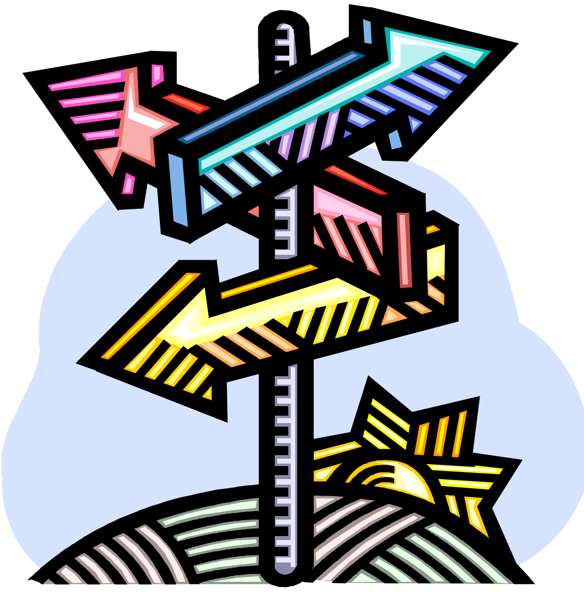
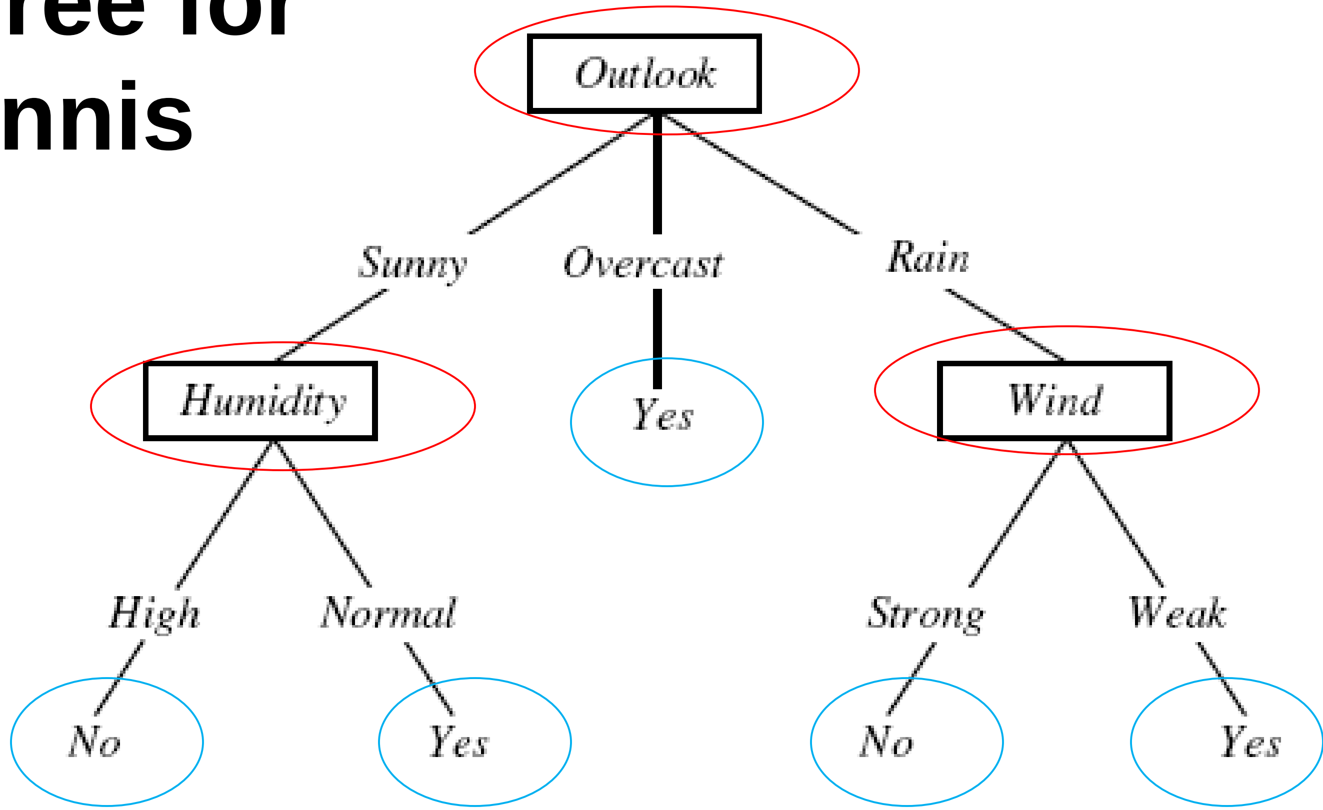
Decision Tree

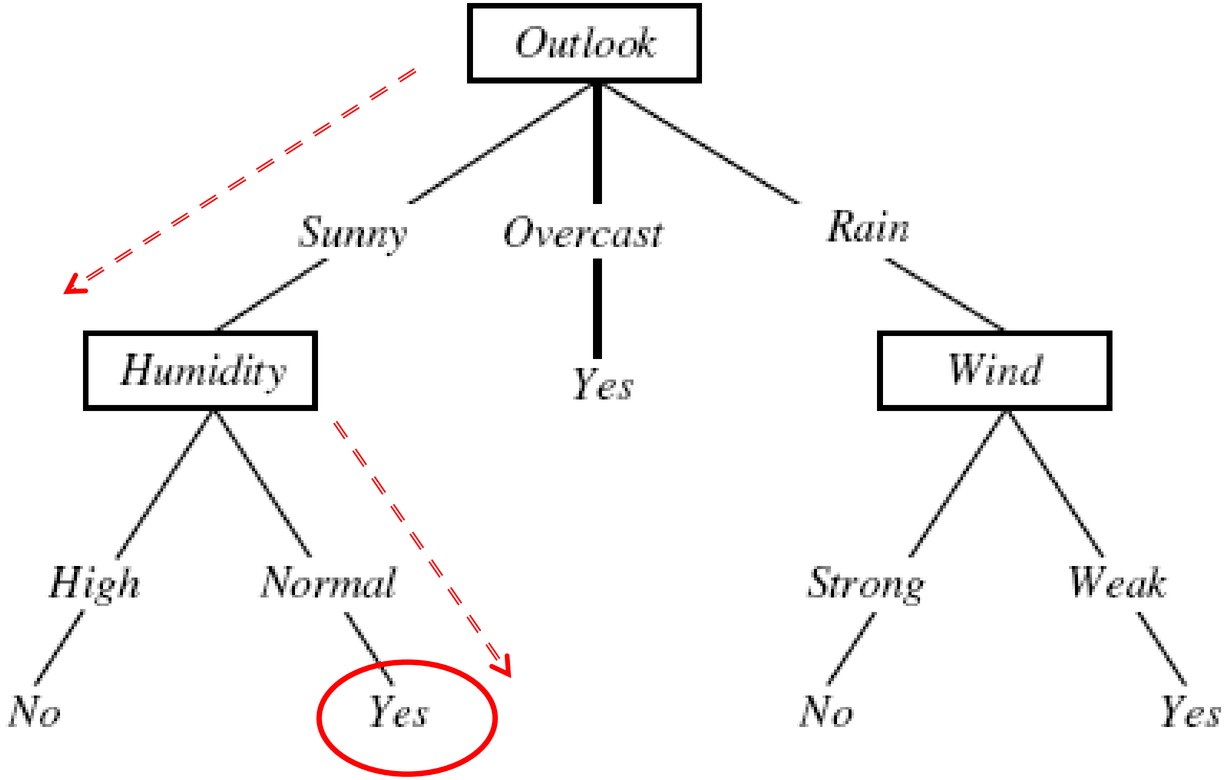


Decision Tree for Playing Tennis



- Each internal node test on an attribute x_i
- Each branch from a node takes a particular value of x_i
- Each leaf node predicts a class label

(outlook=sunny, wind=strong, humidity=normal, ?)



