# IAML: Decision Trees

Victor Lavrenko and Charles Sutton
School of Informatics

Semester 1

## Predict if John will play tennis

- Hard to guess
- Divide & conquer:
  - split into subsets
  - are they pure? (all yes or all no)
  - if yes: stop
  - if not: repeat
- See which subset new data falls into

Training examples: **9 yes / 5 no**

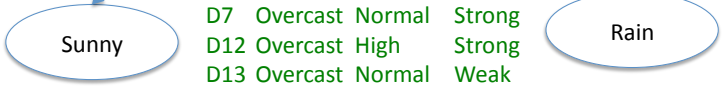
| Day | Outlook | Humidity | Wind | Play |
|---|---|---|---|---|
| D1 | Sunny | High | Weak | No |
| D2 | Sunny | High | Strong | No |
| D3 | Overcast | High | Weak | Yes |
| D4 | Rain | High | Weak | Yes |
| D5 | Rain | Normal | Weak | Yes |
| D6 | Rain | Normal | Strong | No |
| D7 | Overcast | Normal | Strong | Yes |
| D8 | Sunny | High | Weak | No |
| D9 | Sunny | Normal | Weak | Yes |
| D10 | Rain | Normal | Weak | Yes |
| D11 | Sunny | Normal | Strong | Yes |
| D12 | Overcast | High | Strong | Yes |
| D13 | Overcast | Normal | Weak | Yes |
| D14 | Rain | High | Strong | No |

New data:

| | | | | |
|---|---|---|---|---|
| D15 | Rain | High | Weak | ? |



**9 yes / 5 no**




| Day | Outlook | Humid | Wind |
|---|---|---|---|
| D3 | Overcast | High | Weak |
| D7 | Overcast | Normal | Strong |
| D12 | Overcast | High | Strong |
| D13 | Overcast | Normal | Weak |

**4 yes / 0 no**
**pure subset**

| Day | Outlook | Humid | Wind |
|---|---|---|---|
| D1 | Sunny | High | Weak |
| D2 | Sunny | High | Strong |
| D8 | Sunny | High | Weak |
| D9 | Sunny | Normal | Weak |
| D11 | Sunny | Normal | Strong |

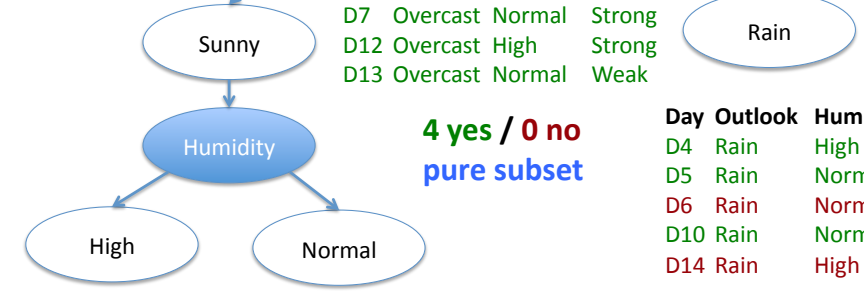
**2 yes / 3 no**
**split further**

| Day | Outlook | Humid | Wind |
|---|---|---|---|
| D4 | Rain | High | Weak |
| D5 | Rain | Normal | Weak |
| D6 | Rain | Normal | Strong |
| D10 | Rain | Normal | Weak |
| D14 | Rain | High | Strong |

**3 yes / 2 no**
**split further**



**9 yes / 5 no**




| Day | Outlook | Humid | Wind |
|---|---|---|---|
| D3 | Overcast | High | Weak |
| D7 | Overcast | Normal | Strong |
| D12 | Overcast | High | Strong |
| D13 | Overcast | Normal | Weak |

