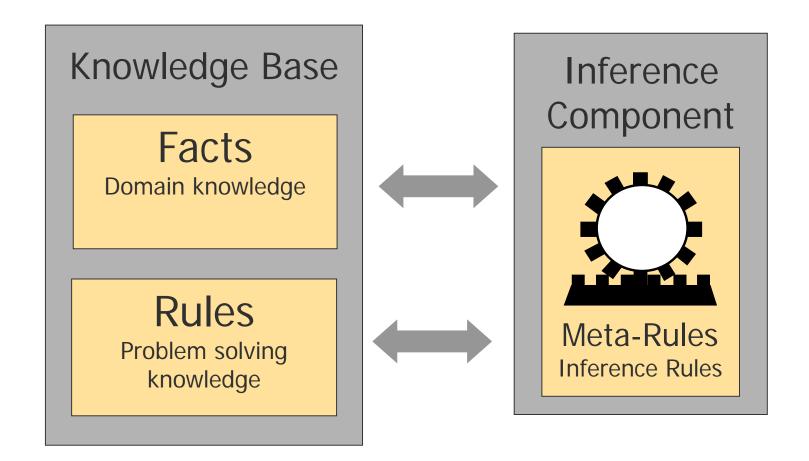
Machine Learning: Learning Rules

Knut Hinkelmann



Knowledge-Based Systems (Rules & Facts)



Creating Knowledge Bases

- Manual: Human experts build rules
 - Rules are often redundant, incomplete, inconsistent or inefficient
 - This is also called Knowledge Engineering
- Machine Learning: automatic derivation of rules from example data
 - this is also called Data Mining or Rule Induction



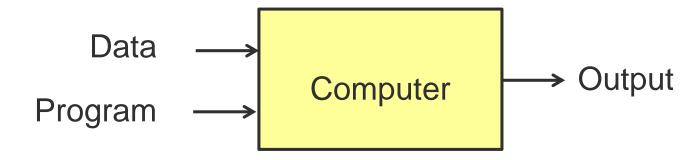
What is Machine Learning?

- Determine rules from data/facts
- Improve performance with experience
- Getting computers to program themselves
- ...

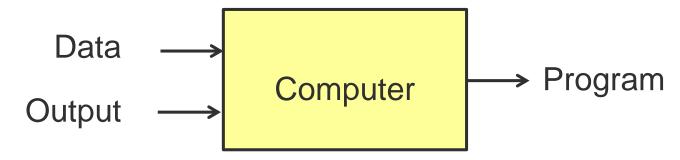


Machine Learning vs. Programming

Computer Application



Machine Learning

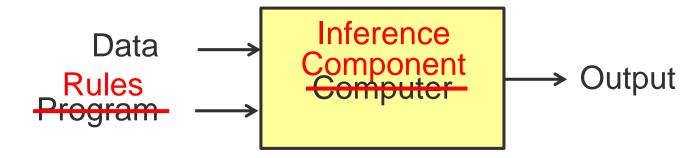


Prof. Dr. Knut Hinkelmann Learning Decision Trees

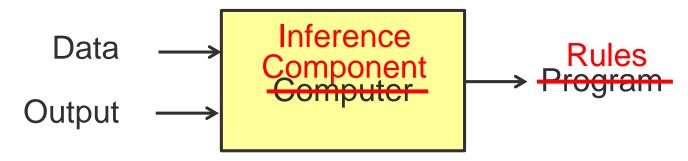


Machine Learning vs. Knowledge-based Systems

Knowledge-based System



Machine Learning





Source: Vibhav Gogate, UT Dallas



Types of Learning

- Supervised learning
 - Solutions/classes for examples are known
 - Criteria for classes are learned
- Unsupervised
 - No prior knowledge
 - classes have to be determined
- Reinforcement
 - occasional rewards



Classification



Task

Assign individuals to known classes

Examples:

credit assessment

Individuals: customers of a bank

Classes: credit worthy

not credit worthy

quality check

Individuals: products

Classes: ok

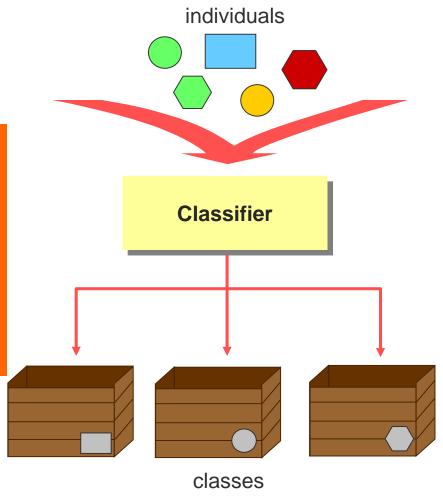
rework defective

optical character recognition (OCR)

Individuals: scan (pixel image)
Classes: ASCII characters



Supervised Learning: Classification Criteria



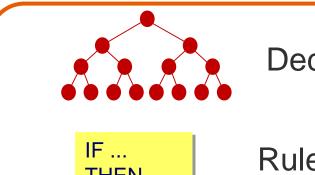
- The classifier decides, which individual belongs to which class
- The classifier is a model of the application
 - The classifier codifies the relevant criteria for the classification: class definitions
- Problems:
 - The criteria for the decision are not always obvious
 - The creation of a classifier requires knowledge and effort
- Learning:
 - Learn the classification criteria from known examples



