Learning by Asking Questions: Decision Trees

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Machine Learning (CS771A)

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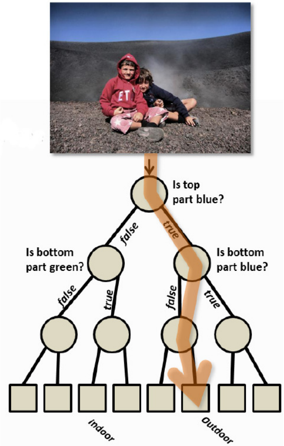
A Classification Problem

Indoor or Outdoor ?

Pic credit: "Decision Forests: A Unified Framework" by Criminisi *et al*

Predicting by Asking Questions



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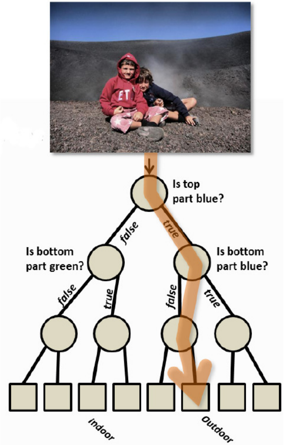

How can we learn this tree using labeled training data?

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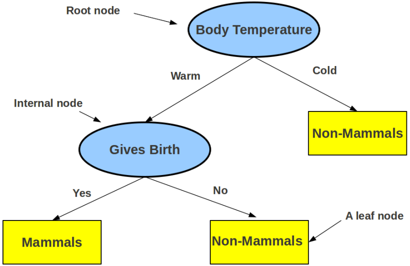
Decision Tree

- Defined by a hierarchy of rules (in form of a tree)



- Rules form the **internal nodes** of the tree (topmost internal node = **root**)
- Each internal node tests the value of some feature and "splits" data across the outgoing branches

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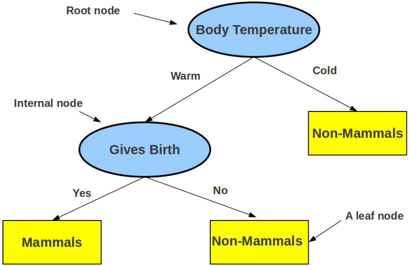

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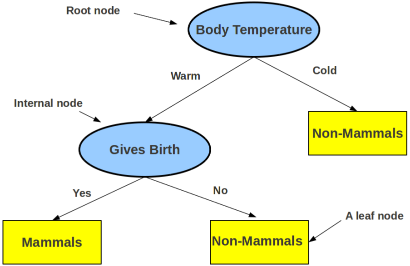

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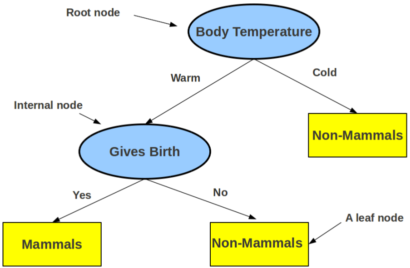

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- The DT can then be used to predict label $\mathbf{y}$ of a test example $\boldsymbol{x}$

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Decision Tree: An Example

- Identifying the region - blue or green - a point lies in (binary classification)
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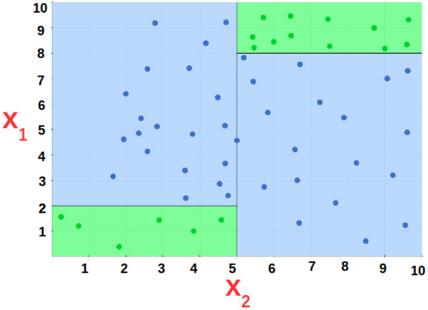
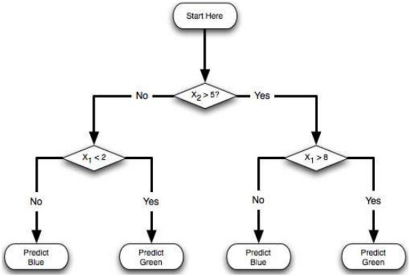
  - Left: Training data, Right: A DT constructed using this data





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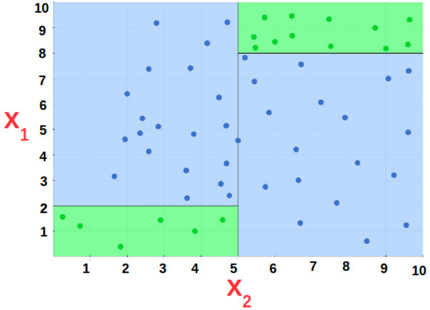

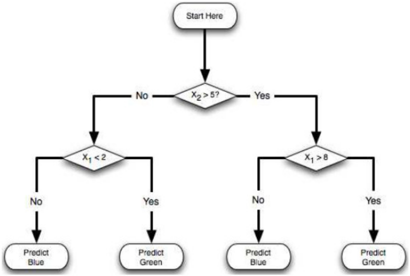

- The DT can be used to predict the region (blue/green) of a new test point
    - By testing the features of the test point
    - In the order defined by the DT (first x_2 and then x_1)

