innovate achieve lead

Machine Learning
DSECL ZG565

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Session Content

- Decision Tree (Tom Mitchell Chapter 3)

Decision trees

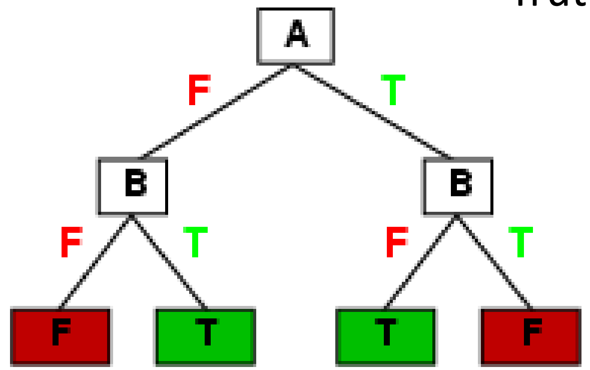
- Decision Trees is one of the most widely used and practical methods of classification
- Method for approximating discrete-valued functions
- Learned functions are represented as decision trees (or if-then-else rules)
- Expressive hypotheses space

Expressiveness

- Decision trees can represent any boolean function of the input attributes

Truth table row → path to leaf

A	B	A xor B
F	F	F
F	T	T
T	F	T
T	T	F



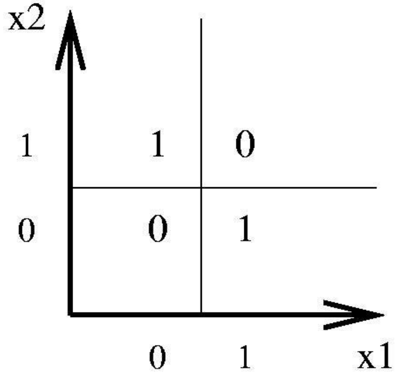
- In the worst case, the tree will require exponentially many nodes

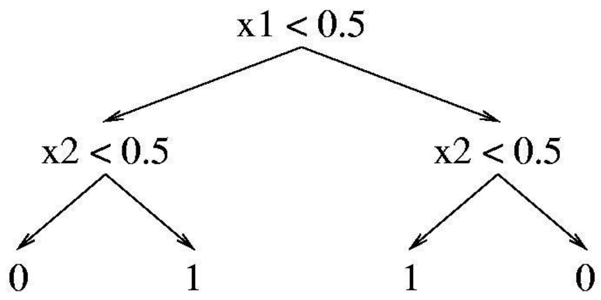
Slide credit : Eric Eaton

Expressiveness

Decision trees have a variable-sized hypothesis space

- As the #nodes (or depth) increases, the hypothesis space grows
  - Depth 1 (“decision stump”): can represent any boolean function of one feature
  - Depth 2: any boolean fn of two features; some involving three features





