

# Lecture 2: Decision Trees

## DD2421

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Autumn, 2021

- Lecture 1: Nearest Neighbour Classifier (Memory-based)
- Lecture 2: Decision Trees (Logical inference, Rule-based)
- Lecture 3: Challenges in Machine Learning

## 1 Decision Trees

- The representation
- Training

## 2 Unpredictability

- Entropy
- Information gain
- Gini impurity

## 3 Overfitting

- Overfitting
- Occam's principle
- Training and validation set approach
- Extensions

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  - The representation
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  - Extensions

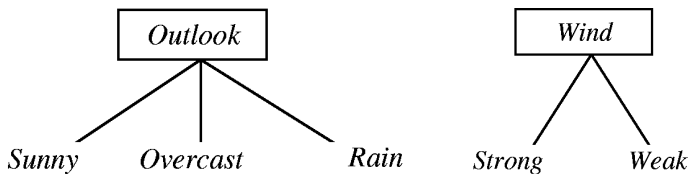
Basic Idea: Test the attributes (features) **sequentially**  
= Ask questions about the target/status **sequentially**

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Example: building a concept of whether someone would like to play tennis.

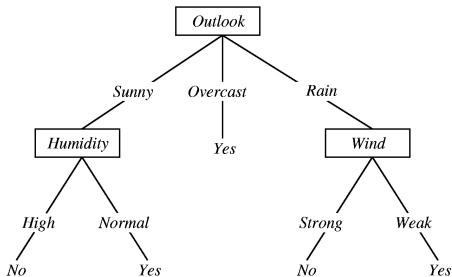
Basic Idea: Test the attributes (features) **sequentially**  
= Ask questions about the target/status **sequentially**

Example: building a concept of whether someone would like to play tennis.



Useful also (but not limited to) when nominal data are involved, e.g. in medical diagnosis, credit risk analysis etc.

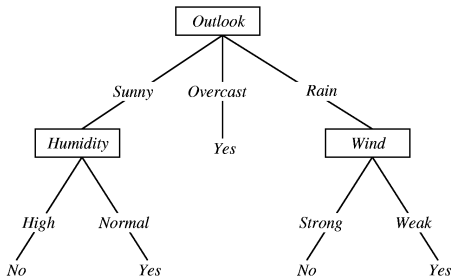
The whole analysis strategy can be seen as a tree.



(T. Mitchell, Machine Learning)

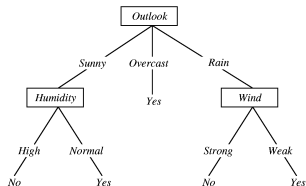


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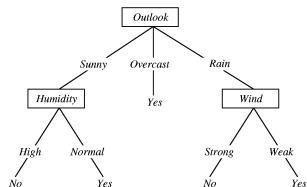


(T. Mitchell, Machine Learning)

Each **leaf node** bears a category label, and the **test pattern** is assigned the category of the leaf node reached.

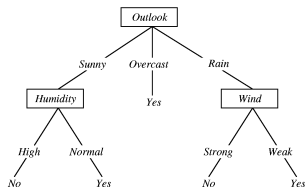


What does the tree encode?



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$(\text{Sunny} \wedge \text{Normal Humidity}) \vee (\text{Cloudy}) \vee (\text{Rainy} \wedge \text{Weak Wind})$



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Logical expressions of the conjunction of decisions along the path.

Arbitrary boolean functions can be represented!

Training: we need to grow a tree from scratch given a set of labeled training data.

How to grow/construct the tree automatically?

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- 2 **Terminate**: call branches with a unique class labels **leaves** (no need for further questions)

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How to grow/construct the tree automatically?

- 1 Choose the **best question** (according to the **information gain**), and split the input data into subsets
- 2 **Terminate**: call branches with a unique class labels **leaves** (no need for further questions)
- 3 **Grow**: recursively extend other branches (with subsets bearing mixtures of labels)



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Quiz time – Game of “sixty-three”

$x$  drawn from  $\{0, 1, 2, 3, 4, \dots, 63\}$

- I pick a number  $x$  from the set.
- You ask me yes/no questions.

