Machine Learning
ZG565

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Lecture No. – 7 | Decision Tree

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Session Content

- Decision Tree
- Handling overfitting
- Continuous values
- Missing Values

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

Decision Tree

- Advantages:

– Inexpensive to construct

– Extremely fast at classifying unknown records

– Easy to interpret for small-sized trees

– Can easily handle redundant or irrelevant attributes (unless the attributes are interacting)

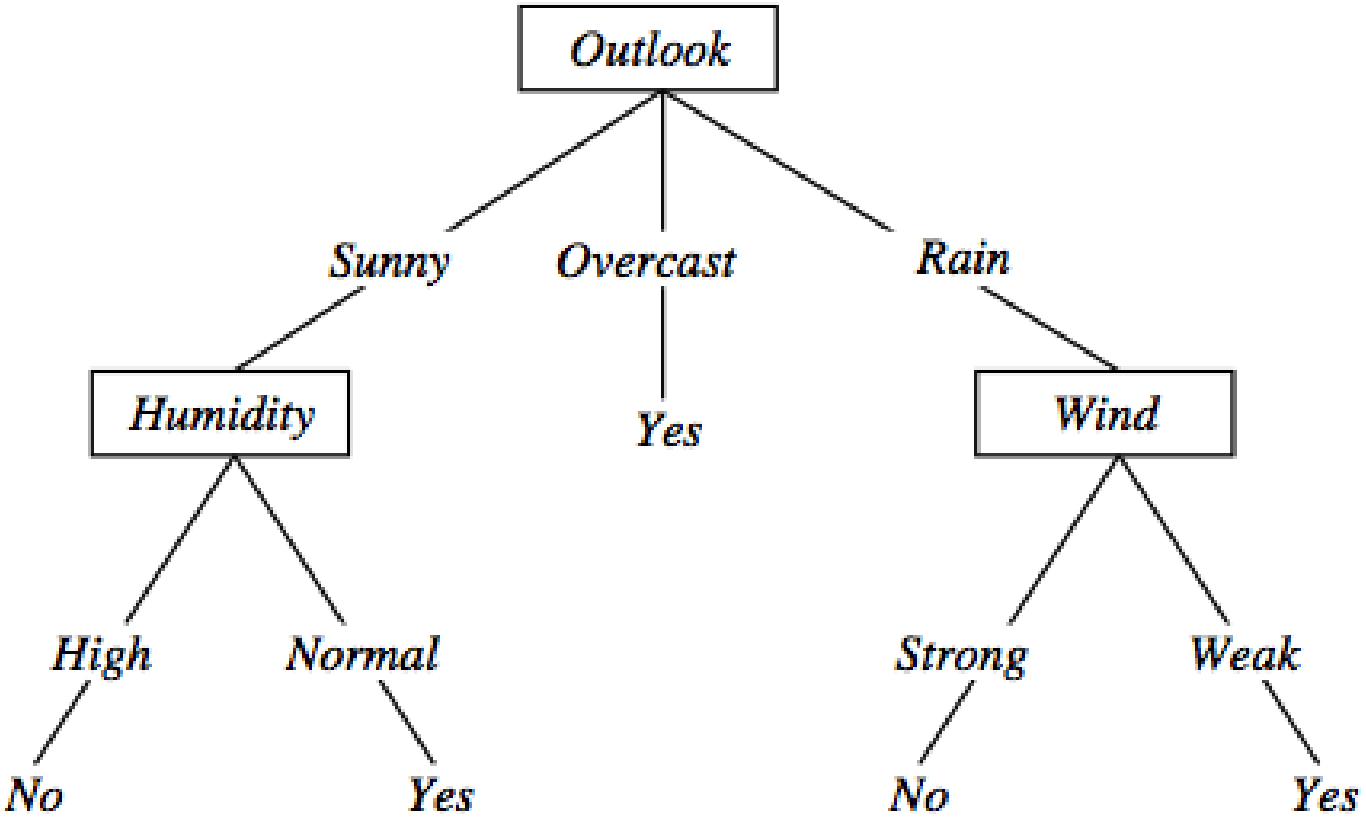
- Disadvantages:

– Space of possible decision trees is exponentially large.
Greedy approaches are often unable to find the best tree.

