# 10-315 Intro to Machine Learning (SCS MAjors)

## Lecture 3: Decision Trees - Overfitting

Leila Wehbe

Carnegie Mellon University

Machine Learning Department

Lecture based on material from Tom Mitchell's **lecture 2**, Nina Balcan's lecture 2, and on on Kilian Weinberger's **lecture 17**

### Lecture outcomes

- What is a decision tree
- How to use information gain as a heuristic to building a short tree
- Notion of overfitting

Links (use the version you need)

- **Notebook**
- **PDF slides**

## Supervised Learning Problem Statement

The goal is to learn a function $c^*$ that maps input variables $X$ to output variables $y$, based on a set of labeled training examples.

- classification: $y$ is binary or multiclass
- regression: $y$ is continuous

**Training Data:** Given a training set of $n$ labeled examples: $\{(X^{(1)}, y^{(1)}), (X^{(2)}, y^{(2)}), \ldots, (X^{(n)}, y^{(n)})\}$, where $X_i \in \mathcal{X}$ represents the input features and $y_i \in \mathcal{Y}$ represents the corresponding labels, the goal is to estimate the optimal function $c^*$ that best predicts the labels for new, unseen data.

**Hypothesis Space:** The function $c^*$ is chosen from a family of hypotheses $\mathcal{H}$. That is, $c^* \in \mathcal{H}$, where $\mathcal{H}$ represents the set of all possible functions that could map inputs to outputs.

**Learning Rule:** A learning rule is applied to select the optimal function $c^*$ from the hypothesis space $\mathcal{H}$. The learning rule is typically defined based on an optimization algorithm that seeks to minimize a cost function over the training data.

## Function approximation

PROBLEM SETTING:

- Set of possible instances $X$
- Unknown target function $f : X \rightarrow Y$
- Set of candidate hypotheses $\mathcal{H} = h|h : X \rightarrow Y$

INPUT:

- Training examples $\langle X^{(i)}, y^{(i)} \rangle$ of unknown target function $f$

OUTPUT:

- Hypothesis $c^* \in H$ that best approximates target function $f$

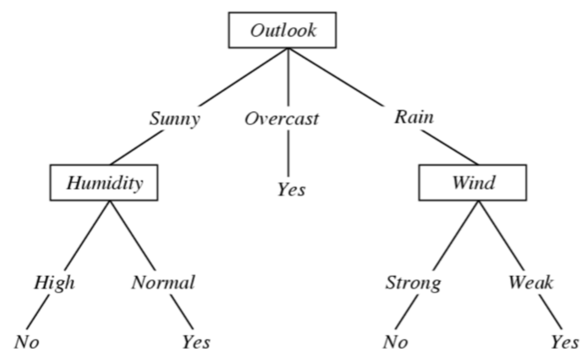
# Decision trees

Learn concept PlayTennis (i.e., decide whether our friend will play tennis in a given day)

| 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 | 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 |

# PLAY TENNIS?

- A Decision tree for $f$: (Outlook, Temperature, Humidity, Wind) $\rightarrow$ PlayTennis?




- Each internal node: test one discrete-valued attribute $X_d$
- Each branch from a node: selects one value for $X_d$
- Each leaf node: predict $Y$ (or $P(Y|X \in \mathrm{leaf})$)

Example: x=(Outlook=sunny, Temperature-Hot, Humidity=Normal,Wind=High), h(x)=Yes

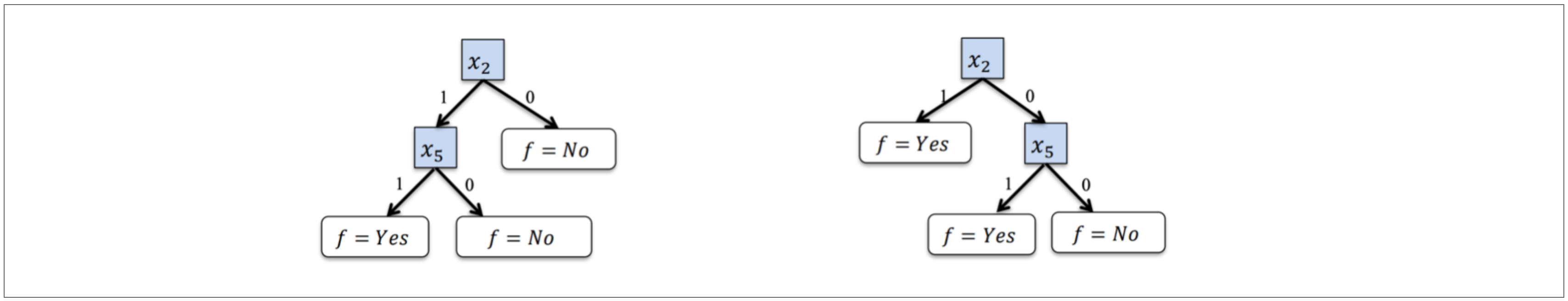
## Function approximation

PROBLEM SETTING:

- Set of possible instances $X$
    - example: Outlook, Temperature, Humidity, Wind
- Unknown target function $f : X \to Y$
    - example: Y is binary (play or not play)
- Set of candidate hypotheses $\mathcal{H} = h|h : X \to Y$
    - example: each $h$ is a decision tree

# Decision tree example

- Suppose $X = (X_1, X_2, \ldots X_n)$ where $X_i$ are boolean-valued variables
- How would you represent $Y = X2 \wedge X5$? $\quad Y = X2 \vee X5$?




How would you represent $X_2X_5 \vee X_3X_4(\neg X_1)$?

## Example with training data

Draw a tree that represents:

| $X_1$ | $X_2$ | $X_3$ | $Y$ |
|---|---|---|---|
| 0 | 0 | 0 | 0 |
| 0 | 0 | 1 | 0 |
| 0 | 1 | 0 | 1 |
| 0 | 1 | 1 | 1 |
| 1 | 0 | 0 | 1 |
| 1 | 0 | 1 | 1 |
| 1 | 1 | 0 | 1 |
| 1 | 1 | 1 | 1 |

- The order we pick the attributes affects the size (and efficiency) of the tree.

## How to choose the best hypothesis?

- How to automatically find a good hypothesis for training data?
    - A core algorithmic question.
- When do we generalize and do well on unseen data?
    - A learning theory question.
    - **Occam's razor**: use the simplest hypothesis consistent with data!
- *Occam's razor: Fewer short hypotheses than long ones*
    - *a short hypothesis that fits the data is less likely to be a statistical coincidence*
    - *highly probable that a sufficiently complex hypothesis will fit the data*
    - *(remember this is a heuristic. read **here** for more discussion)*

## How to choose the best hypothesis?

- How to automatically find a good hypothesis for training data?
    - A core algorithmic question.
- When do we generalize and do well on unseen data?
    - A learning theory question.
    - **Occam's razor**: use the simplest hypothesis consistent with data!
- Other core questions in machine learning:
    - How do we choose a hypothesis space?
        - Often we use prior knowledge to guide this choice
    - How to model applications as machine learning problems?
        - engineering challenge

## How to choose the best Decision Tree?

- How to pick the smallest tree?
  - NP-hard [Hyafil-Rivest'76]!
- Luckily, we have very nice practical heuristics and top down algorithms (e.g, ID3) that can achieve a good solution

## Top-Down Induction of Decision Trees [examples ID3, C4.5, Quinlan]

- ID3: Natural greedy approach to growing a decision tree top-down (from the root to the leaves by repeatedly replacing an existing leaf with an internal node.).
- Algorithm main loop:
    - Pick "best" attribute A to split at a node based on training data.
    - Assign A to this node.
    - For each value of A create new descendent.
    - Split training examples among the descendents.
    - If training examples perfectly classified in new node, stop, else recurse on node.
- How to know which attribute is best?

## Which attribute is best?

- ID3 uses a statistical measure called **information gain** (how well a given attribute separates the training examples according to the target classification)
- Information Gain of variable $A$ is the expected reduction in entropy of target variable $Y$ for data sample $S4$, due to sorting on variable $A$

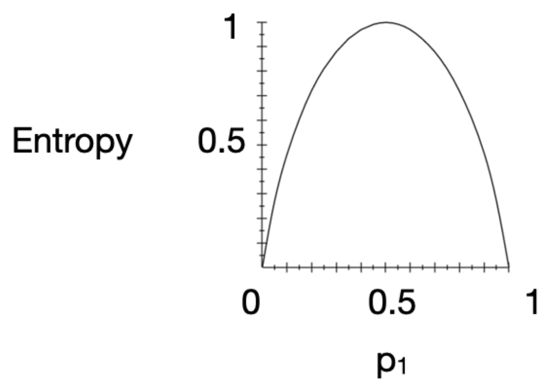
$$\mathrm{Gain}(S, A) = H_S(Y) - H_S(Y|A)$$

- Entropy ($H_S$) is information theoretic measure that characterizes the complexity of a labeled set $S$.