Decision Tree: Another Example

- Deciding whether to play or not to play Tennis on a Saturday
  - A binary classification problem (play vs no-play)
  - Each input (a Saturday) has 4 features: Outlook, Temp., Humidity, Wind

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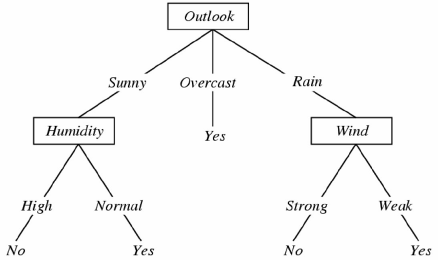

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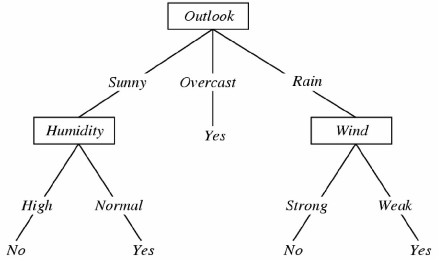

- The DT can be used to predict play vs no-play for a *new* Saturday
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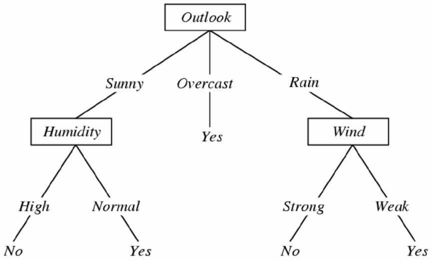

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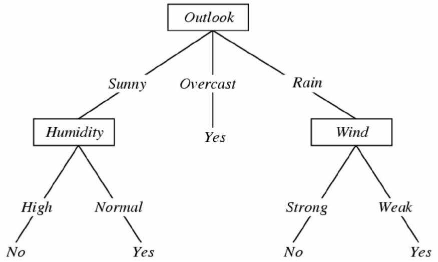

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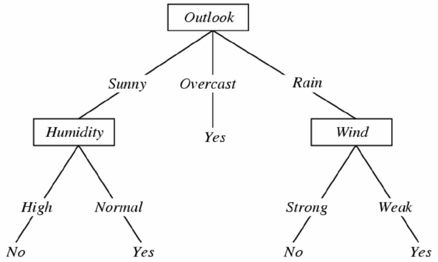

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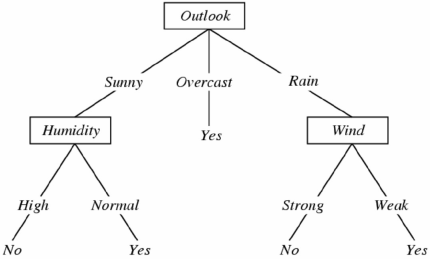

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- **Analogy:** Playing the game 20 Questions (the most useful questions first)

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- We can assess informativeness of each feature by looking at how much it reduces the entropy of the class distribution

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- Information Gain (IG) on knowing the value of some feature 'F'

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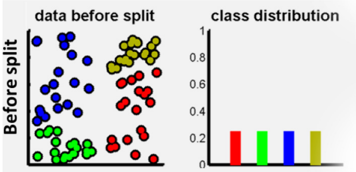
- $IG(S, F)$ denotes the no. of bits saved while encoding S once we know the value of the feature F

Entropy and Information Gain: Pictorially

Assume we have a 4-class problem. Each point has 2 features



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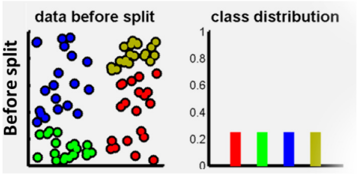

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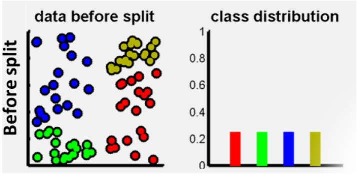

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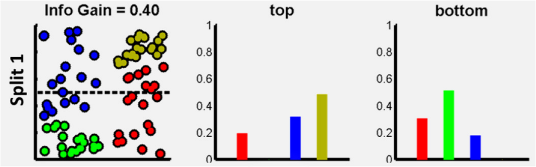

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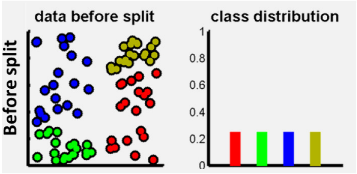

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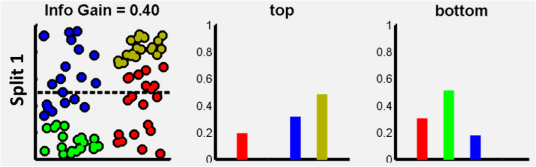

