

Sapienza University of Rome

Master in Artificial Intelligence and Robotics

# 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 the "best" consistent hypothesis wrt  $D$ .

## Solution approach

- Define hypothesis space  $H$
- Implement an algorithm to find  $h^* \in H$ , "best" hypothesis consistent with  $D$

# Decision Trees

Consider a discrete input space described with  $m$  attributes  
 $X = A_1 \times \dots \times A_m$ , with  $A_i$  finite  
and a classification problem for  $f : X \rightarrow C$

Hypothesis space  $H$ : set of decision trees.

## Decision tree

Tree with the following characteristics:

- Each internal node tests an attribute  $A_i$ ;
- Each branch denotes a value of an attribute  $a_j \in A_i$ ;
- Each leaf node assigns a classification value  $c \in C$

## Example *PlayTennis*

Instances  $X = Outlook \times Temperature \times Humidity \times Wind$

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

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

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

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

Classification values:

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

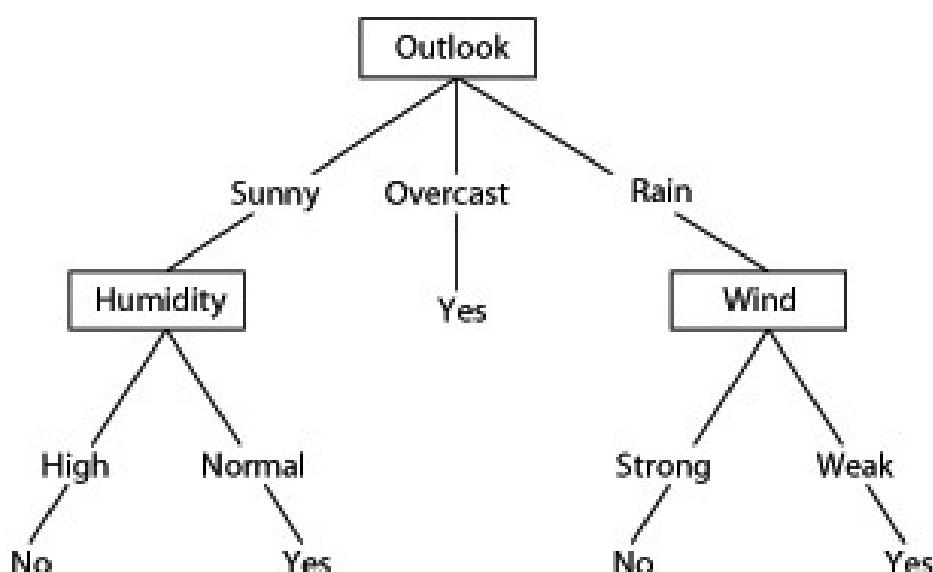
Learning problem:

$$f : Outlook \times Temperature \times Humidity \times Wind \rightarrow PlayTennis$$

# 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.

$$\begin{aligned}
 & (\text{Outlook} = \text{Sunny} \wedge \text{Humidity} = \text{Normal}) \quad \vee \\
 & (\text{Outlook} = \text{Overcast}) \quad \vee \\
 & (\text{Outlook} = \text{Rain} \wedge \text{Wind} = \text{Weak})
 \end{aligned}$$

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         $(\text{Outlook} = \text{Sunny}) \wedge (\text{Humidity} = \text{High})$   
 THEN      $\text{PlayTennis} = \text{No}$

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

...

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  $ID3(Examples_{v_i}, Target\_attribute, Attributes - \{A\})$

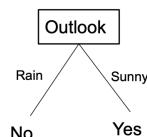
# Which is the best attribute to choose?

Output tree depends on attribute order

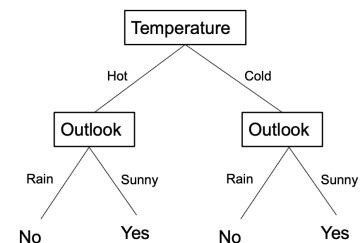
Example (dataset different than previous one):

Day	Outlook	Temperature	PlayTennis
D1	Sunny	Hot	Yes
D2	Sunny	Cold	Yes
D3	Rain	Hot	No
D4	Rain	Cold	No

**Outlook first:**



**Temperature first:**



# Which is the best attribute to choose?

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

Day	Outlook	Temperature	PlayTennis
D1	Sunny	Hot	Yes
D2	Sunny	Cold	Yes
D3	Rain	Hot	No
D4	Rain	Cold	No

Day	Outlook	Temperature	PlayTennis
D1	Sunny	Hot	Yes
D2	Sunny	Cold	Yes
D3	Rain	Hot	No
D4	Rain	Cold	No

