

# Machine Learning

## ITCS 4156

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Decision Trees

CART

Ensembles of DTs

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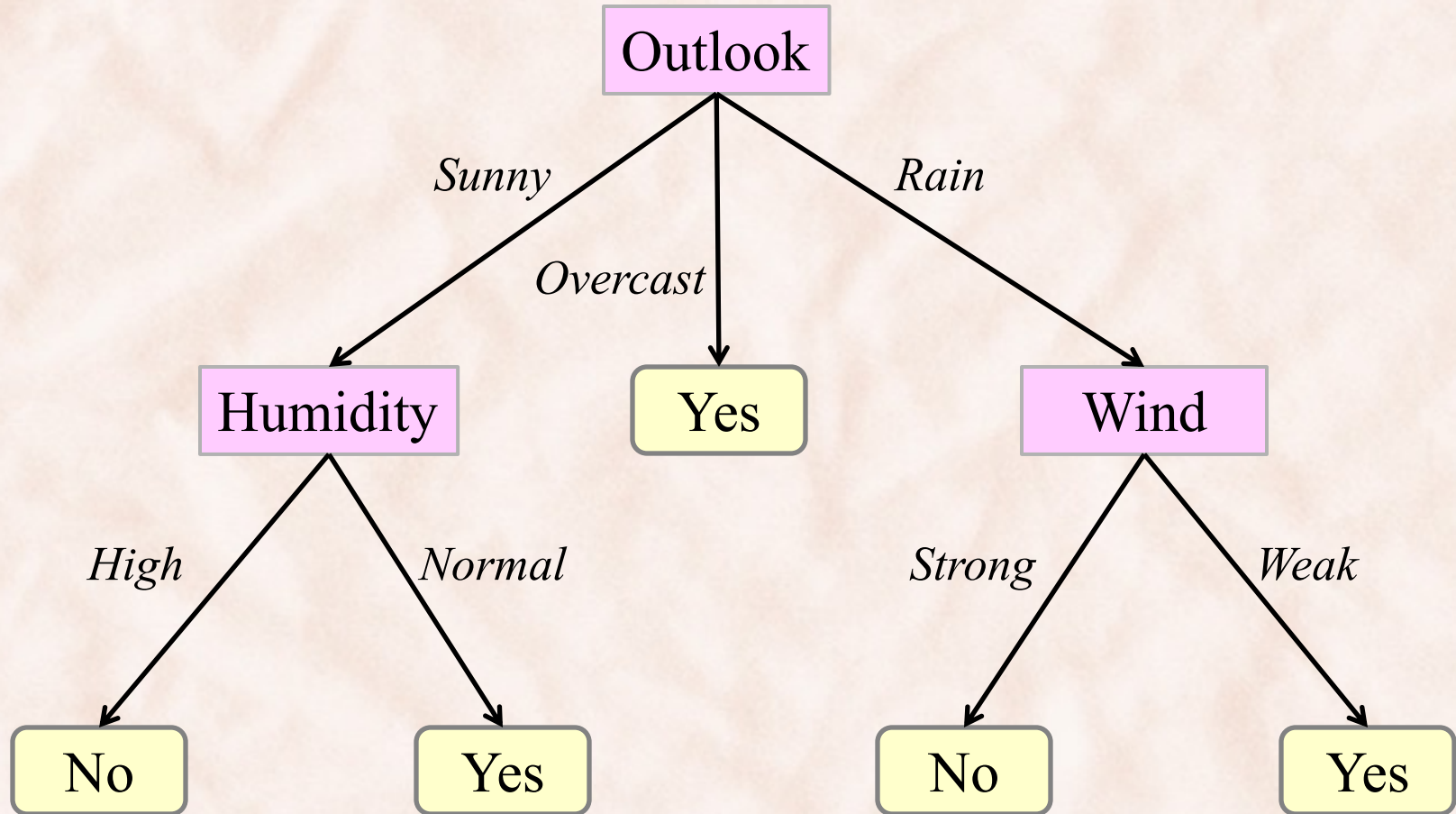
# Decision Tree Learning