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Classification Methods



Decision Trees

Rules



Neuronale Netze



k-Nearest Neighbor



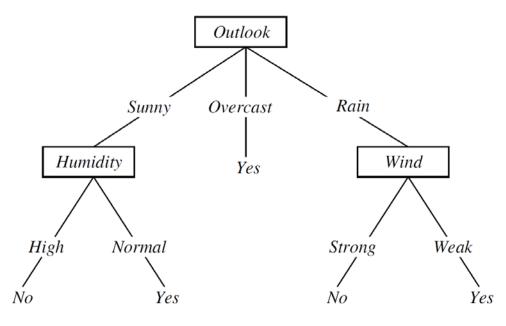
Genetic Algorithms





Decision Trees

Example: Decision tree for playing tennis

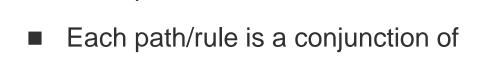


- Decision trees are primarily used for classification
- Decision trees represent classification rules
- Decision tree representation:
 - Each internal node tests an attribute
 - Each branch corresponds to attribute value
 - Each leaf node assigns a classification
- Decision trees classify instances by sorting them down the tree from the root to some leaf node,

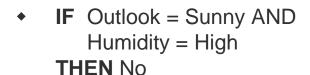




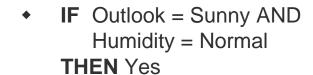
Decision Trees represent Rules



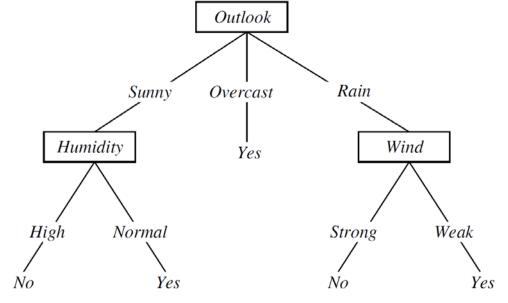
Each path from root to a leaf is a rule



attribute tests:



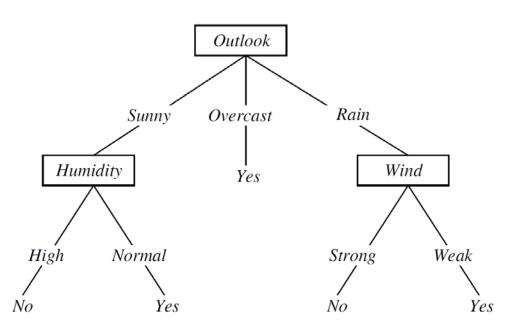
- IF Outlook = OvercastTHEN Yes
- IF Outlook = Rain AND
 Wind = Strong
 THEN No
- IF Outlook = Rain AND Wind = WeakTHEN Yes







Decision Trees represent Rules



- If the classes are boolean, a path can be regarded as a conjunction of attribute tests.
- The tree itself is a disjunction of these conjunctions

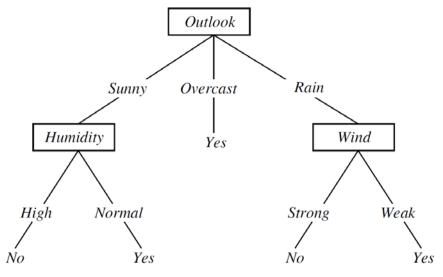
```
( Outlook = Sunny \land Humidity = Normal ) \lor ( Outlook = Overcast ) \lor ( Outlook = Rain \land Wind = Weak )
```





Example: Decision Tree – Decision Table

The decision tree can be represented as a decision table.



Playing Tennis				
	Outlook	Humidity	Wind	Tennis
	Sunny,Overcast, Rain	High, Normal	Strong,Weak	Yes, No
1	Sunny	High		No
2	Sunny	Normal		Yes
3	Overcast			Yes
4	Rain		Strong	No
5	Rain		Weak	Yes

Learning Rules / Decision Trees

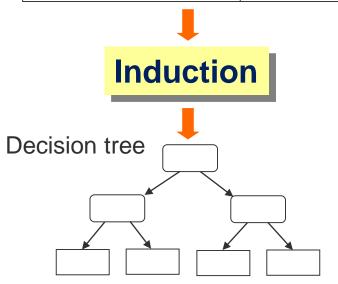
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Learning Decision Trees by Induction



independent			dependent
		•••	
	•••	•••	



Induction = Generalisation from examples





Example

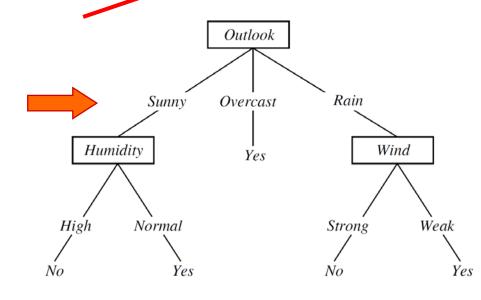
The dependent variable "Tennis" determines if the weather is good for

tennis ("Yes") or not ("No").