How many (and what) questions will you ask me to get the number  $x$  as rapidly as possible?

# Entropy

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$$\log_2 \frac{1}{p_i}$$

( $p_i$  : probability for event  $i$ )

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The Shannon information content of an outcome is:

$$\log_2 \frac{1}{p_i}$$

( $p_i$  : probability for event  $i$ )

The Entropy — measure of **uncertainty (unpredictability)**

$$\text{Entropy} = \sum_i -p_i \log_2 p_i$$

is a sensible measure of expected information content.

# Entropy

Example: tossing a coin

$$p_{\text{head}} = 0.5; \quad p_{\text{tail}} = 0.5$$



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$$\begin{aligned}\text{Entropy} &= \sum_i -p_i \log_2 p_i = \\ &= -0.5 \log_2 0.5 - 0.5 \log_2 0.5\end{aligned}$$



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$$\begin{aligned}\text{Entropy} &= \sum_i -p_i \log_2 p_i = \\ &= -0.5 \underbrace{\log_2 0.5}_{-1} - 0.5 \underbrace{\log_2 0.5}_{-1}\end{aligned}$$

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The result of a coin-toss has **1 bit** of information

# Entropy

Example: rolling a die

$$p_1 = \frac{1}{6}; \quad p_2 = \frac{1}{6}; \dots \quad p_6 = \frac{1}{6}$$



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Example: rolling a die

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$$\begin{aligned} \text{Entropy} &= \sum_i -p_i \log_2 p_i = \\ &= 6 \times \left(-\frac{1}{6} \log_2 \frac{1}{6}\right) \end{aligned}$$

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The result of a die-roll has **2.58 bit** of information

# Entropy

Example: rolling a **fake die**

$$p_1 = 0.1; \dots \quad p_5 = 0.1; \quad p_6 = 0.5$$



$$\text{Entropy} = \sum_i -p_i \log_2 p_i$$



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Example: rolling a **fake die**

$$p_1 = 0.1; \dots \quad p_5 = 0.1; \quad p_6 = 0.5$$



$$\begin{aligned}\text{Entropy} &= \sum_i -p_i \log_2 p_i = \\ &= -5 \cdot 0.1 \log_2 0.1 - 0.5 \log_2 0.5\end{aligned}$$

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$$\begin{aligned}\text{Entropy} &= \sum_i -p_i \log_2 p_i = \\ &= -5 \cdot 0.1 \log_2 0.1 - 0.5 \log_2 0.5 = \\ &\approx 2.16\end{aligned}$$

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A real die is **more unpredictable** (2.58 bit) than a fake (2.16 bit)

# Entropy

Unpredictability of a **dataset**

- 100 examples, 42 positive
- 100 examples, 3 positive

# Entropy

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$$-\frac{58}{100} \log_2 \frac{58}{100} - \frac{42}{100} \log_2 \frac{42}{100} = 0.981$$

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# Entropy

Unpredictability of a **dataset**

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- 100 examples, 3 positive

$$-\frac{97}{100} \log_2 \frac{97}{100} - \frac{3}{100} \log_2 \frac{3}{100} = 0.194$$

# Entropy

Unpredictability of a **dataset** (think of a subset at a node)

- 100 examples, 42 positive

$$-\frac{58}{100} \log_2 \frac{58}{100} - \frac{42}{100} \log_2 \frac{42}{100} = 0.981$$

- 100 examples, 3 positive

$$-\frac{97}{100} \log_2 \frac{97}{100} - \frac{3}{100} \log_2 \frac{3}{100} = 0.194$$

## Back to the decision trees

### Smart idea:

Ask about the attribute which maximizes the expected reduction of the entropy.



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Ask about the attribute which maximizes the expected reduction of the entropy.

