Sapienza University of Rome

Master in Artificial Intelligence and Robotics
Master in Engineering in Computer Science

Machine Learning

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3. Decision Trees

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Overview

- Decision tree representation
- ID3 learning algorithm
- Entropy, Information gain
- Inductive Bias
- Overfitting and pruning

References
T. Mitchell. Machine Learning. Chapter 3

Concept Learning as search

Problem: Given a training set D for a target function c, compute consistent hypotheses wrt D.

Solution approach

- Define hypothesis space H
- Implement an algorithm to search $h \in H$ that are consistent with D

Decision Trees

Hypothesis space: set of decision trees.

Definition

Given an instance space X formed by values coming from a set of attributes, a *decision tree* is a tree with the following characteristics:

- Each internal node tests an attribute
- Each branch denotes a value of an attribute
- Each leaf node assigns a classification value

Example *PlayTennis*

Instances $X = Outlook \times Temperature \times Humidity \times Wind$
tuples of attributes

$$Outlook = \{Sunny, Overcast, Rain\}$$

$$Temperature = \{Hot, Mild, Cold\}$$

$$Humidity = \{Normal, High\}$$

$$Wind = \{Weak, Strong\}$$

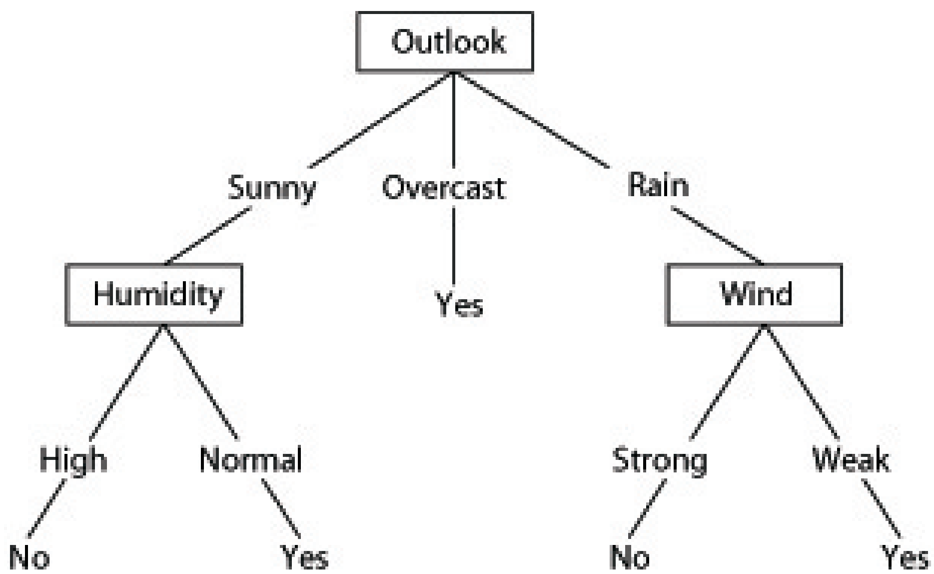
Classification values:

$$PlayTennis = \{Yes, No\}$$

Example *PlayTennis*: Training data

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

Decision Tree for *PlayTennis*



Decision Tree for *PlayTennis*

Decision trees represent a disjunction of conjunctions of constraints on the attribute values of instances.

$$(Outlook = Sunny \wedge Humidity = Normal) \quad \vee$$
$$(Outlook = Overcast) \quad \vee$$
$$(Outlook = Rain \wedge Wind = Weak)$$

Disjunction of conjunctions of all the paths to positive (true) leaf nodes.

Converting a Tree to Rules

A rule is generated for each path to a leaf node.

IF $(Outlook = Sunny) \wedge (Humidity = High)$
THEN $PlayTennis = No$

IF $(Outlook = Sunny) \wedge (Humidity = Normal)$
THEN $PlayTennis = Yes$

...

Decisions are made explicit.