DT for prediction C-section risks

Learned from medical records of 1000 women

Negative examples are C-sections

```
[833+,167-] .83+ .17-
Fetal_Presentation = 1: [822+,116-] .88+ .12-
| Previous_Csection = 0: [767+,81-] .90+ .10-
| | Primiparous = 0: [399+,13-] .97+ .03-
| | Primiparous = 1: [368+,68-] .84+ .16-
| | | Fetal_Distress = 0: [334+,47-] .88+ .12-
| | | | Birth_Weight < 3349: [201+,10.6-] .95+ .
| | | | Birth_Weight >= 3349: [133+,36.4-] .78+
| | | Fetal_Distress = 1: [34+,21-] .62+ .38-
| Previous_Csection = 1: [55+,35-] .61+ .39-
Fetal_Presentation = 2: [3+,29-] .11+ .89-
Fetal_Presentation = 3: [8+,22-] .27+ .73-
```

Characteristics of Decision Trees

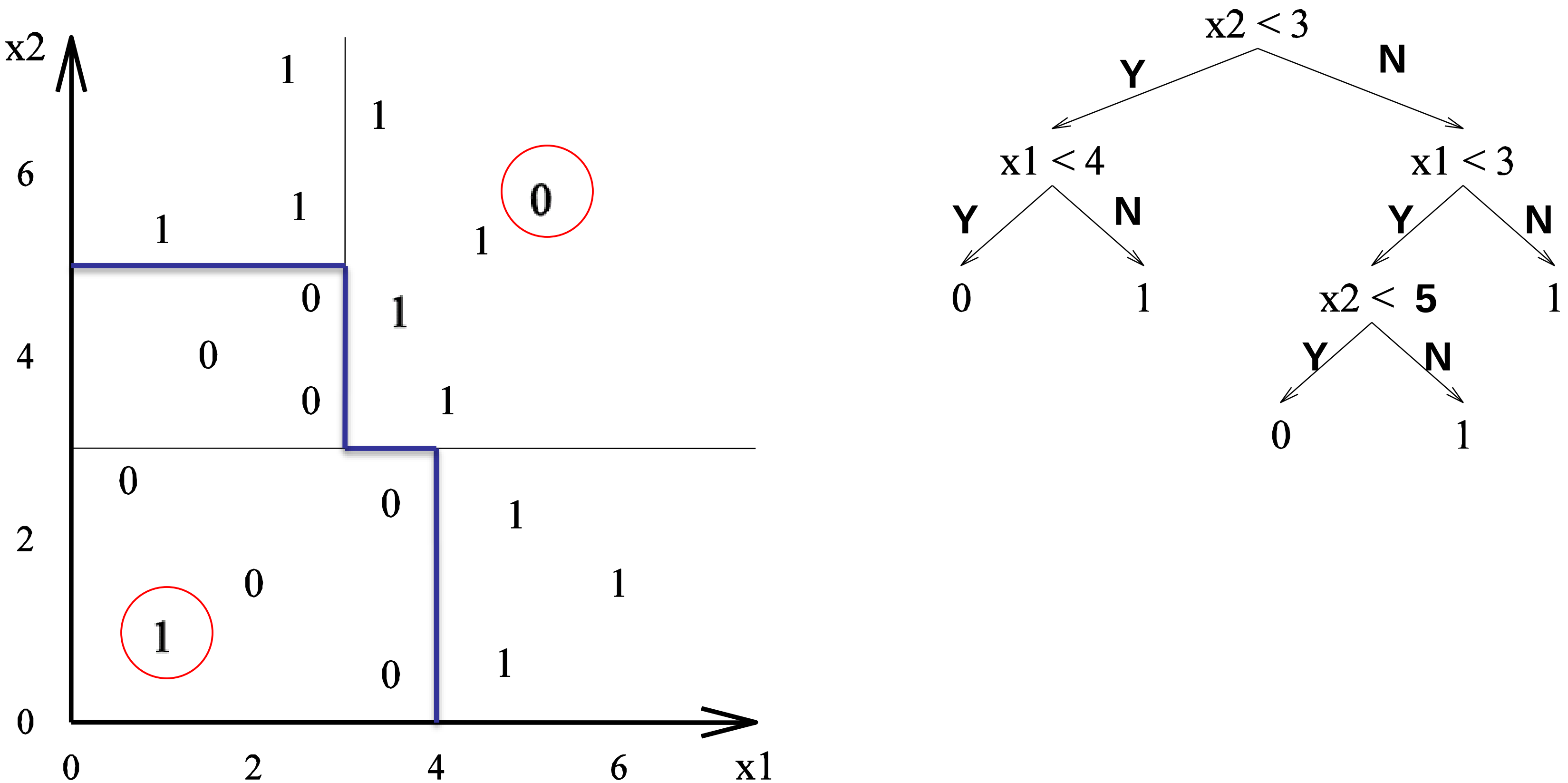
- Decision trees have many appealing properties
  - Similar to human decision process, easy to understand
  - Deal with both **discrete and continuous** features
  - Highly flexible ***hypothesis space***, as the # of nodes (or depth) of the tree increase, decision tree can represent increasingly complex decision boundaries

Definition: ***Hypothesis space H***

The space of solutions that a learning algorithm can possibly output. For example,

- For Perceptron: the hypothesis space is the space of all straight lines
- For nearest neighbor: the hypothesis space is infinitely complex
- For decision tree: it is a flexible space, as we increase the depth of the tree, the hypothesis space grows larger and larger

DT can represent arbitrarily complex decision boundaries



If needed, the tree can keep on growing until all examples are correctly classified! Although it may not be the best idea

How to learn decision trees?

