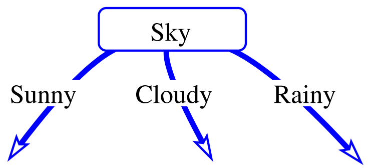
Lecture 2: Decision Trees

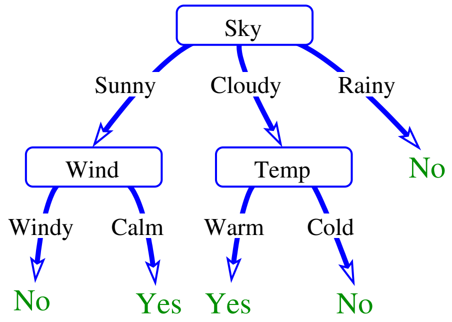
Basic Idea: Test the attributes (features) sequentially
= Ask questions about the target/status sequentially
(the next question depends on the answer to the current)

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

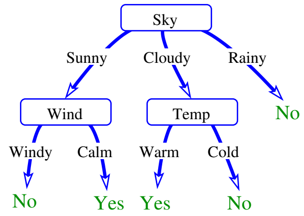
Example: building a concept of whether someone will play tennis.



The whole analysis strategy can be seen as a tree.



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?

$$(\text{Sunny} \land \text{Calm}) \lor (\text{Cloudy} \land \text{Warm})$$

Logical expressions of the conjunction of decisions along the path.

Arbitrary boolean functions can be represented!

Training a decision tree given a set of labeled training data.

How to grow/construct the tree automatically?

1. Choose a test, and split the input data into subsets
2. Terminate: call branches with a unique class labels leaves (no need for further quesitons)
3. Grow: recursively extend other branches (with subsets bearing mixtures of labels)

Greedy approach to choose a test:

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)

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

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

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

$$= -0.5 \log_2 0.5 - 0.5 \log_2 0.5 \quad = -0.5 \underbrace{\log_2 0.5}_{-1} - 0.5 \underbrace{\log_2 0.5}_{-1} =$$

$$= 1$$

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

Entropy

Example: rolling a die
$p_1 = \frac{1}{6}; \quad p_2 = \frac{1}{6}; \ldots \quad p_6 = \frac{1}{6}$

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

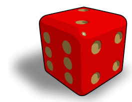
$$= 6 \times (-\frac{1}{6} \log_2 \frac{1}{6}) =$$

$$= -\log_2 \frac{1}{6} = \log_2 6 \approx 2.58$$

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

Entropy

Example: rolling a fake die
$p_1 = 0.1; \ldots \quad p_5 = 0.1; \quad p_6 = 0.5$



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

$$= -5 \cdot 0.1 \log_2 0.1 - 0.5 \log_2 0.5 =$$

$$\approx 2.16$$

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

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.

Information gain

Assume that we ask about attribute A for a dataset S

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

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.

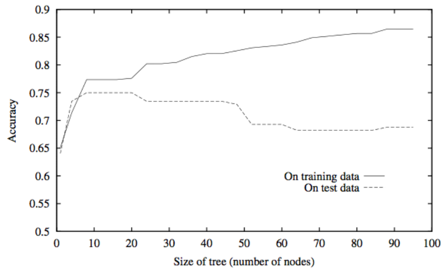
Similar to the entropy but more strongly peaked at equal probabilities.

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



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?

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

Why prefer short hypotheses?

Philosophical argument:
It is more likely that the reality from which the examples come have a simple generating mechanism.

Pragmatic argument:
Simple hypotheses tend to generalize better.

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)

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

- Bootstrap aggregating (bagging)
- Decision Forests