Training Data

Element	Outlook	Temperature	e Humidity	Wind	Tennis
1	Sunny	Hot	High	Weak	No
2	Sunny	Hot	High	Strong	No
3	Overcast	Hot	High	Weak	Yes
4	Rain	Mild	High	Weak	Yes
5	Rain	Cold	Normal	Weak	Yes
6	Rain	Cold	Normal	Strong	No
7	Overcast	Cold	Normal	Strong	Yes
8	Sunny	Mild	High	Weak	No
9	Sunny	Cold	Normal	Weak	Yes
10	Rain	Mild	Normal	Weak	Yes
11	Sunny	Mild	Normal	Strong	Yes
12	Overcast	Mild	High	Strong	Yes
13	Overcast	Hot	Normal	Weak	Yes
14	Rain	Mild	High	Strong	No

Naive approach: Each example data set represents a rule



Induction generalizes the data set → prediction of future case



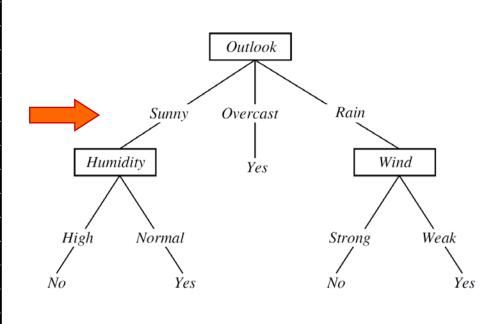


Example

The dependent variable "Tennis" determines if the weather is good for tennis ("Yes") or not ("No").

Training Data

Element	Outlook	Temperature	e Humidity	Wind	Tennis
1	Sunny	Hot	High	Weak	No
2	Sunny	Hot	High	Strong	No
3	Overcast	Hot	High	Weak	Yes
4	Rain	Mild	High	Weak	Yes
5	Rain	Cold	Normal	Weak	Yes
6	Rain	Cold	Normal	Strong	No
7	Overcast	Cold	Normal	Strong	Yes
8	Sunny	Mild	High	Weak	No
9	Sunny	Cold	Normal	Weak	Yes
10	Rain	Mild	Normal	Weak	Yes
11	Sunny	Mild	Normal	Strong	Yes
12	Overcast	Mild	High	Strong	Yes
13	Overcast	Hot	Normal	Weak	Yes
14	Rain	Mild	High	Strong	No



The result of the induction algorithms classifies the data with only three of the four attributes into the classes "Yes" and "No".

Learning Decision Trees



Discussion

What is the difference between the table with the Training Data and the Decision Table?

Element	Outlook	Temperature	Humidity	Wind	Tennis
1	Sunny	Hot	High	Weak	No
2	Sunny	Hot	High	Strong	No
3	Overcast	Hot	High	Weak	Yes
4	Rain	Mild	High	Weak	Yes
5	Rain	Cold	Normal	Weak	Yes
6	Rain	Cold	Normal	Strong	No
7	Overcast	Cold	Normal	Strong	Yes
8	Sunny	Mild	High	Weak	No
9	Sunny	Cold	Normal	Weak	Yes
10	Rain	Mild	Normal	Weak	Yes
11	Sunny	Mild	Normal	Strong	Yes
12	Overcast	Mild	High	Strong	Yes
13	Overcast	Hot	Normal	Weak	Yes
14	Rain	Mild	High	Strong	No

Playing Tennis			17	tani iv
riaying rennis				
	Outlook	Humidity	Wind	Tennis
	Sunny,Overcast, Rain	High, Normal	Strong,Weak	Yes, No
1	Sunny	High		No
2	Sunny	Normal		Yes
3	Overcast			Yes
4	Rain		Strong	No
5	Rain		Weak	Yes



Training Data vs. Decision Tables (Rules)

- Training Data could also be used as decision tables, but
 - Training data are incomplete: only a subset of all possible situations
 - Training data contain input variables, which are not necessary to determin the output
- Decision Tree shall be general, i.e. allow decisions/ predictions for unknown situations
 - Rules only consider combinations of input values, which are necessary to determine the output
 - As a consequence, the decision table does not contain variables, which are not necessary at all (e.g. playing tennis does not depend on the temperature)

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Example: Learning Decision Trees

categorical continuous

Tid	Employed	Marital Status	Taxable Income	accept
1	No	Single	125K	No
2	Yes	Married	160K	Yes
3	Yes	Single	70K	No
4	No	Married	120K	No
5	Yes	Divorced	95K	Yes
6	Yes	Married	60K	No
7	No	Divorced	220K	No
8	Yes	Single	85K	Yes
9	Yes	Married	95K	No
10	Yes	Single	90K	Yes

Decision Tree?