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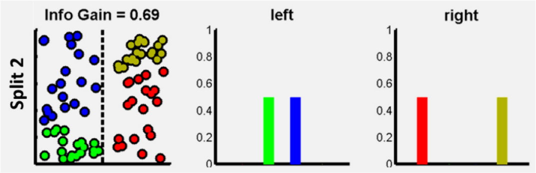

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Computing Information Gain

- Coming back to playing tennis..
- Let's begin with the root node of the DT and compute IG of each feature
- Consider feature "wind" $\in$ {weak,strong} and its IG w.r.t. the root node

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- Root node: $S = [9+, 5-]$ (all training data: 9 play, 5 no-play)
- Entropy: $H(S) = -(9/14)\log_2(9/14) - (5/14)\log_2(5/14) = 0.94$

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- $S_{weak} = [6+, 2-] \implies H(S_{weak}) = 0.811$

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- Root node: $S = [9+, 5-]$ (all training data: 9 play, 5 no-play)
- Entropy: $H(S) = -(9/14)\log_2(9/14) - (5/14)\log_2(5/14) = 0.94$
- $S_{weak} = [6+, 2-] \implies H(S_{weak}) = 0.811$
- $S_{strong} = [3+, 3-] \implies H(S_{strong}) = 1$

Computing Information Gain

- Coming back to playing tennis..
- Let's begin with the root node of the DT and compute *IG* of each feature
- Consider feature "wind" $\in$ {weak,strong} and its *IG* w.r.t. the root node

day	outlook	temperature	humidity	wind	play
1	sunny	hot	high	weak	no
2	sunny	hot	high	strong	no
3	overcast	hot	high	weak	yes
4	rain	mild	high	weak	yes
5	rain	cool	normal	weak	yes
6	rain	cool	normal	strong	no
7	overcast	cool	normal	strong	yes
8	sunny	mild	high	weak	no
9	sunny	cool	normal	weak	yes
10	rain	mild	normal	weak	yes
11	sunny	mild	normal	strong	yes
12	overcast	mild	high	strong	yes
13	overcast	hot	normal	weak	yes
14	rain	mild	high	strong	no

- Root node: $S = [9+, 5-]$ (all training data: 9 play, 5 no-play)
- Entropy: $H(S) = -(9/14)\log_2(9/14) - (5/14)\log_2(5/14) = 0.94$
- $S_{weak} = [6+, 2-] \implies H(S_{weak}) = 0.811$
- $S_{strong} = [3+, 3-] \implies H(S_{strong}) = 1$

$$\begin{aligned} IG(S, \text{wind}) &= H(S) - \frac{|S_{weak}|}{|S|} H(S_{weak}) - \frac{|S_{strong}|}{|S|} H(S_{strong}) \\ &= 0.94 - 8/14 * 0.811 - 6/14 * 1 \\ &= 0.048 \end{aligned}$$

Choosing the most informative feature

- At the root node, the information gains are:
  - $IG(S, \text{wind}) = 0.048$ (we already saw)
  - $IG(S, \text{outlook}) = 0.246$
  - $IG(S, \text{humidity}) = 0.151$
  - $IG(S, \text{temperature}) = 0.029$

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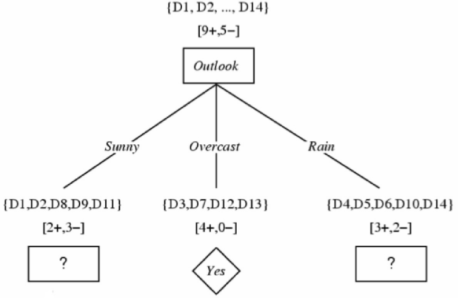

Growing The Tree

- How to decide which feature to test next ?

Growing The Tree

- How to decide which feature to test next ?
- **Rule:** Iterate - for each child node, select the feature with the highest IG

day	outlook	temperature	humidity	wind	play
1	sunny	hot	high	weak	no
2	sunny	hot	high	strong	no
3	overcast	hot	high	weak	yes
4	rain	mild	high	weak	yes
5	rain	cool	normal	weak	yes
6	rain	cool	normal	strong	no
7	overcast	cool	normal	strong	yes
8	sunny	mild	high	weak	no
9	sunny	cool	normal	weak	yes
10	rain	mild	normal	weak	yes
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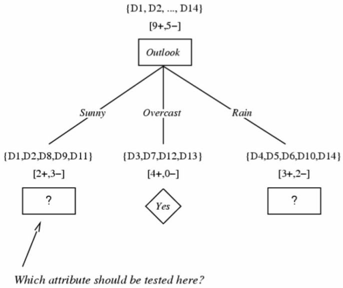
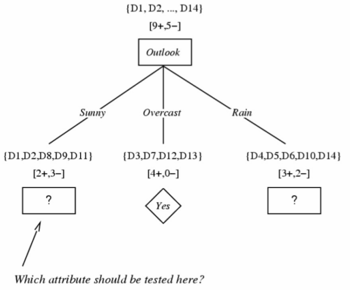
12	overcast	mild	high	strong	yes
13	overcast	hot	normal	weak	yes
14	rain	mild	high	strong	no