– Does not take into account interactions between attributes

– Each decision boundary involves only a single attribute

Decision tree representation (PlayTennis)

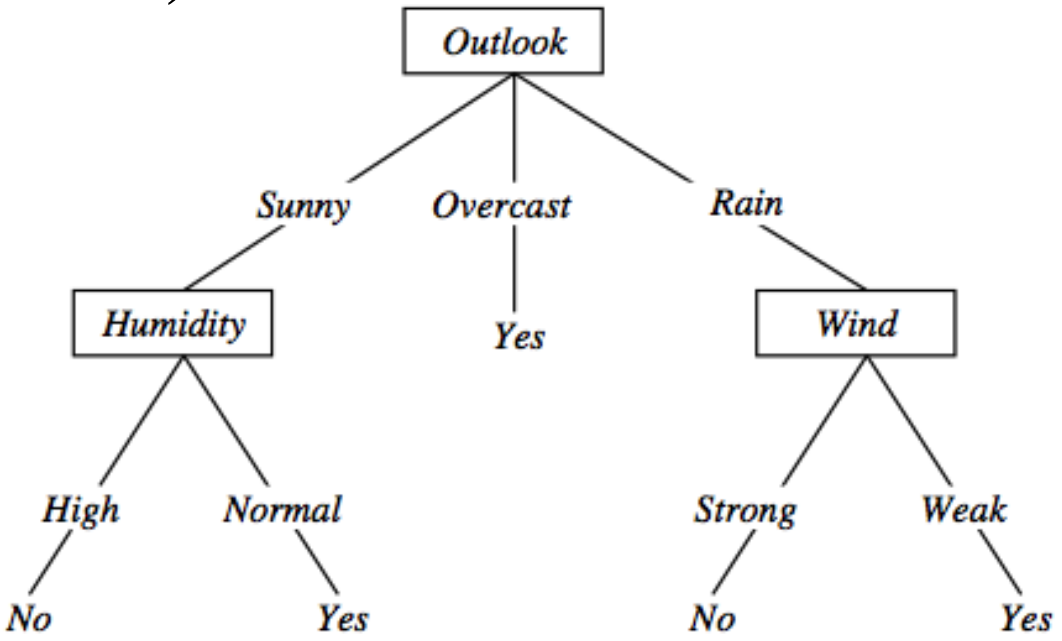


⟨*Outlook=Sunny, Temp=Hot, Humidity=High, Wind=Strong*⟩ No

Decision trees expressivity

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

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



Measure of Information

- 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.

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

Entropy

- Entropy of discrete random variable X={x_1, x_2…x_n}

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

; since: $\log_2(1/P(event)) = -\log_2 P(event)$

- 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 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

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

$$Entropy\,([14+, 0-]) = -14/14 \log_2 (14/14) - 0 \log_2 (0) = 0$$

$$Entropy\,([9+, 5-]) = -9/14 \log_2 (9/14) - 5/14 \log_2 (5/14) = 0.94$$

$$Entropy\,([7+, 7-]) = -7/14 \log_2 (7/14) - 7/14 \log_2 (7/14) =$$

$$= 1/2 + 1/2 = 1 \qquad [\log_2 1/2 = -1]$$

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

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

Information gain as entropy reduction

- *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*

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

$Values(A)$ possible values for A
S_v subset of S for which A has value v

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

Example: Information gain

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

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

- Information gain due to knowing *Wind*:

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

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

$$= 0.048$$

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
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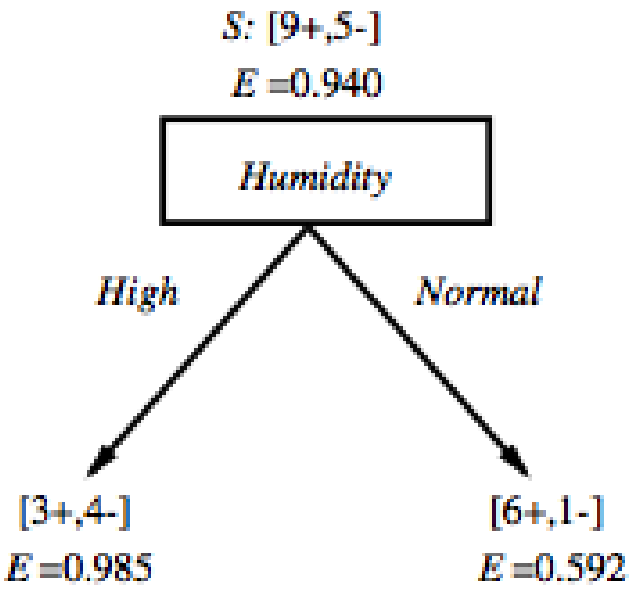
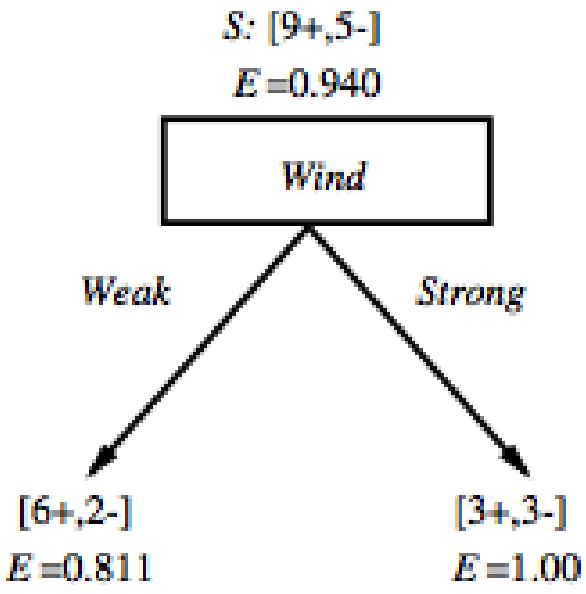
Which attribute is the best classifier?

Which attribute is the best classifier?





Gain (S, Humidity)

= .940 - (7/14).985 - (7/14).592
= .151

Gain (S, Wind)

= .940 - (8/14).811 - (6/14)1.0
= .048

First step: which attribute to test at the root?

- Which attribute should be tested at the root?
  - $Gain(S, Outlook) = 0.246$
  - $Gain(S, Humidity) = 0.151$
  - $Gain(S, Wind) = 0.084$
  - $Gain(S, Temperature) = 0.029$
- *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*