- Possible goal: find a decision tree *h* that achieves minimum error on training data
  - Trivially achievable – if use a large enough tree
- Another possibility: find the smallest decision tree that achieves the minimum training error
  - NP-hard

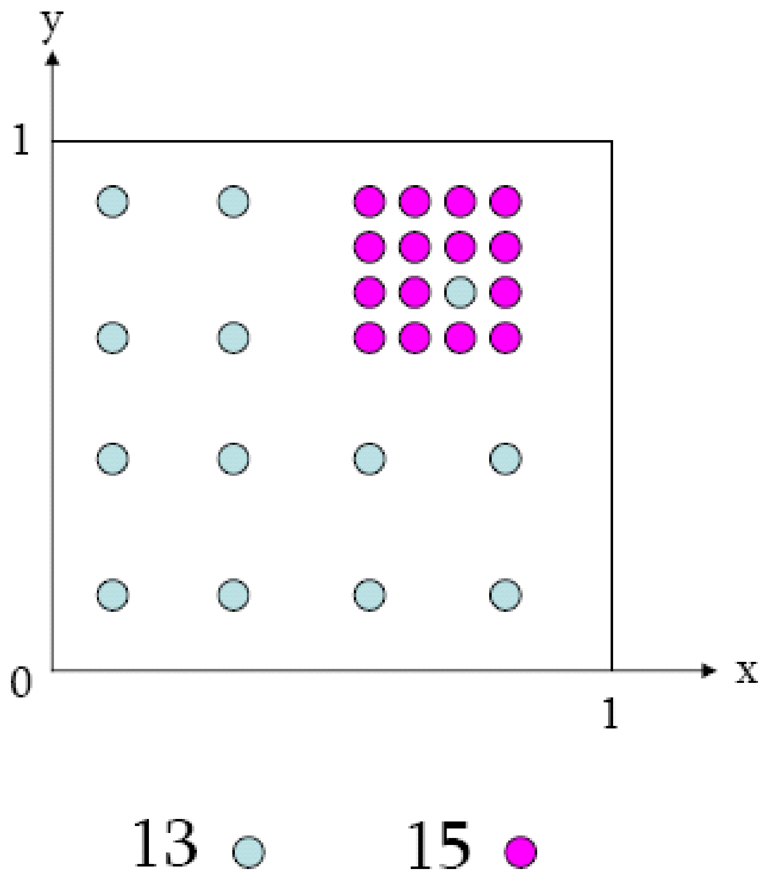
Greedy Learning For DT

We will study a top-down, greedy search approach. Instead of trying to optimize the whole tree together, we try to find one test at a time.

Basic idea: (assuming discrete features, relax later)

1. Choose the best attribute to test on at the root of the tree.
2. Create a descendant node for each possible outcome of the test
3. Training examples in training set S are sent to the appropriate descendent node
4. Recursively apply the algorithm at each descendant node to select the best attribute to test using its associated training examples
   - If all examples in a node belong to the same class, turn it into a leaf node, label with the majority class