Growing The Tree

- How to decide which feature to test next ?
- **Rule:** Iterate - for each child node, select the feature with the highest IG

day	outlook	temperature	humidity	wind	play
1	sunny	hot	high	weak	no
2	sunny	hot	high	strong	no
3	overcast	hot	high	weak	yes
4	rain	mild	high	weak	yes
5	rain	cool	normal	weak	yes
6	rain	cool	normal	strong	no
7	overcast	cool	normal	strong	yes
8	sunny	mild	high	weak	no
9	sunny	cool	normal	weak	yes
10	rain	mild	normal	weak	yes
11	sunny	mild	normal	strong	yes
12	overcast	mild	high	strong	yes
13	overcast	hot	normal	weak	yes
14	rain	mild	high	strong	no

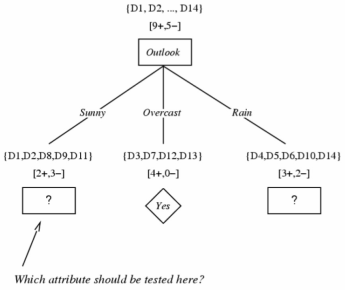


- For level-2, left node: $S = [2+, 3-]$ (days 1,2,8,9,11)
- Compute the Information Gain for each feature (except **outlook**)

Growing The Tree

- How to decide which feature to test next ?
- **Rule:** Iterate - for each child node, select the feature with the highest IG

day	outlook	temperature	humidity	wind	play
1	sunny	hot	high	weak	no
2	sunny	hot	high	strong	no
3	overcast	hot	high	weak	yes
4	rain	mild	high	weak	yes
5	rain	cool	normal	weak	yes
6	rain	cool	normal	strong	no
7	overcast	cool	normal	strong	yes
8	sunny	mild	high	weak	no
9	sunny	cool	normal	weak	yes
10	rain	mild	normal	weak	yes
11	sunny	mild	normal	strong	yes
12	overcast	mild	high	strong	yes
13	overcast	hot	normal	weak	yes
14	rain	mild	high	strong	no



- For level-2, left node: $S = [2+, 3-]$ (days 1,2,8,9,11)
- Compute the Information Gain for each feature (except **outlook**)
- The feature with the highest Information Gain should be chosen for this node

Growing The Tree

day	outlook	temperature	humidity	wind	play
1	sunny	hot	high	weak	no
2	sunny	hot	high	strong	no
3	overcast	hot	high	weak	yes
4	rain	mild	high	weak	yes
5	rain	cool	normal	weak	yes
6	rain	cool	normal	strong	no
7	overcast	cool	normal	strong	yes
8	sunny	mild	high	weak	no
9	sunny	cool	normal	weak	yes
10	rain	mild	normal	weak	yes
11	sunny	mild	normal	strong	yes
12	overcast	mild	high	strong	yes
13	overcast	hot	normal	weak	yes
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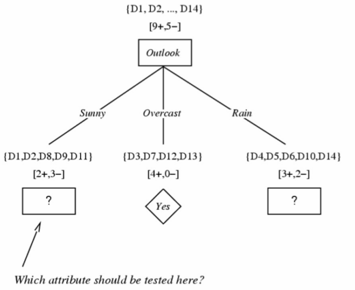
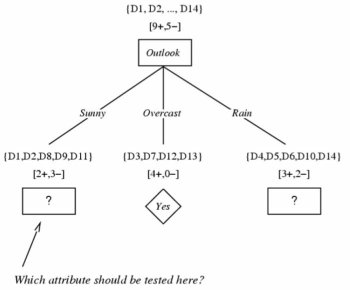


- For this node ($S = [2+, 3-]$), the IG for the feature **temperature**:

$$IG(S, \text{temperature}) \quad = \quad H(S) - \sum_{v \in \{hot, mild, cool\}} \frac{|S_v|}{|S|} H(S_v)$$

Growing The Tree

day	outlook	temperature	humidity	wind	play
1	sunny	hot	high	weak	no
2	sunny	hot	high	strong	no
3	overcast	hot	high	weak	yes
4	rain	mild	high	weak	yes
5	rain	cool	normal	weak	yes
6	rain	cool	normal	strong	no
7	overcast	cool	normal	strong	yes
8	sunny	mild	high	weak	no
9	sunny	cool	normal	weak	yes
10	rain	mild	normal	weak	yes
11	sunny	mild	normal	strong	yes
12	overcast	mild	high	strong	yes
13	overcast	hot	normal	weak	yes
14	rain	mild	high	strong	no



- For this node ($S = [2+, 3-]$), the IG for the feature **temperature**:

$$IG(S, \text{temperature}) \quad = \quad H(S) - \sum_{v \in \{hot, mild, cool\}} \frac{|S_v|}{|S|} H(S_v)$$

- $S = [2+, 3-] \implies H(S) = -(2/5) * \log_2(2/5) - (3/5) * \log_2(3/5) = 0.971$