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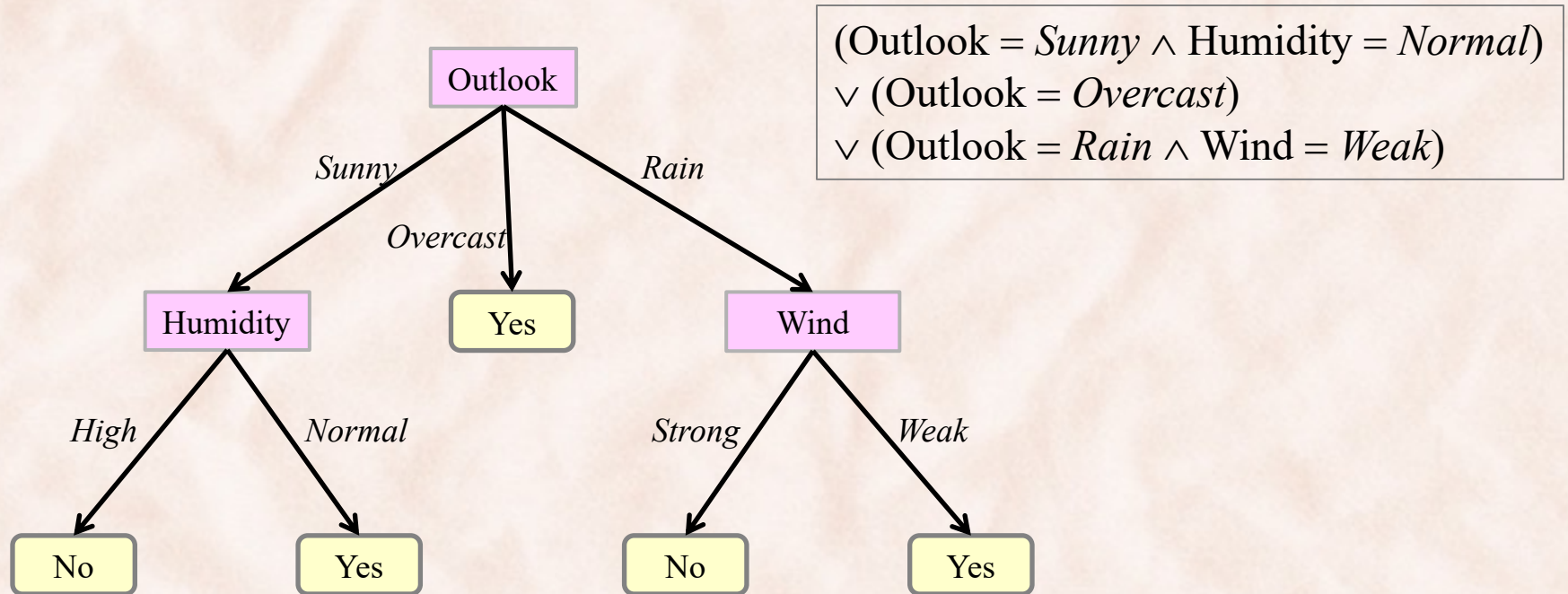
- Target output is discrete (i.e. binary, or multiple classes).
  - $\text{PlayTennis} \in \{\text{Yes}, \text{No}\}$ .
- Features have finite cardinality (i.e. nominal features).
  - $\text{Outlook} \in \{\text{Sunny}, \text{Overcast}, \text{Rain}\}$ .
  - $\text{Temperature} \in \{\text{Cool}, \text{Mild}, \text{Hot}\}$ .
  - $\text{Humidity} \in \{\text{Normal}, \text{High}\}$ .
  - $\text{Wind} \in \{\text{Weak}, \text{Strong}\}$ .
- Target model requires disjunctive description in terms of features  $\Rightarrow$  use **Decision Trees**.