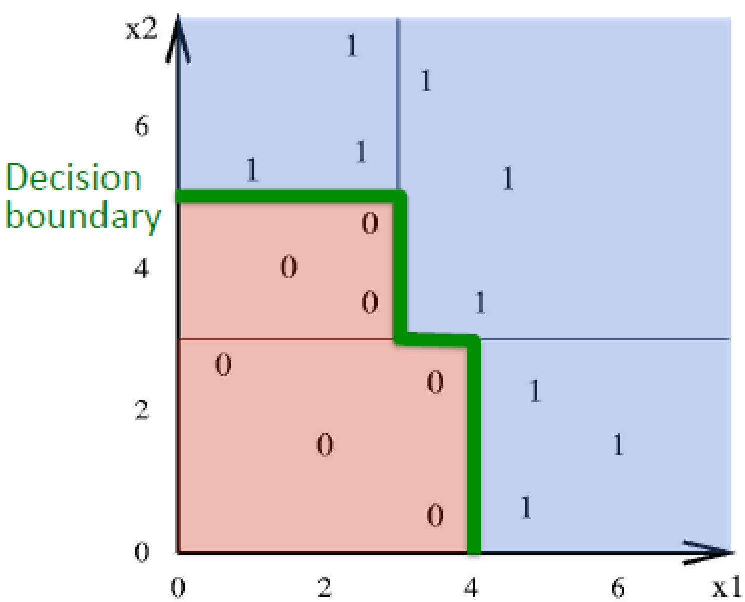
Based on slide by Pedro Domingos

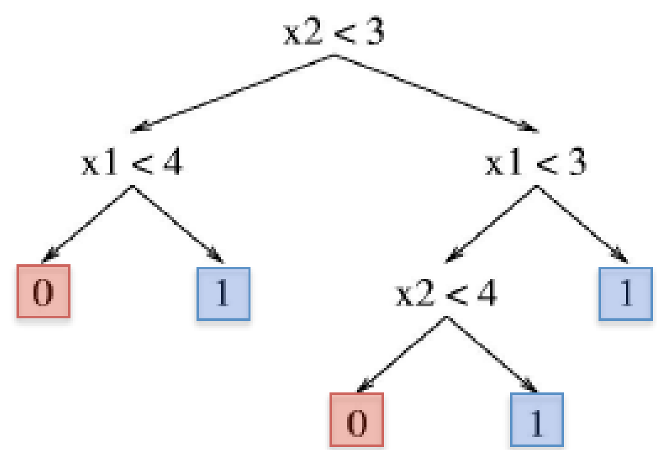
Decision Tree – Decision Boundary

• Decision trees divide the feature space into axis parallel (hyper-)rectangles

• Each rectangular region is labeled with one label

– or a probability distribution over labels



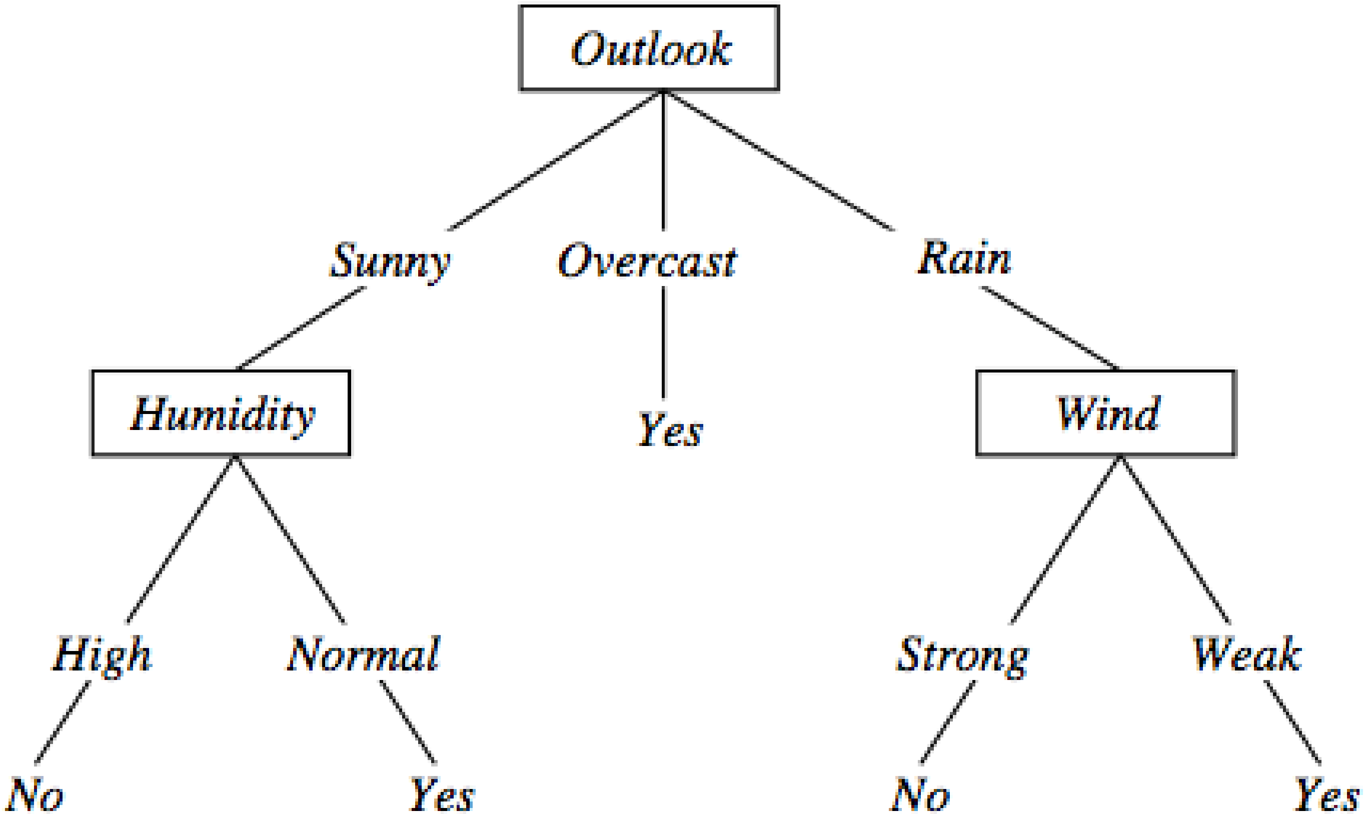


Slide credit : Eric Eaton

Example

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 representation (PlayTennis)