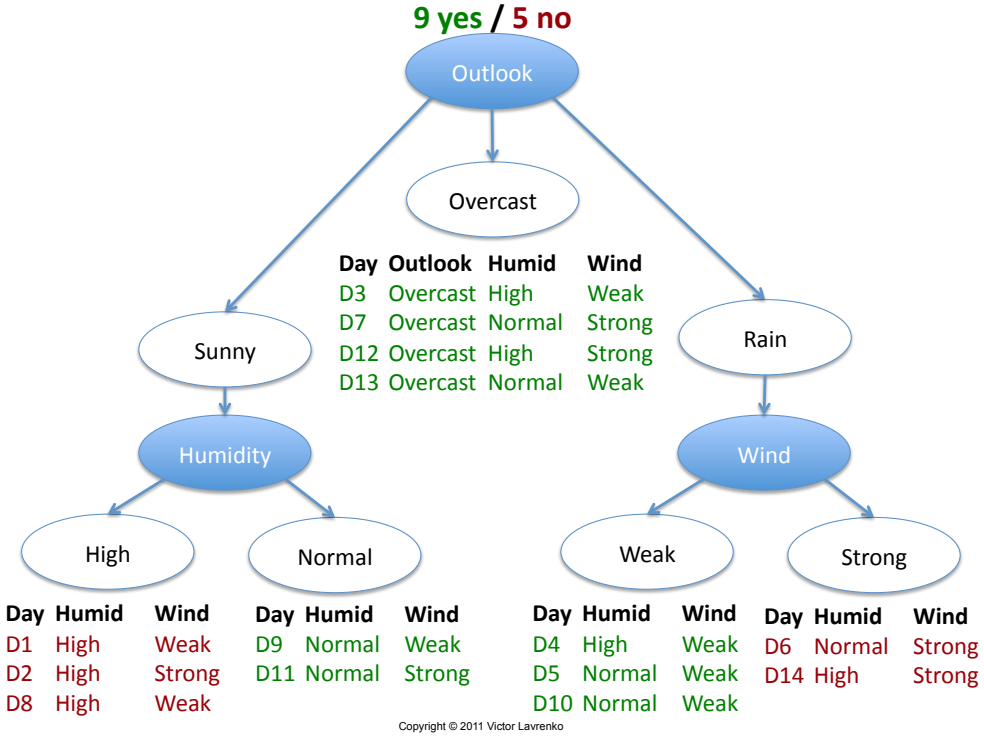
**4 yes / 0 no**
**pure subset**

| Day | Humid | Wind |
|---|---|---|
| D1 | High | Weak |
| D2 | High | Strong |
| D8 | High | Weak |

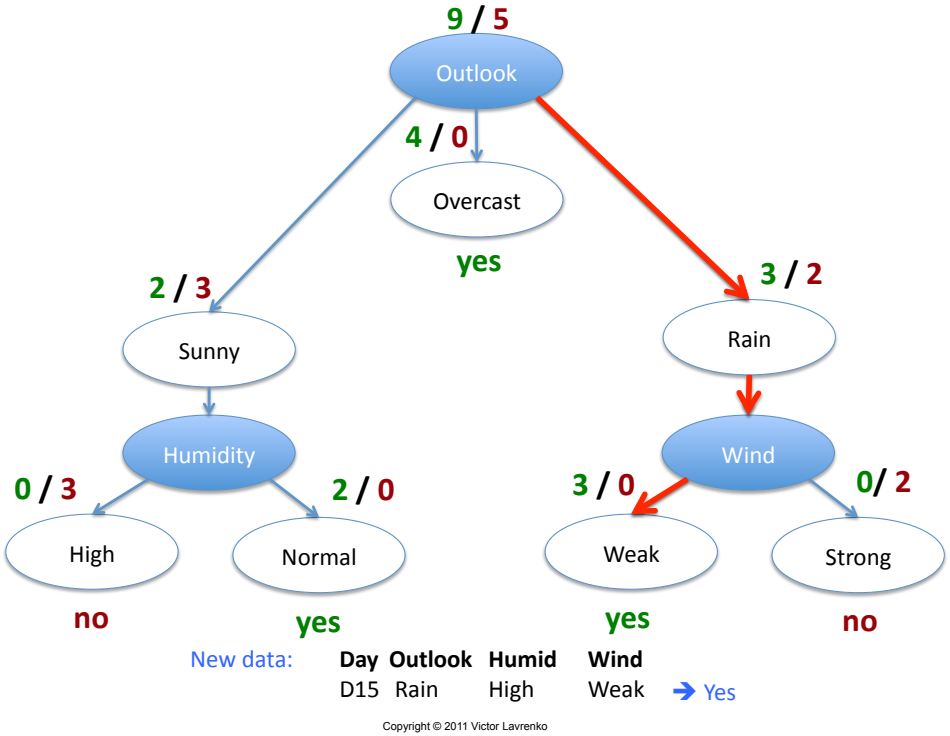
| Day | Humid | Wind |
|---|---|---|
| D9 | Normal | Weak |
| D11 | Normal | Strong |