# Decision Trees

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# Decision Trees



Decision Tree  $\Leftrightarrow$  Disjunction of conjunctions of constraints on the attribute values of instances.

# Decision Tree Learning

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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	Cold	Normal	Weak	Yes
D6	Rain	Cold	Normal	Strong	No
D7	Overcast	Cold	Normal	Strong	Yes
D8	Sunny	Mild	High	Weak	No
D9	Sunny	Cold	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 Learning

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- There may be many decision trees *consistent* with a set of training examples:
  - Q: Which decision tree should be selected?
  - A: Prefer shorter trees over larger trees.
  - ⇒ the **ID3 Algorithm** for learning decision trees.

Occam's razor:

Prefer the simplest hypothesis that fits the data.

$$P(\text{Yes}) = 1$$

$$P(\text{No}) = 0$$

$$\text{min entropy is } H(T) = -1 * \log(1) - 0 * \log(0) = 0 - 0 = 0 \text{ bits}$$

## The ID3 Algorithm

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- At each node:
  - Select the feature that results in the largest *expected reduction in entropy* for the target label.
  - ↔ select the feature with largest *information gain*.
- $D$  = the training data
- $T$  = the random variable corresponding to PlayTennis.

$$\left. \begin{array}{l} p(T = \text{yes}) = \frac{9}{14} \\ p(T = \text{no}) = \frac{5}{14} \end{array} \right\} \Rightarrow H(T; D) = - \sum_i p(x_i) \log p(x_i)$$

$$= - \left\{ \frac{9}{14} \log \frac{9}{14} + \frac{5}{14} \log \frac{5}{14} \right\} \cong 0.940$$

$$P(\text{Yes}) = 0.5$$

$$P(\text{No}) = 0.5$$

$$\text{max entropy is } H(T) = -0.5 * \log_2(1/2) - 0.5 * \log_2(2^{-1}) =$$

$$= -0.5 * -1 - 0.5 * -1 = 1 \text{ bit}$$

# The ID3 Algorithm

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- Suppose we split on feature  $X$  that has  $k$  values  $\{x_1, \dots, x_k\}$
- Let  $D_i$  be the set of instances where  $X = x_i$ .
- The expected reduction in entropy is:

$$IG(X; D) = H(T; D) - \sum_{i=1}^k \frac{|D_i|}{|D|} H(T; D_i)$$

- Choose the feature that maximizes the information gain:

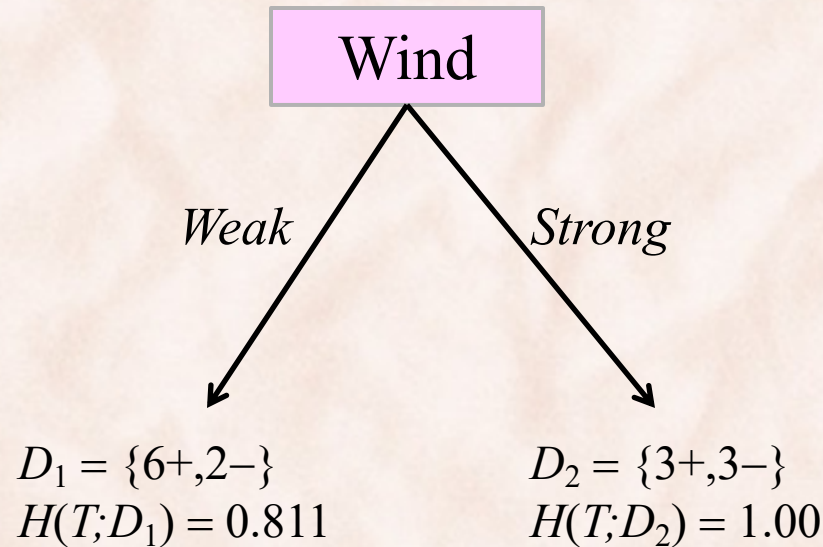
$$\hat{X} = \arg \max_X IG(X; D)$$



# The ID3 Algorithm

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$$D = \{9+, 5-\}$$
$$H(T;D) = 0.940$$