Entropy

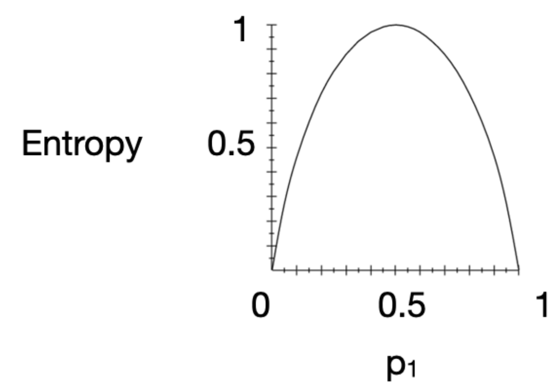
- Sample Entropy of a Labeled Dataset
    - $S$ is a sample of training examples
        - $p_1$ is the proportion of positive examples in $S$
        - $p_0$ the proportion of negative examples in $S$
- Entropy measures the complexity of $S$:

$$H_S = -p_1 \log(p_1) - p_0 \log(p_0)$$



Entropy

$$H_S = -p_1 \log(p_1) - p_0 \log(p_0)$$




- E.g., if all negative, then entropy=0. If all positive, then entropy=0.
- If 50/50 positive and negative then entropy=1.
- If 14 examples with 9 positive and 5 negative, then entropy=.940

If labels not Boolean

$$H_S = -\sum_{k=1}^{c} p_k \log_2(p_k)$$

E.g., if $c$ classes, all equally likely, then $p_k = \frac{1}{c}$ for all $k$ and $H_S = -\log_2 \frac{1}{c}$

## Another way to understand maximizing information gain

- We want to be the farthest possible from all classes being equally likely (let's call this uniform distribution $q_k = \frac{1}{c}$ for all $k$). This can be done by finding another distribution $(p_1, \ldots p_c)$ that maximizes the KL-Divergence (Kullback–Leibler divergence).

$$\mathrm{KL}(p \parallel q) = \sum_{k=1}^{c} p_k \log \frac{p_k}{q_k}$$

- The KL-Divergence is not a metric because it is not symmetric, i.e., $\mathrm{KL}(p||q) \neq \mathrm{KL}(q||p)$.

$$\mathrm{KL}(p \parallel q) = \textstyle\sum_{k=1}^{c} p_k \log \frac{p_k}{q_k} \geq 0 \quad \leftarrow \text{KL-Divergence}$$

$$= \textstyle\sum_k p_k \log(p_k) - p_k \log(q_k) \quad \text{where } q_k = \frac{1}{c}$$

$$= \textstyle\sum_k p_k \log(p_k) + p_k \log(c)$$

$$= \textstyle\sum_k p_k \log(p_k) + \log(c) \sum_k p_k \quad \text{where } \log(c) \text{ is constant, } \sum_k p_k = 1$$

$$\max_p \mathrm{KL}(p \parallel q) = \max_p \textstyle\sum_k p_k \log(p_k)$$

$$= \min_p - \textstyle\sum_k p_k \log(p_k) = \min_p H(s) \quad \leftarrow \text{Entropy}$$

## Information gain of a split

- Information Gain of variable $A$ is the expected reduction in entropy of target variable $Y$ for data sample $S4$, due to sorting on variable $A$ (with $c$ values):

$$\mathrm{Gain}(S, A) = H_S(Y) - H_S(Y|A)$$

$$\mathrm{Gain}(S, A) = \mathrm{Entropy}(S) - \sum_{k=1}^{c} \frac{|S_k|}{S} \mathrm{Entropy}(S_k)$$

- Gain(S,A) is the information provided about the target function, given the value of some other attribute A.