ID3 Algorithm

Input: *Examples*, *Target_attribute*, *Attributes*
Output: *Decision Tree*

1. Create a *Root* node for the tree
2. **if** all *Examples* are positive, **then** return the node *Root* with label $+$
3. **if** all *Examples* are negative, **then** return the node *Root* with label $-$
4. **if** *Attributes* is empty, **then** return the node *Root* with label = most common value of *Target_attribute* in *Examples*
5. Otherwise ...

ID3 Algorithm

5. Otherwise
    - $A \leftarrow$ the "best" decision attribute for *Examples*
    - Assign A as decision attribute for *Root*
    - For each value v_i of A
      - add a new branch from *Root* corresponding to the test $A = v_i$
      - $Examples_{v_i}$ = subset of *Examples* that have value v_i for A
      - **if** $Examples_{v_i}$ is empty **then** add a leaf node with label = most common value of *Target_attribute* in *Examples*
      - **else**
        add the tree ID3($Examples_{v_i}$, *Target_attribute*, *Attributes*$-\{A\}$)

Which is the best attribute to choose?

Information gain measures how well a given attribute separates the training examples according to their target classification.

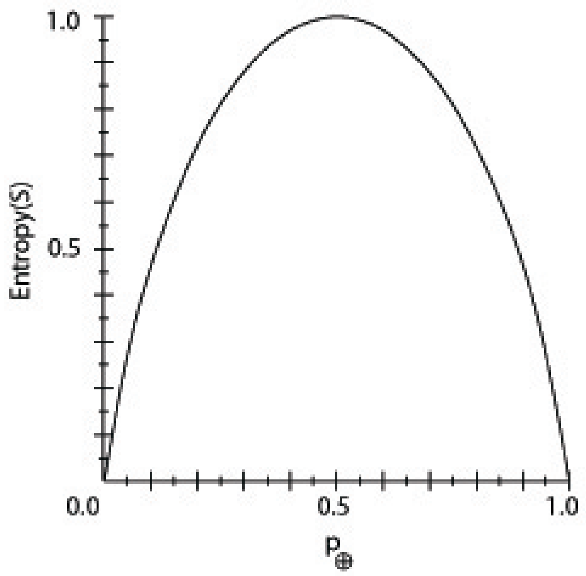
ID3 selects the attribute that has highest information gain.

Information gain measured as reduction in *entropy*.

Entropy

- $p_{\oplus}$ is the proportion of positive examples in S
- $p_{\ominus}$ $(= 1 - p_{\oplus})$ is the proportion of negative examples in S
- Entropy measures the impurity of S

$$Entropy(S) \equiv -p_{\oplus} \log_2 p_{\oplus} - p_{\ominus} \log_2 p_{\ominus}$$



Entropy example

Consider the set $S = [9+, 5-]$ (9 positive examples, 5 negative examples)

$$Entropy(S) = -(9/14)log_2(9/14) - (5/14)log_2(5/14) = 0.940$$

Note: we define $0 log_2 0 = 0$.

Maximum entropy when $p_{\oplus} = 0.5$, minimum when $p_{\oplus} = 0$ or 1.
In case of multi-valued target functions (c-wise classification)

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

Information Gain

$Gain(S, A)$ = expected reduction in entropy of S caused by knowing the value of attribute A.