Growing The Tree

day	outlook	temperature	humidity	wind	play
1	sunny	hot	high	weak	no
2	sunny	hot	high	strong	no
3	overcast	hot	high	weak	yes
4	rain	mild	high	weak	yes
5	rain	cool	normal	weak	yes
6	rain	cool	normal	strong	no
7	overcast	cool	normal	strong	yes
8	sunny	mild	high	weak	no
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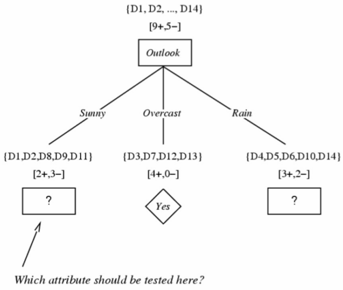

- For this node ($S = [2+, 3-]$), the IG for the feature **temperature**:

$$IG(S, \text{temperature}) \quad = \quad H(S) - \sum_{v \in \{hot, mild, cool\}} \frac{|S_v|}{|S|} H(S_v)$$

- $S = [2+, 3-] \implies H(S) = -(2/5) * \log_2(2/5) - (3/5) * \log_2(3/5) = 0.971$
- $S_{hot} = [0+, 2-] \implies H(S_{hot}) = -0 * \log_2(0) - (2/2) * \log_2(2/2) = 0$

Growing The Tree

day	outlook	temperature	humidity	wind	play
1	sunny	hot	high	weak	no
2	sunny	hot	high	strong	no
3	overcast	hot	high	weak	yes
4	rain	mild	high	weak	yes
5	rain	cool	normal	weak	yes
6	rain	cool	normal	strong	no
7	overcast	cool	normal	strong	yes
8	sunny	mild	high	weak	no
9	sunny	cool	normal	weak	yes
10	rain	mild	normal	weak	yes
11	sunny	mild	normal	strong	yes
12	overcast	mild	high	strong	yes
13	overcast	hot	normal	weak	yes
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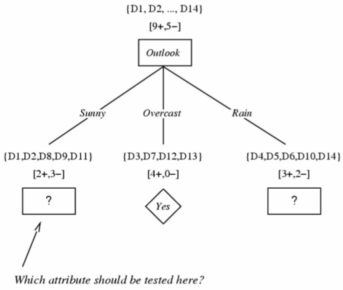

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$$IG(S, \text{temperature}) \quad = \quad H(S) - \sum_{v \in \{hot, mild, cool\}} \frac{|S_v|}{|S|} H(S_v)$$

- $S = [2+, 3-] \implies H(S) = -(2/5) * \log_2(2/5) - (3/5) * \log_2(3/5) = 0.971$
- $S_{hot} = [0+, 2-] \implies H(S_{hot}) = -0 * \log_2(0) - (2/2) * \log_2(2/2) = 0$
- $S_{mild} = [1+, 1-] \implies H(S_{mild}) = -(1/2) * \log_2(1/2) - (1/2) * \log_2(1/2) = 1$

Growing The Tree

day	outlook	temperature	humidity	wind	play
1	sunny	hot	high	weak	no
2	sunny	hot	high	strong	no
3	overcast	hot	high	weak	yes
4	rain	mild	high	weak	yes
5	rain	cool	normal	weak	yes
6	rain	cool	normal	strong	no
7	overcast	cool	normal	strong	yes
8	sunny	mild	high	weak	no
9	sunny	cool	normal	weak	yes
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13	overcast	hot	normal	weak	yes
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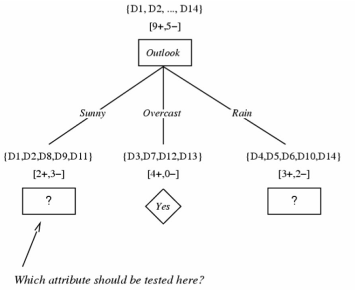

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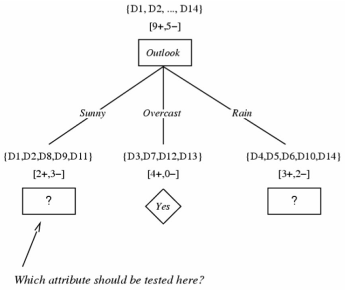
- $S_{mild} = [1+, 1-] \implies H(S_{mild}) = -(1/2) * \log_2(1/2) - (1/2) * \log_2(1/2) = 1$
- $S_{cool} = [1+, 0-] \implies H(S_{cool}) = -(1/1) * \log_2(1/1) - (0/1) * \log_2(0/1) = 0$

Growing The Tree

day	outlook	temperature	humidity	wind	play
1	sunny	hot	high	weak	no
2	sunny	hot	high	strong	no
3	overcast	hot	high	weak	yes
4	rain	mild	high	weak	yes
5	rain	cool	normal	weak	yes
6	rain	cool	normal	strong	no
7	overcast	cool	normal	strong	yes
8	sunny	mild	high	weak	no
9	sunny	cool	normal	weak	yes
10	rain	mild	normal	weak	yes
11	sunny	mild	normal	strong	yes
12	overcast	mild	high	strong	yes
13	overcast	hot	normal	weak	yes
14	rain	mild	high	strong	no



