Lecture 3: Decision Trees

Cognitive Systems II - Machine Learning
SS 2005

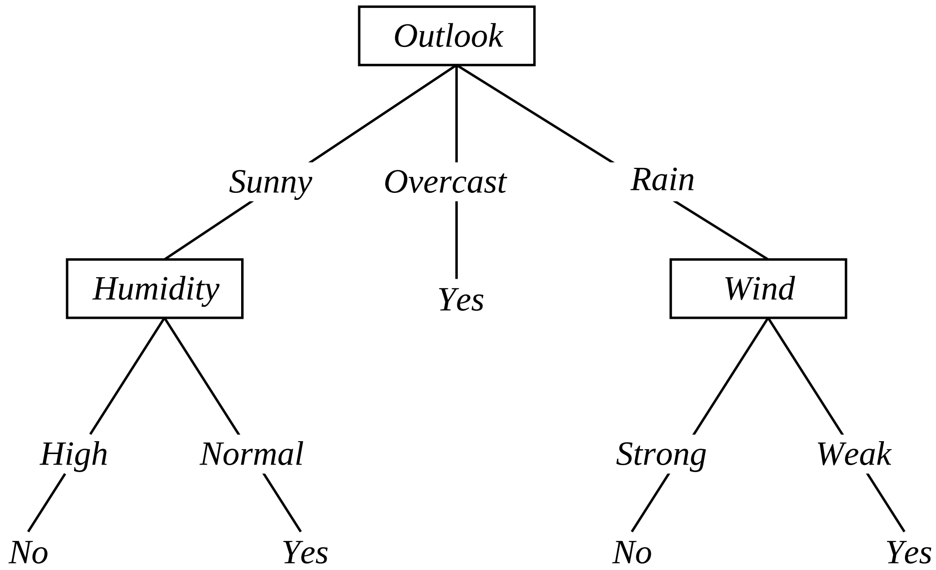
Part I: Basic Approaches of Concept Learning

ID3, Information Gain, Overfitting, Pruning

Decision Tree Representation

- classification of instances by sorting them down the tree from the root to some leaf note
  - **node** $\approx$ test of some attribute
  - **branch** $\approx$ one of the possible values for the attribute
- decision trees represent a **disjunction of conjunctions of constraints on the attribute values of instances**
  - i.e., $(\ldots \wedge \ldots \wedge \ldots) \vee (\ldots \wedge \ldots \wedge \ldots) \vee \ldots$
- equivalent to a set of if-then-rules
  - each branch represents one if-then-rule
    - **if-part**: conjunctions of attribute tests on the nodes
    - **then-part**: classification of the branch

Decision Tree Representation



- This decision tree is equivalent to:

  if $(Outlook = Sunny) \wedge (Humidity = Normal)$ then Yes;

  if $(Outlook = Overcast)$ then Yes;

  if $(Outlook = Rain) \wedge (Wind = Weak)$ then Yes;

Appropriate Problems

- Instances are represented by attribute-value pairs, e.g. (Temperature, Hot)
- Target function has discrete output values, e.g. yes or no
- **Disjunctive descriptions** may be required
- Training data may **contain errors**
- Training data may contain **missing attribute values**

$\Rightarrow$ last three points make Decision Tree Learning more attractive than CANDIDATE-ELIMINATION

ID3

- learns decision trees by constructing them **top-down**
- employs a **greedy search algorithm without backtracking** through the space of all possible decision trees
  - ⇒ finds the shortest but not neccessarily the best decision tree
- **key idea:**
  - selection of the next attribute according to a statistical measure
  - all examples are considered at the same time (simultaneous covering)
  - recursive application with reduction of selectable attributes until each training example can be classified unambiguously