Day	Outlook	Temperature	PlayTennis
D1	Sunny	Hot	Yes
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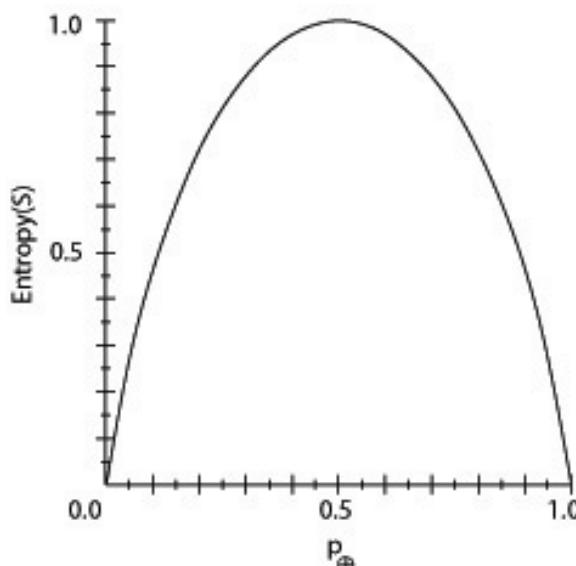
ID3 selects the attribute that induces **highest information gain**.

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  $S$

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



## Entropy example

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

$$\text{Entropy}(S) = -(9/14)\log_2(9/14) - (5/14)\log_2(5/14) = 0.940$$

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)

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

# Information Gain

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

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

$Values(A)$  : set of all possible values of  $A$

$$S_v = \{s \in S | A(s) = v\}$$

## Information Gain example

$$Values(Wind) = \{Weak, Strong\}$$

$$S = [9+, 5-]$$

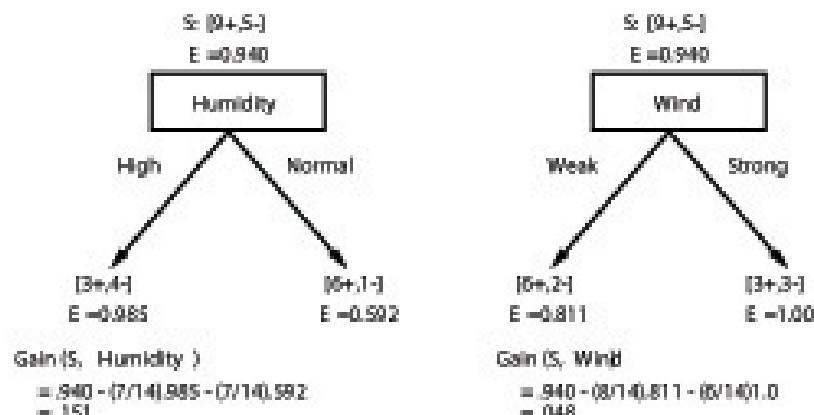
$$S_{Weak} = [6+, 2-]$$

$$S_{Strong} = [3+, 3-]$$

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

# Selecting the Next Attribute

Which attribute is the best classifier?



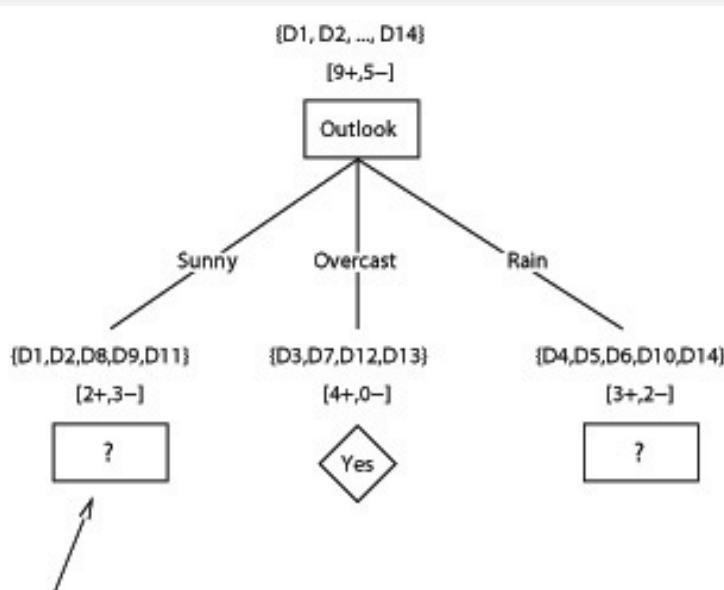
$$\text{Gain}(S, \text{Outlook}) = 0.246$$

$$\text{Gain}(S, \text{Humidity}) = 0.151$$

$$\text{Gain}(S, \text{Wind}) = 0.048$$

$$\text{Gain}(S, \text{Temperature}) = 0.029$$

# Selecting the Next Attribute



Which attribute should be tested here?