| Day | Outlook | Humid | Wind |
|---|---|---|---|
| D4 | Rain | High | Weak |
| D5 | Rain | Normal | Weak |
| D6 | Rain | Normal | Strong |
| D10 | Rain | Normal | Weak |
| D14 | Rain | High | Strong |

**3 yes / 2 no**
**split further**







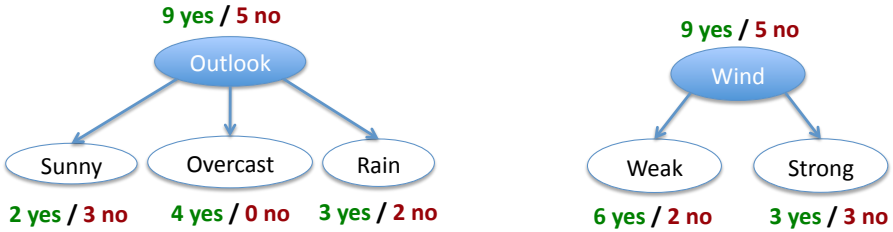


# ID3 algorithm

- Split (node, {examples} ):
  1. A ← the best attribute for splitting the {examples}
  2. Decision attribute for this node ← A
  3. For each value of A, create new child node
  4. Split training {examples} to child nodes
  5. If examples perfectly classified: STOP
     else: iterate over new child nodes
     Split (child_node, {subset of examples} )
- Ross Quinlan (ID3: 1986), (C4.5: 1993)
- Breimanetal (CaRT: 1984) from statistics



# Which attribute to split on?




- Want to measure "purity" of the split
  - more certain about Yes/No after the split
    - pure set (4 yes / 0 no) => completely certain (100%)
    - impure (3 yes / 3 no) => completely uncertain (50%)
  - can't use P("yes" | set):
    - must be symmetric: 4 yes / 0 no as pure as 0 yes / 4 no

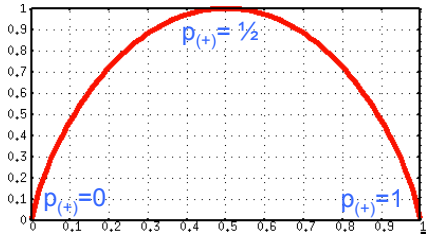
# Entropy

- Entropy: $H(S) = - p_{(+)} \log_2 p_{(+)} - p_{(-)} \log_2 p_{(-)}$ bits
  - S … subset of training examples
  - $p_{(+)}$ / $p_{(-)}$ … % of positive / negative examples in S
- Interpretation: assume item X belongs to S
  - how many bits need to tell if X positive or negative
- impure (3 yes / 3 no):

$$H(S) = -\frac{3}{6}\log_2\frac{3}{6} - \frac{3}{6}\log_2\frac{3}{6} = 1 \text{ bits}$$