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Training Data

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Learning Decision Trees: Generalisation of Data

categorical continuous

Tid	Employed	Marital Status	Taxable Income	accept
1	No	Single	125K	No
2	Yes	Married	160K	Yes
3	Yes	Single	70K	No
4	No	Married	120K	No
5	Yes	Divorced	95K	Yes
6	Yes	Married	60K	No
7	No	Divorced	220K	No
8	Yes	Single	85K	Yes
9	Yes	Married	95K	No
10	Yes	Single	90K	Yes

l <mark>oyed</mark> Yes	
MarSt	
Divorced M	larried
Inc	TaxInc
> 80K ≤ 100K	∕
YES	YES
	MarSt Divorced Inc 80K ≤ 100K

Credit Worthiness				
	Employed	Marital Status	Taxable Income	Accept
	Yes, No	Single, Divorced, Married	Integer	Yes, No
1	No			No
2	Yes	Single	> 80K	Yes
3	Yes	Divorced	> 80K	Yes
4	Yes	Single	≤ 80K	No
5	Yes	Divorced	≤ 80K	No
6	Yes	Married	> 100K	Yes
7	Yes	Married	≤ 100K	No

Training Data

Model: Decision Tree/Table

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The model uses intervals instead of concrete numerical data

Predictive Model for Classification

- Given a collection of training records (*training set*)
 - Each record consists of *attributes*, one of the attributes is the *class*
 - The class is the dependent attribute, the other attributes are the independent attributes
- Find a model for the class attribute as a function of the values of the other attributes.
- Goal: to assign a class to **previously unseen records** as accurately as possible.

- Generalisation of data if training set does not cover all possible cases or data are too specific
 - → Induction

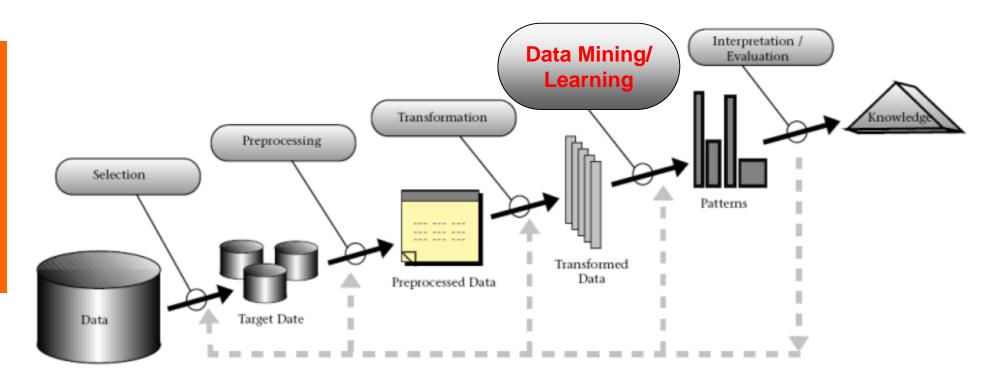


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Knowledge Discovery in Data

 Data Mining/Machine Learning is a step to discover knowledge in data



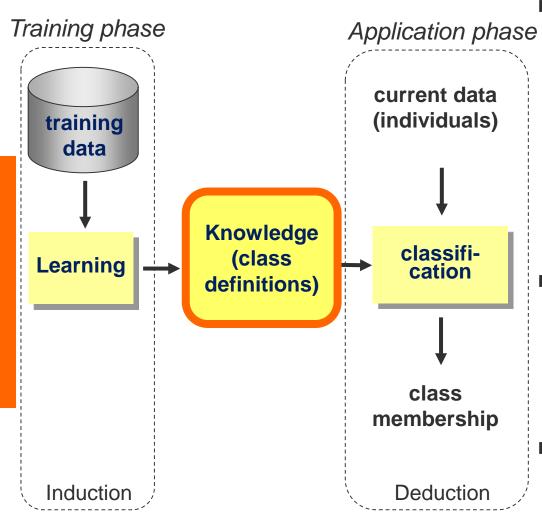
Knowledge is then used in processes and applications.

(Fayyad et al., 1996)





Training and Application Phase



- Training: Learning the criteria for the assignment of individuals to classes
 - Given: a sample set of individuals
 - described by attribute values (independent variables)
 - class membership (dependent variables)
 - Result: class definitions (decision tree, rules, model)
- Application: Assignment of individuals to classes (classification)
 - Given: Description of individuals by attribute values
 - Result: class membership
- During training the class membership is given, during application the class membership is calculated



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Induction of Decision Tree

- Enumerative approach
 - Create all possible decision trees
 - Choose the tree with the least number of questions

This approach finds the best classifying tree, but it is inefficient.

- Heuristic approach:
 - Start with an empty root and extend the tree step by step with new decision nodes
 - Stop, if the desired homogenity is achieved

This approach is efficient, but does not necessariy find the best classifying tree.





Sketch of an Induction Algorithmus

Heuristic Approach

Learning a Decision Tree

- Calculate for each attribute, how *good* it classifies the elements of the training set
- Classify with the *best* attribute
- Repeat for each resulting subtree the first two steps
- Stop this recursive process as soon as a termination condition is satisfied

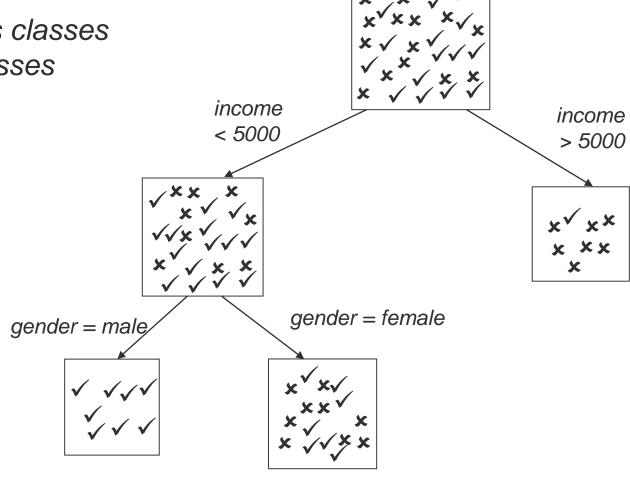
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Learning of Decision Tree

