

Lecture 2: Decision Trees

DD2421

Atsuto Maki

Autumn, 2017

- 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
- 4 Applications

- 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
- 4 Applications

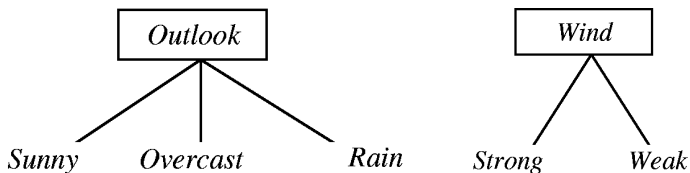
Basic Idea: Test the attributes (features) **sequentially**
= Ask questions about the target/status **sequentially**

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.

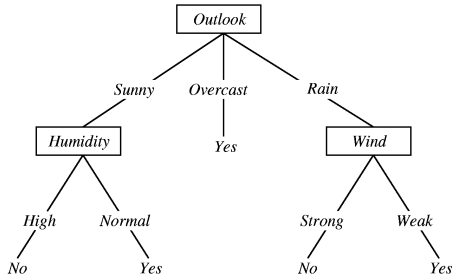
Basic Idea: Test the attributes (features) **sequentially**
= Ask questions about the target/status **sequentially**

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



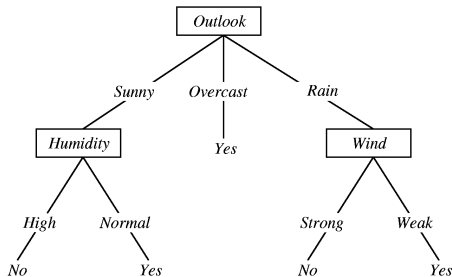
Useful also (but not limited to) when nominal data are involved, e.g. in medical diagnosis, credit risk analysis etc.

The whole analysis strategy can be seen as a tree.



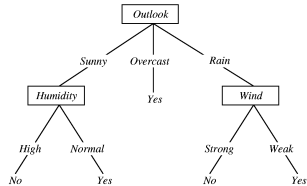
(T. Mitchell, Machine Learning)

The whole analysis strategy can be seen as a tree.

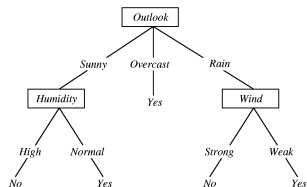


(T. Mitchell, Machine Learning)

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

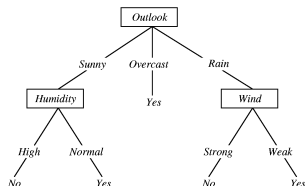


What does the tree encode?



What does the tree encode?

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



What does the tree encode?

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

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?

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

How to grow/construct the tree automatically?

- 1 Choose the **best question** (according to the **information gain**), and split the input data into subsets

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

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)

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

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)

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

4 Applications

Entropy

How to measure **information gain**?

Entropy

How to measure **information gain**?

The Shannon information content of an outcome is:

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

(p_i : probability for event i)

Entropy

How to measure **information gain**?

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

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



Entropy

Example: tossing a coin

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



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

Entropy

Example: tossing a coin

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



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

Entropy

Example: tossing a coin

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



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

Entropy

Example: tossing a coin

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



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

Entropy

Example: tossing a coin

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



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

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

Entropy

Example: rolling a die

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



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

Entropy

Example: rolling a die

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



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

Entropy

Example: rolling a die

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



$$\begin{aligned} \text{Entropy} &= \sum_i -p_i \log_2 p_i = \\ &= 6 \times \left(-\frac{1}{6} \log_2 \frac{1}{6}\right) = \\ &= -\log_2 \frac{1}{6} = \log_2 6 \approx 2.58 \end{aligned}$$

Entropy

Example: rolling a die

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



$$\begin{aligned} \text{Entropy} &= \sum_i -p_i \log_2 p_i = \\ &= 6 \times \left(-\frac{1}{6} \log_2 \frac{1}{6}\right) = \\ &= -\log_2 \frac{1}{6} = \log_2 6 \approx 2.58 \end{aligned}$$

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

Entropy

Example: rolling a **fake die**

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



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

Entropy

Example: rolling a **fake die**

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



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

Entropy

Example: rolling a **fake die**

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



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

Entropy

Example: rolling a **fake die**

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



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

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

Unpredictability of a **dataset**

- 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

Entropy

Unpredictability of a **dataset**

- 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

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

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.

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 $\text{Ent}(S)$,

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

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	
○	●	●	○	+
●	●	○	○	+
○	○	○	○	
○	○	●	●	+
○	●	○	○	+
●	○	●	○	
○	●	●	○	+
○	○	○	○	
●	○	○	○	
○	●	●	○	+
○	○	○	●	+
○	○	●	○	
●	●	●	○	+
○	●	○	●	
○	○	○	○	
○	○	●	○	
○	●	●	●	
○	●	○	○	+
○	○	●	○	
●	○	○	○	
○	●	○	○	+
○	○	●	●	+
●	●	○	○	+
○	○	○	○	
○	○	●	○	

