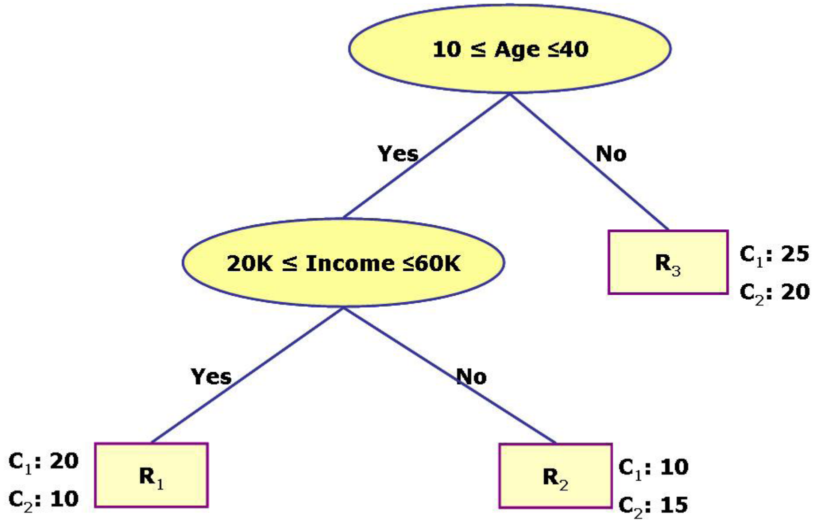
- The three measures, are commonly used and in general, return good results but
  - Information gain Gain(S,A):
    - biased towards multivalued attributes
  - Gain ratio GainRatio(S,A) :
    - tends to prefer unbalanced splits in which one partition is much smaller than the others
  - Gini index:
    - biased to multivalued attributes
    - has difficulty when # of classes is large
    - tends to favor tests that result in equal-sized partitions and purity in both partitions
- Several other measures exist

Hypothesis search space (by ID3)

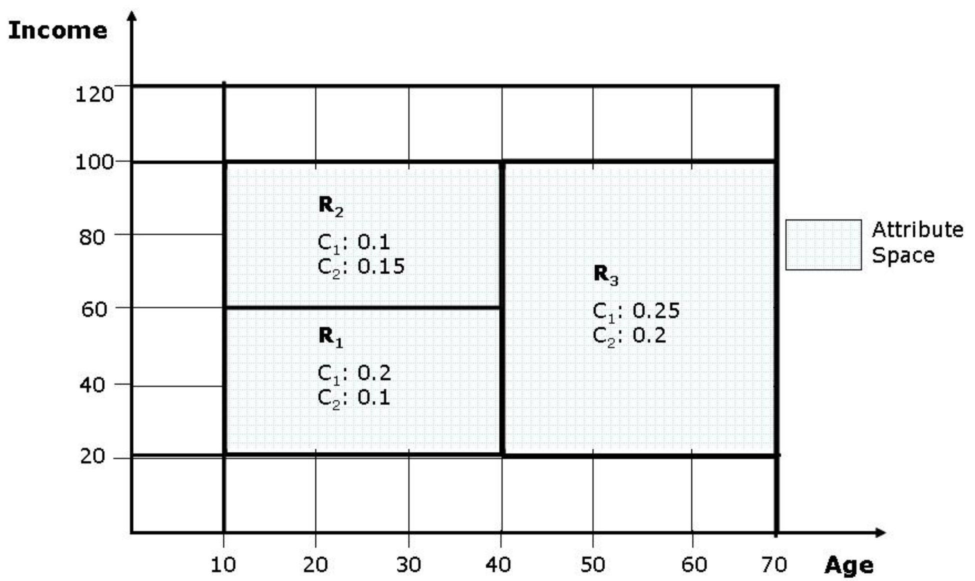


- Hypothesis space is complete
  - Solution is surely in there
- Greedy approach
- No back tracking
  - Local minima
- Outputs a single hypothesis