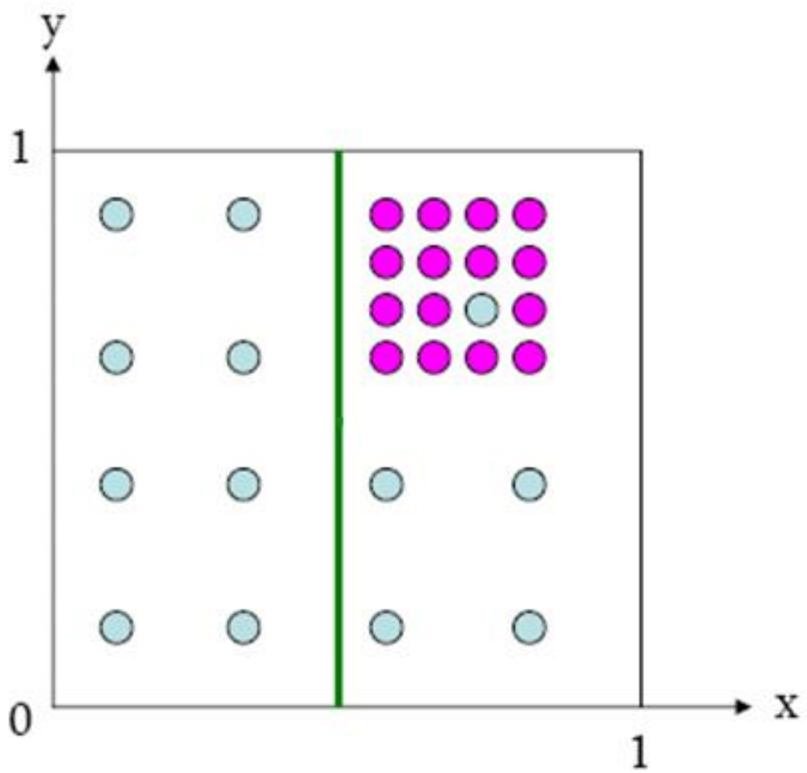
Building DT: an example

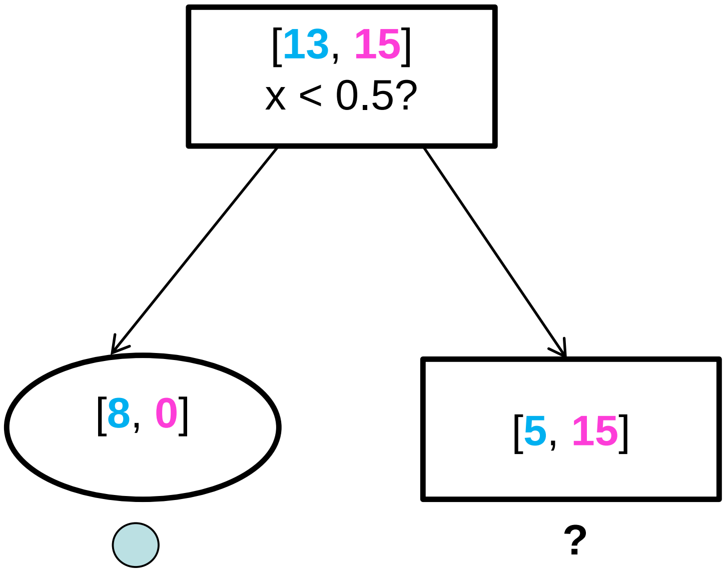


Training data contains

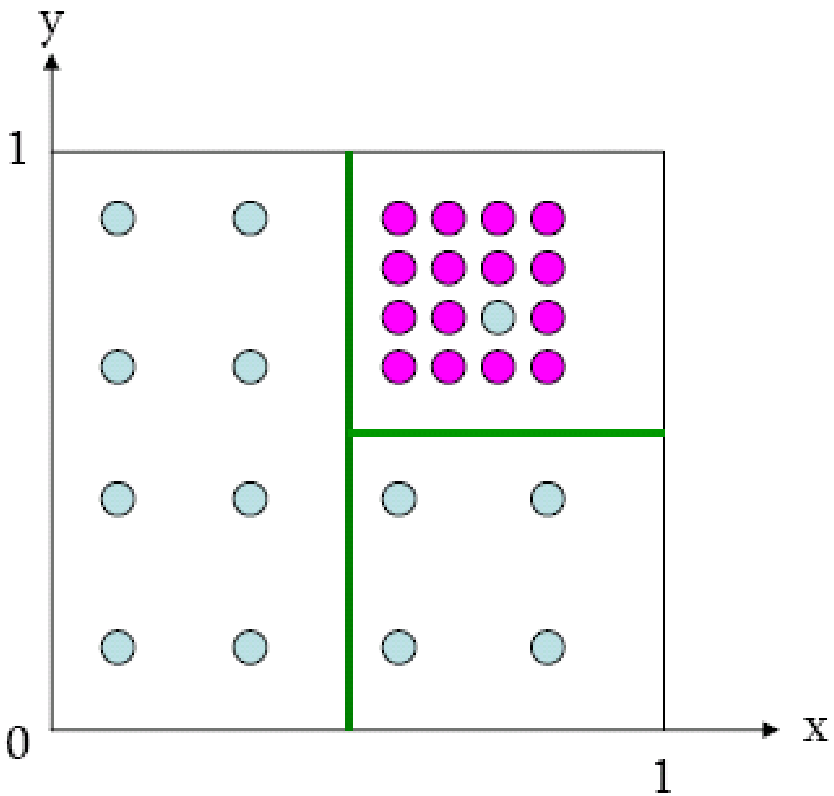
13 ● 15 ●

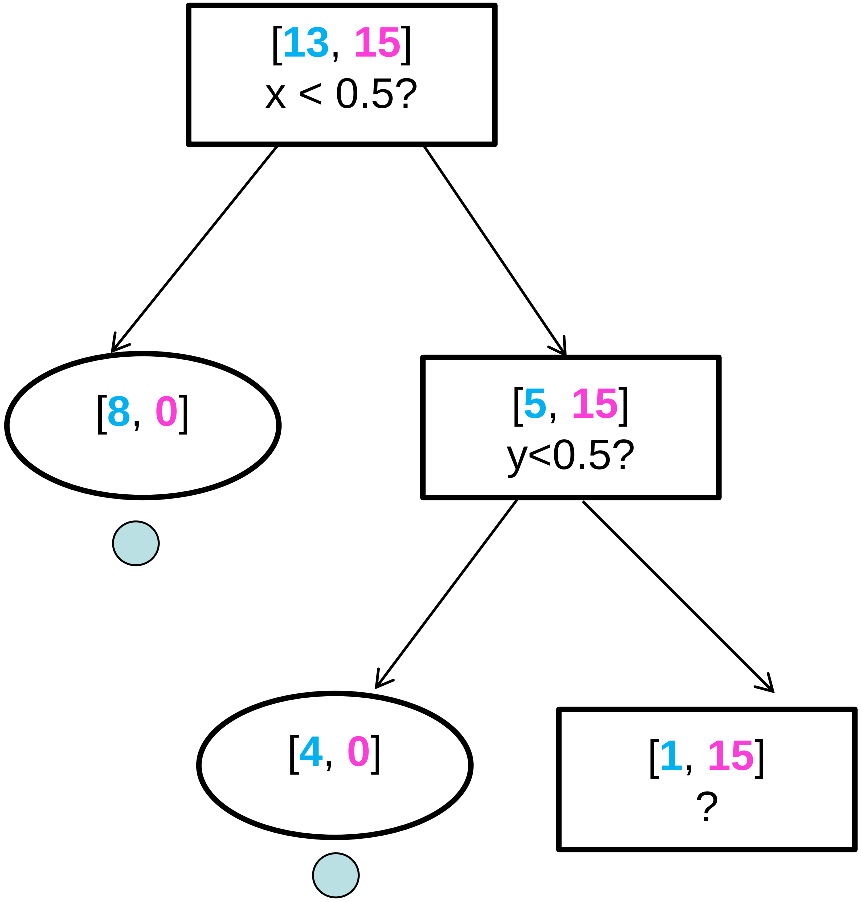
One possible question: is x <0.5?





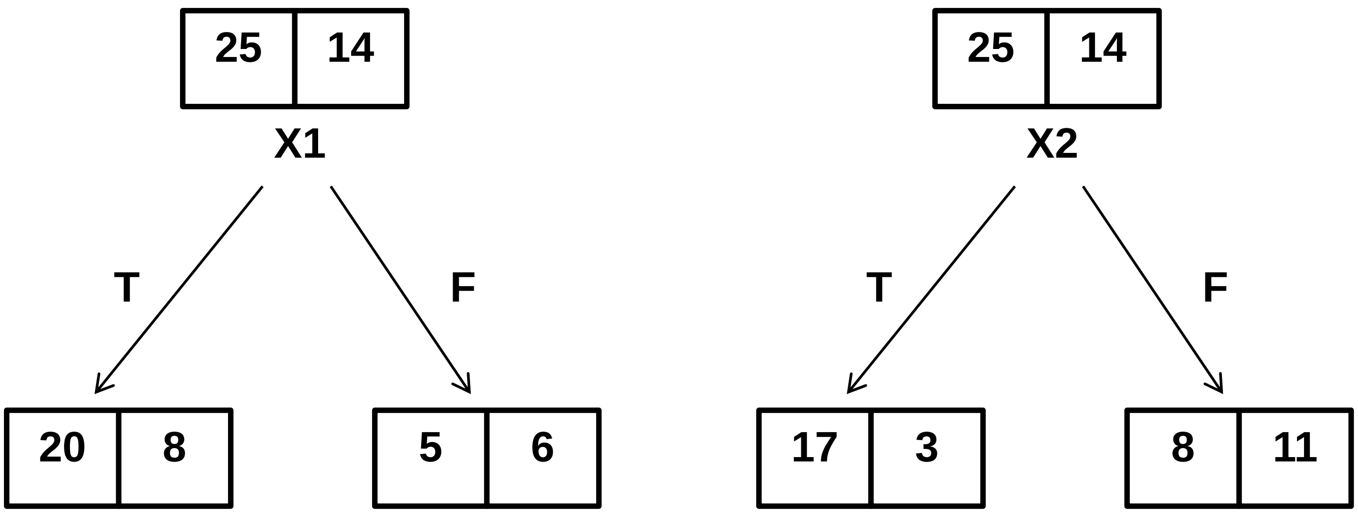
Continue





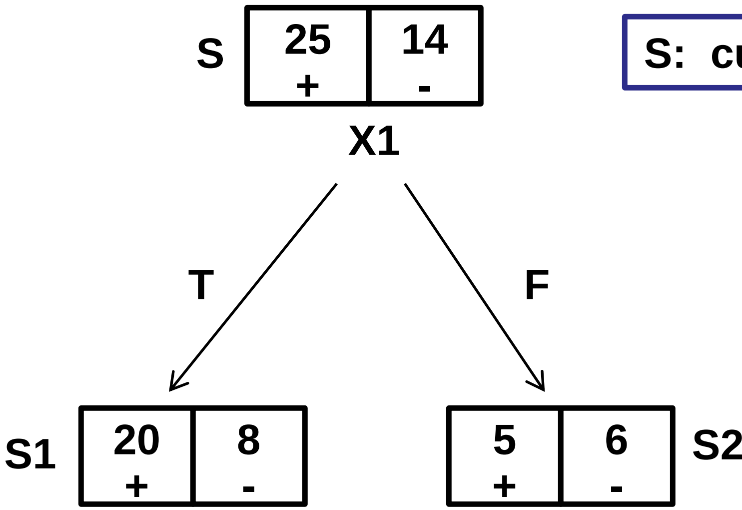
This could keep on going, until all examples are correctly classified.

Choosing the best test



Which one is better?