Information gain

Ask about attribute  $A$  for a data set  $S$  that has Entropy  $\text{Ent}(S)$ ,

$$\text{Gain} = \underbrace{\text{Ent}(S)}_{\text{before}} -$$

Back to the decision trees

Smart idea:

Ask about the attribute which maximizes the expected reduction of the entropy.

Information gain

Ask about attribute  $A$  for a data set  $S$  that has Entropy  $\text{Ent}(S)$ , and get subsets  $S_v$  according to the value of  $A$

$$\text{Gain} = \underbrace{\text{Ent}(S)}_{\text{before}} - \underbrace{\sum_{v \in \text{Values}(A)} \frac{|S_v|}{|S|}}_{\text{weighted sum}} \underbrace{\text{Ent}(S_v)}_{\text{after}}$$

What is the entropy of this binary dataset (attributes= $\{A, B, C, D\}$ ,  $n = 25$ )?

A	B	C	D	
○	●	●	○	+
●	●	○	○	+
○	○	○	○	
○	○	●	●	+
○	●	○	○	+
●	○	●	○	
○	●	●	○	+
○	○	○	○	
●	○	○	○	
○	●	●	○	+
○	○	○	●	+
○	○	●	○	
●	●	●	○	+
○	●	○	●	
○	○	○	○	
○	○	●	○	
○	●	●	●	
○	●	○	○	+
○	○	●	○	
●	○	○	○	
○	●	○	○	+
○	○	●	●	+
●	●	○	○	+
○	○	○	○	
○	○	●	○	

What is the entropy of this binary dataset (attributes= $\{A, B, C, D\}$ ,  $n = 25$ )?

$$\text{Ent} = -\frac{12}{25} \log_2 \frac{12}{25} - \frac{13}{25} \log_2 \frac{13}{25} \approx \mathbf{0.9988}$$

A	B	C	D	
○	●	●	○	+
●	●	○	○	+
○	○	○	○	
○	○	●	●	+
○	●	○	○	+
●	○	●	○	
○	●	●	○	+
○	○	○	○	
●	○	○	○	
○	●	●	○	+
○	○	○	●	+
○	○	●	○	
●	●	●	○	+
○	●	○	●	
○	○	○	○	
○	○	●	○	
○	●	●	●	
○	●	○	○	+
○	○	●	○	
●	○	○	○	
○	○	○	○	
○	●	○	○	+
○	○	●	●	+
●	●	○	○	+
○	○	○	○	
○	○	●	○	

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$$A = \bullet: \frac{3}{6} \text{ positive} \rightarrow 1.0$$

$$A = \circ: \frac{9}{19} \text{ positive} \rightarrow 0.9980$$

$$\text{Expected: } \frac{6}{25} \cdot 1.0 + \frac{19}{25} \cdot 0.9980 \approx \mathbf{0.9985}$$

A	B	C	D	
○	●	●	○	+
●	●	○	○	+
○	○	○	○	
○	○	●	●	+
○	●	○	○	+
●	○	●	○	
○	●	●	○	+
○	○	○	○	
●	○	○	○	
○	●	●	○	+
○	○	○	●	+
○	○	●	○	
●	●	●	○	+
○	●	○	●	
○	○	○	○	
○	○	●	○	
○	●	●	●	
○	●	○	○	+
○	○	●	○	
●	○	○	○	
○	●	○	○	+
○	○	●	●	+
●	●	○	○	+
○	○	○	○	
○	○	●	○	

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Expected:  $\frac{6}{25} \cdot 1.0 + \frac{19}{25} \cdot 0.9980 \approx \mathbf{0.9985}$

$$B = \bullet: \frac{9}{11} \text{ positive} \rightarrow 0.684$$
$$B = \circ: \frac{3}{14} \text{ positive} \rightarrow 0.750$$