Learn concept PlayTennis (i.e., decide whether our friend will play tennis in a given day)

| 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 | 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 |

| Day | Outlook | Temperature | Humidity | Wind | Play Tennis |
|---|---|---|---|---|---|
| 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 |

# Which attribute is the best classifier?

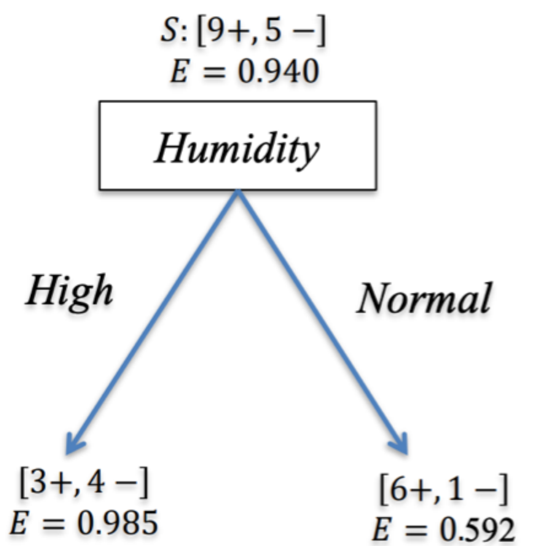
$$\text{Gain}(S, A) = \text{Entropy}(S) - \sum_{k=1}^{c} \frac{|S_k|}{S} \text{Entropy}(S_k)$$

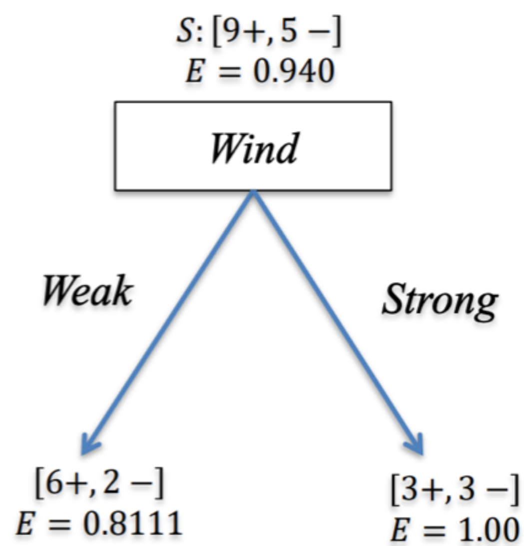
$$Entropy[9+, 5-] = -\left(\frac{9}{14}\right)\log_2\left(\frac{9}{14}\right) - \left(\frac{5}{14}\right)\log_2\left(\frac{5}{14}\right) = .940$$

| Day | Outlook | Temperature | Humidity | Wind | Play Tennis |
|---|---|---|---|---|---|
| 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 |

# Which attribute is the best classifier?

$$\text{Gain}(S, A) = \text{Entropy}(S) - \sum_{k=1}^{c} \frac{|S_k|}{S} \text{Entropy}(S_k)$$




$Gain(S, Humidity)$

$$= .940 - \left(\frac{7}{14}\right).985 - \left(\frac{7}{14}\right).592$$

$$= .151$$

$Gain(S, Wind)$

$$= .940 - \left(\frac{8}{14}\right).811 - \left(\frac{6}{14}\right)1.0$$

$$= .048$$

## Which attribute is the best classifier?

$$\text{Gain}(S, A) = \text{Entropy}(S) - \sum_{k=1}^{c} \frac{|S_k|}{S} \text{Entropy}(S_k)$$

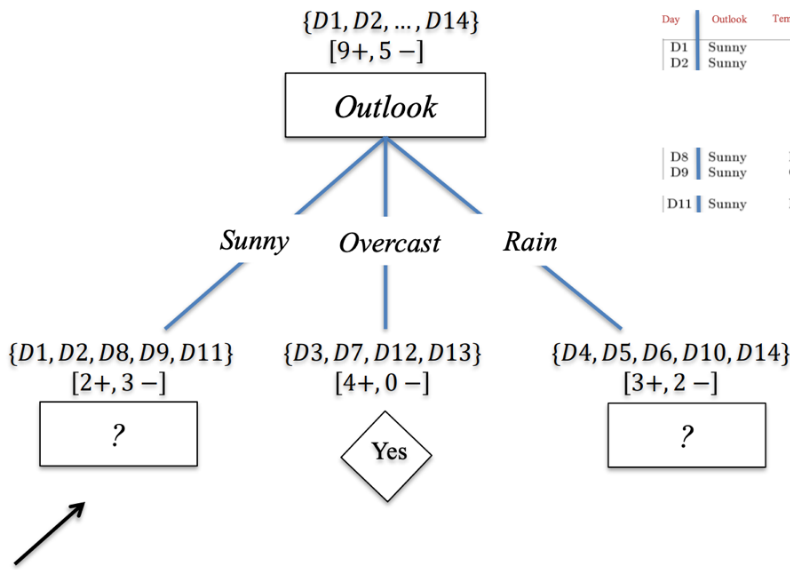
| Day | Outlook | Temperature | Humidity | Wind | Play Tennis |
|---|---|---|---|---|---|
| D1 | Sunny | Hot | High | Weak | No |
| D2 | Sunny | Hot | High | Strong | No |
| D3 | Overcast | Hot | High | Weak | Yes |
| D4 | Rain | Mild | High | Weak | Yes |
| D5 | Rain | Cool | Normal | Weak | Yes |
| 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 |