$$IG(\text{Wind};D) = 0.940 - (8/14)*0.811 - (6/14)*1.00 = 0.048$$

# The ID3 Algorithm

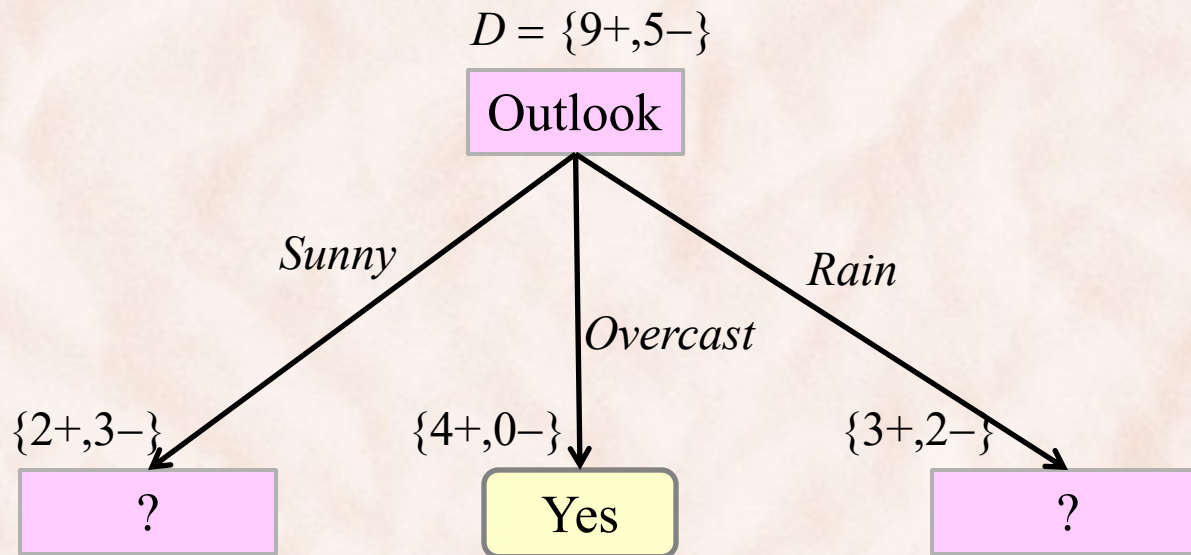
$$IG(\text{Wind}; D) = 0.048$$

$$IG(\text{Humidity}; D) = 0.151$$

$$IG(\text{Temperature}; D) = 0.029$$

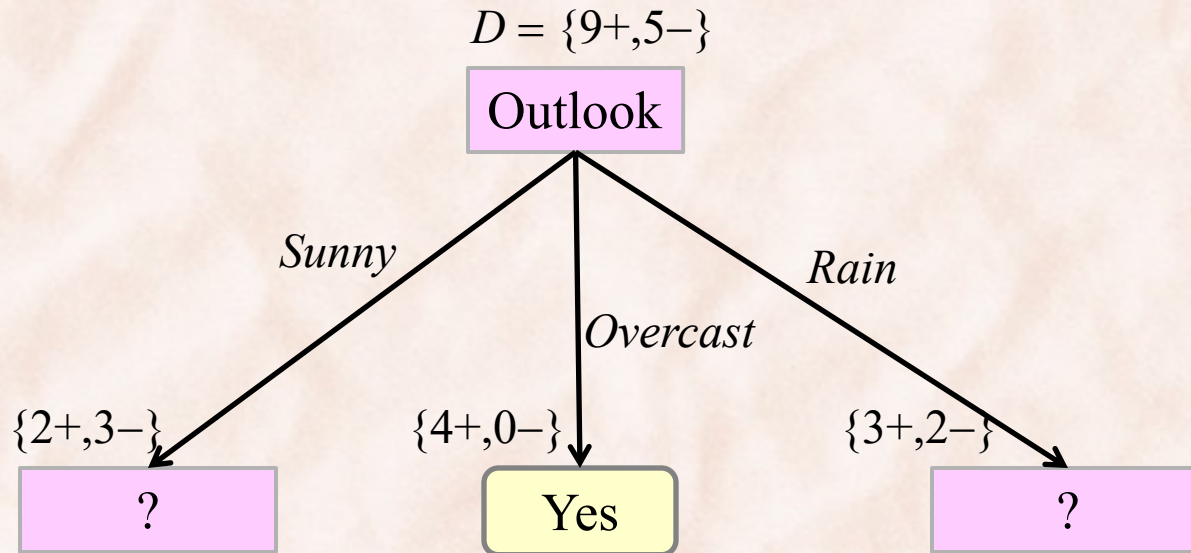
$$IG(\text{Outlook}; D) = 0.246$$

}  $\Rightarrow$  select  $X = \text{Outlook}$  to split at the root.



# The ID3 Algorithm

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- Repeatedly apply the Information Gain criterion to select the best attribute for each nonterminal node.
  - set  $D$  to the training examples for that node.
  - use only remaining attributes.

# The ID3 Algorithm

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Algorithm ID3(Training data  $D$ , Features  $F$ ):