Expected: **0.721**

A	B	C	D	
○	●	●	○	+
●	●	○	○	+
○	○	○	○	
○	○	●	●	+
○	●	○	○	+
●	○	●	○	
○	●	●	○	+
○	○	○	○	
●	○	○	○	
○	●	●	○	+
○	○	○	●	+
○	○	●	○	
●	●	●	○	+
○	●	○	●	
○	○	○	○	
○	○	●	○	
○	●	●	●	
○	●	○	○	+
○	○	●	○	
●	○	○	○	
○	●	○	○	+
○	○	●	●	+
●	●	○	○	+
○	○	○	○	
○	○	●	○	

$$\text{Ent} = -\frac{12}{25} \log_2 \frac{12}{25} - \frac{13}{25} \log_2 \frac{13}{25} \approx \mathbf{0.9988}$$

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$$C = \bullet: \frac{6}{12} \text{ positive} \rightarrow 1.0$$
$$C = \circ: \frac{6}{13} \text{ positive} \rightarrow 0.9957$$

Expected: **0.9977**

A	B	C	D	
○	●	●	○	+
●	●	○	○	+
○	○	○	○	
○	○	●	●	+
○	●	○	○	+
●	○	●	○	
○	●	●	○	+
○	○	○	○	
●	○	○	○	
○	●	●	○	+
○	○	○	●	+
○	○	●	○	
●	●	●	○	+
○	●	○	●	
○	○	○	○	
○	○	●	○	
○	●	●	●	
○	●	○	○	+
○	○	●	○	
●	○	○	○	
○	●	○	○	+
○	○	●	●	+
●	●	○	○	+
○	○	○	○	
○	○	●	○	

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$$B = \bullet: \frac{9}{11} \text{ positive} \rightarrow 0.684$$

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$$C = \circ: \frac{6}{13} \text{ positive} \rightarrow 0.9957$$

Expected: **0.9977**

$$D = \bullet: \frac{3}{5} \text{ positive} \rightarrow 0.9710$$

$$D = \circ: \frac{9}{20} \text{ positive} \rightarrow 0.9928$$

Expected: **0.9884**

A	B	C	D	
○	●	●	○	+
●	●	○	○	+
○	○	○	○	
○	○	●	●	+
○	●	○	○	+
●	○	●	○	
○	●	●	○	+
○	○	○	○	
●	○	○	○	
○	●	●	○	+
○	○	○	●	+
○	○	●	○	
●	●	●	○	+
○	●	○	●	
○	○	○	○	
○	○	●	○	
○	●	●	●	
○	●	○	○	+
○	○	●	○	
●	○	○	○	
○	●	○	○	+
○	○	●	●	+
●	●	○	○	+
○	○	○	○	
○	○	●	○	



$$\text{Gain}(A) = 0.9988 - 0.9985 = \mathbf{0.0003}$$

$$\text{Gain}(B) = 0.9988 - 0.7210 = \mathbf{0.2778}$$

$$\text{Gain}(C) = 0.9988 - 0.9977 = \mathbf{0.0011}$$

$$\text{Gain}(D) = 0.9988 - 0.9884 = \mathbf{0.0104}$$

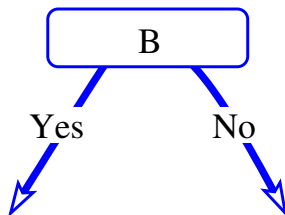
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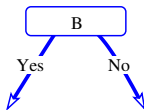
$$\text{Gain}(B) = 0.9988 - 0.7210 = \mathbf{0.2778}$$