After first step

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
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D7	Overcast	Cool	Normal	Strong	Yes
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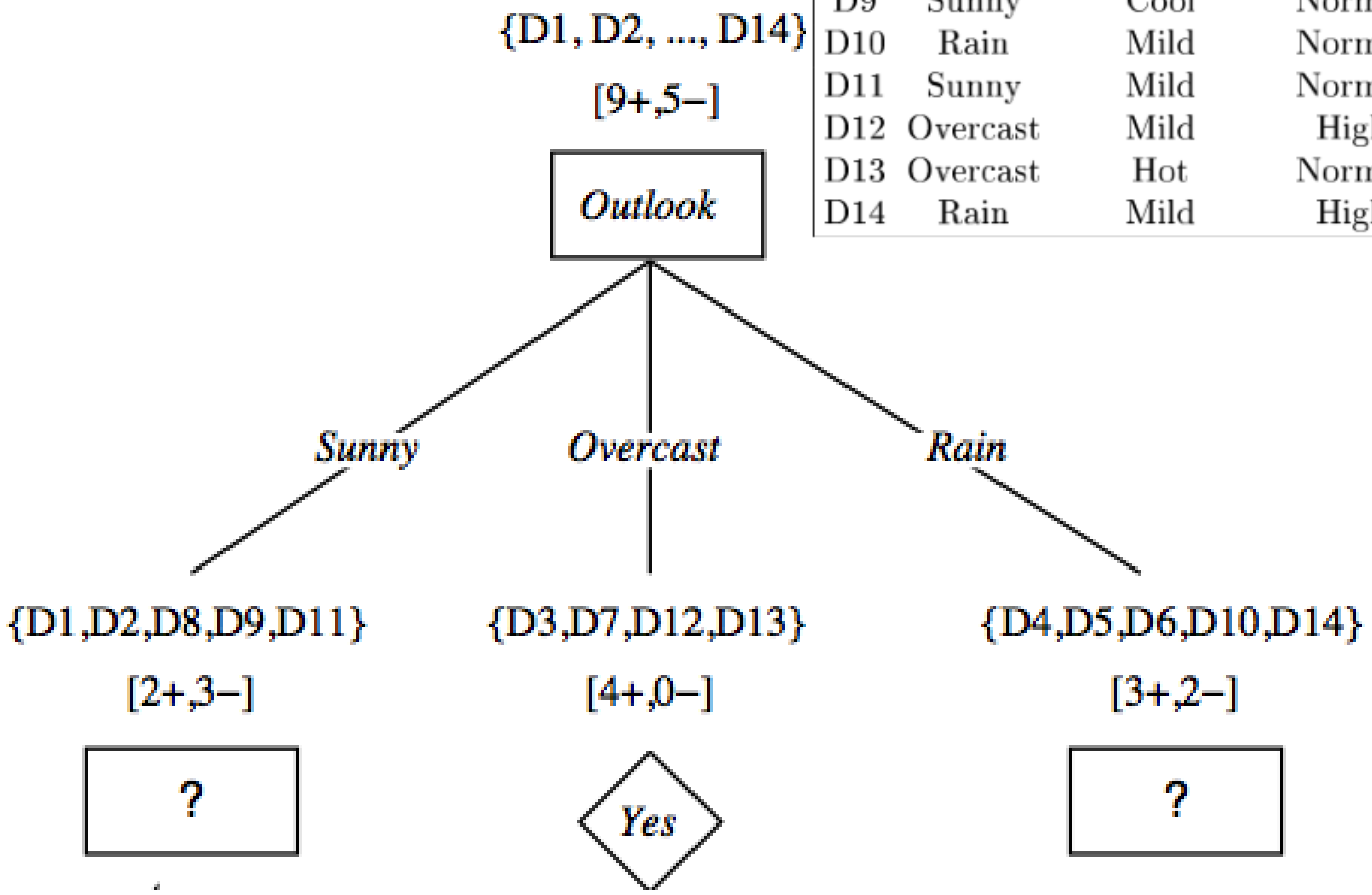

Second step

- Working on *Outlook=Sunny* node:

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

  $Gain(S_{Sunny}, Wind) = 0.970 - 2/5 \times 1.0 - 3.5 \times 0.918 = 0\ .019$

  $Gain(S_{Sunny}, Temp.) = 0.970 - 2/5 \times 0.0 - 2/5 \times 1.0 - 1/5 \times 0.0 = 0.570$

