Machine Learning
[RN2] Sec 18.1-18.4
[RN3] Sec 18.1-18.4

CS 486/686

University of Waterloo

Lecture 13: June 12, 2017

Outline

- Inductive learning
- Decision trees

What is Machine Learning?

- Definition:
  - A computer program is said to **learn** from experience E with respect to some class of tasks T and performance measure P, if its performance at tasks in T, as measured by P, improves with experience E.

[T Mitchell, 1997]

Examples

- Backgammon (reinforcement learning):
  - T: playing backgammon
  - P: percent of games won against an opponent
  - E: playing practice games against itself
- Handwriting recognition (supervised learning):
  - T: recognize handwritten words within images
  - P: percent of words correctly recognized
  - E: database of handwritten words with given classifications
- Customer profiling (unsupervised learning):
  - T: cluster customers based on transaction patterns
  - P: homogeneity of clusters
  - E: database of customer transactions

Representation

- Representation of the learned information is important
  - Determines how the learning algorithm will work

- Common representations:
  - Linear weighted polynomials
  - Propositional logic
  - First order logic
  - Bayes nets
  - …

Inductive learning (aka concept learning)

- Induction:
  - Given a training set of examples of the form (x,f(x))
    - x is the input, f(x) is the output
  - Return a function h that approximates f
    - h is called the hypothesis

Classification

- Training set:

Sky	Humidity	Wind	Water	Forecast	EnjoySport
Sunny	Normal	Strong	Warm	Same	Yes
Sunny	High	Strong	Warm	Same	Yes
Sunny	High	Strong	Warm	Change	No
Sunny	High	Strong	Cool	Change	Yes

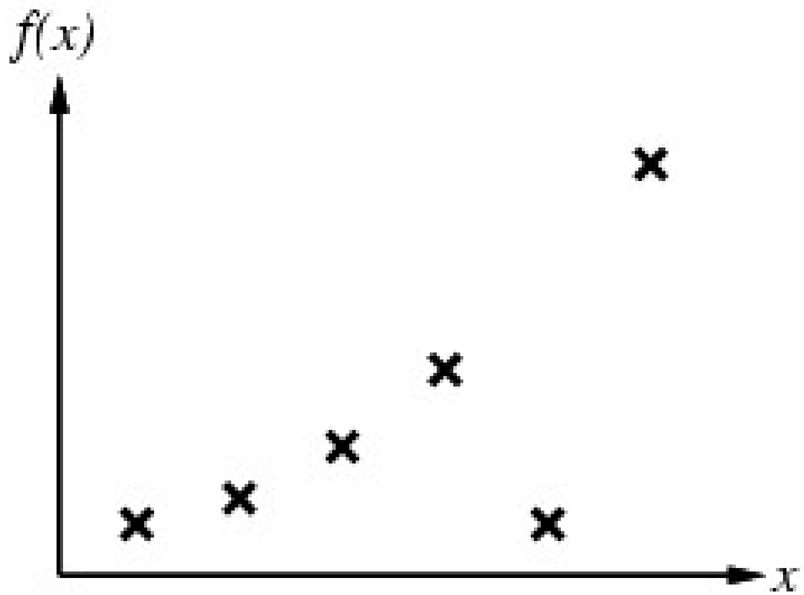
x

f(x)

- Possible hypotheses:
  - h_1: S=sunny → ES=yes
  - h_2: Wa=cool or F=same → enjoySport

Regression

- Find function **h** that fits f at instances x



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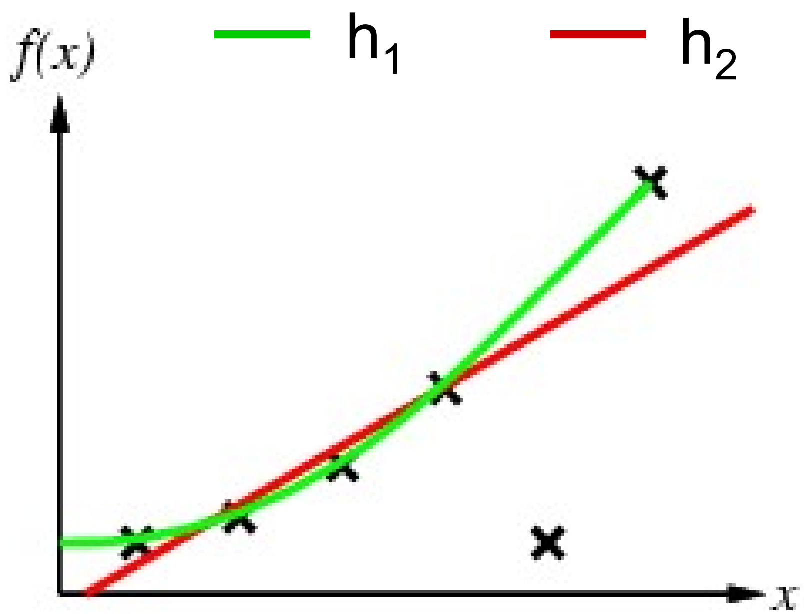


Hypothesis Space

- Hypothesis space H
  - Set of all hypotheses h that the learner may consider
  - Learning is a search through hypothesis space
- Objective:
  - Find hypothesis that agrees with training examples
  - But what about unseen examples?