Choosing the Best test: A General View



S: current set of training examples

m branches, one for each possible outcome of the test

$S_1, S_2, \ldots S_m$: m subsets of training examples

p_i: The portion of examples in S that takes branch i

Benefit of split = $U(S) - \underbrace{\sum_i^m p_i U(S_i)}_{\text{Total Expected Remaining Uncertainty after the test}}$

Uncertainty of the class label in S

Uncertainty Measure: Entropy

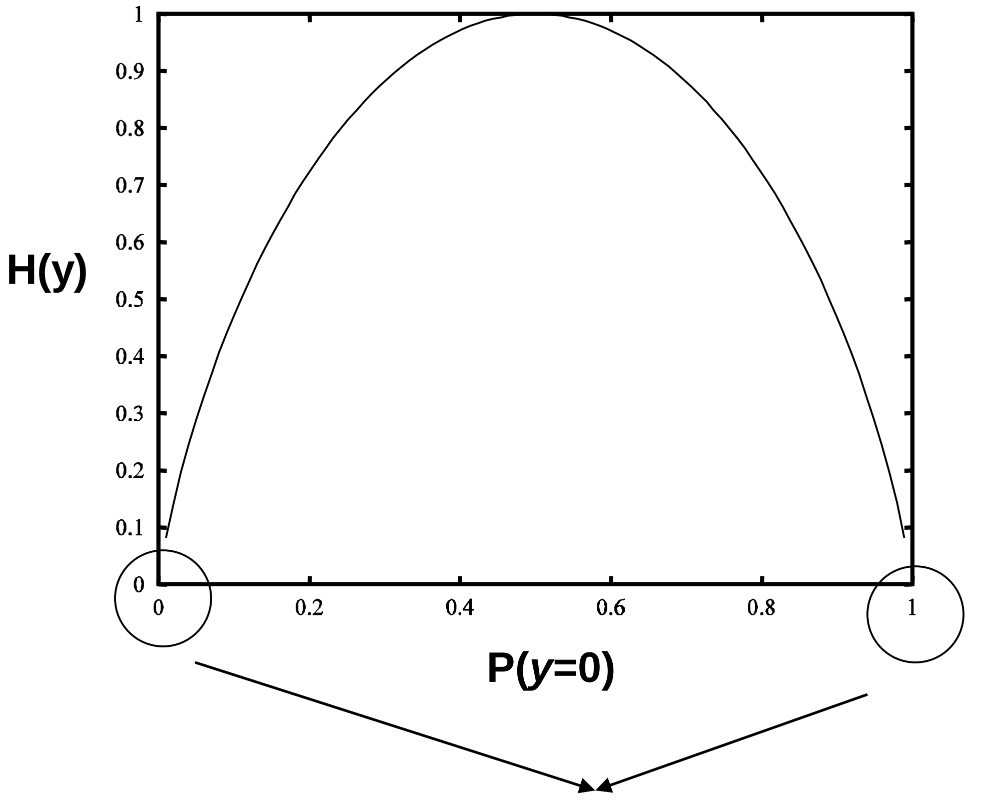
- Given a set of training examples S
  - Let y denote the label of an example randomly drawn from S
  - If all examples belong to one class, *y* has zero uncertainty
  - If y takes the positive and negative values with a 50%-50% chance, we have the highest amount of uncertainty in y
- In information theory, ***entropy*** is the measure of uncertainty of a random variable

Definition
Let y be a categorical random variable that can take k different values: $v_1, v_2, \dots, v_k$; and $p_i = P(y = v_i)$ for $i = 1, \dots, k$.
The ***entropy*** of y, denoted $H(y)$, is defined as

$$H(y) = \sum_{i=1}^{k} p_i \log_2 \frac{1}{p_i} = -\sum_{i=1}^{k} p_i \log_2 p_i$$

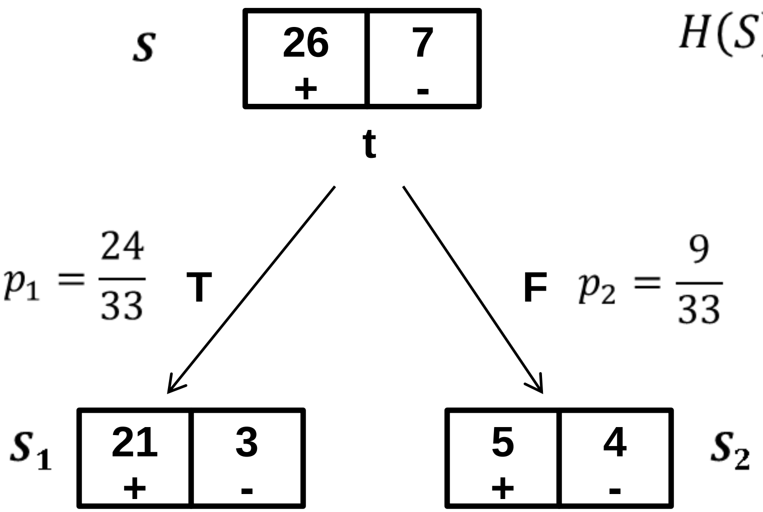
Entropy of a Binary y

- Entropy is a concave function downward



Minimum uncertainty occurs when p_0=0 or 1

The **Information Gain** approach: Measuring uncertainty using entropy:



$$H(S) = -\frac{26}{33}\log_2\frac{26}{33} - \frac{7}{33}\log_2\frac{7}{33} = 0.7455$$

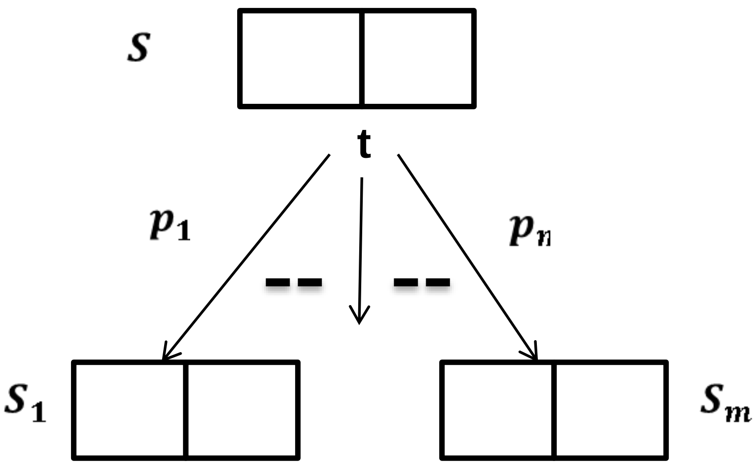
$$H(S_1) = -\frac{21}{24}\log_2\frac{21}{24} - \frac{3}{24}\log_2\frac{3}{24} = 0.5436$$

$$H(S_2) = -\frac{5}{9}\log_2\frac{5}{9} - \frac{4}{9}\log_2\frac{4}{9} = 0.9911$$

$$H(S) - (p_1 H(S_1) + p_2 H(S_2))$$
$$= 0.7455 - \frac{24}{33} * 0.5436 - \frac{9}{33} * 0.9911 = 0.0799$$

- This measures the ***Mutual information*** between t and y $I(t, y)$
- Hence the name information gain