**if** all examples in  $D$  have the same label:

**return** a leaf node with that label

**let**  $X \in F$  be the feature with the largest information gain

**let**  $T$  be a tree root labeled with feature  $X$ .

**let**  $D_1, D_2, \dots, D_k$  be the partition produced by splitting  $D$  on feature  $X$

**for each**  $D_i \in \{D_1, D_2, \dots, D_k\}$ :

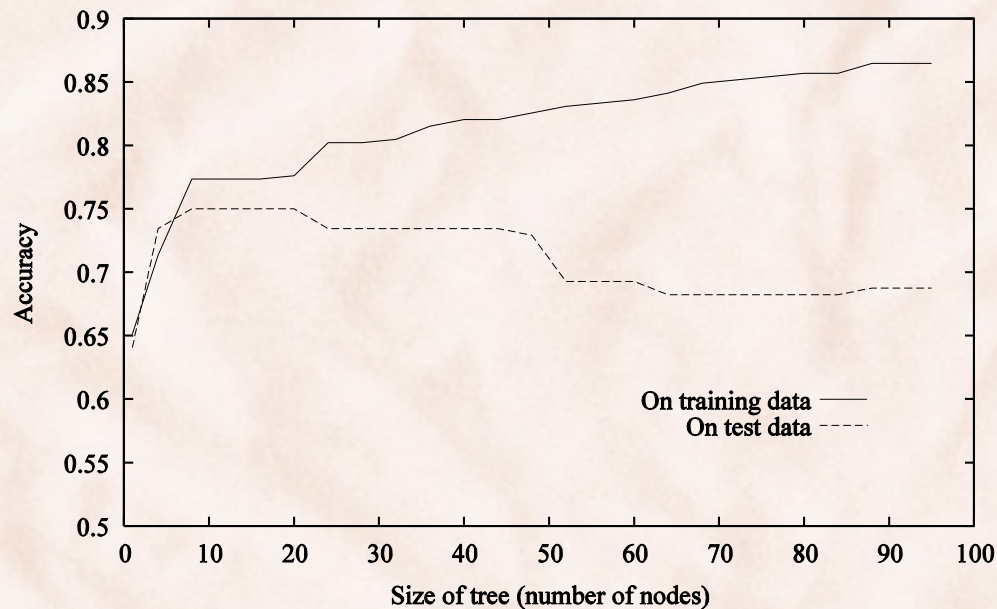
**let**  $T_i = \text{ID3}(D_i, F - \{X\})$

    add  $T_i$  as a new branch of  $T$

**return**  $T$

# Overfitting

- ID3 learns a tree that classifies the training data perfectly.
- The learned tree may not lead to the tree with the best generalization performance on unseen (test) data.