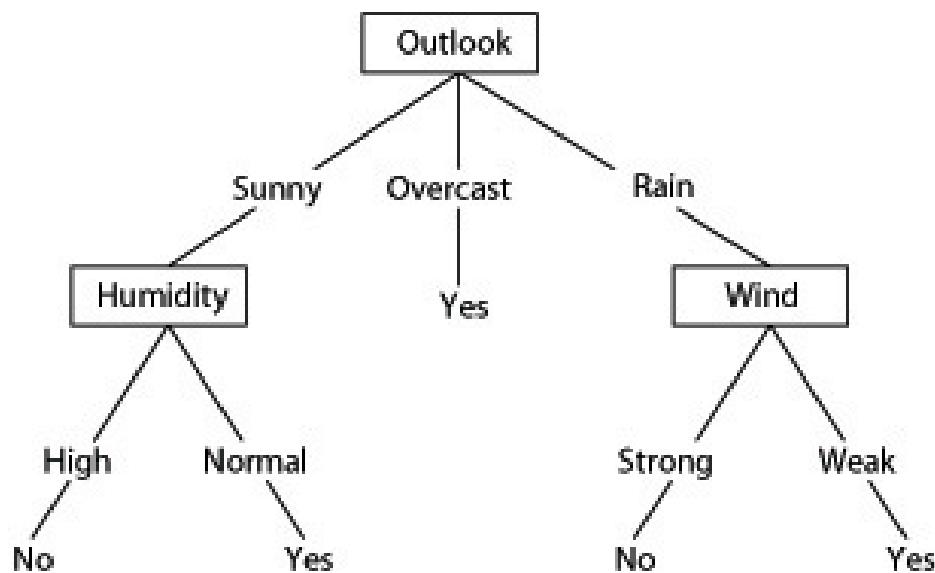
$$S_{\text{sunny}} = [D1, D2, D8, D9, D11]$$

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

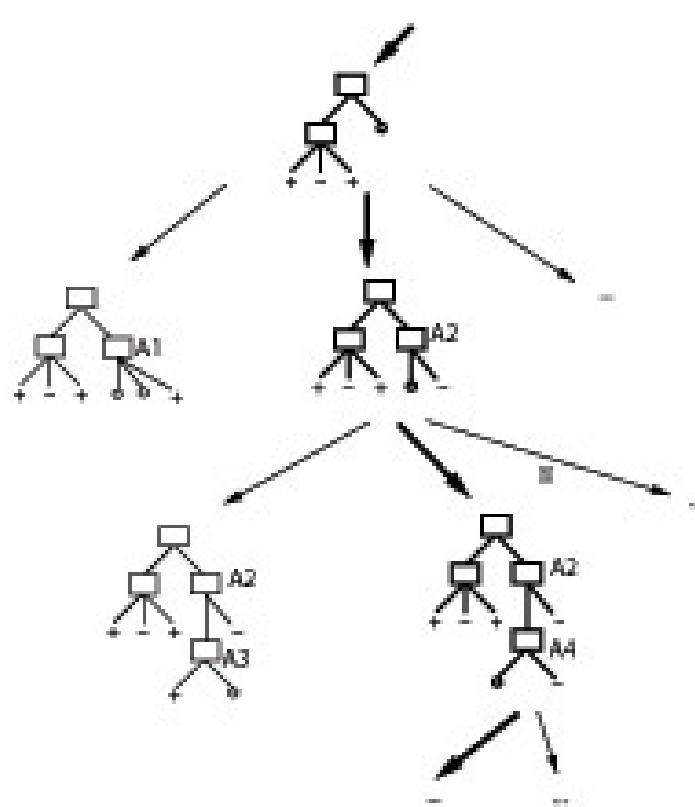
$$\text{Gain}(S_{\text{sunny}}, \text{Temperature}) = .970 - (2/5)0.0 - (2/5)1.0 - (1/5)0.0 = .570$$

$$\text{Gain}(S_{\text{sunny}}, \text{Wind}) = .970 - (2/5)1.0 - (3/5)0.918 = .019$$

# Decision Tree for *PlayTennis*



## Hypothesis Space Search by ID3



# 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:

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

ID3 will generate a different tree  $T'$

Note:  $T$  consistent with  $D$  and  $T'$  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 a large dataset  $D$  containing noisy data, two decision trees  $T$  and  $T'$  obtained with different configurations of an ID3-like algorithm with