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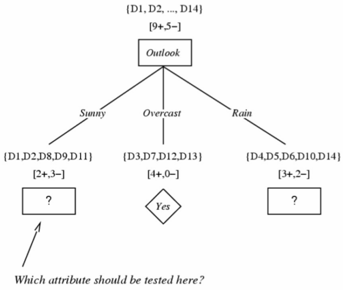
$$IG(S, \text{temperature}) \quad = \quad H(S) - \sum_{v \in \{hot, mild, cool\}} \frac{|S_v|}{|S|} H(S_v)$$

- $S = [2+, 3-] \implies H(S) = -(2/5) * \log_2(2/5) - (3/5) * \log_2(3/5) = 0.971$
- $S_{hot} = [0+, 2-] \implies H(S_{hot}) = -0 * \log_2(0) - (2/2) * \log_2(2/2) = 0$
- $S_{mild} = [1+, 1-] \implies H(S_{mild}) = -(1/2) * \log_2(1/2) - (1/2) * \log_2(1/2) = 1$
- $S_{cool} = [1+, 0-] \implies H(S_{cool}) = -(1/1) * \log_2(1/1) - (0/1) * \log_2(0/1) = 0$
- $IG(S, \text{temperature}) = 0.971 - 2/5 * 0 - 2/5 * 1 - 1/5 * 0 = 0.570$

Growing The Tree

day	outlook	temperature	humidity	wind	play
1	sunny	hot	high	weak	no
2	sunny	hot	high	strong	no
3	overcast	hot	high	weak	yes
4	rain	mild	high	weak	yes
5	rain	cool	normal	weak	yes
6	rain	cool	normal	strong	no
7	overcast	cool	normal	strong	yes
8	sunny	mild	high	weak	no
9	sunny	cool	normal	weak	yes
10	rain	mild	normal	weak	yes
11	sunny	mild	normal	strong	yes
12	overcast	mild	high	strong	yes
13	overcast	hot	normal	weak	yes
14	rain	mild	high	strong	no



- For this node ($S = [2+, 3-]$), the IG for the feature **temperature**:

$$IG(S, \text{temperature}) = H(S) - \sum_{v \in \{hot, mild, cool\}} \frac{|S_v|}{|S|} H(S_v)$$

- $S = [2+, 3-] \implies H(S) = -(2/5) * \log_2(2/5) - (3/5) * \log_2(3/5) = 0.971$
- $S_{hot} = [0+, 2-] \implies H(S_{hot}) = -0 * \log_2(0) - (2/2) * \log_2(2/2) = 0$
- $S_{mild} = [1+, 1-] \implies H(S_{mild}) = -(1/2) * \log_2(1/2) - (1/2) * \log_2(1/2) = 1$
- $S_{cool} = [1+, 0-] \implies H(S_{cool}) = -(1/1) * \log_2(1/1) - (0/1) * \log_2(0/1) = 0$
- $IG(S, \text{temperature}) = 0.971 - 2/5 * 0 - 2/5 * 1 - 1/5 * 0 = 0.570$
- Likewise we can compute: $IG(S, \text{humidity}) = 0.970$, $IG(S, \text{wind}) = 0.019$

Growing The Tree

day	outlook	temperature	humidity	wind	play
1	sunny	hot	high	weak	no
2	sunny	hot	high	strong	no
3	overcast	hot	high	weak	yes
4	rain	mild	high	weak	yes
5	rain	cool	normal	weak	yes
6	rain	cool	normal	strong	no
7	overcast	cool	normal	strong	yes
8	sunny	mild	high	weak	no
9	sunny	cool	normal	weak	yes
10	rain	mild	normal	weak	yes
11	sunny	mild	normal	strong	yes
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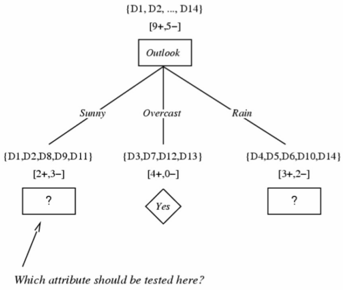
14	rain	mild	high	strong	no



- For this node ($S = [2+, 3-]$), the IG for the feature **temperature**:

$$IG(S, \text{temperature}) \quad = \quad H(S) - \sum_{v \in \{hot, mild, cool\}} \frac{|S_v|}{|S|} H(S_v)$$

- $S = [2+, 3-] \Longrightarrow H(S) = -(2/5) * \log_2(2/5) - (3/5) * \log_2(3/5) = 0.971$
- $S_{hot} = [0+, 2-] \Longrightarrow H(S_{hot}) = -0 * \log_2(0) - (2/2) * \log_2(2/2) = 0$
- $S_{mild} = [1+, 1-] \Longrightarrow H(S_{mild}) = -(1/2) * \log_2(1/2) - (1/2) * \log_2(1/2) = 1$
- $S_{cool} = [1+, 0-] \Longrightarrow H(S_{cool}) = -(1/1) * \log_2(1/1) - (0/1) * \log_2(0/1) = 0$
- $IG(S, \text{temperature}) = 0.971 - 2/5 * 0 - 2/5 * 1 - 1/5 * 0 = 0.570$
- Likewise we can compute: $IG(S, \text{humidity}) = 0.970$, $IG(S, \text{wind}) = 0.019$
- Therefore, **we choose "humidity"** (with highest $IG = 0.970$) for the level-2 left node