- pure set (4 yes / 0 no):

$$H(S) = -\frac{4}{4}\log_2\frac{4}{4} - \frac{0}{4}\log_2\frac{0}{4} = 0 \text{ bits}$$






# Information Gain

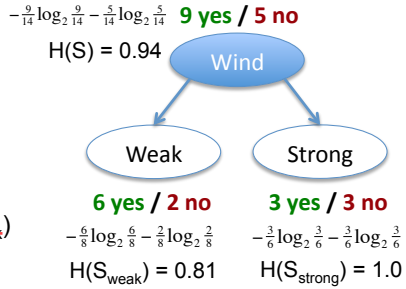
- Want many items in pure sets
- Expected drop in entropy after split:

$$Gain(S,A) = H(S) - \sum_{V \in Values(A)} \frac{|S_V|}{|S|} H(S_V)$$

V … possible values of A
S … set of examples {X}
$S_v$ … subset where $X_A$ = V

- Mutual Information
  - between attribute A and class labels of S

Gain (S, Wind)
= H(S) – $^8/_{14}$ H($S_{weak}$) – $^6/_{14}$ H($S_{strong}$)
= 0.94 – $^8/_{14}$ * 0.81 – $^6/_{14}$ * 1.0
= 0.049






# Overfitting in Decision Trees

- Can always classify training examples perfectly
  - keep splitting until each node contains 1 example
  - singleton = pure
- Doesn't work on new data

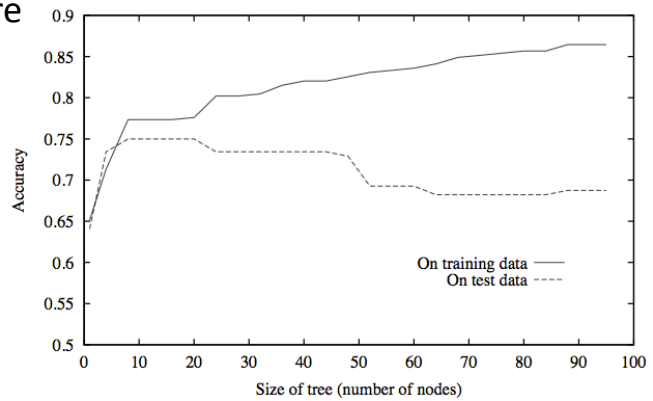





Figure credit: Tom Mitchell, 1997

# Avoid overfitting

- Stop splitting when not statistically significant
- Grow, then post-prune
  - based on validation set
- Sub-tree replacement pruning (WF 6.1)
  - for each node:
    - pretend remove node + all children from the tree
    - measure performance on validation set
  - remove node that results in greatest improvement
  - repeat until further pruning is harmful

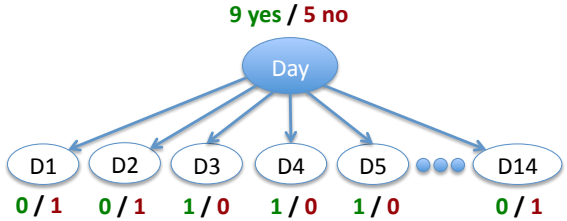
# General Structure

- **Task:** classification, discriminative
- **Model structure:** decision tree
- **Score function**
  - information gain at each node
  - preference for short trees
  - preference for high-gain attributes near the root
- **Optimization / search** method
  - greedy search from simple to complex
  - guided by information gain



# Problems with Information Gain

- Biased towards attributes with many values
- Won't work for new data: D15 Rain High Weak
- Use GainRatio:




all subsets perfectly pure => optimal split

$$SplitEntropy(S,A) = -\sum_{V \in Values(A)} \frac{|S_V|}{|S|} \log \frac{|S_V|}{|S|}$$

A … candidate attribute
V … possible values of A
S … set of examples {X}
$S_v$ … subset where $X_A = V$