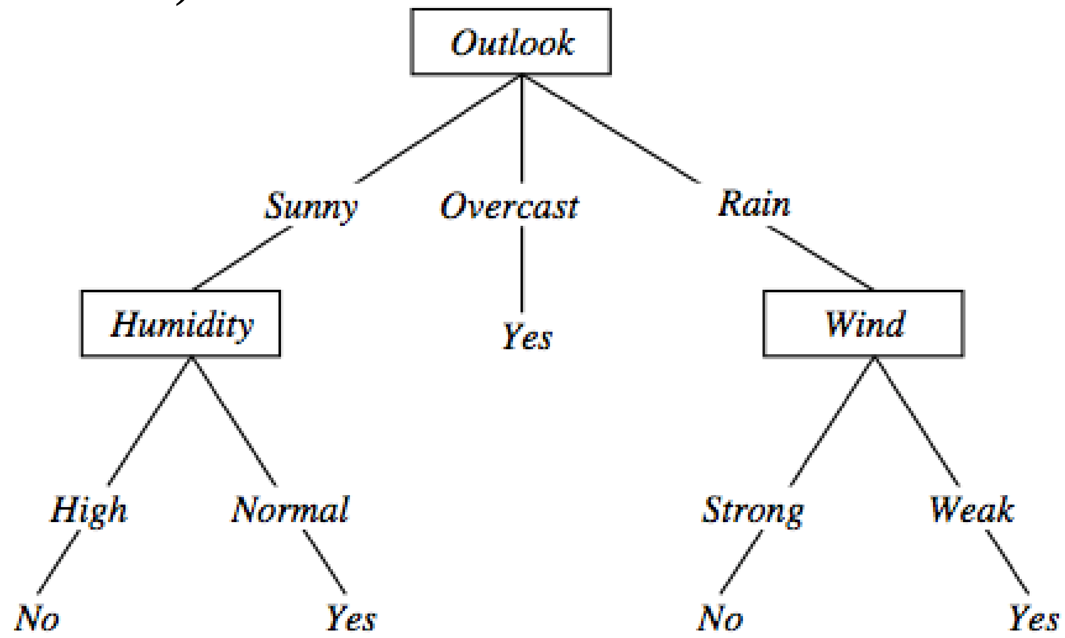


⟨*Outlook=Sunny, Temp=Hot, Humidity=High, Wind=Strong*⟩ No

Decision trees expressivity

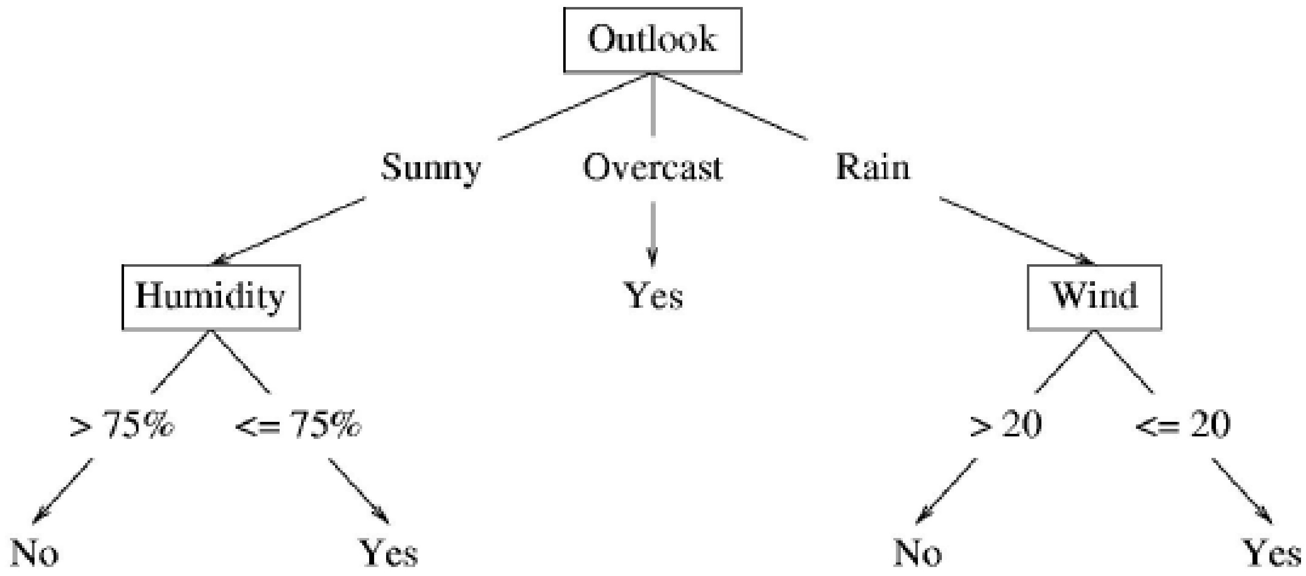
- Decision trees represent a disjunction of conjunctions on constraints on the value of attributes:

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



Dealing with continuous-valued attributes

If features are continuous, internal nodes can test the value of a feature against a threshold



Dealing with continuous-valued attributes

- Given a continuous-valued attribute A, dynamically create a new attribute A_c

  $$A_c = \text{True } \textit{if } A < c, \text{ False } \textit{otherwise}$$
- How to determine threshold value *c* ?
- Example. *Temperature* in the *PlayTennis* example
  - Sort the examples according to *Temperature*

Temperature	40	48	|	60	72	80	|	90
PlayTennis	No	No	*54*	Yes	Yes	Yes	*85*	No

  - Determine candidate thresholds by averaging consecutive values where there is a change in classification:

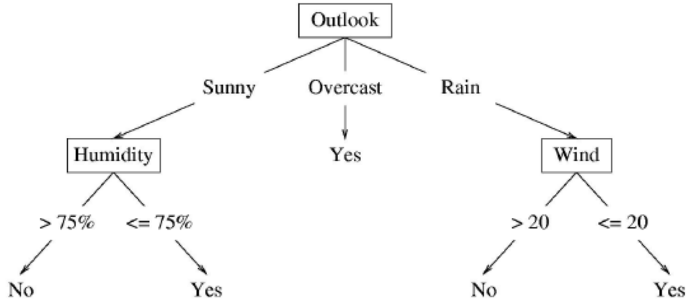
    (48+60)/2=54 and (80+90)/2=85

Problem Setting

Set of possible instances *X*

- each instance *x* in *X* is a feature vector
- e.g., *<Humidity=low, Wind=weak, Outlook=rain, Temp=hot>*

- Unknown target function *f* : *X* -> *Y*
  - *Y* is discrete valued
- Set of function hypotheses *H*={ *h* | *h* : *X*->*Y* }
  - each hypothesis *h* is a decision tree
  - trees sorts *x* to leaf, which assigns *y*