Growing The Tree

day	outlook	temperature	humidity	wind	play
1	sunny	hot	high	weak	no
2	sunny	hot	high	strong	no
3	overcast	hot	high	weak	yes
4	rain	mild	high	weak	yes
5	rain	cool	normal	weak	yes
6	rain	cool	normal	strong	no
7	overcast	cool	normal	strong	yes
8	sunny	mild	high	weak	no
9	sunny	cool	normal	weak	yes
10	rain	mild	normal	weak	yes
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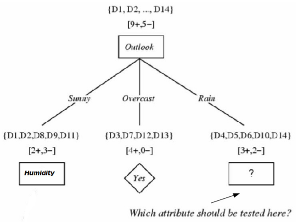

Growing The Tree

day	outlook	temperature	humidity	wind	play
1	sunny	hot	high	weak	no
2	sunny	hot	high	strong	no
3	overcast	hot	high	weak	yes
4	rain	mild	high	weak	yes
5	rain	cool	normal	weak	yes
6	rain	cool	normal	strong	no
7	overcast	cool	normal	strong	yes
8	sunny	mild	high	weak	no
9	sunny	cool	normal	weak	yes
10	rain	mild	normal	weak	yes
11	sunny	mild	normal	strong	yes
12	overcast	mild	high	strong	yes
13	overcast	hot	normal	weak	yes
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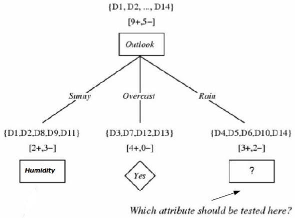
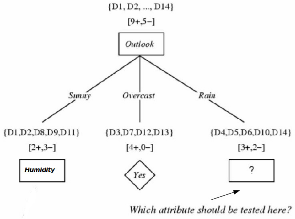


- Level-2, middle node: no need to grow (already a leaf)

Growing The Tree

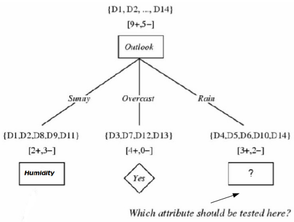
day	outlook	temperature	humidity	wind	play
1	sunny	hot	high	weak	no
2	sunny	hot	high	strong	no
3	overcast	hot	high	weak	yes
4	rain	mild	high	weak	yes
5	rain	cool	normal	weak	yes
6	rain	cool	normal	strong	no
7	overcast	cool	normal	strong	yes
8	sunny	mild	high	weak	no
9	sunny	cool	normal	weak	yes
10	rain	mild	normal	weak	yes
11	sunny	mild	normal	strong	yes
12	overcast	mild	high	strong	yes
13	overcast	hot	normal	weak	yes
14	rain	mild	high	strong	no



- Level-2, middle node: no need to grow (already a leaf)
- Level-2, right node: repeat the same exercise!

Growing The Tree

day	outlook	temperature	humidity	wind	play
1	sunny	hot	high	weak	no
2	sunny	hot	high	strong	no
3	overcast	hot	high	weak	yes
4	rain	mild	high	weak	yes
5	rain	cool	normal	weak	yes
6	rain	cool	normal	strong	no
7	overcast	cool	normal	strong	yes
8	sunny	mild	high	weak	no
9	sunny	cool	normal	weak	yes
10	rain	mild	normal	weak	yes
11	sunny	mild	normal	strong	yes
12	overcast	mild	high	strong	yes
13	overcast	hot	normal	weak	yes
14	rain	mild	high	strong	no



- Level-2, middle node: no need to grow (already a leaf)
- Level-2, right node: repeat the same exercise!
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Growing The Tree

day	outlook	temperature	humidity	wind	play
1	sunny	hot	high	weak	no
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4	rain	mild	high	weak	yes
5	rain	cool	normal	weak	yes
6	rain	cool	normal	strong	no
7	overcast	cool	normal	strong	yes
8	sunny	mild	high	weak	no
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10	rain	mild	normal	weak	yes
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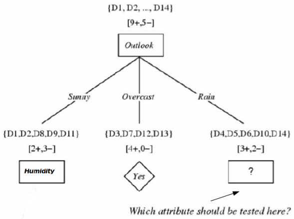

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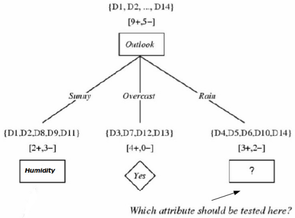