Principle: From heterogeous classes to homogeous classes





Types of Data

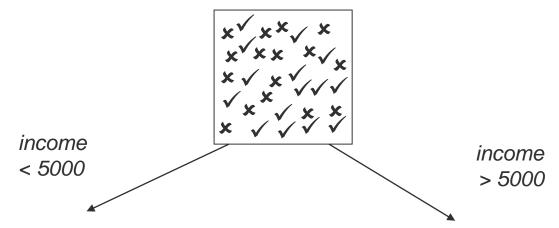
- Discrete: final number of possible values
 - Examples: marital status, gender
 - Splitting: selection of values or groups of values
- Numeric infinite number of values on which an order is defined
 - Examples: age, income
 - Splitting: determine interval boundaries

For which kind of attributes is splitting easier?





Determine how to split the Records in a Decision Tree



Attribute selection

- Which attributes separate best in which order?
 - e.g. income before marital status

■ Test condition

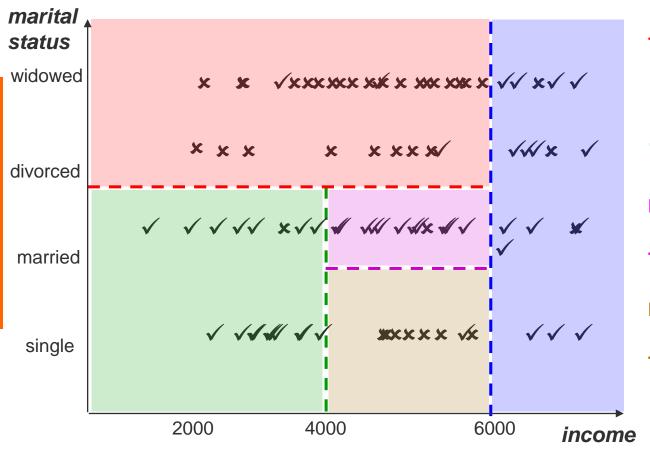
- Which values separate best?
 - select value, e.g. single or married
 - determine number: e.g. income < 5000 instead of < 6000?



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Creation of Decision Trees

Each decision divides the area in sections



IF income > 6000 THEN accept

income < 6000 and marital status = widowed or marital status = divorced

THEN reject

income < 4000 and marital status = single or marital status = married

THEN accept

income > 4000 and income < 6000 and marital status = married

THEN accept

income > 4000 and income < 6000 and marital status = single

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THEN reject



Generating Decision Trees

- ID3 is a basic decision learning algorithm.
- It recursively selects test attributes and begins with the question "which attribute should be tested at the root of the tree?"
- ID3 selects the attribute with the highest
 - Information Gain
- To calculate the information gain of an attribute one needs
 - the Entropy of a classification
 - the Expectation Value of the attribute



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ID3 Algorithm in English

The algorithm looks at each feature within the featurelist and determines which will provide the largest information gain (**X**). Once **X** is found it can be removed from the list of candidates to be considered.

A **newfeaturelist** and a **newdata_subset** are created which are subsets of the original **featurelist** and **newdata_subset** respectively (exluding feature **X**). Each possible value of the feature **X** is recursively called with the **newfeaturelist** and the narrowed down examples of **newdata_subset**, so the algorithm will continue performing the steps indicated.

The base case is reached when a **featurelist** is provided that has no features in it (so the features have been exhausted), or where the entropy is equal to 0 (there's complete certainty). For these cases, the algorithm returns a leaf node consisting of the most probable outcome.

https://computersciencesource.wordpress.com/2010/01/28/year-2-machine-learning-decision-trees-and-entropy/



feature = attribute = independent variable



Building the Decision Tree

Decision trees can be constructed using the ID3 algorithm that splits the data by the feature with the maximum information gain recursively for each branch.

```
maketree (featurelist, examples) returns
BASE CASE: if featurelist is empty, or entropy = 0
return an empty tree with leaf = majority answer in examples
RECURSION:
find the feature X with the largest information gain,
list subset = remove X from the featurelist
create an empty tree T
for each possible value 'x' of feature X
data_subset = get all examples where X = 'x'
t = maketree( list subset, data subset )
add t as a new sub-branch to T
endfor
return T
```



https://computersciencesource.wordpress.com/2010/01/28/year-2-machine-learning-decision-trees-and-entropy/

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A basic Decision Tree Learning Algorithm

ID3(Examples, Target-attribute, Attributes)

```
/* Examples: The training examples; */
/* Target-attribute:The attribute whose value is to be predicted by the tree; */
/* Attributes: A list of other attributes that may be tested by the learned decision tree. */
/* Return a decision tree that correctly classifies the given Examples */
Step 1: Create a Root node for the tree
Step 2: If all Examples are positive, Return the single-node tree Root, with label = +
Step 3: If all Examples are negative, Return the single-node tree Root, with label = -
Step 4: If Attributes is empty, Return the single-node tree Root, with label = most common value of Target-attribute in Examples
Step 5: Otherwise Begin
```