Measure of Information

- It rained heavily in Shillong yesterday
- There was a heavy rainfall in Rajasthan last night.
- The amount of information (surprise element) conveyed by a message is inversely proportional to its probability of occurrence. That is

$$I_k \,\alpha\, \frac{1}{p_k}$$

- The mathematical operator satisfies above properties is the logarithmic operator.

$$I_k = \log_r \frac{1}{p_k} \quad units$$

Entropy

- Entropy of discrete random variable $X=\{x_1, x_2 \ldots x_n\}$

$$\mathrm{H}(X) = \mathrm{E}[\mathrm{I}(X)] = \mathrm{E}[-\log(\mathrm{P}(X))].$$

since: $\log_2(1/P(\text{event})) = -\log_2 P(\text{event})$

- As uncertainty increases, entropy increases
- Entropy across all values

$$\mathrm{H}(X) = -\sum_{i=1}^{n} \mathrm{P}(x_i) \log_b \mathrm{P}(x_i)$$

- Entropy measures the amount of information in a random variable

Entropy in general

- Entropy measures the amount of information in a random variable

$$H(X) = -p_+ \log_2 p_+ - p_- \log_2 p_- \qquad X = \{+, -\}$$

for binary classification [two-valued random variable]

$$H(X) = -\sum_{i=1}^{c} p_i \log_2 p_i = \sum_{i=1}^{c} p_i \log_2 1/p_i \qquad X = \{i, \ldots, c\}$$

for classification in *c* classes

Entropy in binary classification

- Entropy measures the *impurity* of a collection of examples. It depends from the distribution of the random variable *p.*
  - S is a collection of training examples
  - p_+ the proportion of positive examples in S
  - p_- the proportion of negative examples in S

$$Entropy\ (S) \equiv -p_+ \, log_2 \, p_+ - p_- log_2 \, p_- \quad [0 \; log_2 0 = 0]$$

Entropy in binary classification

Note: the log of a number < 1 is negative, $0 \le p \le 1$, $0 \le entropy \le 1$

$$Entropy\ (S) \equiv -p_+ \log_2 p_+ - p_- \log_2 p_- \quad [0 \log_2 0 = 0]$$

Example:

- https://www.easycalculation.com/log-base2-calculator.php

Information gain as entropy reduction

- Information Gain (also called mutual information) between input attribute A and target variable
- **It is a measure of the effectiveness of an attribute in classifying the training data.**
- *Information gain* is the *expected* reduction in entropy caused by partitioning the examples on an attribute.
- The higher the information gain the more effective the attribute in classifying training data.
- Expected reduction in entropy knowing *A*

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

Values(A) is the set of all possible values for attribute A, and $\boldsymbol{S_v}$ is the subset of S for which attribute A has value v

- **First term is the entropy of the original collection *S*, and the second term is the expected value of the entropy after *S* is partitioned using attribute *A*.**

Example

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

- information gain due to sorting the original ***14*** examples by the attribute ***Wind***