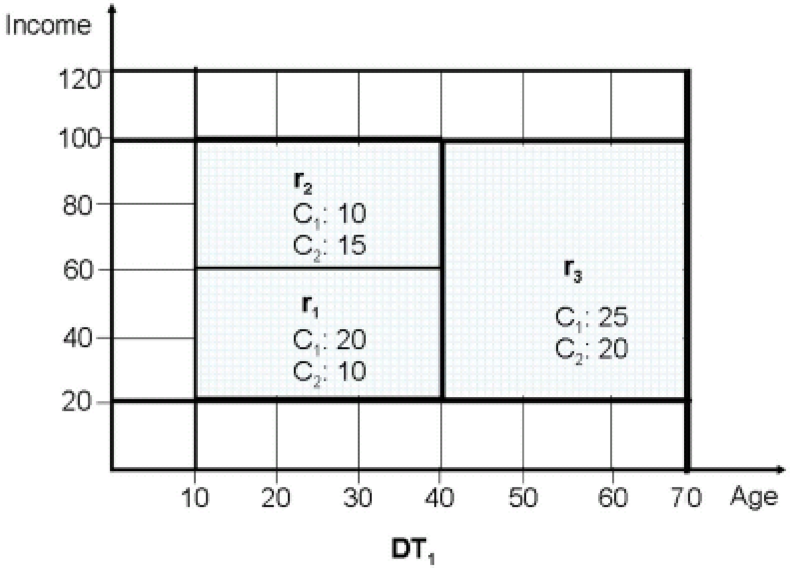
Space partitioning

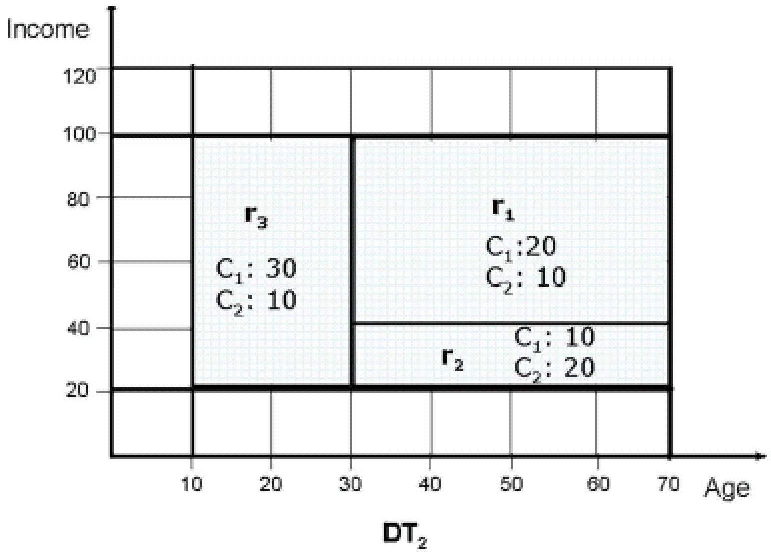


- Decision boundary: The border line between two neighboring regions of different classes
- Decision regions: Axis parallel hyper-rectangles



Comparing DTs/ partitionings





Overfitting

Consider adding a *noisy* training example D_{15} to the training set

How the earlier tree (built upon D_1-D_{14}) would be effected?

Training set

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D1	Sunny	Hot	High	Weak	No
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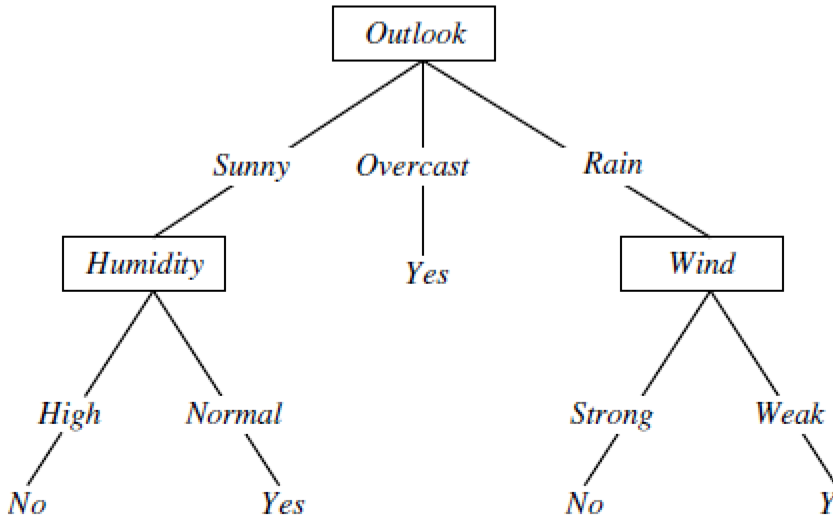
D14	Rain	Mild	High	Strong	No
D15	Sunny	Hot	Normal	Strong	No