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

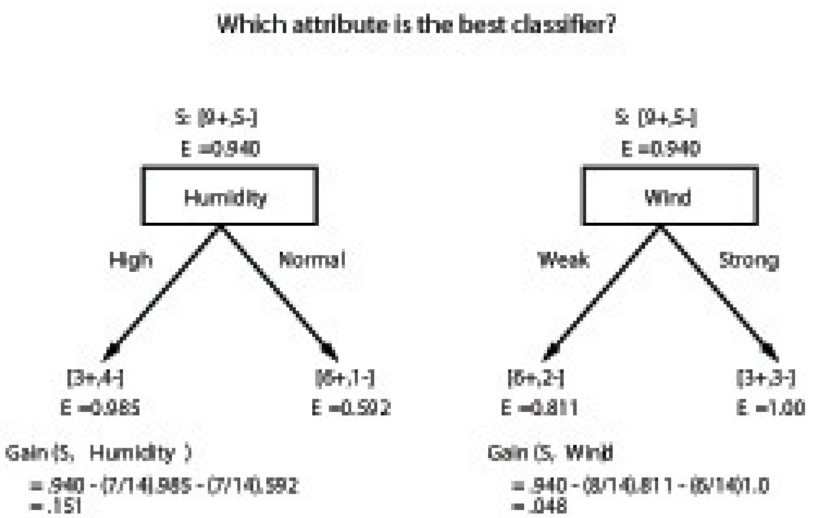
$Values(A)$: set of all possible values of A
$S_v = \{s \in S | A(s) = v\}$

Information Gain example

$$
\begin{aligned}
Values(Wind) &= \{Weak, Strong\} \\
S &= [9+, 5-] \\
S_{Weak} &= [6+, 2-] \\
S_{Strong} &= [3+, 3-]
\end{aligned}
$$

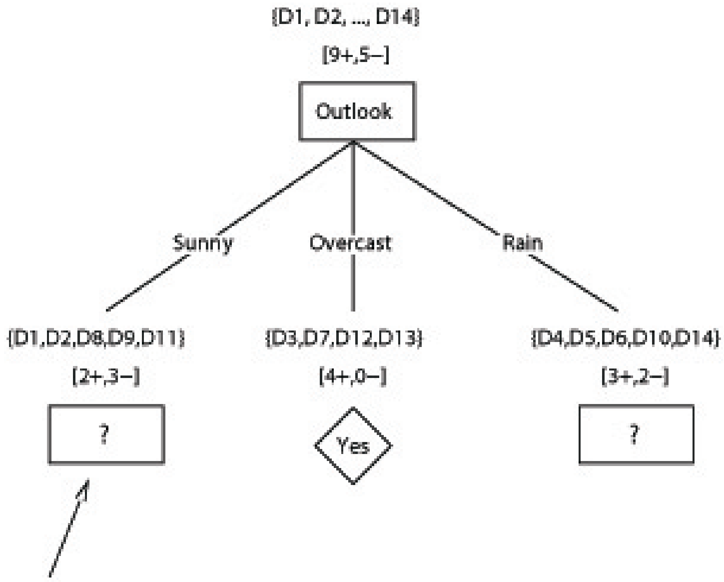
$$
\begin{aligned}
Gain(S, Wind) &= Entropy(S) - \frac{8}{14} Entropy(S_{Weak}) - \frac{6}{14} Entropy(S_{Strong}) \\
&= 0.940 - \frac{8}{14} 0.811 - \frac{6}{14} 1.00 \\
&= 0.048
\end{aligned}
$$

Selecting the Next Attribute



$$
\begin{aligned}
\text{Gain(S,Outlook)} &= 0.246 \\
\text{Gain(S,Humidity)} &= 0.151 \\
\text{Gain(S,Wind)} &= 0.048 \\
\text{Gain(S,Temperature)} &= 0.029
\end{aligned}
$$

Selecting the Next Attribute



Which attribute should be tested here?