ID3 algorithm

$ID3(Examples, Target\_attribute, Attributes)$

- Create a $Root$ for the tree
- If all examples are **positive**, Return single-node tree $Root$, with $label = +$
- If all examples are **negative**, Return single-node tree $Root$, with $label = -$
- If $Attributes$ is empty, Return single-node tree $Root$, with $label =$ most common value of $Target\_attribute$ in $Examples$
- **otherwise**, Begin
  - $A \leftarrow$ attribute in $Attributes$ that best classifies $Examples$
  - decision attribute for $Root \leftarrow A$
  - **For each possible value v_i of A**
    - Add new branch below $Root$ with $A = v_i$
    - Let $Examples_{v_i}$ be the subset of $Examples$ with v_i for A
    - If $Examples$ is empty
      - Then add a leaf node with label = most common value of $Target\_attribute$ in $Examples$
      - Else add ID3($Examples_{v_i}, Target\_Attribute, Attributes - \{A\}$)
- Return $Root$

The best classifier

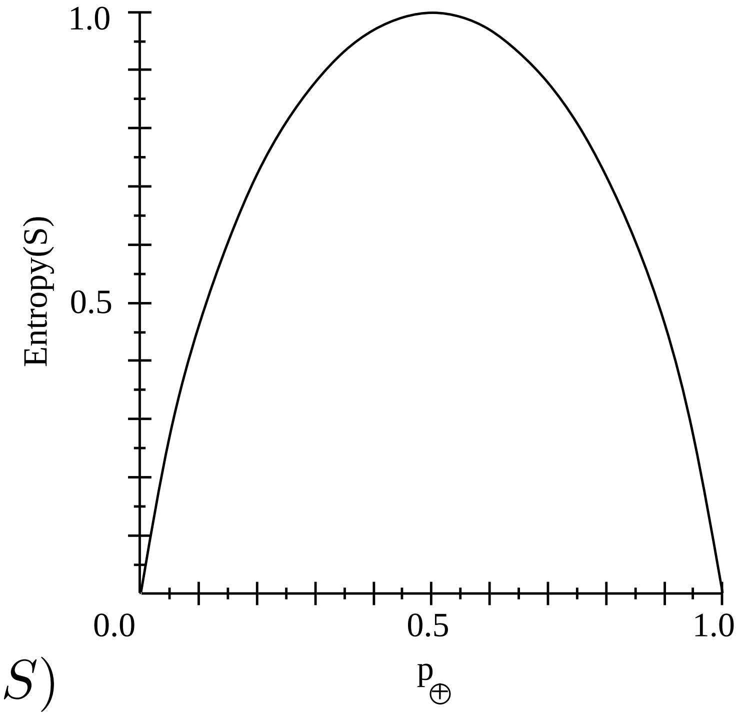
- **central choice**: Which attribute classifies the examples best?
- ID3 uses the **information gain**
  - statistical measure that indicates how well a given attribute separates the training examples according to their target classification
  - $$Gain(S,A) = \underbrace{Entropy(S)}_{\text{original entropy of S}} - \underbrace{\sum_{v \in values(A)} \frac{|S_v|}{|S|} \cdot Entropy(S_v)}_{\text{relative entropy of S}}$$
  - interpretation:
    - denotes the reduction in entropy caused by partitioning S according to A
    - alternative: number of saved yes/no questions (i.e., bits)

⇒ attribute with $\max_A Gain(S,A)$ is selected!

Entropy

- statistical measure from information theory that **characterizes (im-)purity** of an arbitrary collection of examples S
- for binary classification: $H(S) \equiv -p_{\oplus} \log_2 p_{\oplus} - p_{\ominus} \log_2 p_{\ominus}$
- for n-ary classification: $H(S) \equiv \sum_{i=1}^{n} -p_i \log_2 p_i$
- **interpretation:**
  - specification of the minimum number of bits of information needed to encode the classification of an arbitrary member of S
  - alternative: number of yes/no questions