Overfitting

- An induced tree may overfit the training data
  - Too many branches, some may reflect anomalies due to noise or outliers
  - Poor accuracy for unseen samples

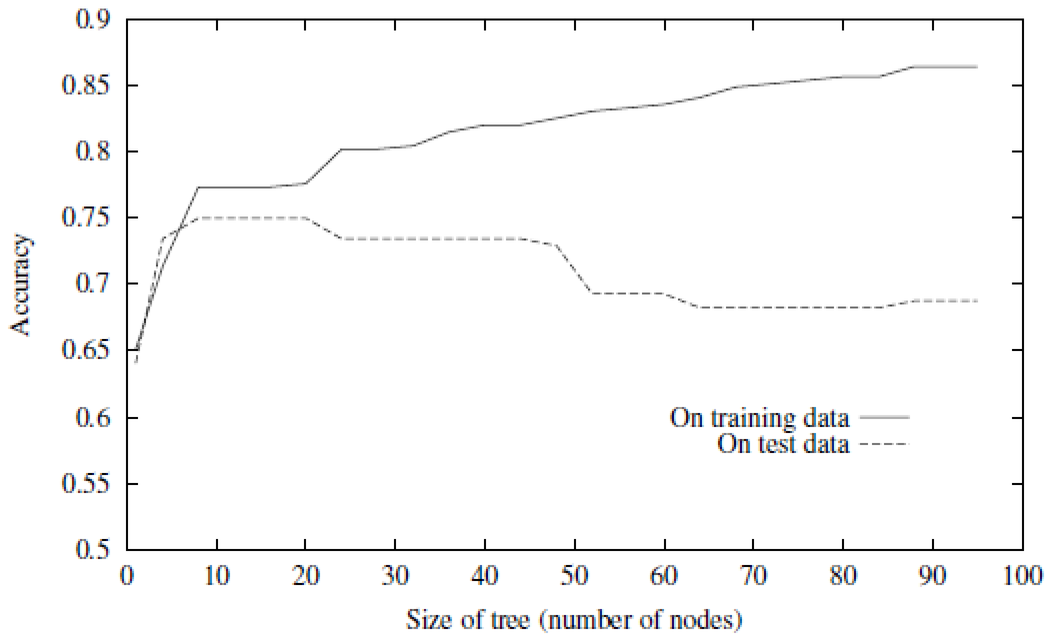
- Overfitting: Consider an hypothesis h
  - $error_{train}(h)$: the error of h in training set
  - $error_D(h)$: the error of h in the entire distribution D of data
  - Hypothesis h overfits training data if there is an alternative hypothesis h' in H such that:

$$error_{train}(h) < error_{train}(h')$$

and

$$error_{\mathcal{D}}(h) > error_{\mathcal{D}}(h')$$

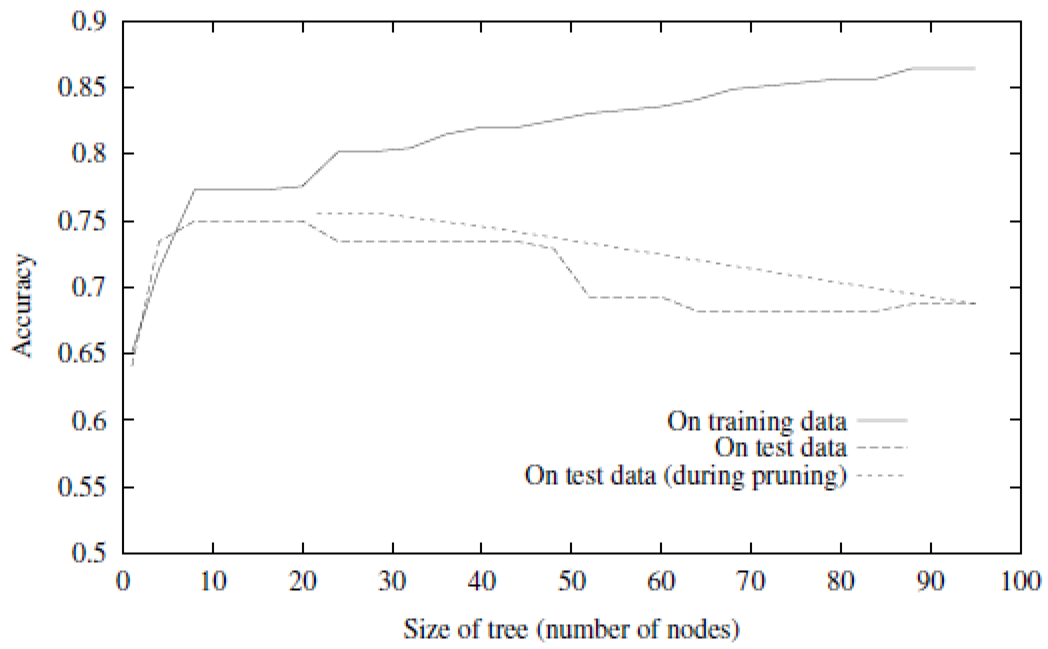
Overfitting



Avoiding overfitting

- Two approaches to avoid overfitting
  - Prepruning: Halt tree construction early—do not split a node if this would result in the goodness measure falling below a threshold
    - Difficult to choose an appropriate threshold
  - Postpruning: Remove branches from a “fully grown” tree—get a sequence of progressively pruned trees
    - Use a set of data different from the training data to decide which is the “best pruned tree”
      - Test set

Effect of prunning



Dealing with continuous-valued attributes

- Let attribute A be a continuous-valued attribute
- Must determine the *best split point* t for A, (A ≤ t)
  - Sort the value A in increasing order
  - Identify adjacent examples that differ in their target classification
    - Typically, every such pair suggests a potential split threshold t= $(a_i+a_{i+1})/2$
  - Select threshold t that yields the best value of the splitting criterion.

Temperature:	40	48	60	72	80	90
PlayTennis:	No	No	Yes	Yes	Yes	No

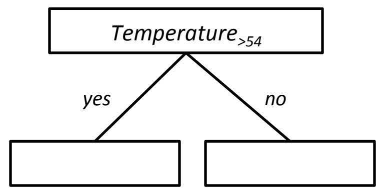
t=(48+60)/2=54 *t =(80+90)/2=85*

2 potential thresholds:Temperature$_{>54}$, *Temperature* $_{>85}$
Compute the attribute selection measure (e.g. information gain) for both
Choose the best (Temperature$_{>54}$ *here)*

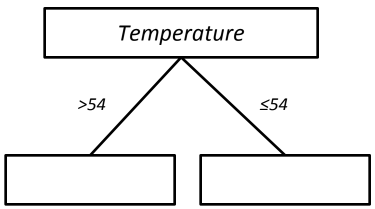
Continuous-valued attributes cont’

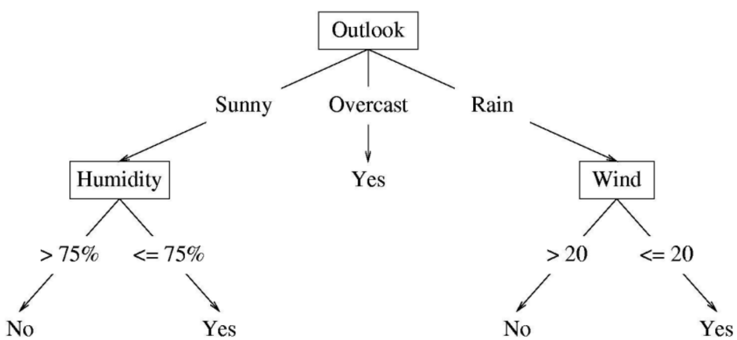
- Let t be the threshold chosen from the previous step
- Create a boolean attribute based on A and threshold t with two possible outcomes: yes, no
  - S_1 is the set of tuples in S satisfying (A >t), and S_2 is the set of tuples in S satisfying (A ≤ t)