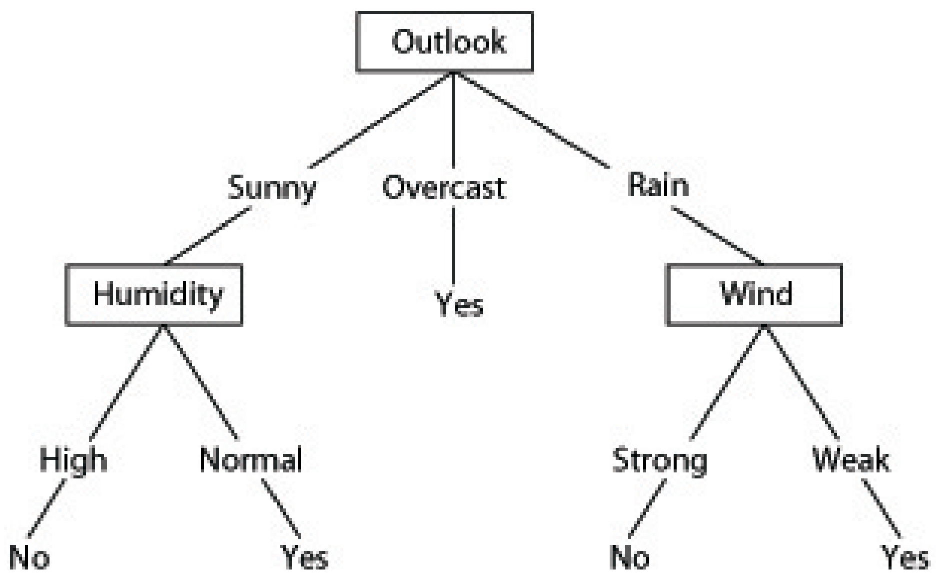
$S_{sunny} = \{D1,D2,D8,D9,D11\}$

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

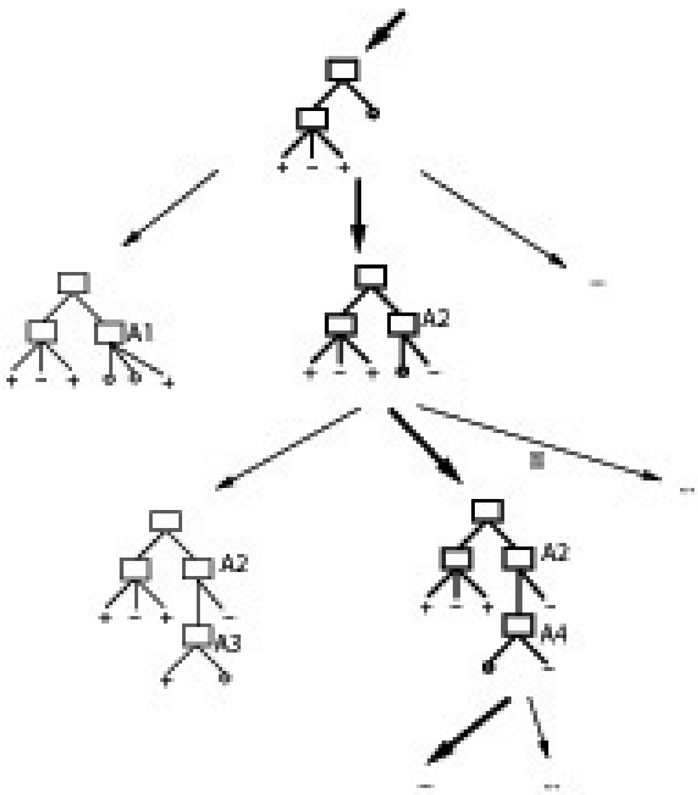
$Gain(S_{sunny}, Temperature) = .970 - (2/5)\ 0.0 - (2/5)\ 1.0 - (1/5)\ 0.0 = .570$

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

Decision Tree for *PlayTennis*



Hypothesis Space Search by ID3



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Hypothesis Space Search by ID3

- Hypothesis space is complete (target concept is there!)
- Outputs a single hypothesis (cannot determine how many DTs are consistent!)
- No back tracking (local minima!)
- Statistically-based search choices (robust to noisy data!)
- Uses all the training examples at each step (not incremental!)