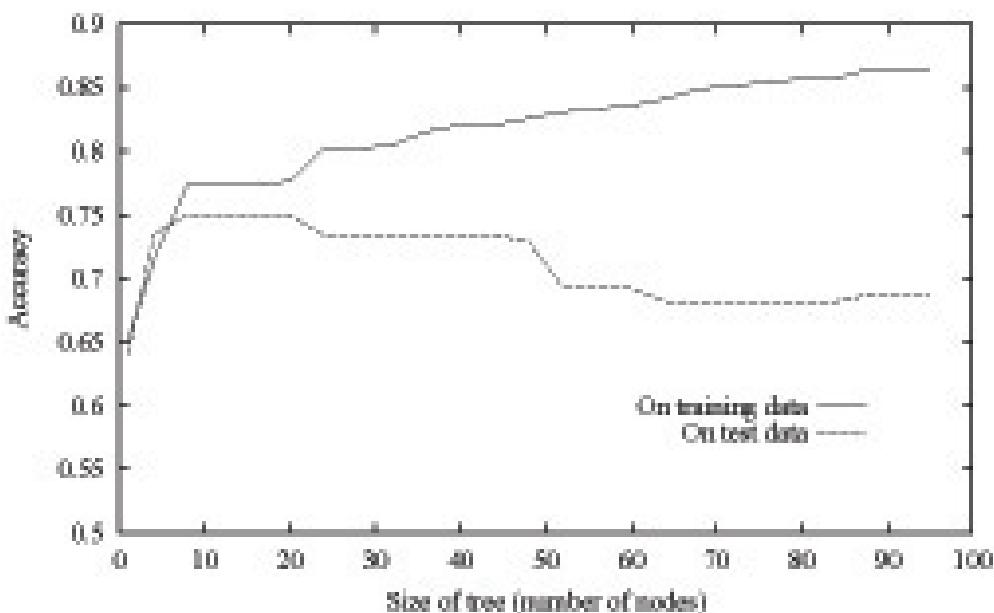
$$\text{accuracy}_D(T') \geq \text{accuracy}_D(T)$$

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

Using a test set  $S$

$$\text{accuracy}_S(T') > ? \text{ accuracy}_S(T)$$

# 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 Post-Pruning

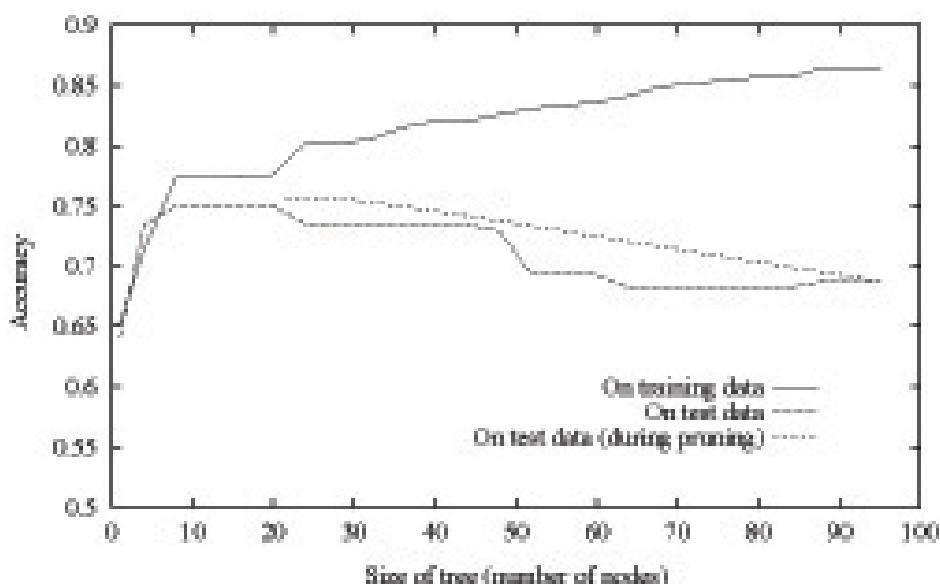
**Pruning:** replace a sub-tree with a leaf node labelled as the most common class among samples filtered to the node.

## Post-Pruning:

- ① Split data into *training* and *validation* set
- ② Generate a tree using the *training* set
- ③ Do until further pruning is harmful (decreases accuracy):
  - Evaluate impact (\*) on *validation* set of pruning each possible node (remove all the subtree and assign the most common classification)
  - Greedily remove the one that most improves *validation* set accuracy

(\*) e.g., cost-complexity measure [Breiman et al., 1984]

## 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

In general, rule post-pruning allows for better generalization.

# Decision Tree Pruning

DT pruning is greedy, efficient, but cannot guarantee global optimality

Optimal DT Algorithms are computationally very expensive.

Some methods aim at trade off between optimality and efficiency

## Continuous Valued Attributes

Create a discrete attribute to test continuous variables

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

<i>Temperature:</i>	40	48	60	72	80	90
<i>PlayTennis:</i>	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

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

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

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

# 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)

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

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

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

# 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** (explainable)
- 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