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

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

$S = [9+, 5-]$

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

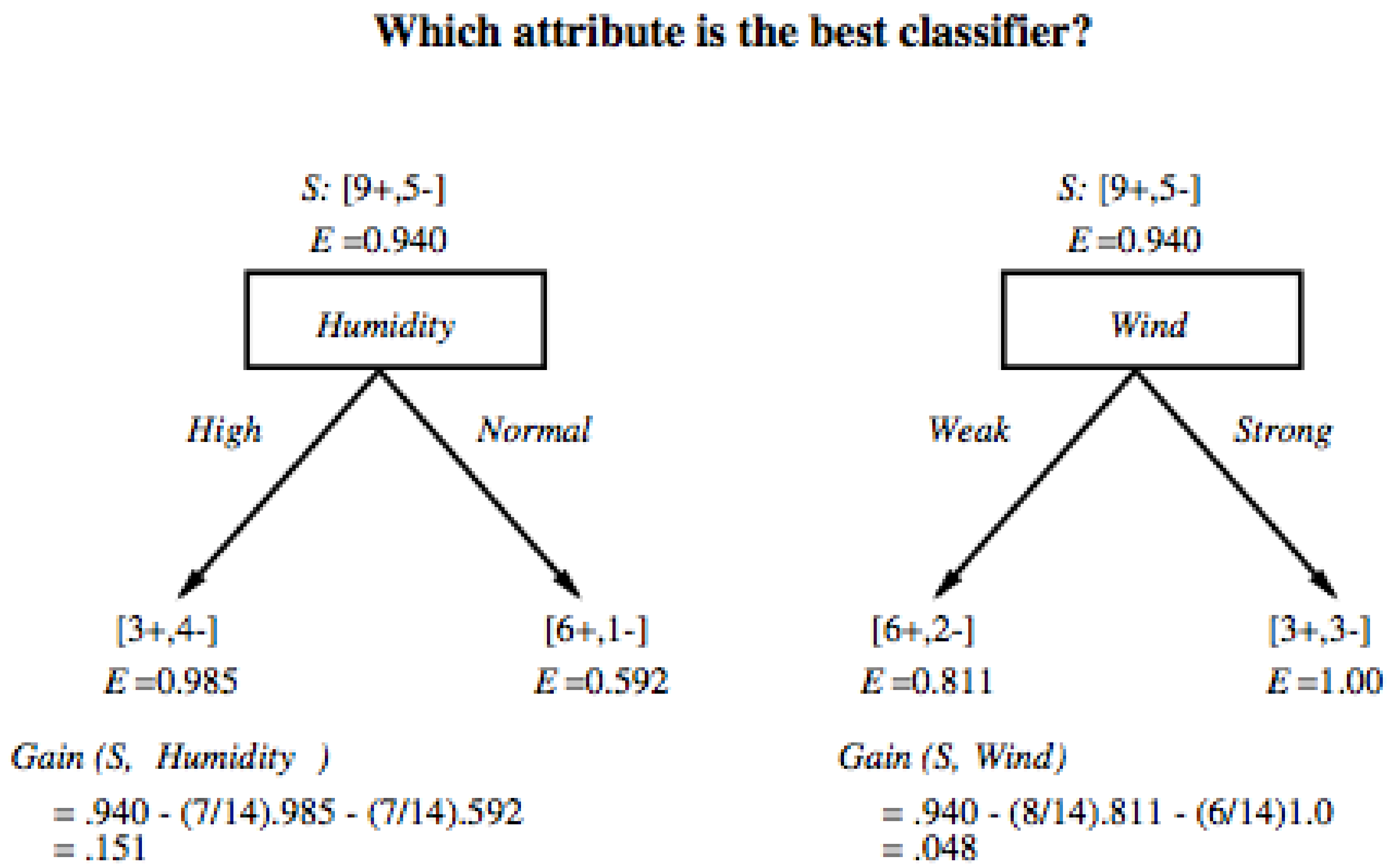
$S_{Strong} = [3+, 3-]$

$$Gain(S, Wind) = Entropy(S) - 8/14\ Entropy(S_{Weak}) - 6/14\ Entropy(S_{Strong})$$

$$= 0.94 - 8/14 \times 0.811 - 6/14 \times 1.00$$

$$= 0.048$$

Which attribute is the best classifier?



First step: which attribute to test at the root?

- Which attribute should be tested at the root?
  - $Gain(S, Outlook) = 0.246$
  - $Gain(S, Humidity) = 0.151$
  - $Gain(S, Wind) = 0.048$
  - $Gain(S, Temperature) = 0.029$
- *Outlook* provides the best prediction for the target
- Lets grow the tree:
  - add to the tree a successor for each possible value of *Outlook*
  - partition the training samples according to the value of *Outlook*

Example

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
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D10	Rain	Mild	Normal	Weak	Yes
D11	Sunny	Mild	Normal	Strong	Yes
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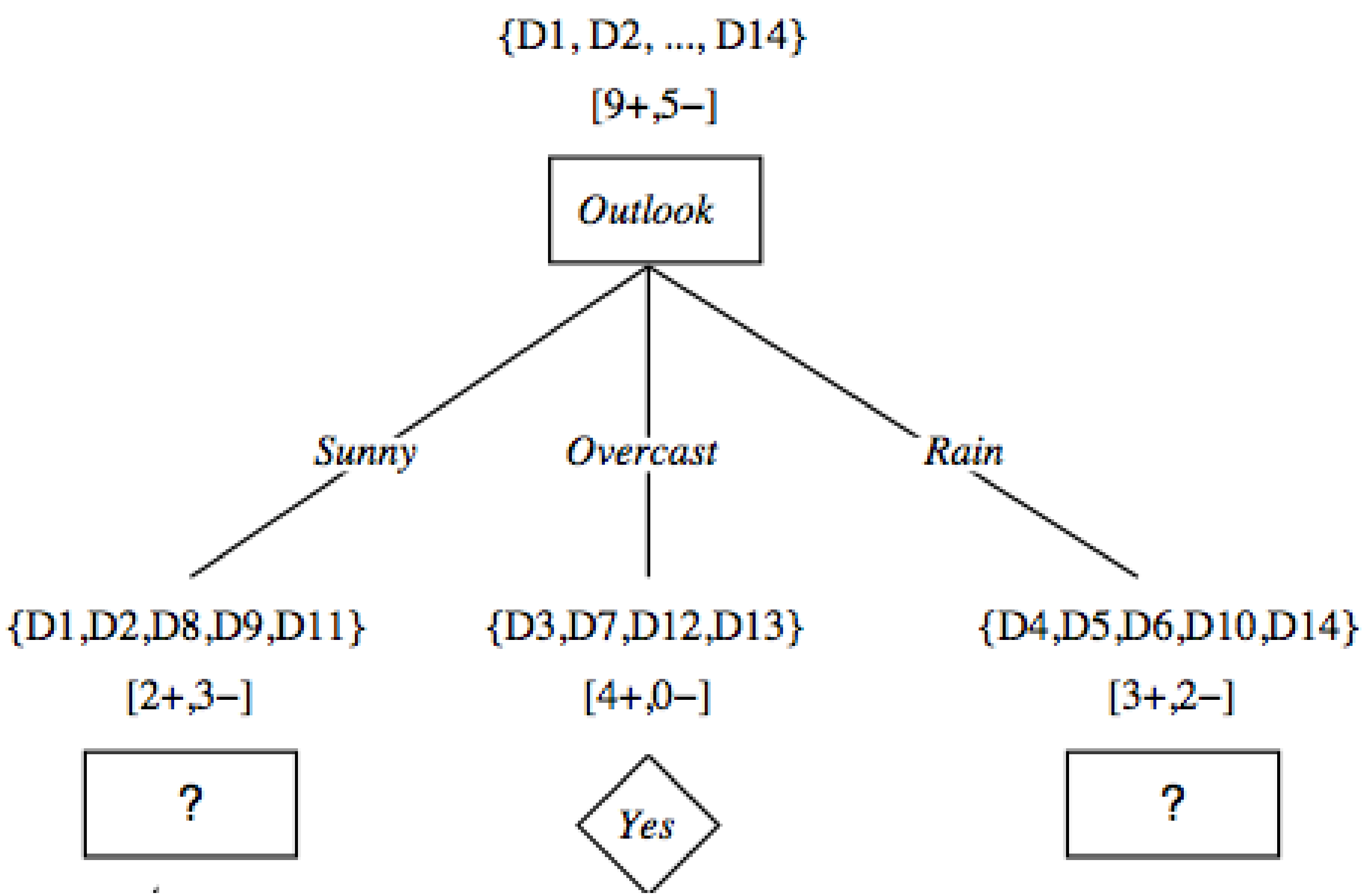
D13	Overcast	Hot	Normal	Weak	Yes
D14	Rain	Mild	High	Strong	No