$$\text{Gain}(C) = 0.9988 - 0.9977 = \mathbf{0.0011}$$

$$\text{Gain}(D) = 0.9988 - 0.9884 = \mathbf{0.0104}$$

Attribute *B* gives most information gain



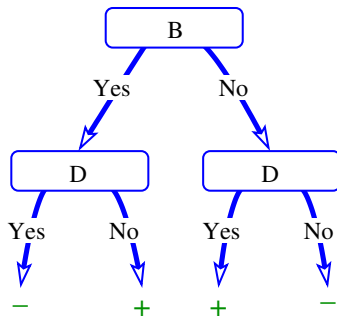


Examples where  
 $B = \bullet$

A	B	C	D	
○	●	●	○	+
●	●	○	○	+
○	●	○	○	+
○	●	●	○	+
○	●	●	○	+
●	●	●	○	+
○	●	○	●	
○	●	●	●	
○	●	○	○	+
○	●	○	○	+
●	●	○	○	+

Examples where  
 $B = \circ$

A	B	C	D	
○	○	○	○	
○	○	○	●	+
●	○	●	○	
○	○	○	○	
●	○	○	○	
○	○	○	●	+
○	○	●	○	
○	○	○	○	
○	○	●		
○	○	○	○	
●	○	○	○	
○	○	●	○	
○	○	●	●	+
○	○	○	○	
○	○	●	○	



Greedy approach to choose a question:

Choose the attribute which tells us most about the answer

In sum, we need to find good questions to ask.  
(more than one attribute could be involved in one question)

Gini impurity: Another definition of predictability (impurity).

$$\sum_i p_i(1 - p_i) = 1 - \sum_i p_i^2$$

( $p_i$  : probability for event  $i$ )

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( $p_i$  : probability for event  $i$ )

The expected error rate at a node,  $N$ , if the category label is randomly selected from the class distribution present at  $N$ .

Gini impurity: Another definition of predictability (impurity).

$$\sum_i p_i(1 - p_i) = 1 - \sum_i p_i^2$$

( $p_i$  : probability for event  $i$ )

The expected error rate at a node,  $N$ , if the category label is randomly selected from the class distribution present at  $N$ .

Similar to the entropy but more strongly peaked at equal probabilities.



## 1 Decision Trees

- The representation
- Training

## 2 Unpredictability

- Entropy
- Information gain
- Gini impurity

## 3 Overfitting

- Overfitting
- Occam's principle
- Training and validation set approach
- Extensions

## Overfitting

When the learned models are overly specialized for the training samples.

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Good results on training data, but generalizes poorly.

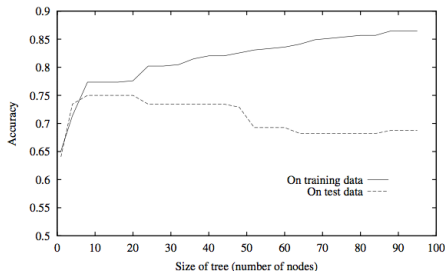
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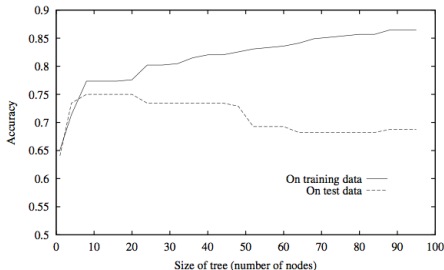
When does this occur?

- Non-representative sample
- Noisy examples
- Too complex model



(T. Mitchell, Machine Learning)

What can be done about it?



(T. Mitchell, Machine Learning)

What can be done about it?

Choose a simpler model and accept some errors for the training examples

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William from Ockham, Theologian and Philosopher  
(1288–1348)

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**Occam's principle** (Occam's razor)

William from Ockham, Theologian and Philosopher  
(1288–1348)

"Entities should not be multiplied beyond necessity"

The **simplest explanation** compatible with data  
tends to be the right one

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- *Training set*  $T$ : to form the learned model
- *Validation set*  $V$ : to evaluate the accuracy of this model

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( $V$  need be large enough to provide statistically meaningful instances)

# Reduced-Error Pruning

Split data into *training* and *validation* set

Do until further pruning is harmful:

- Evaluate impact on *validation* set of pruning each possible node (plus those below it)
- Greedily remove the one that most improves *validation* set accuracy

Produces smallest version of most accurate subtree

## Possible ways of improving/extending the decision trees

- Avoid overfitting
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## A collection of trees (Ensemble learning: in Lecture 10)

- Bootstrap aggregating (bagging)
- Decision Forests