$$Gain(S, Humidity) = .151$$

$$Gain(S, Wind) = .048$$

$$Gain(S, Outlook) = .246$$

$$Gain(S, Temperature) = .029$$




| Day | Outlook | Temperature | Humidity | Wind | Play Tennis |
|---|---|---|---|---|---|
| D1 | Sunny | Hot | High | Weak | No |
| D2 | Sunny | Hot | High | Strong | No |
| D8 | Sunny | Mild | High | Weak | No |
| D9 | Sunny | Cool | Normal | Weak | Yes |
| D11 | Sunny | Mild | Normal | Strong | Yes |

*Which attribute should be tested here?*

$$s_{sunny} = \{D1, D2, D8, D9, D11\}$$

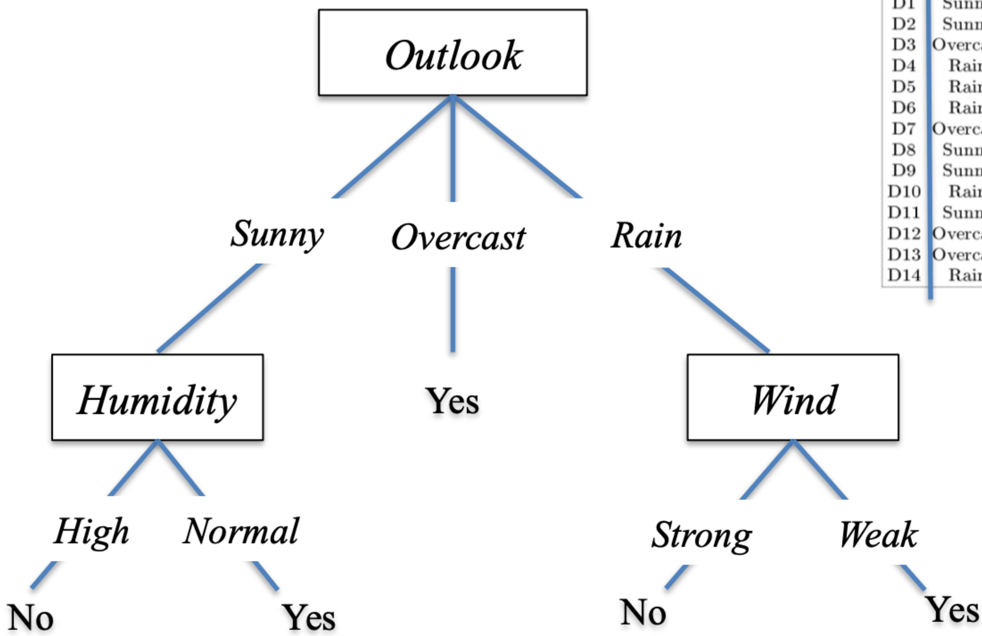
$$Gain(s_{sunny}, Humidity) = .970 - \left(\frac{3}{5}\right)0.0 - \left(\frac{2}{5}\right)0.0 = .970$$

$$Gain(s_{sunny}, Temperature) = .970 - \left(\frac{2}{5}\right)0.0 - \left(\frac{2}{5}\right)1.0 - \left(\frac{1}{5}\right)0.0 = .570$$

$$Gain(s_{sunny}, Wind) = .970 - \left(\frac{2}{5}\right)1.0 - \left(\frac{3}{5}\right).918 = .019$$