Issues in Decision Tree Learning

- Determining how deeply to grow the DT
- Handling continuous attributes
- Choosing appropriate attribute selection measures
- Handling training data with missing attribute values
- Handling attributes with different costs

Overfitting in Decision Trees

Consider a new data set $D' = D \cup d_{15}$ adding a training example:

$$d_{15} = \langle Sunny,\ Hot,\ Normal,\ Strong,\ PlayTennis = No \rangle$$

ID3 will generate a different tree T'

Note: T is consistent with D and T' is consistent with D' (i.e., accuracy $= 100\%$)

Is T' in general a better solution for our learning problem?

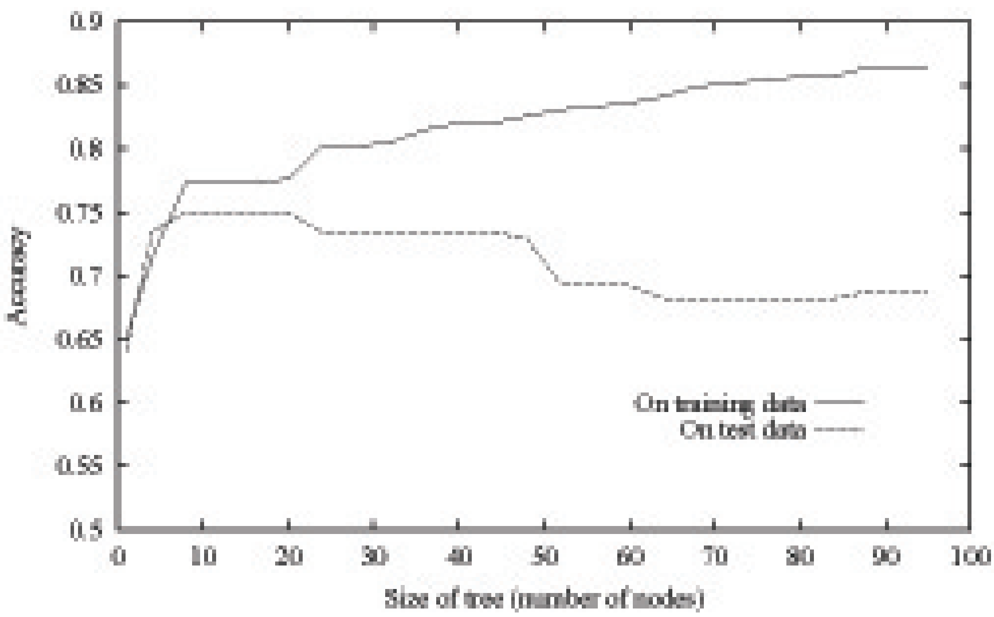
Overfitting in Decision Trees

Let's consider a more complex problem with $|D| \gg 15$ and containing noisy data and two decision trees T and T' obtained with different configuration of an ID3-like algorithm.

$$accuracy_D(T') > accuracy_D(T)$$

Is T' in general a better solution for our learning problem?

Overfitting in Decision Tree Learning



Avoiding Overfitting

How can we avoid overfitting?

- stop growing when data split not statistically significant
- grow full tree, then post-prune

To determine the correct tree size

- use a separate set of examples (distinct from the training examples) to evaluate the utility of post-pruning
- apply a statistical test to estimate accuracy of a tree on the entire data distribution
- using an explicit measure of the complexity for encoding the examples and the decision trees.