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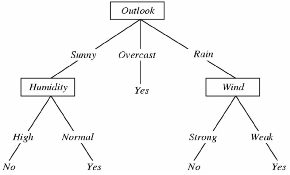
  - Compute *IG* for each feature (except outlook)
  - **Exercise:** Verify that wind has the highest *IG* for this node
- Level-2 expansion gives us the following tree:



Growing The Tree: Stopping Criteria

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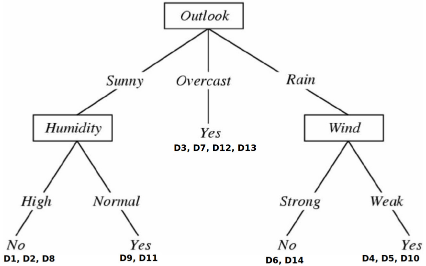

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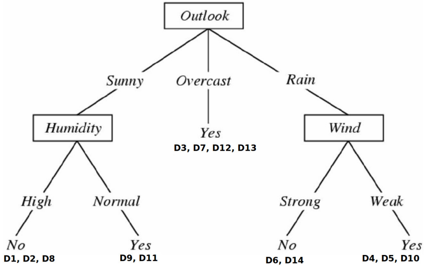

- Stop expanding a node further when:

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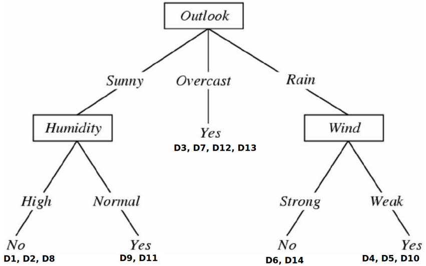

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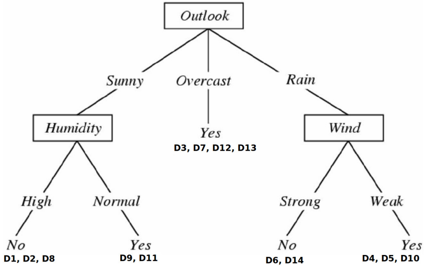

- Stop expanding a node further when:
  - It consist of examples all having the same label (the node becomes "pure")
  - Or we run out of features to test!

Decision Tree Learning Algorithm

A recursive algorithm:

$\mathrm{DT}(\textit{Examples}, \textit{Labels}, \textit{Features})$:

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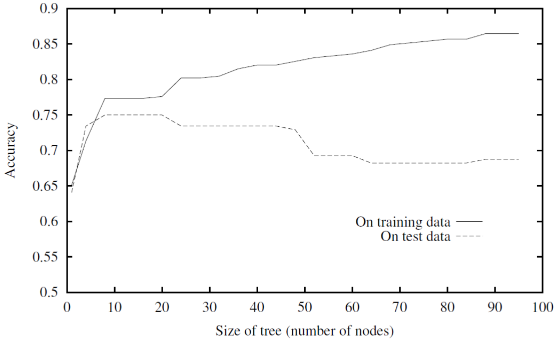
    - Otherwise, add the following subtree below this branch:

$$\mathrm{DT}(\mathit{Examples}_f, \mathit{Labels}_f, \mathit{Features} - \{F\})$$

    - Note: $\mathit{Features} - \{F\}$ removes feature F from the feature set *Features*

Overfitting in Decision Trees

- Overfitting Illustration



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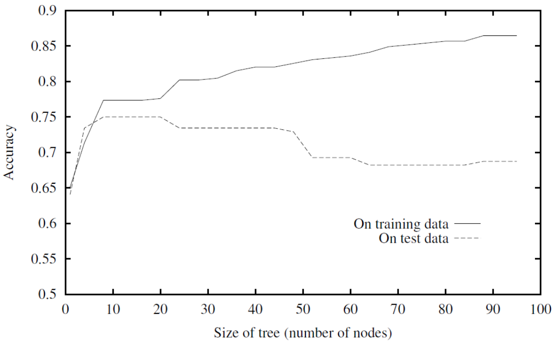

- High training accuracy doesn't necessarily imply high test accuracy

Avoiding Overfitting: Decision Tree Pruning

- Desired: a DT that is not too big in size, yet fits the training data reasonably

- Mainly two approaches

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    - Minimum Description Length (MDL): more details when we cover Model Selection

Decision Tree Extensions

- Real-valued features can be dealt with using thresholding

[2] Breiman, Leo; Friedman, J. H.; Olshen, R. A.; Stone, C. J. (1984). Classification and regression trees

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Some Aspects about Decision Trees

Some key strengths:

- Simple and each to interpret
- Do not make any assumption about distribution of data
- Easily handle different types of features (real, categorical/nominal, etc.)
- Very fast at test time (just need to check the features, starting the root node and following the DT until you reach a leaf node)
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Some key weaknesses:

- Learning the optimal DT is NP-Complete. The existing algorithms are heuristics (e.g., greedy selection of features)
- Can be unstable if some labeled examples are noisy
- Can sometimes become very complex unless some pruning is applied

Next Class:
Learning as Optimization