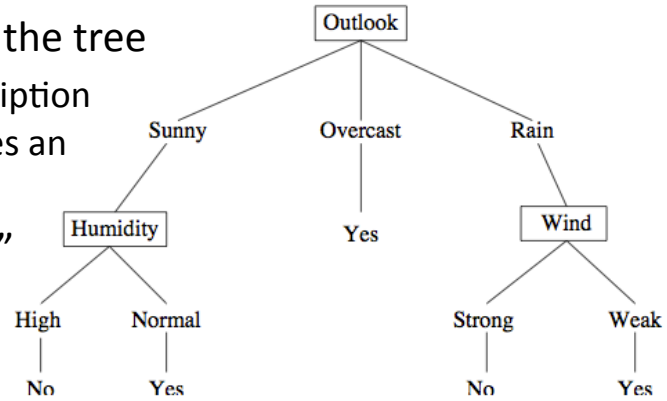
$$GainRatio(S,A) = \frac{Gain(S,A)}{SplitEntropy(S,A)}$$

penalizes attributes with many values



# Trees are interpretable

- Read rules off the tree
  - concise description of what makes an item positive
- No "black box"
  - important for users



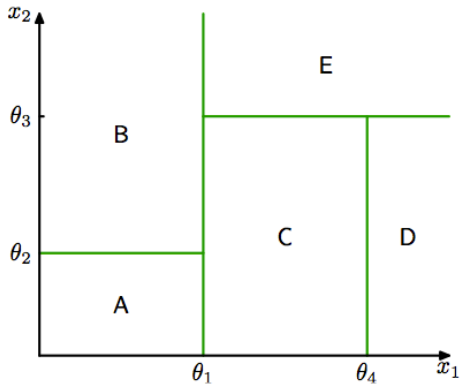

Rule: (Outlook = Overcast) ∨
(Outlook = Rain ∧ Wind = Weak) ∨
(Outlook = Sunny ∧ Humidity = Normal)



Figure credit: Tom Mitchell, 1997

# Continuous Attributes

- Dealing with continuous-valued attributes:
  - create a split: (Temperature > 72.3) = True,False
- Threshold can be optimized (WF 6.1)



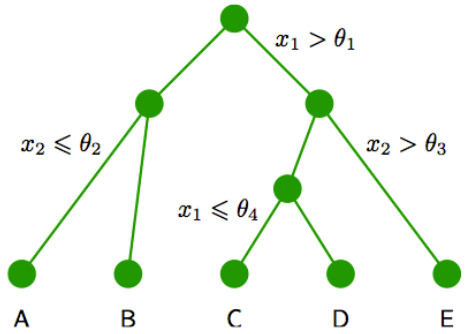




Figure credit: Chris Bishop, PRML

# Multi-class and Regression

- Multi-class classification:
  - predict most frequent class in the subset
  - entropy: $H(S) = - \Sigma_c p_{(c)} \log_2 p_{(c)}$
  - $p_{(c)}$ … % of examples of class c in S
- Regression:
  - predicted output = mean of the training examples in the subset
  - requires a different definition of entropy
  - can use linear regression at the leaves (WF 6.5)



# Random Decision Forest

- Grow K different decision trees:
  - pick a random subset $S_r$ of training examples
  - grow a full ID3 tree (no prunning):
    - when splitting: pick from $d << D$ random attributes
    - compute gain based on $S_r$ instead of full set
  - repeat for r = 1 … K
- Given a new data point X:
  - classify X using each of the K trees
  - use majority vote: class predicted most often
- Fast, scalable, state-of-the-art performance



# Summary

- ID3: grows decision tree from the root down
  - greedily selects next best attribute (Gain)
- Searches a complete hypothesis space
  - prefers smaller trees, high gain at the root
- Overfitting addressed by post-prunning
  - prune nodes, while accuracy ⇧ on validation set
- Can handle missing data (see WF 6.1)
- Easily handles irrelevant variables
  - Information Gain = 0 => will not be selected