Entropy



- **minimum** of $H(S)$
  - for minimal impurity $\longrightarrow$ point distribution
  - $H(S) = 0$
- **maximum** of $H(S)$
  - for maximal impurity $\longrightarrow$ uniform distribution
  - for binary classification: $H(S) = 1$
  - for n-ary classification: $H(S) = \log_2 n$

Illustrative Example

- example days

Day	$Sunny$	$Temp.$	$Humidity$	$Wind$	$PlayTennis$
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

Illustrative Example

- entropy of S

  $S = \{D1, ..., D14\} = [9+, 5-]$

  $H(S) = -\frac{9}{14} \cdot \log_2 \frac{9}{14} - \frac{5}{14} \cdot \log_2 \frac{5}{14} = 0.940$

- information gain (e.g. $Wind$)

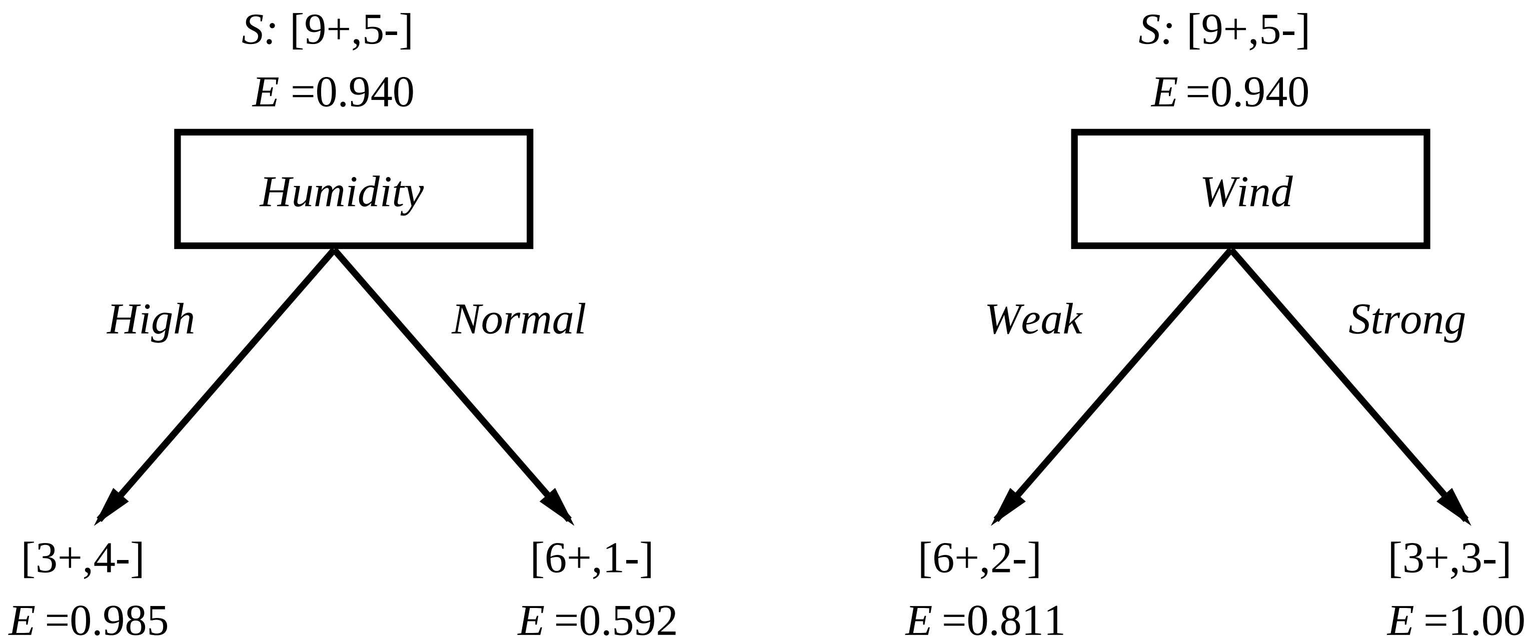
  $S_{Weak} = \{D1, D3, D4, D5, D8, D9, D10, D13\} = [6+, 2-]$