- *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

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
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D13	Overcast	Hot	Normal	Weak	Yes
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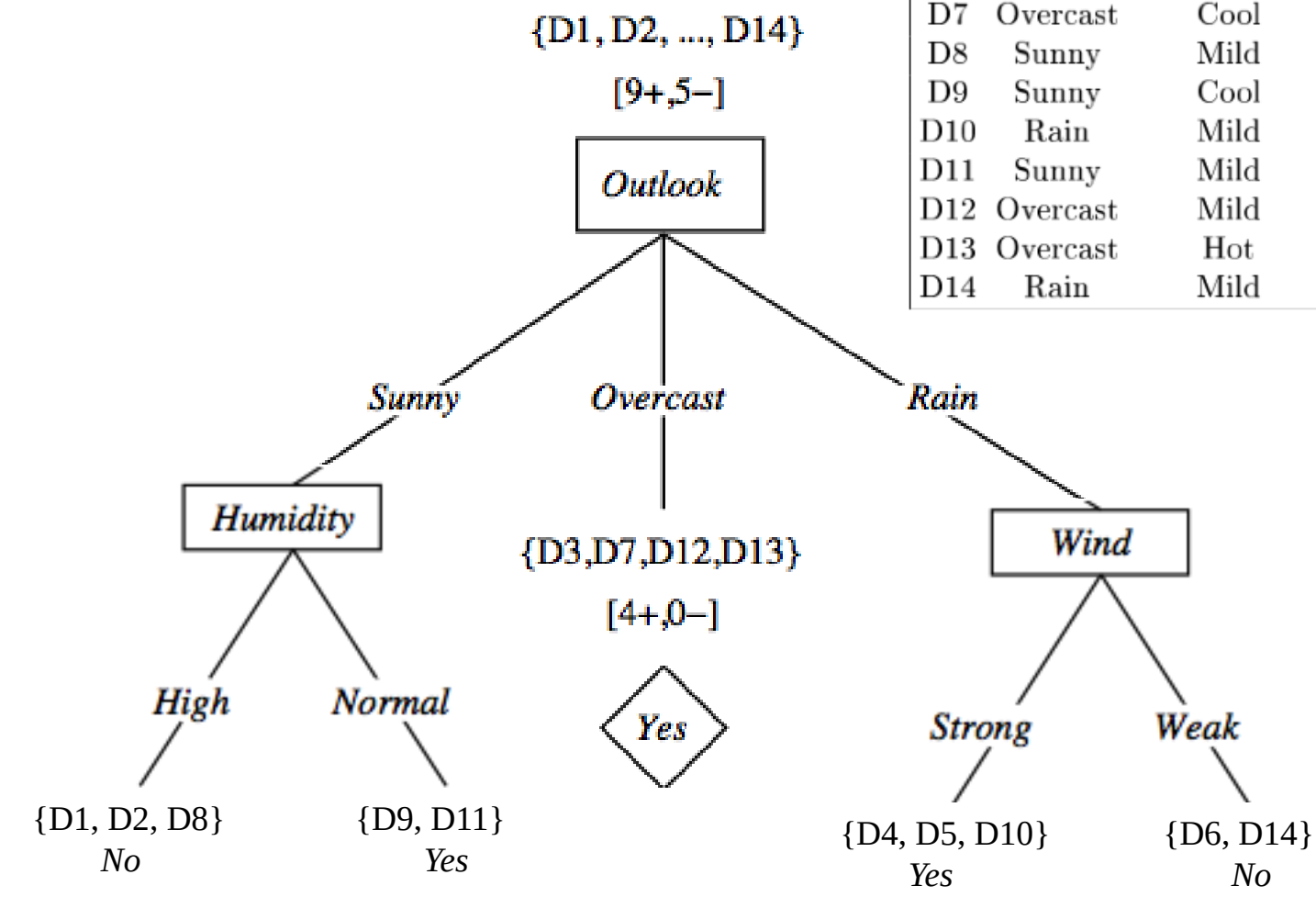

ID3: algorithm

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

Overfitting: definition

- **overfitting** is "the production of an analysis that corresponds too closely or exactly to a particular set of data
- Building trees that “adapt too much” to the training examples may lead to “overfitting”.
- May therefore fail to fit additional data or predict future observations reliably
- **overfitted model** is a statistical model that contains more parameters than can be justified by the data