After first step



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

Day	Outlook	Temperature	Humidity	Wind	PlayTennis
D1	Sunny	Hot	High	Weak	No
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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

Second step

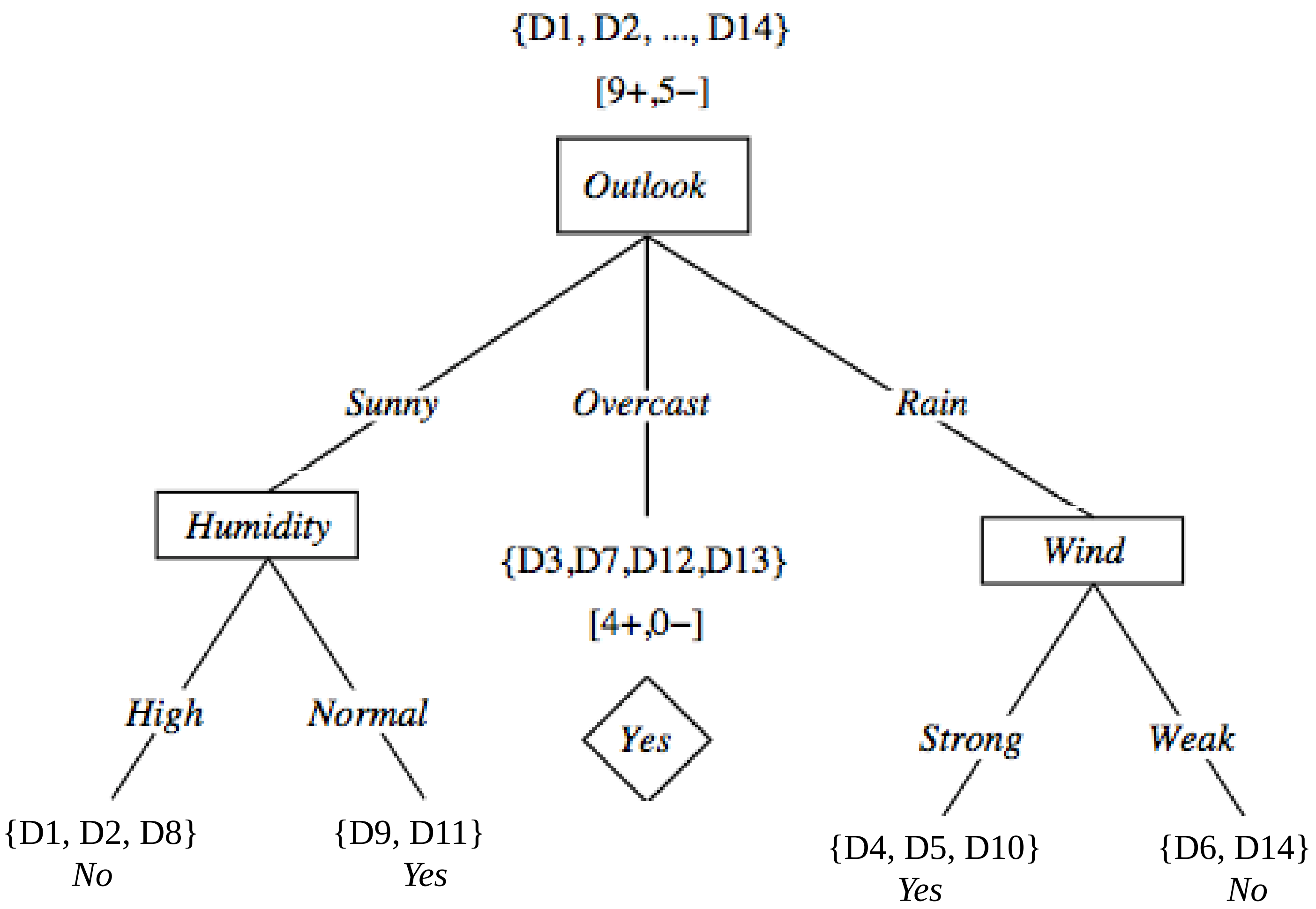
- Working on *Outlook=Sunny* node:

  $Gain(S_{Sunny}, Humidity) = 0.970 – 3/5 \times 0.0 – 2/5 \times 0.0 = 0.970$

  $Gain(S_{Sunny}, Wind) = 0.970 – 2/5 \times 1.0 – 3.5 \times 0.918 = 0 .014$

  $Gain(S_{Sunny}, Temp.) = 0.970 – 2/5 \times 0.0 – 2/5 \times 1.0 – 1/5 \times 0.0 = 0.570$
- *Humidity* provides the best prediction for the target
- Lets grow the tree:
  - add to the tree a successor for each possible value of *Humidity*
  - partition the training samples according to the value of *Humidity*