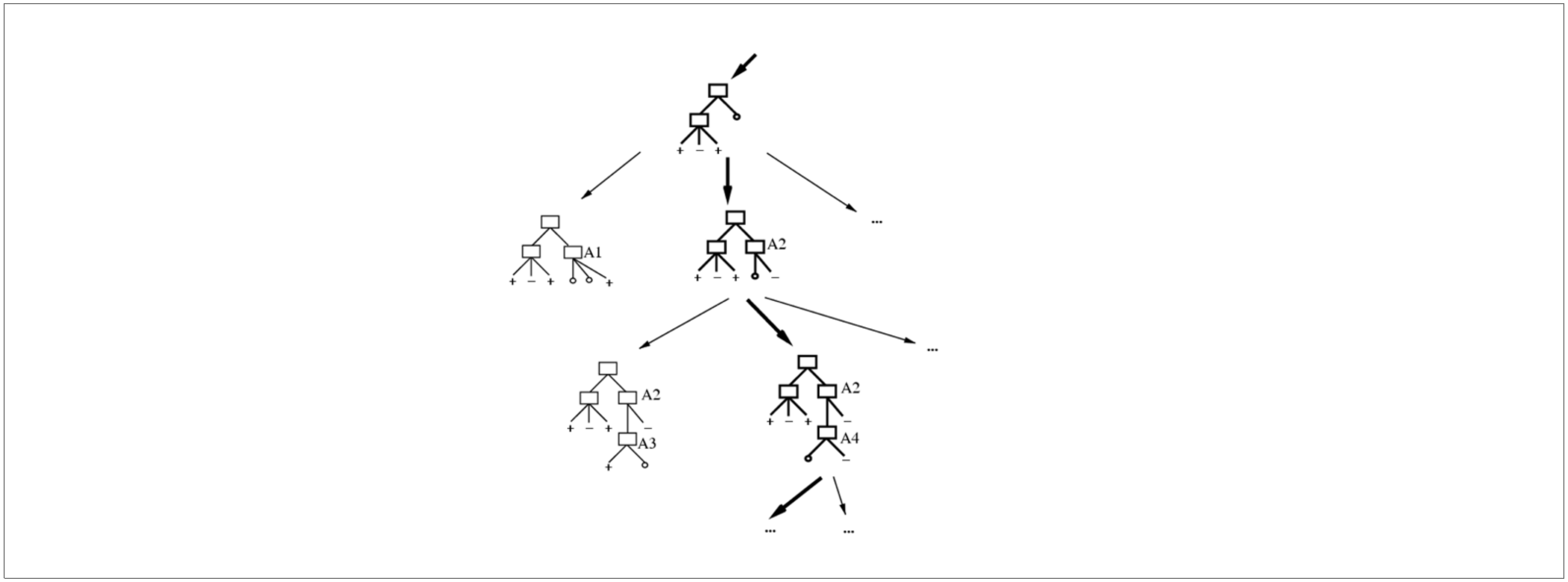
Final decision tree

f: <Outlook, Temperature, Humidity, Wind> → PlayTennis?




| Day | Outlook | Temperature | Humidity | Wind | Play Tennis |
|---|---|---|---|---|---|
| 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 |

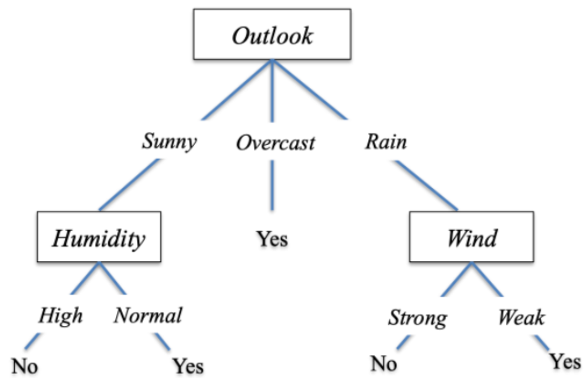
## Properties of ID3




- ID3 performs heuristic search through space of decision trees.
- It stops at smallest acceptable tree. (Occam's razor).
- Still a greedy approach, might not find the shortest tree.