- A \leftarrow the attribute from Attributes that best (i.e., highest information gain) classifies Examples;
- The decision attribute for $Root \leftarrow A$;
- For each possible value, v_i , of A,
 - Add a new tree branch below *Root*, corresponding to the test $A=v_i$;
 - Let $Examples(v_i)$ be the subset of Examples that have value v_i for A;
 - If $Examples(v_i)$ is empty
 - * Then below this new branch add a leaf node with label = most common value of Target-attribute in Examples

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* Else below this new branch add the subtree $ID3(Examples(v_i), Target-attribute, Attributes- A))$

End

Return Root



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Entropy ("disorder")

- Entropy is a measure of unpredictability of information content.
 - The higher the information content, the lower the entropy
- The more classification information a decision tree contains, the smaller the entropy
- The goal of ID3 is to create a tree with minimal entropy



Entropy increases with increasing Equality of Distribution

- Assume there are two classes + und -
- An uninformed classifier will assign the individuals randomly to the classes + and –
- It is thus plausible, that the entropy is smaller the more the frequencies p (of +) and n (of –) for each class are different from equal distribution.
- The more unequal p and n, the smaller is the entropy





Calculation of the Entropy for binary Classification

- Assume a decision tree which classifies the training set into to classes + (positive) and – (negative)
- The entropy is calculated by

Entropy (S) =
$$-p + * log_2 (p+) - p- * log_2 (p-)$$

S = p + n is the number of all elements

p frequency of elements of class +

n frequency of elements of class -

p+=p/S and p-=n/S are the relative frequencies, i.e. the proportions of values of classes + and –



Entropy Calculation for different Distributions

■ The more different p and n, the lower is the entropy

p	n	p+	<i>Id(p+)</i>	p-	Id(p-)	Entropy(p+n)
7	7	0.5	-1	0.5	-1	1
6	8	0.43	-1.22	0.57	-0.81	0.99
5	9	0.36	-1.49	0.64	-0.64	0.94
4	10	0.29	-1.81	0.71	-0.49	0.86
3	11	0.21	-2.22	0.79	-0.35	0.75
2	12	0.14	-2.81	0.86	-0.22	0.59
1	13	0.07	-3.81	0.93	-0.11	0.37

 $Id = log_2$ (logarithmus dualis)

Id(0) cannot be calculated, but for p = 0 or n = 0 no classification is necessary





Expectation Value

The expectation value measures the information, which is needed for classification with attribute A



Expectation Value

- Let A be an attribute with m possible values v₁, ..., v_i, ... v_m
 - Values(A) is the set of all possible values for attribute A
 - S_v is the subset of S for which attribute A has value v
- The attribute A divides the elements into m partitions (subtrees)
- Entropy(S_v) = entropy of the subtree created by the attribute value v with respect to the classification (entropy for p and n)
- Expectation Value EV_A of the required information for the classification of the root attribute A

$$EV(A) := \sum_{v \in Values(A)} \frac{|S_v|}{|S|} Entropy(S_v)$$

■ The expectation value is the weighted average of the entropies of the subtrees created by v_i





Information Gain

- The information gain measures how well a given attribute A separates the training examples according to their target classification.
- The information gain is calculated by subtracting the expectation value of the subtrees created by A from the entropy of the tree with root A

$$GAIN(S, A) = Entropy(S) - EV(A)$$

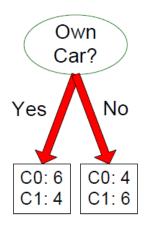
$$= Entropy(S) - \left(\sum_{v \in Values(A)} \frac{|S_v|}{|S|} Entropy(S_v)\right)$$

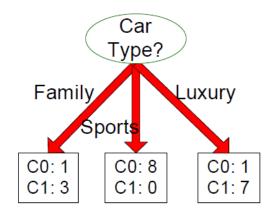


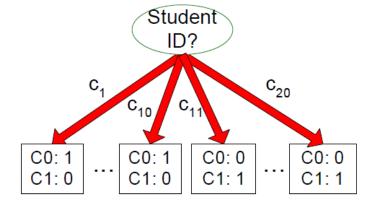


Exercise

Before Splitting: 10 records of class 0, 10 records of class 1







Which test condition is the best?