How it looks



or





An example of a tree for the play tennis problem when attributes Humidity and Wind are continuous

When to consider decision trees

- Instances are represented by attribute-value pairs
  - Instances are represented by a fixed number of attributes, e.g. outlook, humidity, wind and their values, e.g. (wind=strong, outlook =rainy, humidity=normal)
  - The easiest situation for a DT is when attributes take a small number of disjoint possible values, e.g. wind={strong, weak}
  - There are extensions for numerical attributes also, e.g. temperature, income.
- The class attribute has discrete output values
  - Usually binary classification, e.g. {yes, no}, but also for more class values, e.g. {pos, neg, neutral}
- The training data might contain errors
  - DTs are robust to errors: both errors in the class values of the training examples and in the attribute values of these examples
- The training data might contain missing values
  - DTs can be used even when some training examples have some unknown attribute values

Outline

- Introduction
- The classification process
- Classification (supervised) vs clustering (unsupervised)
- Decision trees
- Evaluation of classifiers
- Things you should know
- Homework/tutorial

Classifier evaluation

- The quality of a classifier is evaluated over a *test set*, different from the training set
- For each instance in the test set, we know its true class label
- Compare the predicted class (by some classifier) with the true class of the test instances
- Terminology
  - Positive tuples: tuples of the main class of interest
  - Negative tuples: all other tuples

- A useful tool for analyzing how well a classifier performs is the *confusion matrix*
- For an m-class problem, the matrix is of size m x m
- An example of a matrix for a 2-class problem:

Predicted class

Actual class

	C_1	C_2	totals
C_1	TP (true positive)	FN (false negative)	P
C_2	FP(false positive)	TN (true negative)	N
Totals	P'	N'	

Classifier evaluation measures

	C_1	C_2	totals
C_1	TP (true positive)	FN (false negative)	P
C_2	FP(false positive)	TN (true negative)	N
Totals	P'	N'	

- Accuracy/ Recognition rate:
  % of test set instances correctly classified

$$accuracy(M) = \frac{TP + TN}{P + N}$$

classes	buy_computer = yes	buy_computer = no	total	recognition(%)
buy_computer = yes	6954	46	7000	
buy_computer = no	412	2588	3000	
total	7366	2634	10000	95.42

- Error rate/ Missclassification rate: error_rate(M)=1-accuracy(M)

$$accuracy(M) = \frac{FP + FN}{P + N}$$

- More effective when the class distribution is relatively balanced

Classifier evaluation measures cont'

	C_1	C_2	totals
C_1	TP (true positive)	FN (false negative)	P
C_2	FP(false positive)	TN (true negative)	N
Totals	P'	N'	

If classes are imbalanced:

- Sensitivity/ True positive rate/ recall:
  % of positive tuples that are correctly recognized

$$sensitivity(M) = \frac{TP}{P}$$

- Specificity/ True negative rate : % of negative tuples that are correctly recognized

$$specificity(M) = \frac{TN}{N}$$

classes	buy_computer = yes	buy_computer = no	total	recognition(%)
buy_computer = yes	6954	46	7000	99.34
buy_computer = no	412	2588	3000	86.27
total	7366	2634	10000	95.42

Classifier evaluation measures cont'

	C_1	C_2	totals
C_1	TP (true positive)	FN (false negative)	P
C_2	FP(false positive)	TN (true negative)	N
Totals	P'	N'	

- Precision: % of tuples labeled as positive which are actually positive

$$precision(M) = \frac{TP}{TP + FP}$$

- Recall: % of positive tuples labeled as positive

$$recall(M) = \frac{TP}{TP + FN} = \frac{TP}{P}$$

  – Precision does not say anything about misclassified instances
  – Recall does not say anything about possible instances from other classes labeled as positive