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
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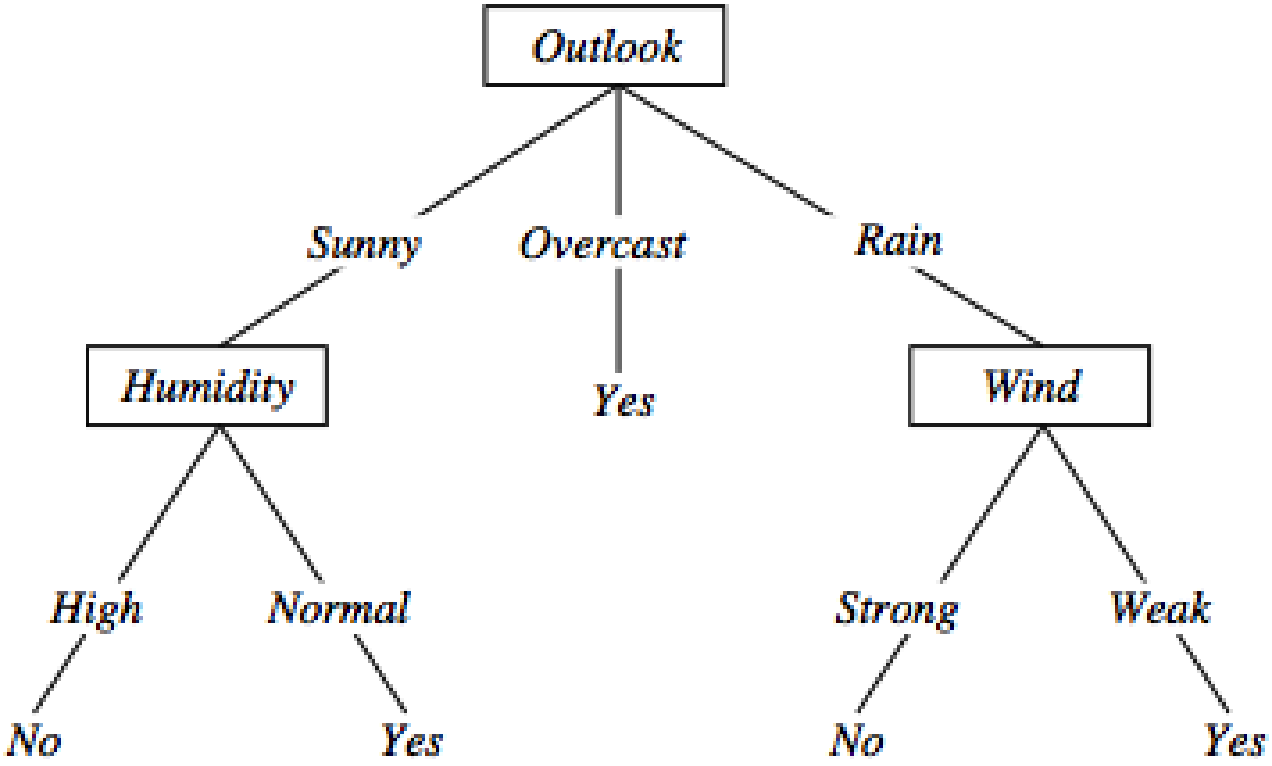
D10	Rain	Mild	Normal	Weak	Yes
D11	Sunny	Mild	Normal	Strong	Yes
D12	Overcast	Mild	High	Strong	Yes
D13	Overcast	Hot	Normal	Weak	Yes
D14	Rain	Mild	High	Strong	No
D15	Sunny	Hot	Normal	Strong	No

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 the tree, 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*