*learning which patients  
have a form of diabetes.*

<http://www.cs.cmu.edu/afs/cs/project/theo-11/www/decision-trees.html>

# Overfitting

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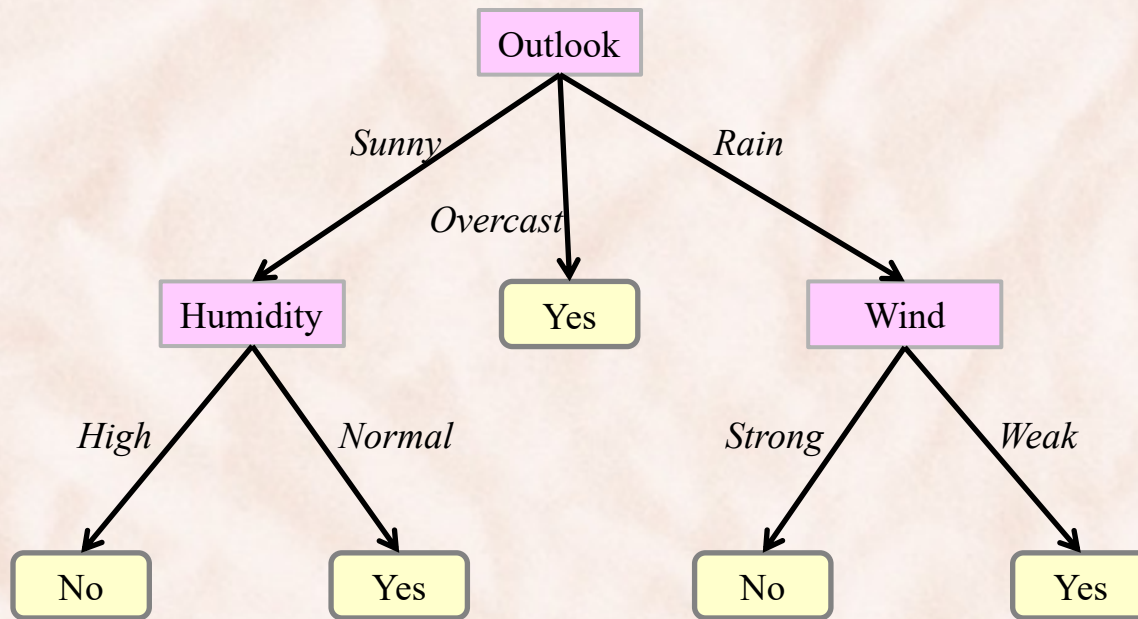
1. Maximum number of leaf nodes is  $N = \#$  training examples  
 $\Rightarrow$  no generalization outside of the training data.
2. When small number of examples are associated with leaf nodes:
  - some attribute that is unrelated to the actual target function happens to partition the examples very well.
3. When training examples contain random noise:
  - consider adding (false) negative example:

Day	Outlook	Temperature	Humidity	Wind	PlayTennis
D15	Sunny	Hot	Normal	Strong	No

# Overfitting

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Day	Outlook	Temperature	Humidity	Wind	PlayTennis
D15	Sunny	Hot	Normal	Strong	No



{+D<sub>9</sub>, +D<sub>11</sub>, -D<sub>15</sub>}

# Methods for Reducing Overfitting

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- Two types of methods:
  - 1) Stop growing the tree before it perfectly classifies the training data.
  - 2) Allow the tree to overfit the data, then prune the tree.
  - 3) Use ensembles of trees: **bagged trees** & **random forests**.
- 1. Criteria for determining the right size of the tree:
  - Use a validation set to evaluate utility of pruning nodes.
  - Use a statistical test ( $\chi^2$ ) to determine whether expanding a particular node is likely to produce improvement over entire instance distribution.
  - Minimal Description Length (MDL): determine if additional nodes leads to less complex hypothesis than just remembering any exceptions that result from pruning.