  $S_{Strong} = \{D2, D6, D7, D11, D12, D4\} = [3+, 3-]$

$$
\begin{aligned}
Gain(S, Wind) &= H(S) - \sum_{v \in Wind} \frac{|S_v|}{|S|} \cdot H(S_v) \\
&= H(S) - \frac{8}{14} \cdot H(S_{Weak}) - \frac{6}{14} \cdot H(S_{Strong}) \\
&= 0.940 - \frac{8}{14} \cdot 0.811 - \frac{6}{14} 1.000 \\
&= 0.048
\end{aligned}
$$

Illustrative Example

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

Illustrative Example

- informations gains for the four attributes:

  $Gain(S, Outlook) = 0.246$

  $Gain(S, Humidity) = 0.151$

  $Gain(S, Wind) = 0.048$

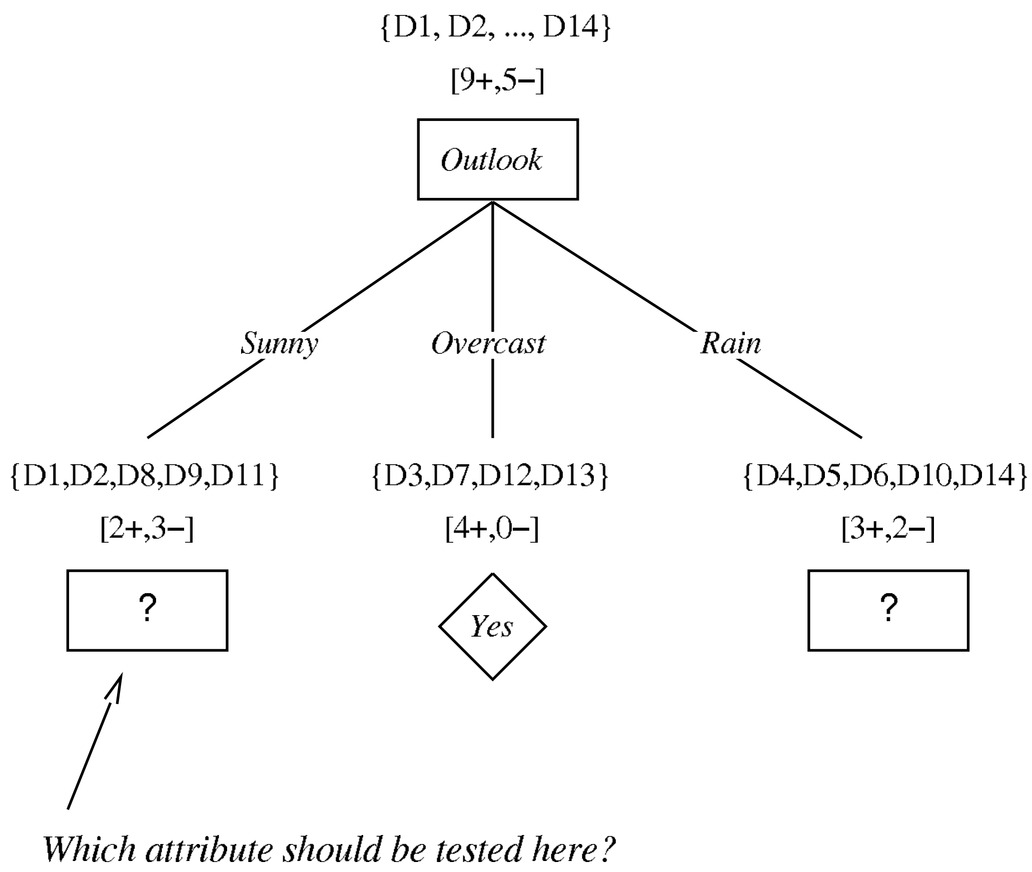
  $Gain(S, Temperature) = 0.029$

⇒ $Outlook$ is selected as best classifier and is therefore $Root$ of the tree

⇒ now branches are created below the root for each possible value

  - because every example for which $Outlook = Overcast$ is positive, this node becomes a leaf node with the classification Yes
  - the other descendants are still ambiguous (e.g. $H(S) \neq 0$)
  - hence, the decision tree has to be further elaborated below these nodes