Thanks to Nadeem Qaisar Mehmood

ID3: Information Gain for Attribute Selection

ID3 uses the Information Gain to select the test attribute

On each level of the tree select the attribute with the highest information gain

- The recursive calculation of the attributes stops when either
 - all partitions contain only positive or only negative elements or
 - a user-defined threshold is achieved



Computing Entropy: Example

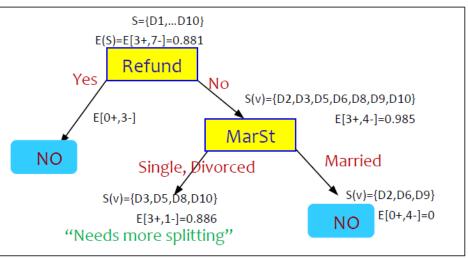
Tid	Refund	Marital Status	Taxable Income	Cheat
D1	Yes	Single	125K	No
D2	No	Married	100K	No
D3	No	Single	70K	No
D4	Yes	Married	120K	No
D5	No	Divorced	95K	Yes
D6	No	Married	60K	No
D7	Yes	Divorced	220K	No
D8	No	Single	85K	Yes
D9	No	Married	75K	No
D10	No	Single	90K	Yes

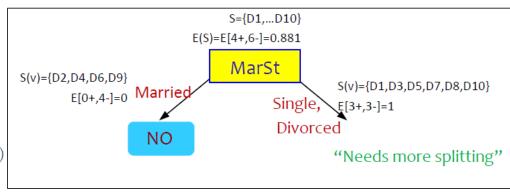
Training Data (S)

 $E(S)=E[3+,7-]=-(3/10)\log(3/10)-(7/10)\log(7/10)$

 $=-(0.3)\log(0.3)-(0.7)\log(0.7)$

=0.881





[Tan&Steinbach's "Intro to Data Mining"]

Thanks to Nadeem Qaisar Mehmood





Get Information Gain using Entropy

- Measures Reduction in Entropy achieved because of the split.
- Choose the split that achieves most reduction in entropy

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

☐ Gain (S,Refund)

$$=0.881-\{(3/10)(0)+(7/10)(0.985)\}$$

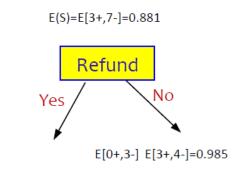
=0.1915

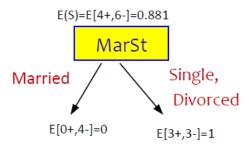
☐ Gain(S, MarStatus)

$$=0.881-\{(4/10)(0)+(6/10)(1)\}$$

=0.281

Since with marital status provides more gain, therefore in this case it will be the root node.





Thanks to Nadeem Qaisar Mehmood

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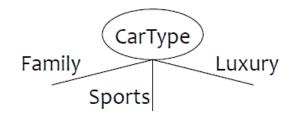
How to specify Attribute Test Conditions

Specification of the test condition depends on

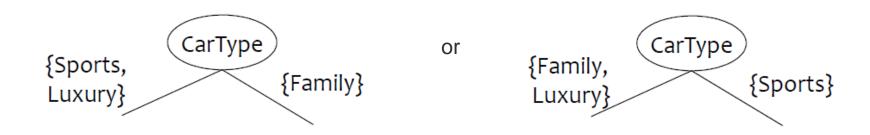
- attribute types
 - **Nominal**
 - **Ordinal**
 - Continuous
- number of ways to split
 - 2-way split
 - Multi-way split

Splitting for Nominal Attributes

Multi-way split: Use as many partitions as distinct values.

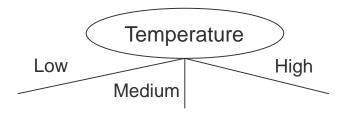


Binary split: Divides values into two subsets. Need to find optimal partitioning.

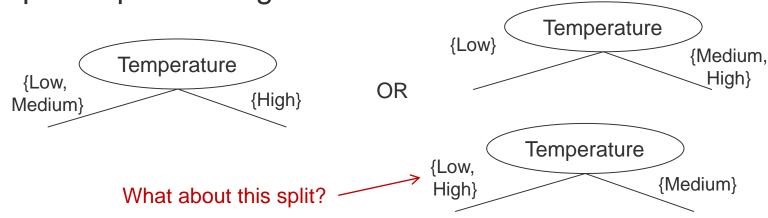


Splitting for Ordinal Attributes

Multi-way split: Use as many partitions as distinct values.



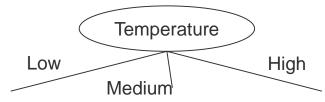
 Binary split: Divides values into two subsets. Need to find optimal partitioning.



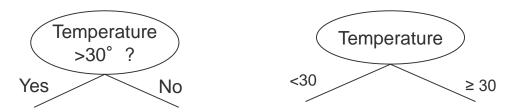


Splitting for Continuous Attributes

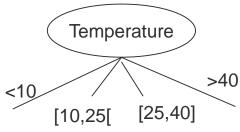
- Different ways of handling
 - Discretization to form an ordinal categorical attribute



Binary Decision: (A < v) or (A ≥ v)



Multi-way Split: Intervals

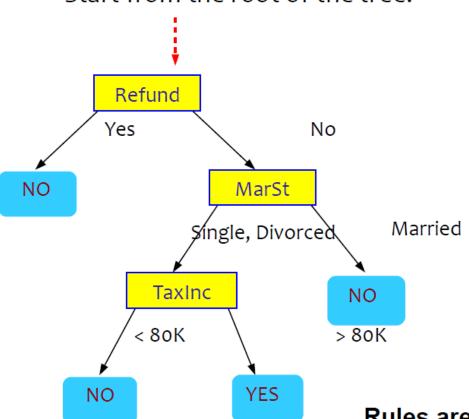


considering all possible splits and finding the best cut can be computing intensive



Decision Tree represented in Rules form

Start from the root of the tree.