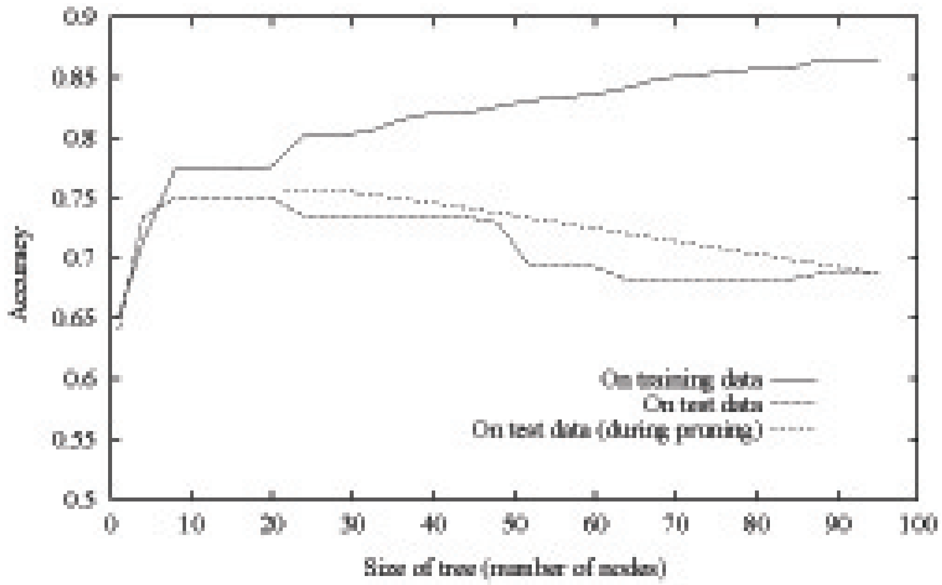
Reduced-Error Pruning

Split data into *training* and *validation* set

Do until further pruning is harmful (decreases accuracy):

1. Evaluate impact on *validation* set of pruning each possible node (remove all the subtree and assign the most common classification)
2. Greedily remove the one that most improves *validation* set accuracy

Effect of Reduced-Error Pruning



Remarks on Reduced-Error Pruning

- it produces smallest version of most accurate subtree (removing sub-trees added due to coincidental irregularities).
- When data set is limited, reducing the set of training examples (used as validation examples) can give bad results.

Rule Post-Pruning (C4.5)

1. Infer the decision tree allowing for overfitting
2. Convert the learned tree into an equivalent set of rules
3. Prune (generalize) each rule independently of others
4. Sort final rules into desired sequence for use

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Continuous Valued Attributes

Create a discrete attribute to test continuous variables

- $Temperature = 82.5$
- $(Temperature > 72.3) = t, f$

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

Attributes with Many Values

Problem:

- If attribute has many values, *Gain* will select it
- Imagine using $Date = Jun\_3\_1996$ as attribute

One approach: use *GainRatio* instead

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

$$SplitInformation(S, A) \equiv - \sum_{i=1}^{c} \frac{|S_i|}{|S|} \log_2 \frac{|S_i|}{|S|}$$

where S_i is subset of S for which A has value v_i

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Attributes with Costs

Consider

- medical diagnosis, *BloodTest* has cost \$150
- robotics, $Width\_from\_1ft$ has cost 23 sec.

How to learn a consistent tree with low expected cost?
Replace gain by

- Tan and Schlimmer (1990)

$$\frac{Gain^2(S, A)}{Cost(A)}$$

- Nunez (1988) ($w \in [0, 1]$ determines importance of cost)

$$\frac{2^{Gain(S,A)} - 1}{(Cost(A) + 1)^w}$$

Unknown Attribute Values

What if some examples missing values of A?
Use training example anyway, sort through tree

- If node n tests A, assign most common value of A among other examples sorted to node n
- assign most common value of A among other examples with same target value
- assign probability p_i to each possible value v_i of A
  - assign fraction p_i of example to each descendant in tree

Classify new examples in same fashion

Other algorithms based on Decision Trees

Random Forest: ensemble method that generates a set of decision trees with some random criteria and integrates their values into a final result.

Random criteria: 1) random subsets of data (bagging), 2) random subset of attributes (feature selection), ...

Integration of results: majority vote (most common class returned by all the trees).

Random Forests are less sensitive to overfitting.

Summary

- Decision Trees can represent classification function by **making decisions explicit**
- Learning as search in the hypothesis space with heuristics based on information gain
- Statistical method (some robustness to noisy data)
- Overfitting and pruning
- Used as basis of randomized ensemble methods