Illustrative Example



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

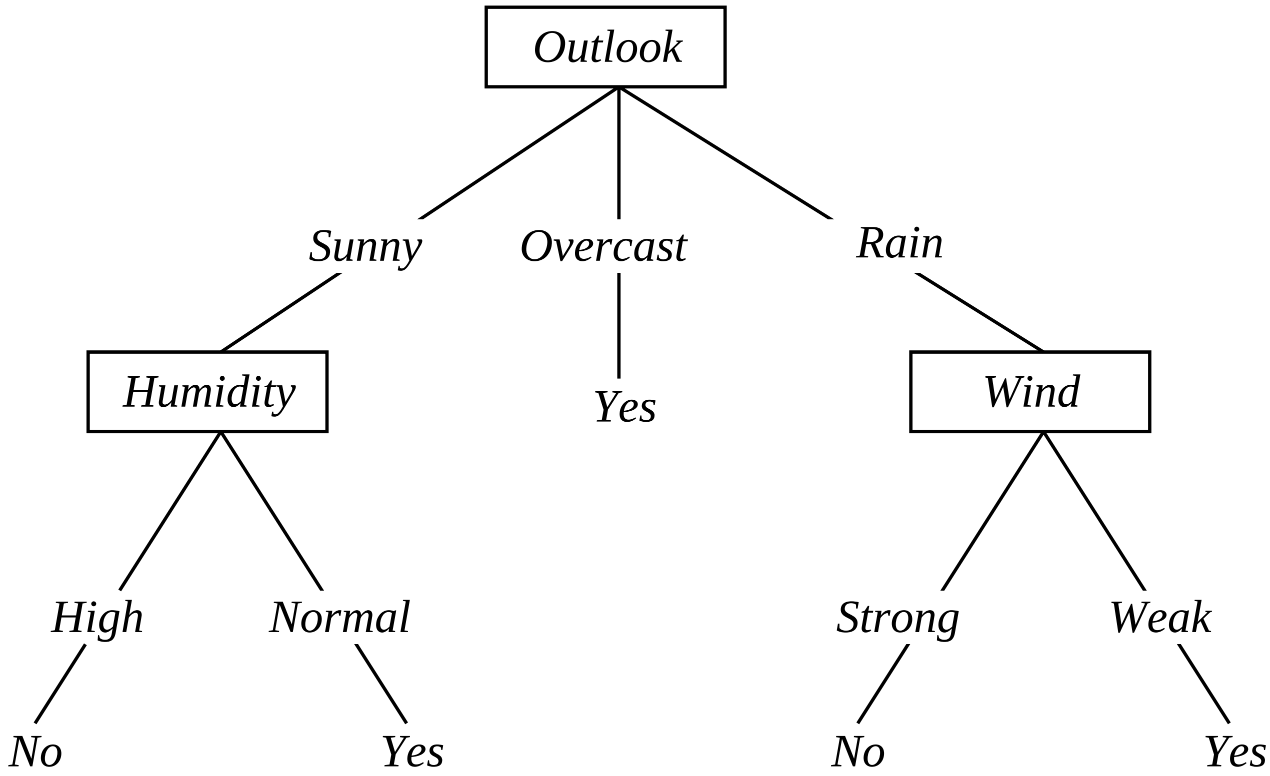
$Gain(S_{sunny}, Humidity) = .970 - (3/5)\ 0.0 - (2/5)\ 0.0 = .970$