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

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

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

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

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

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

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

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

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	
○	●	●	○	+
●	●	○	○	+
○	○	○	○	
○	○	●	●	+
○	●	○	○	+
●	○	●	○	
○	●	●	○	+
○	○	○	○	
●	○	○	○	
○	●	●	○	+
○	○	○	●	+
○	○	●	○	
●	●	●	○	+
○	●	○	●	
○	○	○	○	
○	○	●	○	
○	●	●	●	
○	●	○	○	+
○	○	●	○	
●	○	○	○	
○	●	○	○	+
○	○	●	●	+
●	●	○	○	+
○	○	○	○	
○	○	●	○	

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

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

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

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

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

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

$$B = \circ: \frac{3}{14} \text{ positive} \rightarrow 0.750$$

$$\text{Expected: } \mathbf{0.721}$$

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

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

$$\text{Expected: } \mathbf{0.9977}$$

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

$$\text{Ent} = -\frac{12}{25} \log_2 \frac{12}{25} - \frac{13}{25} \log_2 \frac{13}{25} \approx \mathbf{0.9988}$$
$$A = \circ: \frac{9}{19} \text{ positive} \rightarrow 0.9980$$

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**

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

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	
○	●	●	○	+
●	●	○	○	+
○	○	○	○	
○	○	●	●	+
○	●	○	○	+
●	○	●	○	
○	●	●	○	+
○	○	○	○	
●	○	○	○	
○	●	●	○	+
○	○	○	●	+
○	○	●	○	
●	●	●	○	+
○	●	○	●	
○	○	○	○	
○	○	●	○	
○	●	●	●	
○	●	○	○	+
○	○	●	○	
●	○	○	○	
○	●	○	○	+
○	○	●	○	
●	○	○	○	
○	●	○	○	+
○	○	●	○	+
●	●	○	○	+
○	○	○	○	
○	○	●	○	

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

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

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

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

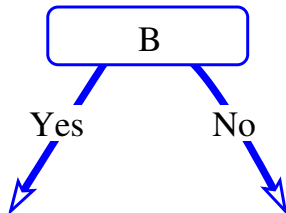
$$\text{Gain}(A) = 0.9988 - 0.9985 = \mathbf{0.0003}$$

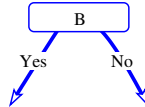
$$\text{Gain}(B) = 0.9988 - 0.7210 = \mathbf{0.2778}$$

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

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

Attribute *B* gives most information gain



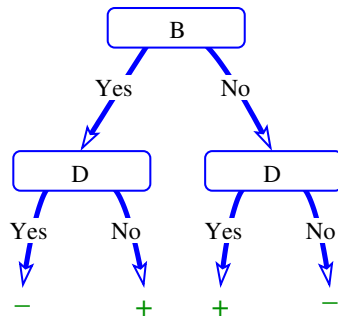


Examples where
 $B = \bullet$

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)

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 .

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

4 Applications

Overfitting

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

Overfitting

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

Good results on training data, but generalizes poorly.

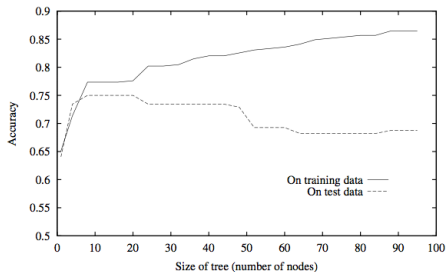
Overfitting

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

Good results on training data, but generalizes poorly.

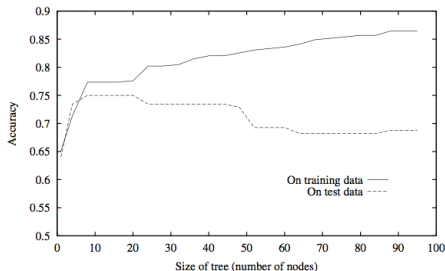
When does this occur?

- 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

Which hypothesis should be preferred when several are compatible with the data?

Which hypothesis should be preferred when several are compatible with the data?

Occam's principle (Occam's razor)

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

"Entities should not be multiplied beyond necessity"

Which hypothesis should be preferred when several are compatible with the data?

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

Separate the available data into two sets of examples

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

Separate the available data into two sets of examples

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

The motivations:

- The training may be misled by random errors, but the validation set is unlikely to exhibit the same random fluctuations
- The validation set to provide a safety check against overfitting the spurious characteristics of the training set

Separate the available data into two sets of examples

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

The motivations:

- The training may be misled by random errors, but the validation set is unlikely to exhibit the same random fluctuations
- The validation set to provide a safety check against overfitting the spurious characteristics of the training set

(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
 - Stop growing when data split not statistically significant
 - Grow full tree, then post-prune (e.g. Reduced error pruning)

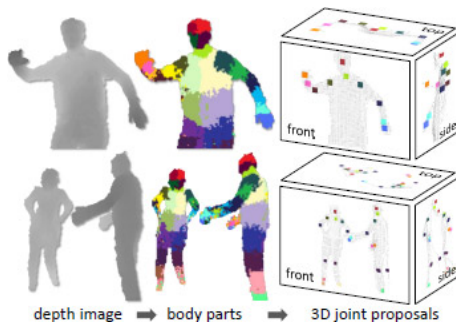
Possible ways of improving/extending the decision trees

- Avoid overfitting
 - Stop growing when data split not statistically significant
 - Grow full tree, then post-prune (e.g. Reduced error pruning)

A collection of trees (Ensemble learning: in Lecture 10)

- Bootstrap aggregating (bagging)
- Decision Forests

Example: Human pose estimation



(Picture courtesy of J. Shotton et al)