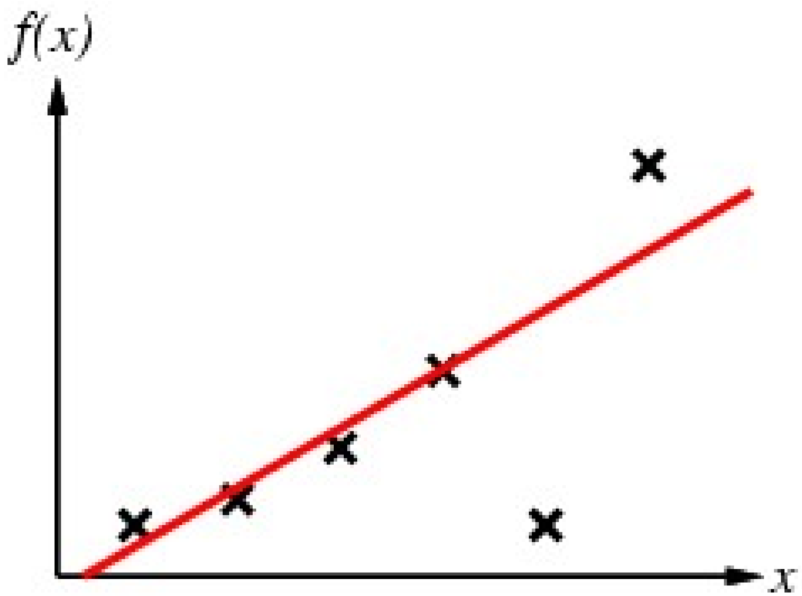
Generalization

- A good hypothesis will generalize well (i.e. predict unseen examples correctly)

- Usually…
  - Any hypothesis h found to approximate the target function f well over a sufficiently large set of training examples will also approximate the target function well over any unobserved examples

Inductive learning

- Construct/adjust h to agree with f on training set
- (h is consistent if it agrees with f on all examples)
- E.g., curve fitting:



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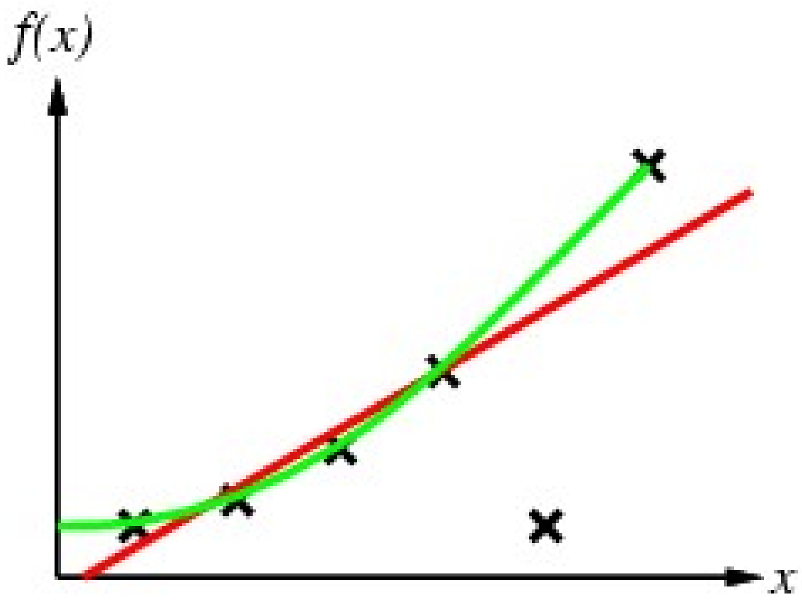