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

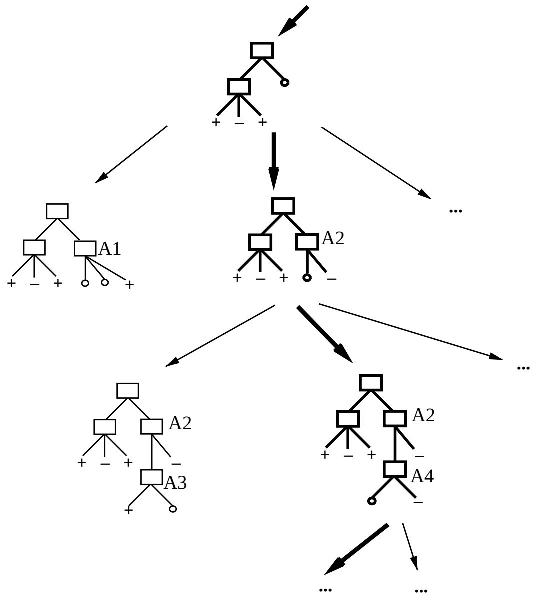
$Gain(S_{sunny}, Wind) = .970 - (2/5)\ 1.0 - (3/5)\ .918 = .019$

Illustrative Example

- Resulting decision tree



Hypothesis Space Search

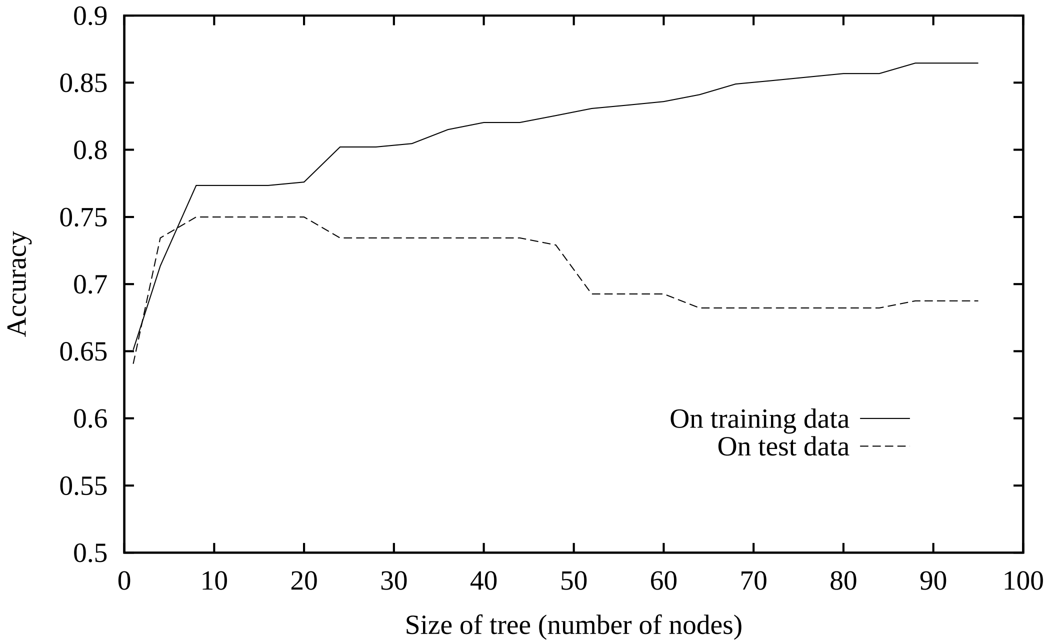


- $H \approx$ *complete* space of finite discrete functions, relative to the available attributes (i.e. all possible decision trees)
- **capabilites and limitations:**
  - returns just one single consistent hypothesis
  - performs greedy search (i.e., $\max_A Gain(S, A)$)
  - susceptible to the usual risks of hill-climbing without backtracking
  - uses all training examples at each step $\Rightarrow$ simultaneous covering