Choosing the Best Feature: Summary



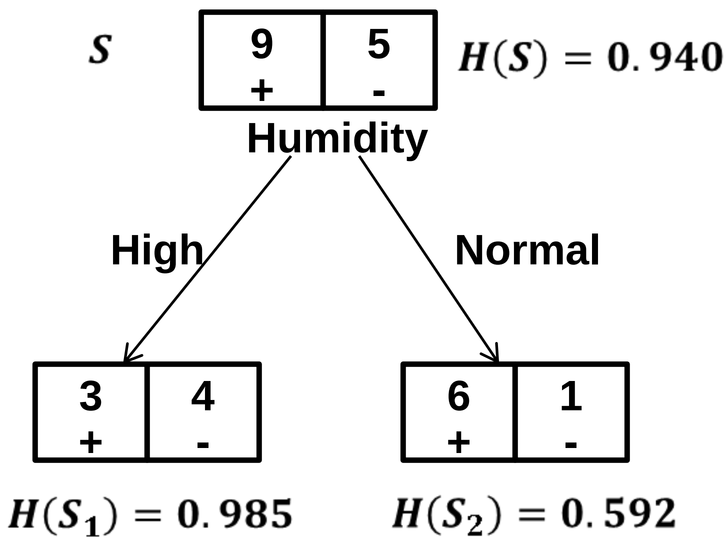
Benefit of split = $\underbrace{U(S)}_{\text{Original uncertainty}} - \underbrace{\sum_i^m p_i U(S_i)}_{\text{Total Expected Remaining Uncertainty after the test}}$

Measures of Uncertainty	
Error	$\min(p_+, p_-)$
Entropy	$-p_+ \log_2 p_+ - p_- \log_2 p_-$
Gini Index	$p_+ p_-$

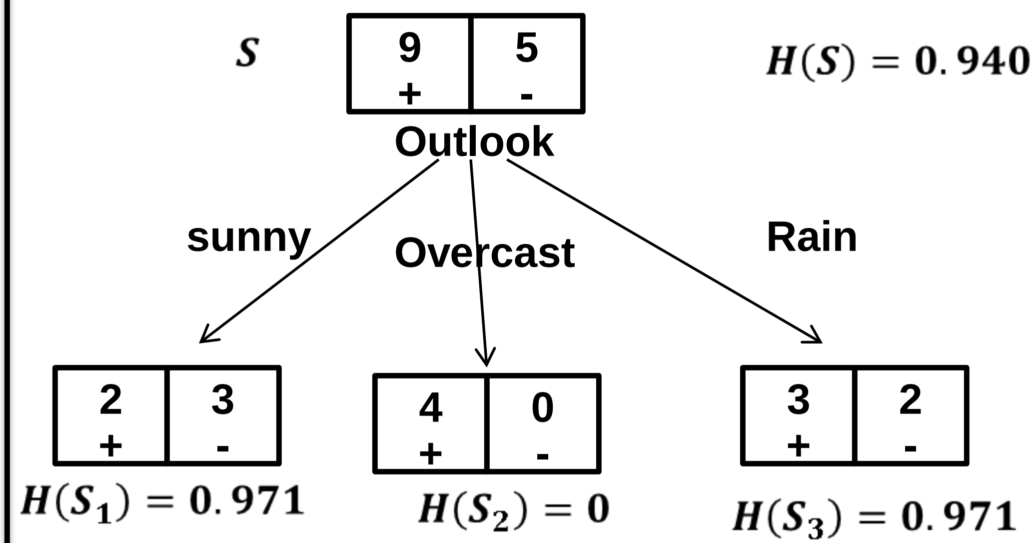
Example

Day	Outlook	Temperature	Humidity	Wind	PlayTen
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

Selecting the root test using information gain

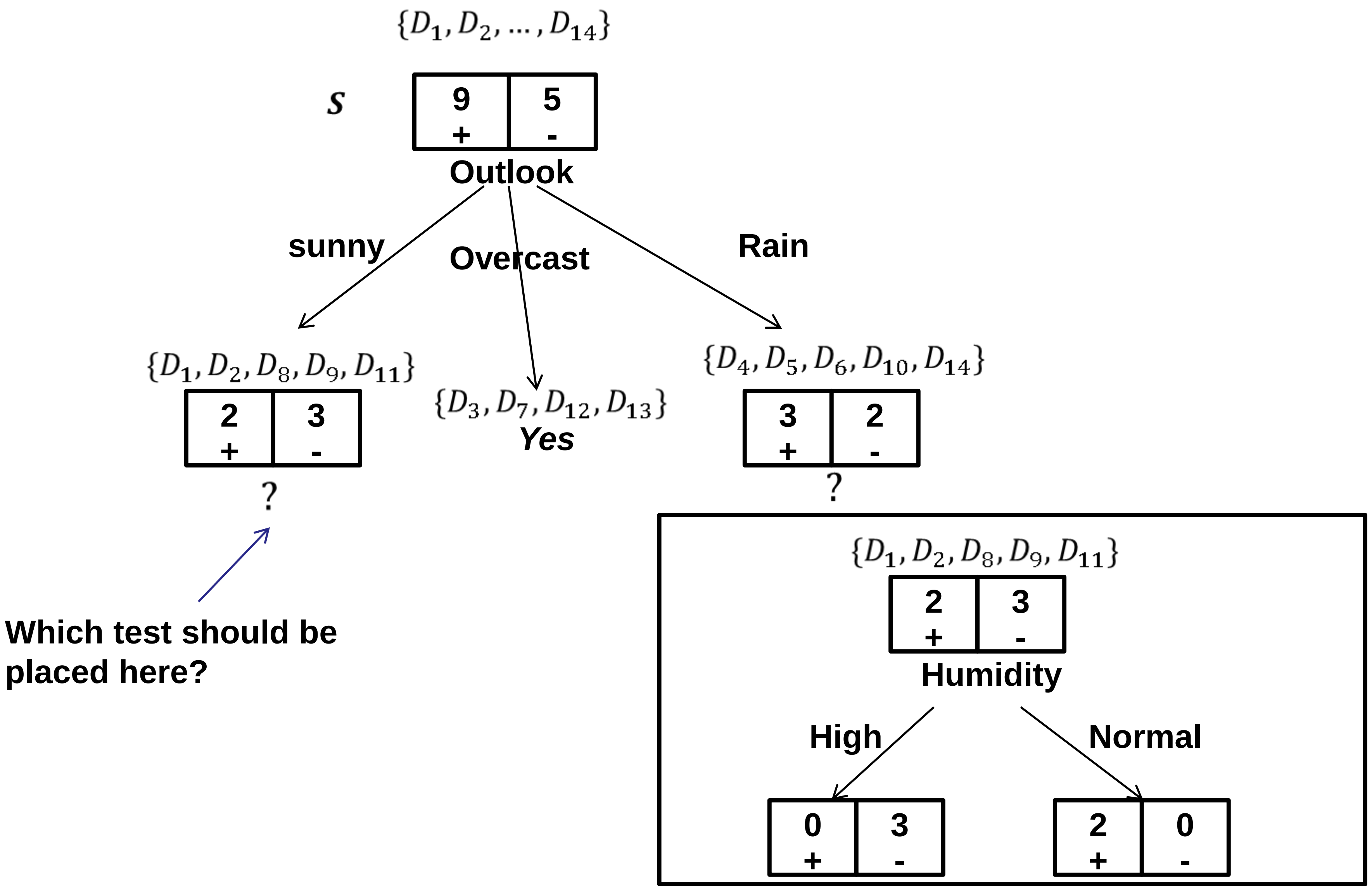


$$Gain(humidity) = 0.940 - \frac{1}{2}0.985 - \frac{1}{2}0.592 = 0.151$$



$$Gain(Outlook) = 0.940 - \frac{5}{14}0.971 - \frac{5}{14}0.971 = 0.2464$$

Continue building the tree



Issues with Multi-nomial Features

- Multi-nomial features: more than 2 possible values
- Consider two features, one is binary, the other has 100 possible values, which one you expect to have higher information gain?
- Conditional entropy of Y given the 100-valued feature will be low – why?
- This bias will prefer multinomial features to binary features
  - Test for one value, e.g., Outlook = sunny?