Classification Rules

(Refund=Yes) ==> No

(Refund=No, Marital Status={Single,Divorced}, Taxable Income<80K) ==> No

(Refund=No, Marital Status={Single,Divorced}, Taxable Income>80K) ==> Yes

(Refund=No, Marital Status={Married}) ==> No

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Rules are mutually exclusive and exhaustive
Rule set contains as much information as the tree



Preference for Short Trees

- Preference for short trees over larger trees, and for those with high information gain attributes near the root
- Occam's Razor: Prefer the simplest hypothesis that fits the data.
- Arguments in favor:
 - a short hypothesis that fits data is unlikely to be a coincidence
 - compared to long hypothesis
- Arguments opposed:
 - There are many ways to define small sets of hypotheses



Overfitting

- When there is noise in the data, or when the number of training examples is too small to produce a representative sample of the true target function, the rule set (hypothesis) overfits the training examples!!
- Consider error of hypothesis h over
 - training data: errortrain(h)
 - entire distribution D of data: errorD(h)
- Hypothesis h OVERFITS training data if there is an alternative hypothesis h0 such that
 - errortrain(h) < errortrain(h0)
 - errorD(h) > errorD(h0)



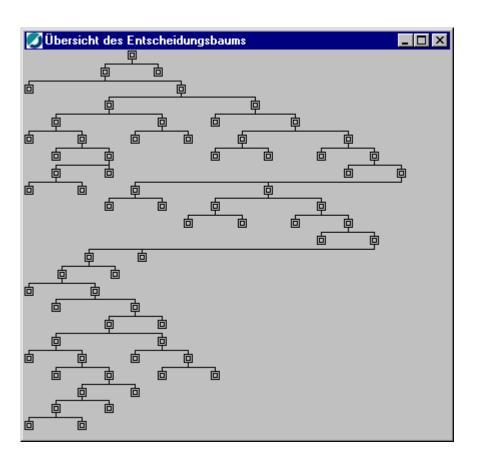
Avoiding Overfitting by Pruning

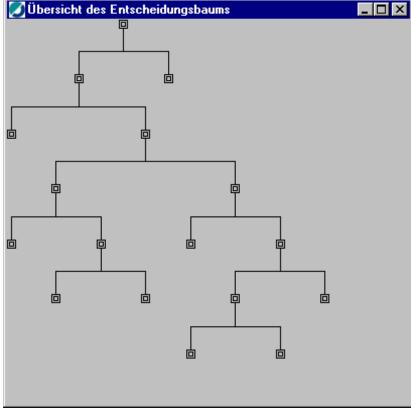
- The classification quality of a tree can be improved by cutting weak branches
- Reduced error pruning
 - remove the subtree rooted at that node,
 - make it a leaf,
 - assign it the most common classification of the training examples afiliated with that node.
- To test accuracy, the data are separated in training set and valication set. Do until further pruning is harmful:
 - Evaluate impact on validation set of pruning each possible node
 - Greedily remove the one that most improves validation set accuracy



Pruning

These figures shoe the structure of a decision tree before and after pruning







Training and Validation

Attrib1 Attrib2 Attrib3 Class Yes 125K Large No 2 No Medium 100K No 3 Small 70K No No 4 Yes Medium 120K No No Large 95K Yes No Medium 60K No No Yes Large 220K No Small 85K Yes No Medium 75K No No Small 90K Yes

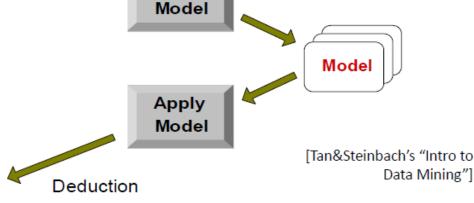
Training Set

Tid	Attrib1	Attrib2	Attrib3	Class
11	No	Small	55K	?
12	Yes	Medium	80K	?
13	Yes	Large	110K	?
14	No	Small	95K	?
15	No	Large	67K	?

Test Set

Usually, the given data set is divided into

- training set (used to build the model)
- 2. test set (used to validate it)
 The *test set* is used to determine the accuracy of the model.



Learning

algorithm

Learn

Induction



Generalisations

- Multiple Classes
 - Although the examples had only two classes, decision tree learning can be done also for more than two classes
 - Example: Quality
 - okay, rework, defective
- Probability
 - The examples only had Boolean decisions
 - Example: **IF** income > 5000 and age > 30 **THEN** creditworthy
 - Generalisation: Probabilties for classification
 - Example: **IF** income > 5000 and age > 30 **THEN** creditworthy with probability 0.92



Algorithms for Decision Tree Learning

- Examples os algorithms for learning decision trees
 - C4.5 (successor of ID3, predecessor of C5.0)
 - CART (Classification and Regression Trees)
 - CHAID (CHI-squared Automatic Interaction Detection)
- A comparison 1) of various algorithms showed that
 - the algorithms are similar with respect to classification performance
 - pruning increases the performance
 - performance depends on the data and the problem.

¹⁾ D. Michie, D.J. Spiegelhalter und C.C. Taylor: Machine Learning, Neural and Statistical Classificaiton, Ellis Horwood 199