Second and third steps



ID3: algorithm

ID3(X, T, $Attrs$) X: training examples:
T: target attribute (e.g. *PlayTennis*),
$Attrs$: other attributes, initially all attributes

Create *Root* node
If all X's are +, *return* *Root* with class +
If all X's are –, *return* *Root* with class –
If *Attrs* is empty *return* *Root* with class most common value of T in X
else
$A \leftarrow$ best attribute; decision attribute for Root $\leftarrow A$
For each possible value v_i of A:
- add a new branch below *Root,* for test $A = v_i$
- $X_i \leftarrow$ subset of X with $A = v_i$
- *If* X_i is empty *then* add a new leaf with class the most common value of T in X
else add the subtree generated by ID3(X_i, T, $Attrs - \{A\}$)

return *Root*

Prefer shorter hypotheses: Occam's razor

- Why prefer shorter hypotheses?
- Arguments in favor:
  - There are fewer short hypotheses than long ones
  - If a short hypothesis fits data unlikely to be a coincidence
  - Elegance and aesthetics
- Arguments against:
  - Not every short hypothesis is a reasonable one.
- Occam's razor says that when presented with competing hypotheses that make the **same** predictions, one should select the solution which is simple"

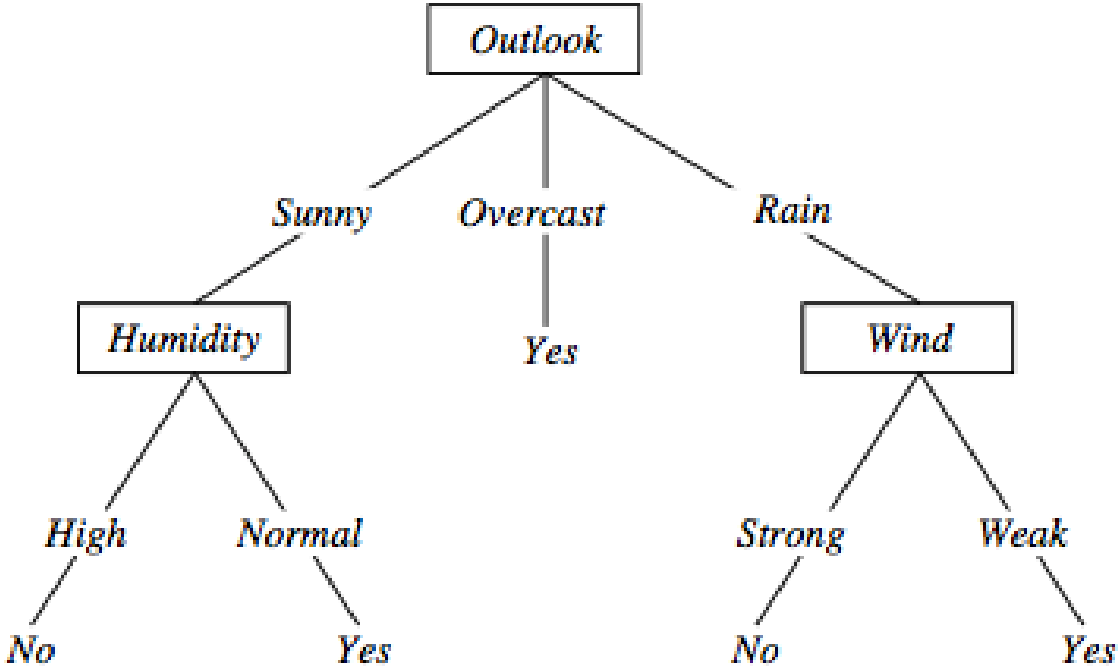
Issues in decision trees learning

- Overfitting
  - Reduced error pruning
  - Rule post-pruning
- Extensions
  - Continuous valued attributes
  - Handling training examples with missing attribute values

Example

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
D15	Sunny	Hot	Normal	Strong	No

Overfitting in decision trees



$\langle$*Outlook=Sunny, Temp=Hot, Humidity=Normal, Wind=Strong, PlayTennis=No* $\rangle$

New noisy example causes splitting of second leaf node.