Dealing with Continuous Features

- Test against a threshold
- How to compute the best threshold θ_j for x_j?
  - Sort the examples according to x_j.
  - Move the threshold θ from the smallest to the largest value
  - Select θ that gives the best information gain
  - Trick: only need to compute information gain when class label changes

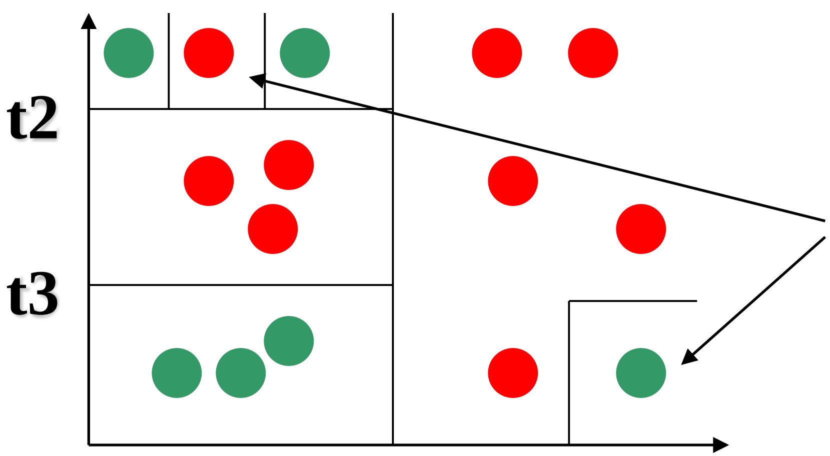
- Note that continuous features can be tested for multiple times on the same path in a DT

Considering both discrete and continuous features

- If a data set contains both types of features, do we need special handling?
- No, we simply consider all possibly splits in every step of the decision tree building process, and choose the one that gives the highest information gain
  - This include all possible (meaningful) thresholds

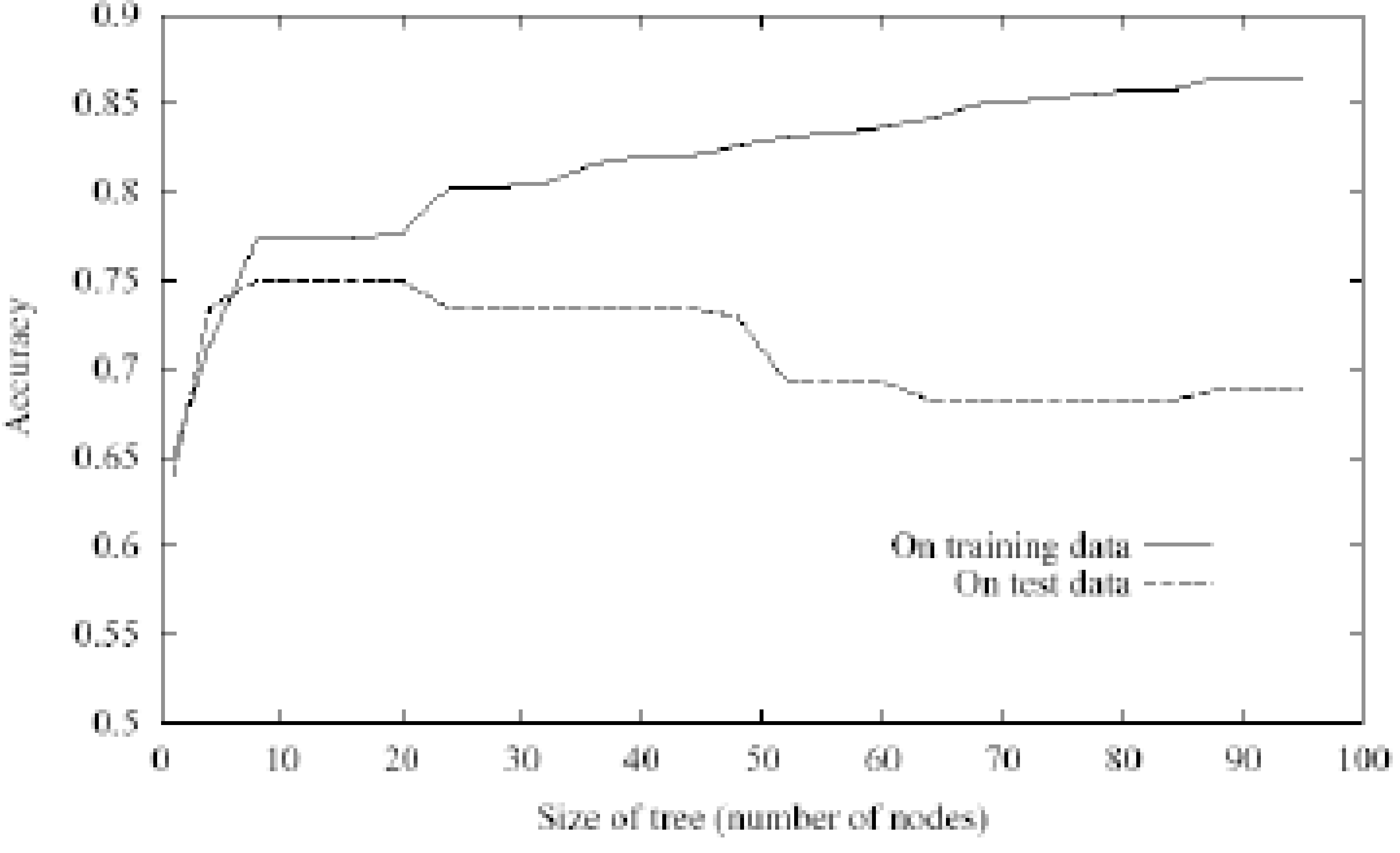
Issue of Over-fitting

- Decision tree has a very flexible hypothesis space
- As the nodes increase, we can represent arbitrarily complex decision boundaries
- This can lead to over-fitting