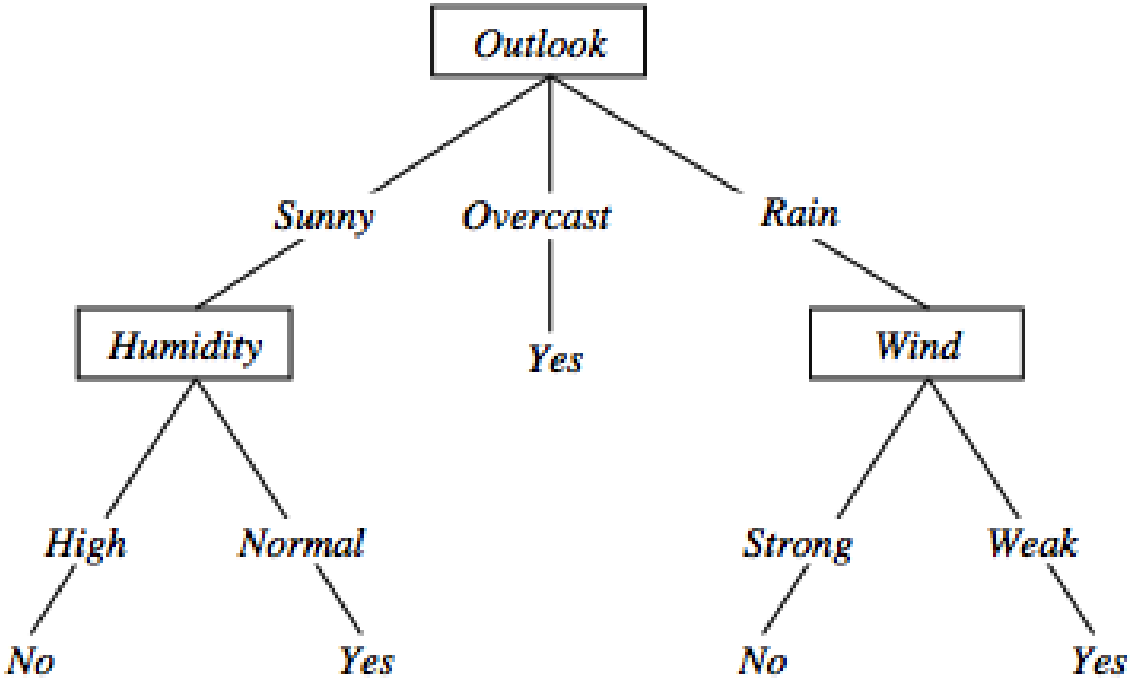
Reduced-error pruning

- 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 on the validation set.
- Nodes are pruned iteratively: at each iteration the node whose removal most increases accuracy on the validation set is pruned.
- Pruning stops when no pruning increases accuracy

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 improves accuracy …
   - … over validation set
4. Sort the rules in estimated order of accuracy, and consider them in sequence when classifying new instances

Converting to rules



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

Rule Post-Pruning

- Convert tree to rules (one for each path from root to a leaf)
- For each antecedent in a rule, remove it if error rate on validation set does not decrease
- Sort final rule set by accuracy

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

Compare first rule to:

```
Outlook=sunny->No
Humidity=high->No
```

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
- In rule form, tests are not ordered and there is no book-keeping involved when conditions (nodes) are removed
- Converting to rules improves readability for humans

Dealing with continuous-valued attributes

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

$$A_c = \text{True } if\ A < c, \text{ False } otherwise$$

- 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	Yes	Yes	Yes	No

  - Determine candidate thresholds by averaging consecutive values where there is a change in classification: (48+60)/2=54 and (80+90)/2=85

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

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

- S_i are the sets obtained by partitioning on value i of A
- *SplitInformation* measures the entropy of S with respect to the values of A. The more uniformly dispersed the data the higher it is.

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

- *GainRatio* penalizes attributes that split examples in many small classes such as *Date*. 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, and 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

Random Forest

- https://www.stat.berkeley.edu/~breiman/RandomForests/