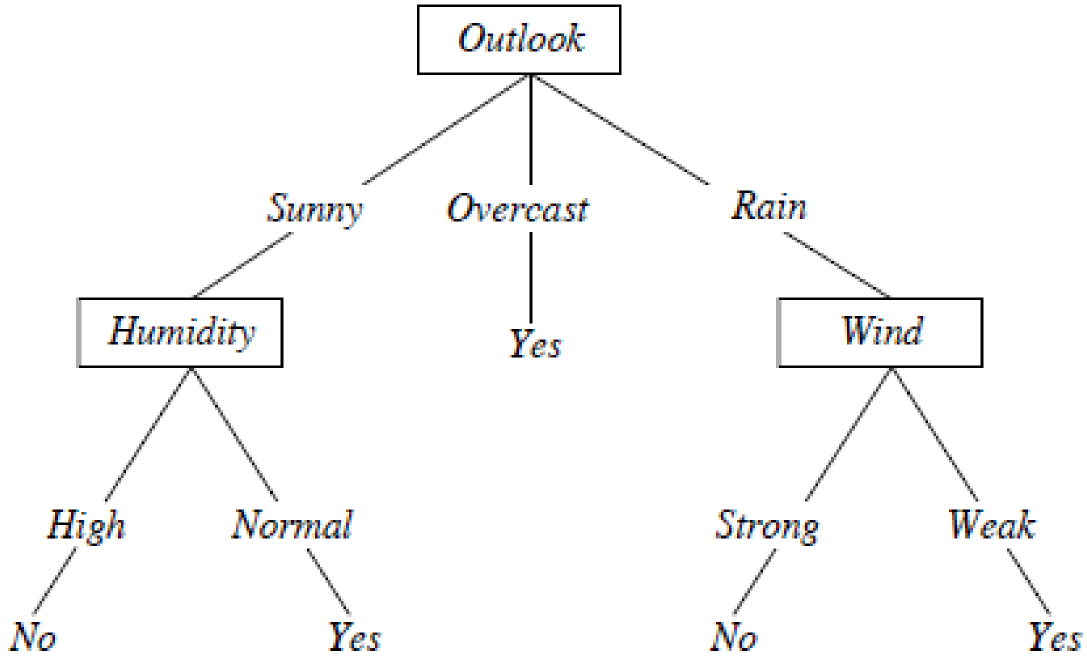
Avoid overfitting in Decision Trees

- Two strategies:
  1. Stop growing the tree earlier , before perfect classification
  2. Allow the tree to *overfit* the data, and then *post-prune* the tree
- Training and validation set
  - split the training in two parts (training and validation) and use validation to assess the utility of *post-pruning*
    - *Reduced error pruning*
    - *Rule post pruning*

Reduced-error pruning

- Each node is a candidate for pruning
- *Pruning* consists in removing a subtree rooted in a node: the node becomes a leaf and is assigned the most common classification
- Nodes are removed only if the resulting tree performs no worse than the original on the validation set.
- Nodes are pruned iteratively, always choosing the node whose removal most increases the decision tree accuracy over the validation set
- Pruning of nodes continues until the accuracy of the tree over the validation set decreases

Decision Tree as set of rules



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

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

Rule post-pruning

1. Create the decision tree from the training set
2. Convert the tree into an equivalent set of rules
   – Each path corresponds to a rule
   – Each node along a path corresponds to a pre-condition
   – Each leaf classification to the post-condition
3. Prune (generalize) each rule by removing those preconditions whose removal does not worsen accuracy …
   – … over validation set
4. Sort the rules in estimated order of accuracy, and consider them in sequence when classifying new instances

Rule Post-Pruning - example


```
Outlook=sunny ^ humidity=high -> No
Outlook=sunny ^ humidity=normal -> Yes
Outlook=overcast -> Yes
Outlook=rain ^ wind=strong -> No
Outlook=rain ^ wind=weak -> Yes
```

Remove first two preconditions

```
    Outlook=sunny
    Humidity=high
```

Calculate accuracy of 3 rules based on validation set and pick best version.

Why converting to rules?

- Each distinct path produces a different rule: a condition removal may be based on a local (contextual) criterion. Node pruning is global and affects all the rules
- Provides flexibility of not removing entire node
- Converting to rules improves readability for humans

Problems with information gain

- Natural bias of information gain: it favors attributes with many possible values.
- Consider the attribute *Date* in the *PlayTennis* example.
  - *Date* would have the highest information gain since it perfectly separates the training data.
  - It would be selected at the root resulting in a very broad tree
  - Very good on the training, this tree would perform poorly in predicting unknown instances. Overfitting.
- The problem is that the partition is too specific, too many small classes are generated.
- We need to look at alternative measures …

An alternative measure: gain ratio

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

- *SplitInformation* measures the entropy of *S* with respect to the values of *A*. The more uniformly dispersed the data the higher it is.

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

where S_1 through S_c, are the ***c*** subsets of examples resulting from partitioning S by the c-valued attribute A.

- *GainRatio* penalizes attributes that split examples in many small classes such as *Date by incorporating split information.*
- Let $|S| = n$, *Date* splits examples in n classes
  - $SplitInformation(S, Date) = -[(1/n \log_2 1/n) + \ldots + (1/n \log_2 1/n)] = -\log_2 1/n = \log_2 n$
- Compare with A, which splits data in two even classes:
  - $SplitInformation(S, A) = -[(1/2 \log_2 1/2) + (1/2 \log_2 1/2)] = -[-1/2 - 1/2] = 1$

Handling missing values training data

- How to cope with the problem that the value of some attribute may be missing?
- The strategy: use other examples to guess attribute
  1. Assign the value that is most common among the training examples at the node
  2. Assign a probability to each value, based on frequencies, assign values to missing attribute, according to this probability distribution

Applications

Suited for following classification problems:

- Applications whose Instances are represented by attribute-value pairs.
- The target function has discrete output values
- Disjunctive descriptions may be required
- The training data may contain missing attribute values

Real world applications

- Biomedical applications
- Manufacturing
- Banking sector
- Make-Buy decisions

Good References

Decision Tree

- https://www.youtube.com/watch?v=eKD5gxPPeY0&list=PLBv09BD7ez_4temBw7vLA19p3tdQH6FYO&index=1

Overfitting

- https://www.youtube.com/watch?time_continue=1&v=t56Nid85Thg
- https://www.youtube.com/watch?v=y6SpA2Wuyt8