Inductive Bias

- as mentioned above, ID3 searches
  - *complete* space of possible, but not *completely*
  - ⇒ Preference Bias
- **Inductive bias**: Shorter trees are prefered to longer trees. Trees that place high information gain attributes close to the root are also prefered.
- Why prefer shorter hypotheses?
  - **Occam's Razor**: Prefer the simplest hypothesis that fits the data!
  - see Minimum Description Length Principle (Bayesian Learning)
  - e.g., if there are two decision trees, one with 500 nodes and another with 5 nodes, the second one should be prefered
  - ⇒ better chance to avoid overfitting

Overfitting



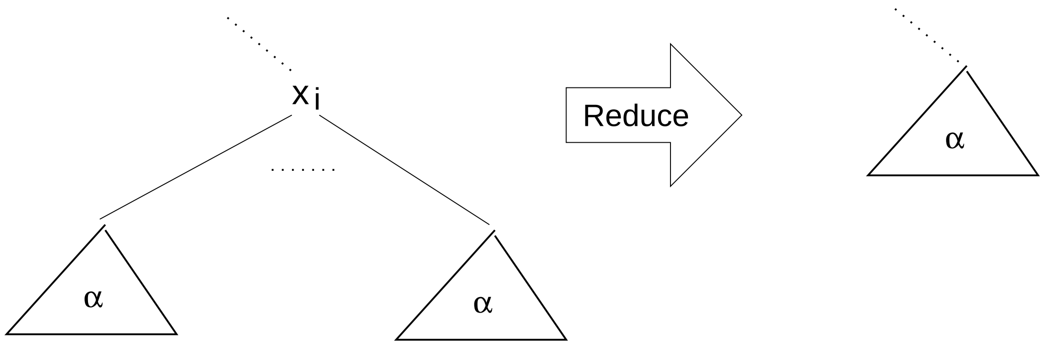
- Given a hypothesis space H, a hypothesis $h \in H$ is said to **overfit** the training data if there exists some alternative hypothesis $h' \in H$, such that h has smaller error than h' over the training, but h' has smaller error than h over the entire distribution of instances.

Overfitting

- **reasons for overfitting:**
  - noise in the data
  - number of training examples is to small too produce a representative sample of the target function
- **how to avoid overfitting:**
  - **stop the tree grow earlier**, before it reaches the point where it perfectly classifies the training data
  - allow overfitting and then **post-prune** the tree (more successful in practice!)
- **how to determine the perfect tree size:**
  - separate validation set to evaluate utility of post-pruning
  - apply statistical test to estimate whether expanding (or pruning) produces an improvement