## ID3 might still overfit!

- Overfitting could occur because of noisy data and because ID3 is not guaranteed to output a small hypothesis even if one exists.
- Consider adding a noisy example:
    - Sunny, Hot, Normal, Strong, PlayTennis = No
- The tree we learned would not be compatible with the training data



# Overfitting

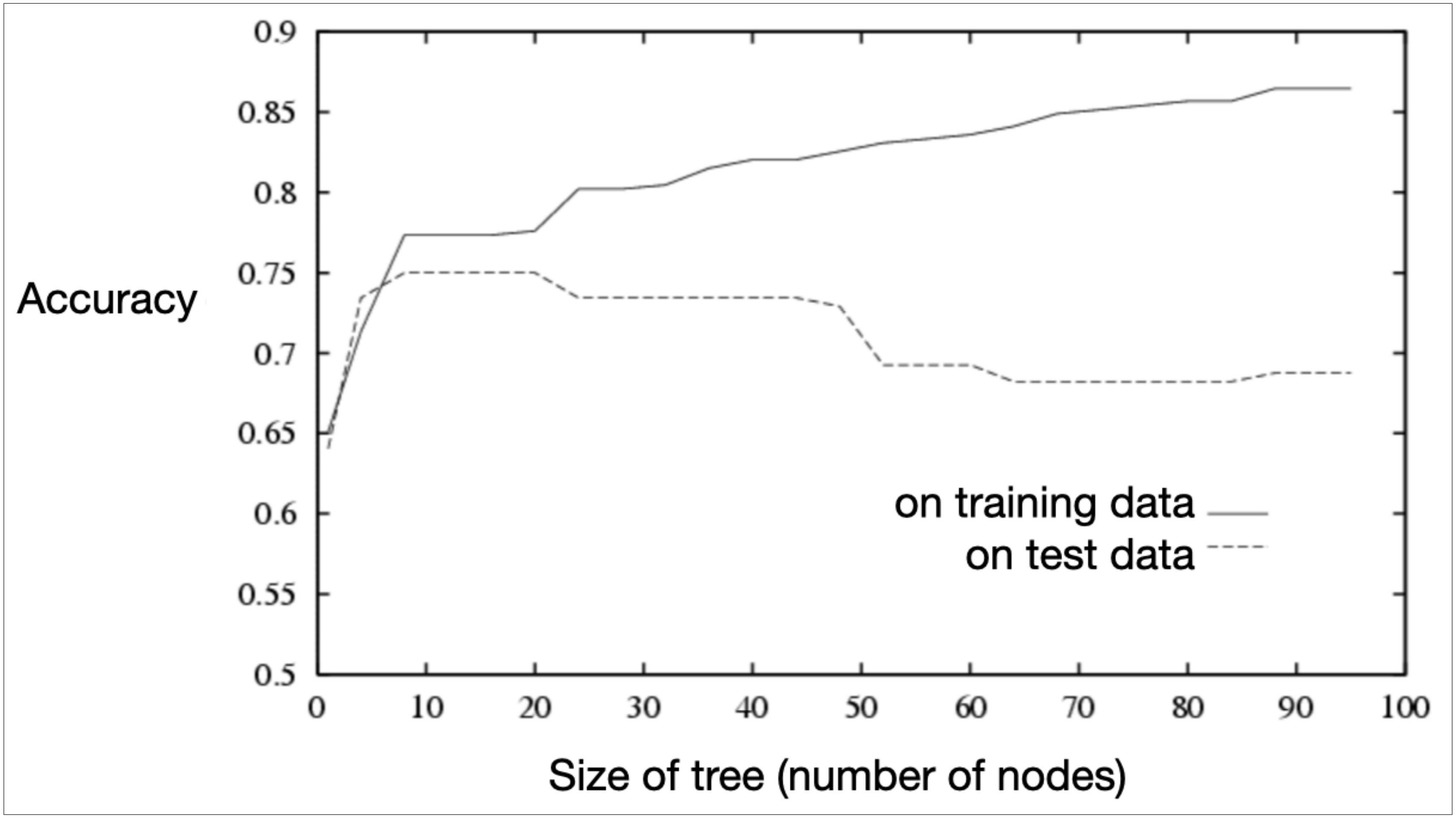
- Consider a hypothesis h and its
  - Error rate over training data: $error\_train(h)$
  - True error rate over all data: $error\_true(h)$

- We say h overfits the training data if $error\_true(h) > error\_train(h)$
  - We typically don't know $error\_true(h)$ but we can estimate $error\_test(h)$ on a heldout set from the same distribution as the training data.

- Amount of overfitting = $error\_true(h) - error\_train(h)$

Example of overfitting in ID3

Task: learning which medical patients have a form of diabetes.