Possibly just noise, but the tree is grown larger to capture these examples

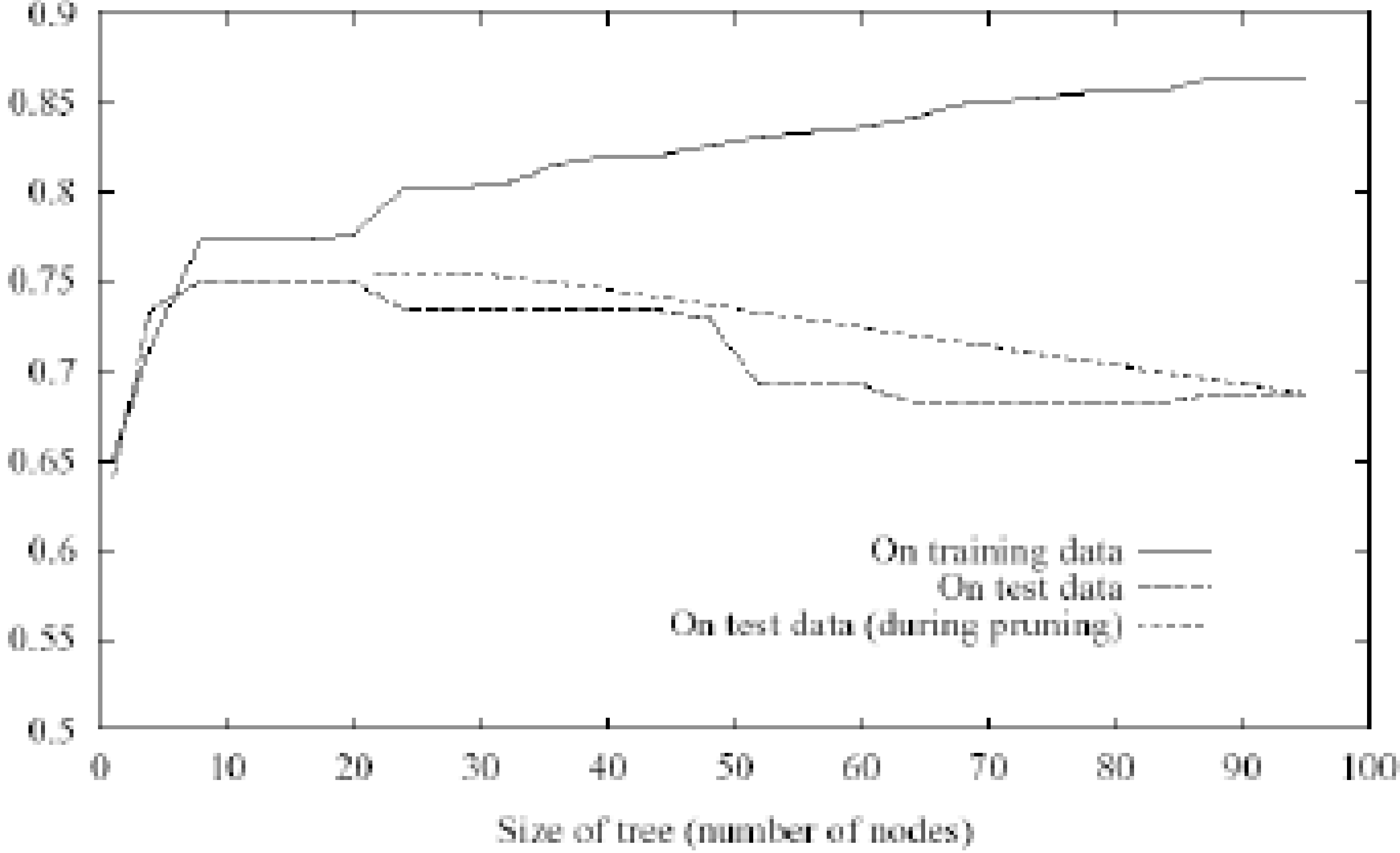
Over-fitting



Avoid Overfitting

- Early stop
  - Stop growing the tree when data split does not offer large benefit (e.g., compare information gain to a threshold, or perform statistical testing to decide if the gain is significant)
- Post pruning
  - Separate training data into **training set** and **validating set**
  - Evaluate impact on validation set when pruning each possible node
  - Greedily prune the node that most improves the validation set performance

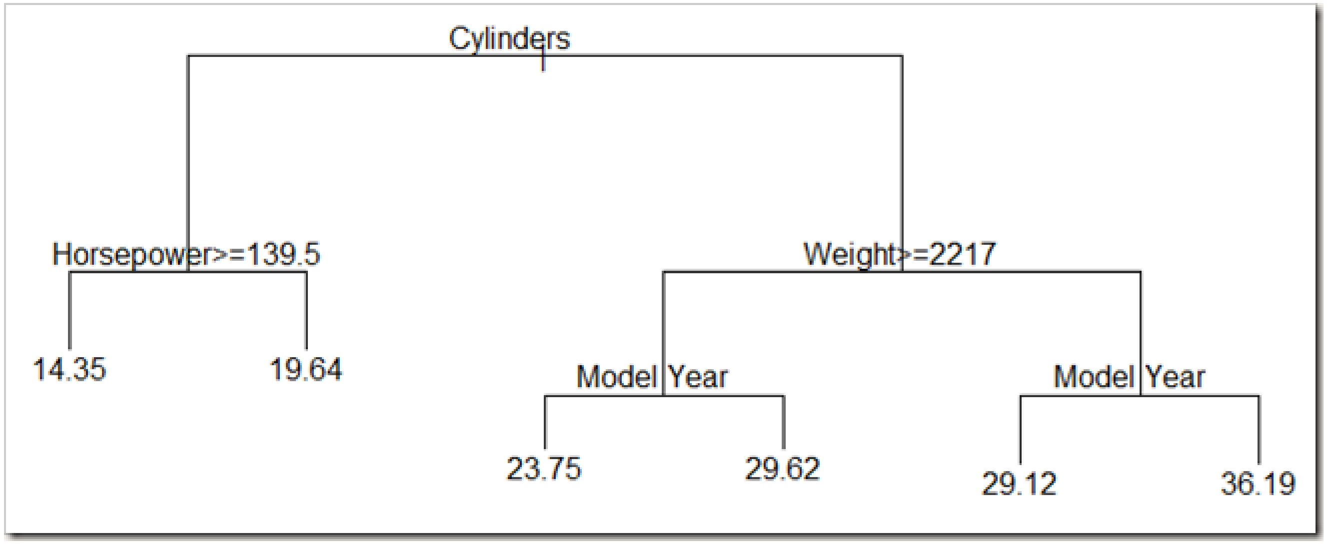
Effect of Pruning



Regression Tree

- Similar ideas can be applied for regression problems
- Prediction is computed as the <u>average of the target values</u> of all examples in the leave node
- Uncertainty is measured by sum of squared errors

Example Regression Tree



Predicting MPG of a car given its # of cylinders, horsepower, weight, and model year

Summary

- Decision tree is a very flexible classifier
  - Can model arbitrarily complex decision boundaries
  - By changing the depth of the tree (or # of nodes in the tree), we can increase of decrease the model complexity
  - Handling both continuous and discrete features
- Learning of the decision tree
  - Greedy top-down induction
  - Not guaranteed to find an optimal decision tree
- DT can overfitting to noise and outliers
  - Can be controlled by early stopping or post pruning