## 2. Reduced Error Pruning

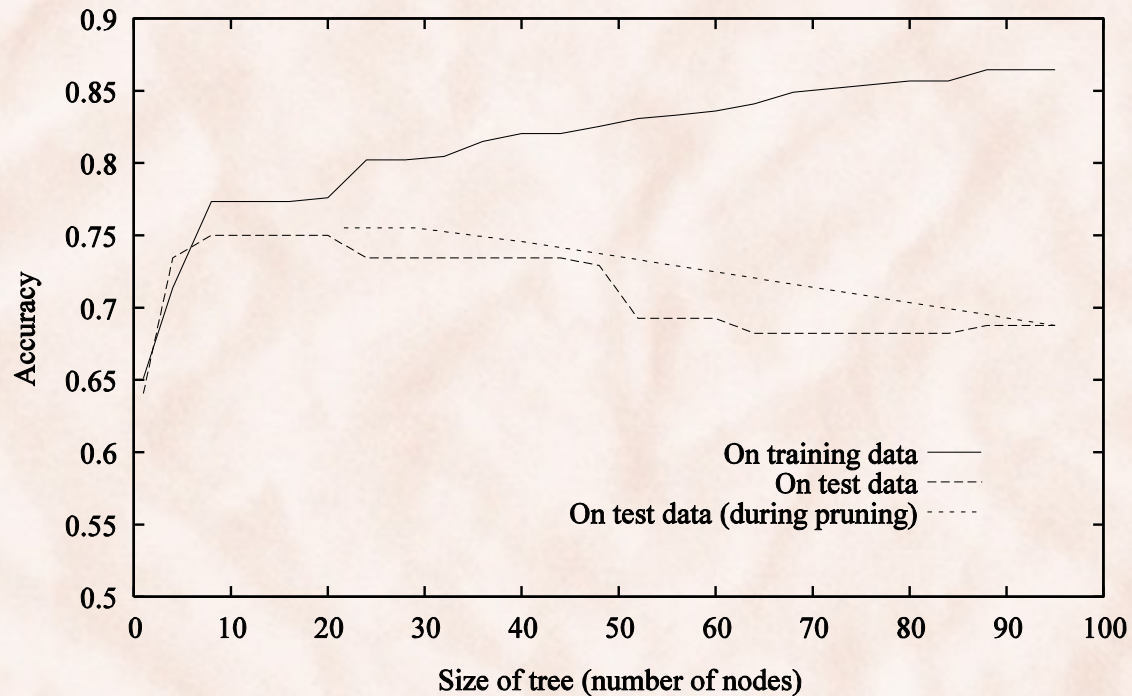
[Quinlan, 1987]

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1. grow a complete tree from the training data
  2. **while** accuracy on validation set is non-decreasing:
  3.     **for each** internal node in the tree:
  4.         temporarily prune the subtree and replace it with a leaf labeled with the majority class
  5.         measure the accuracy of the pruned tree on validation set
  6.         permanently prune the node that results in greatest accuracy.
- ⇒ leaf nodes created due to chance regularities in training data are likely to be pruned.
- Drawback: “wastes” validation dataset, instead of using it for training.

## 2. Reduced Error Pruning

[Quinlan, 1987]



## 3. Bagged Decision Trees

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- Training set has  $N$  examples, each example has  $K$  features.
  1. for  $t = 1$  to  $T$ :
    2. draw  $n < N$  samples with replacement.
    3. train a decision tree  $D_t$  on the  $n$  samples.
  4. construct final classifier by majority voting over trees  $D_t$ .
    - for regression, average predictions of trees  $D_t$ .

## 3. Random Forests

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- Training set has  $N$  examples, each example has  $K$  features.
  1. for  $t = 1$  to  $T$ :
    2. draw  $n < N$  samples with replacement.
    3. sample  $k < K$  features at random.
    4. train a decision tree  $D_t$  on the  $n$  samples and  $k$  features.
    5. construct final classifier by majority voting over trees  $D_t$ .
      - for regression, average predictions of trees  $D_t$ .