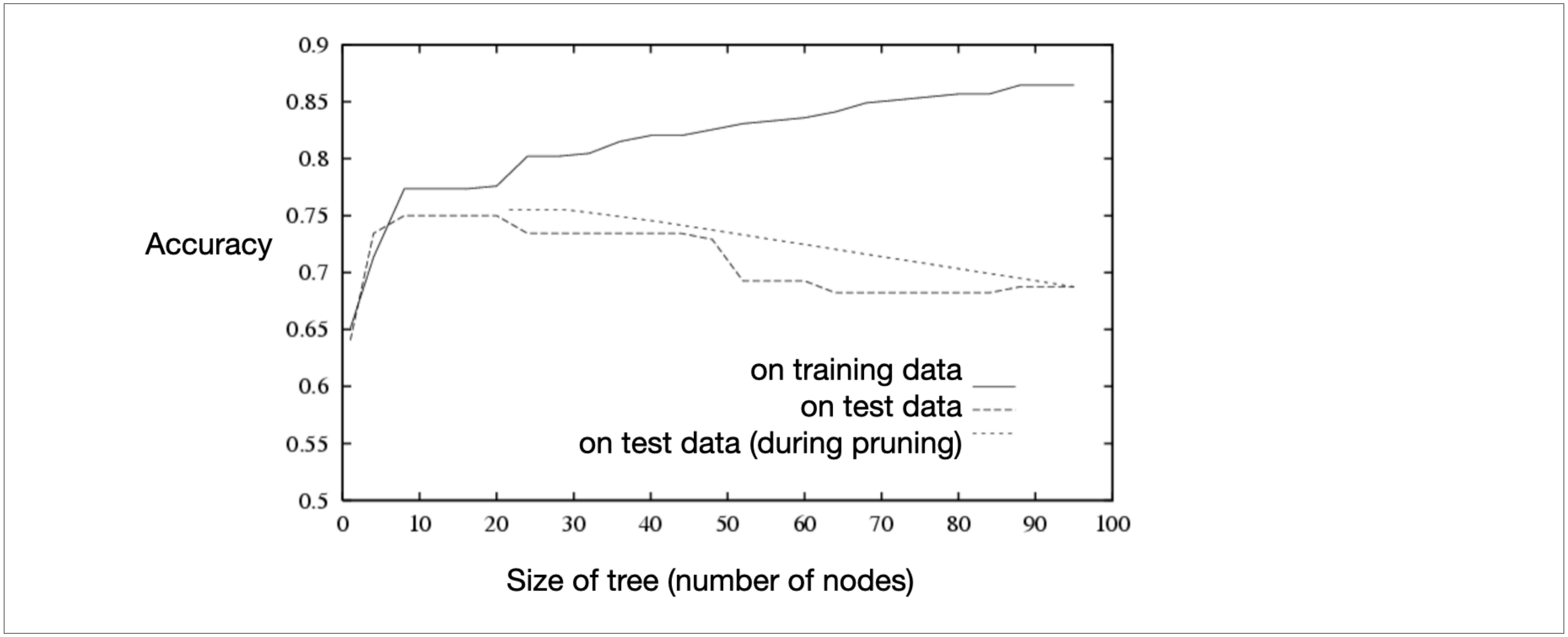


## How can we avoid overfitting?

- Stop growing when data split not statistically significant
- Grow full tree, then prune it

- example: Reduced Error Pruning
    - Split data into training set and validation set
    - Train a tree to classify training set as well as possible
    - Do until further pruning is harmful:
        1. For each internal tree node, consider making it a leaf node (pruning the tree below it)
        2. Greedily chose the above pruning step that best improves error over validation set
    - Produces smallest version of the most accurate pruned tree

## Effect of reduced error pruning




NOTE: THE TEST SET SHOULD NEVER BE USED FOR TRAINING. A SEPARATE VALIDATION SET IS USED FOR MAKING DECISIONS ABOUT PRUNING.

What if my attributes $x$ are real valued?

- Use a decision stump: for each attribute, consider splitting above, below
  - e.g. (is Temperature $\geq$ 72)

| | | | | | | |
|---|---|---|---|---|---|---|
| *Temperature*: | 40 | 48 | 60 | 72 | 80 | 90 |
| *PlayTennis*: | No | No | Yes | Yes | Yes | No |

## Ensemble learning, bagging

- Using ensemble learning with trees makes them work very well in practice
    - instead of one tree, create a forest of trees and combine their prediction

- Bagging: resample the training dataset with replacement and average the trees
- Random forests: use subsets of the data (different features)

- Will see ensemble learning later in the couse