- F-measure/ F_1 score/F-score combines both

$$F(M) = \frac{2 * precision(M) * recall(M)}{precision(M) + recall(M)}$$

It is the harmonic mean of precision and recall

- F_β-measure is a weighted measure of precision and recall

$$F_\beta(M) = \frac{(1+\beta^2) * precision(M) * recall(M)}{\beta^2 * precision(M) + recall(M)}$$

Common values for β:
β=2
β=0.5

Classifier evaluation methods

- Holdout method
  - Given data is randomly partitioned into two independent sets
    - Training set (e.g., 2/3) for model construction
    - Test set (e.g., 1/3) for accuracy estimation
  - It takes no longer to compute (+)
  - It depends on how data are divided (-)
  - Random sampling: a variation of holdout
    - Repeat holdout k times, accuracy is the avg accuracy obtained

Classifier evaluation methods cont'

- Cross-validation (*k*-fold cross validation, k = 10 usually)
  - Randomly partition the data into *k mutually exclusive* subsets $D_1, \ldots, D_k$ each approximately equal size
  - Training and testing is performed k times
    - At the *i*-th iteration, use D_i as test set and others as training set
  - Accuracy is the avg accuracy over all iterations
  - Does not rely so much on how data are divided (+)
  - The algorithm should re-run from scratch k times (-)

  - Leave-one-out: k folds where k = #of tuples, so only one sample is used as a test set at a time; for small sized data

  - Stratified cross-validation: folds are stratified so that class distribution in each fold is approximately the same as that in the initial data
    - Stratified 10 fold cross-validation is recommended

Classifier evaluation methods cont'

- Bootstrap: Samples the given training data uniformly with replacement
  - i.e., each time a tuple is selected, it is equally likely to be selected again and re-added to the training set
  - Works well with small data sets
- Several boostrap methods, and a common one is .632 boostrap
  - Suppose we are given a data set of #d tuples.
  - The data set is sampled #d times, with replacement, resulting in a training set of #d samples (also known as *bootstrap sample*):
    - It is very likely that some of the original tuples will occur more than once in this set
  - The data tuples that did not make it into the training set end up forming the test set.
  - On average, 36.8 of the tuples will not be selected for training and thereby end up in the test set; the remaining 63.2 will form the train test
    - Each sample has a probability 1/d of being selected and (1-1/d) of not being chosen. We repeat d times, so the probability for a tuple to not be chosen during the whole period is $(1-1/d)^d$.
    - For large d: $\left(1-\frac{1}{n}\right)^n \approx e^{-1} \approx 0.368$
  - Repeat the sampling procedure k times, report the overall accuracy of the model:

$$acc(M) = \sum_{i=1}^{k} (0.632 \times acc(M_i)_{test\_set} + 0.368 \times acc(M_i)_{train\_set})$$

Accuracy of the model obtained by bootstrap sample i when it is applied on test set i.

Accuracy of the model obtained by bootstrap sample i when it is applied over all cases

Classifier evaluation summary

- Accuracy measures
  - accuracy, error rate, sensitivity, specificity, precision, F-score, F_β
- Other parameters
  - Speed (construction time, usage time)
  - Robustness to noise, outliers and missing values
  - Scalability for large data sets
  - Interpretability from humans

Things you should know

- What is classification
- Class attribute, attributes
- Train set, test set, new unknown instances
- Supervised vs unsupervised
- Decision tree induction algorithm
- Choosing the best attribute for splitting
- Overfitting
- Dealing with continuous attributes
- Evaluation of classifiers

Homework/ Tutorial

Tutorial: No tutorial this Thursday (Christi Himmelfahrt)

- Repeat exercises from the previous tutorials
- Get familiar with Weka/ Elki/ R/ SciPy.

Homework:

- Run decision tree classification in Weka
- Implement a decision tree classifier ☺

Suggested reading:

- Han J., Kamber M., Pei J. *Data Mining: Concepts and Techniques 3rd ed., Morgan Kaufmann, 2011* (Chapter 8)
- Tom Mitchel, *Machine Learning*, McGraw Hill, 1997 (Chapter 3)