Reduced Error Pruning

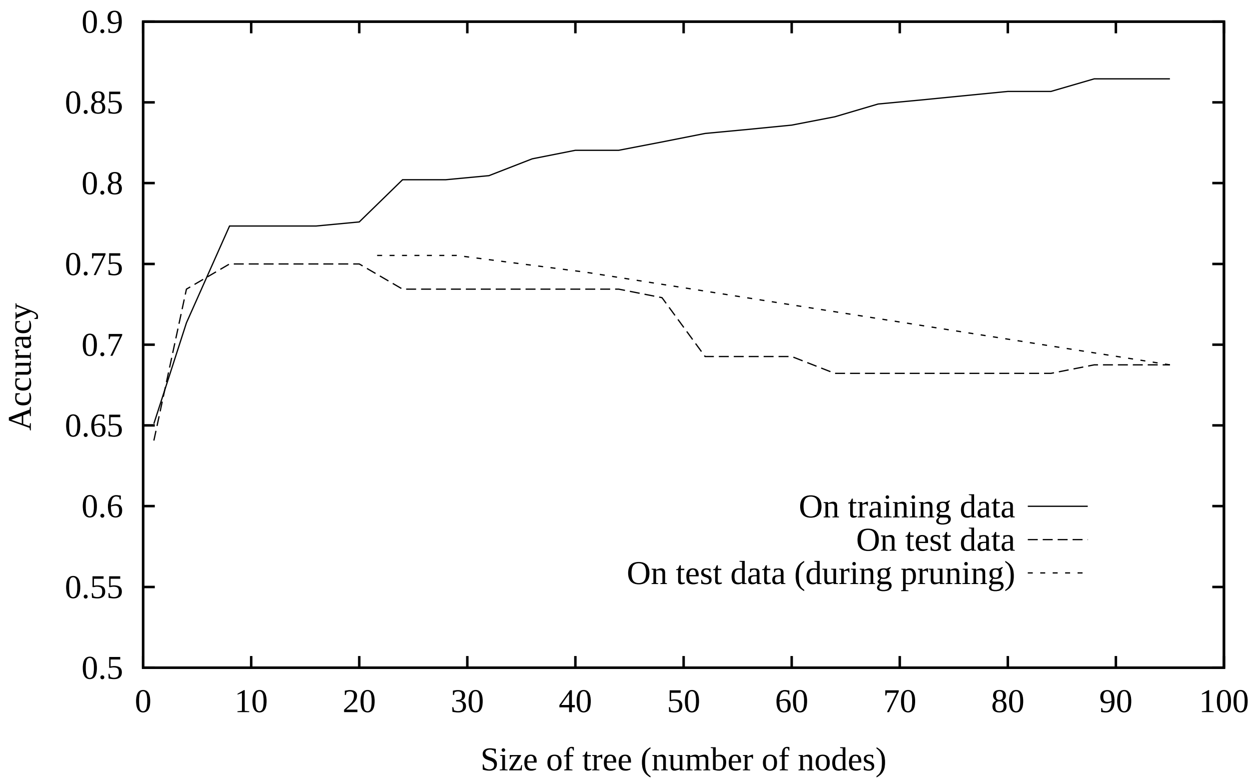
- each of the decision nodes is considered to be candidate for pruning



- **pruning** a decision node consists of removing the subtree rootet at the node, making it a leaf node and assigning the most common classification of the training examples affiliated with that node
- nodes are removed only if the resulting tree performs **not worse** than the original tree over the validation set
- pruning starts wit the node whose removal most increases accuracy and continues until further pruning is harmful

Reduced Error Pruning

- **effect of reduced error pruning:**



- any node added to coincidental regularities in the training set is likely to be pruned

Rule Post-Pruning

- rule post-pruning involves the following steps:
  1. Infer the decision tree from the training set (Overfitting allowed!)
  2. Convert the tree into a set of rules
  3. Prune each rule by removing any preconditions that result in improving its estimated accuracy
  4. Sort the pruned rules by their estimated accuracy
- one method to estimate rule accuracy is to use a separate validation set
- pruning rules is more precise than pruning the tree itself

Alternative measures

- natural bias in information gain favors attributes with many values over those with few values

- e.g. attribute $Date$
  - very large number of values (e.g. March 21, 2005)
  - inserted in the above example, it would have the highest information gain, because it perfectly separates the training data
  - but the classification of unseen examples would be impossible

- alternative measure: $GainRatio$
  - $GainRatio(S, A) = \frac{Gain(S,A)}{SplitInformation(S,A)}$

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

  - $SplitInformation(S, A)$ is sensitive to how broadly and uniformly A splits S (entropy of S with respect to the values of A)

  $\Rightarrow$ $GainRatio$ penalizes attributes such as $Date$

Summary

- practical and intuitively understandable method for concept learning
- able to learn disjunctive, discrete-valued conepts
- noise in the data is allowed
- **ID3** is a simultaneous covering algorithm based on information gain that performs a greedy top-down search through the space of possible decision trees
- **Inductive Bias**: Short trees are prefered (Occam's razor)
- overfitting is an important issue and can be reduced by pruning