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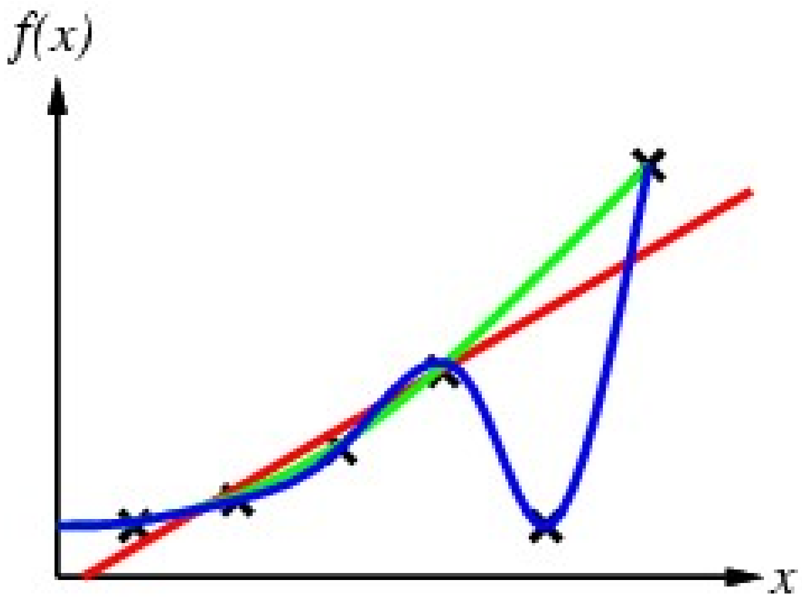

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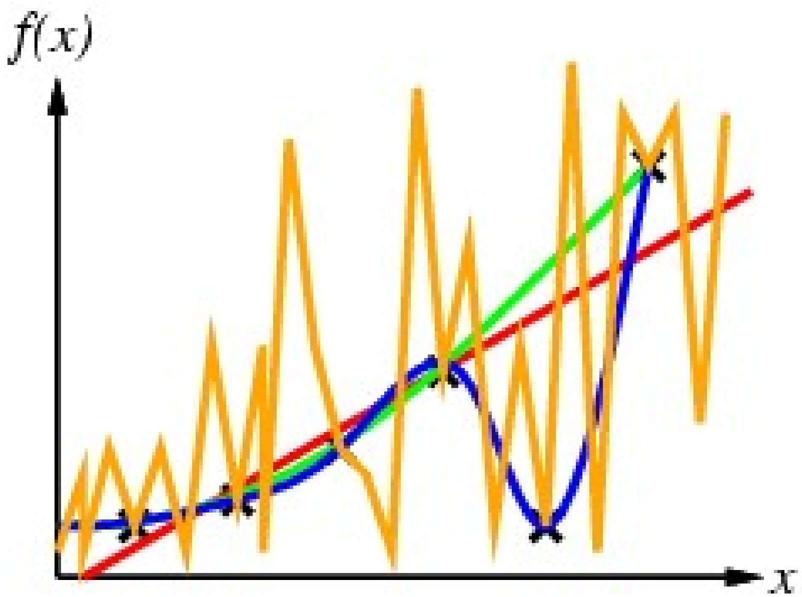

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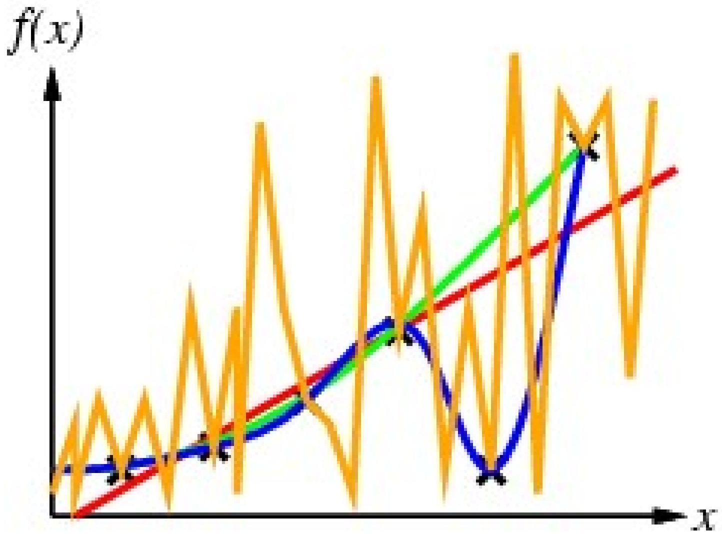


- Ockham's razor: prefer the simplest hypothesis consistent with data

Inductive learning

- Finding a consistent hypothesis depends on the hypothesis space
  - For example, it is not possible to learn exactly $f(x)=ax+b+x\sin(x)$ when H=space of polynomials of finite degree

- A learning problem is realizable if the hypothesis space contains the true function, otherwise it is unrealizable
  - Difficult to determine whether a learning problem is realizable since the true function is not known

Inductive learning

- It is possible to use a very large hypothesis space
  - For example, H=class of all Turing machines

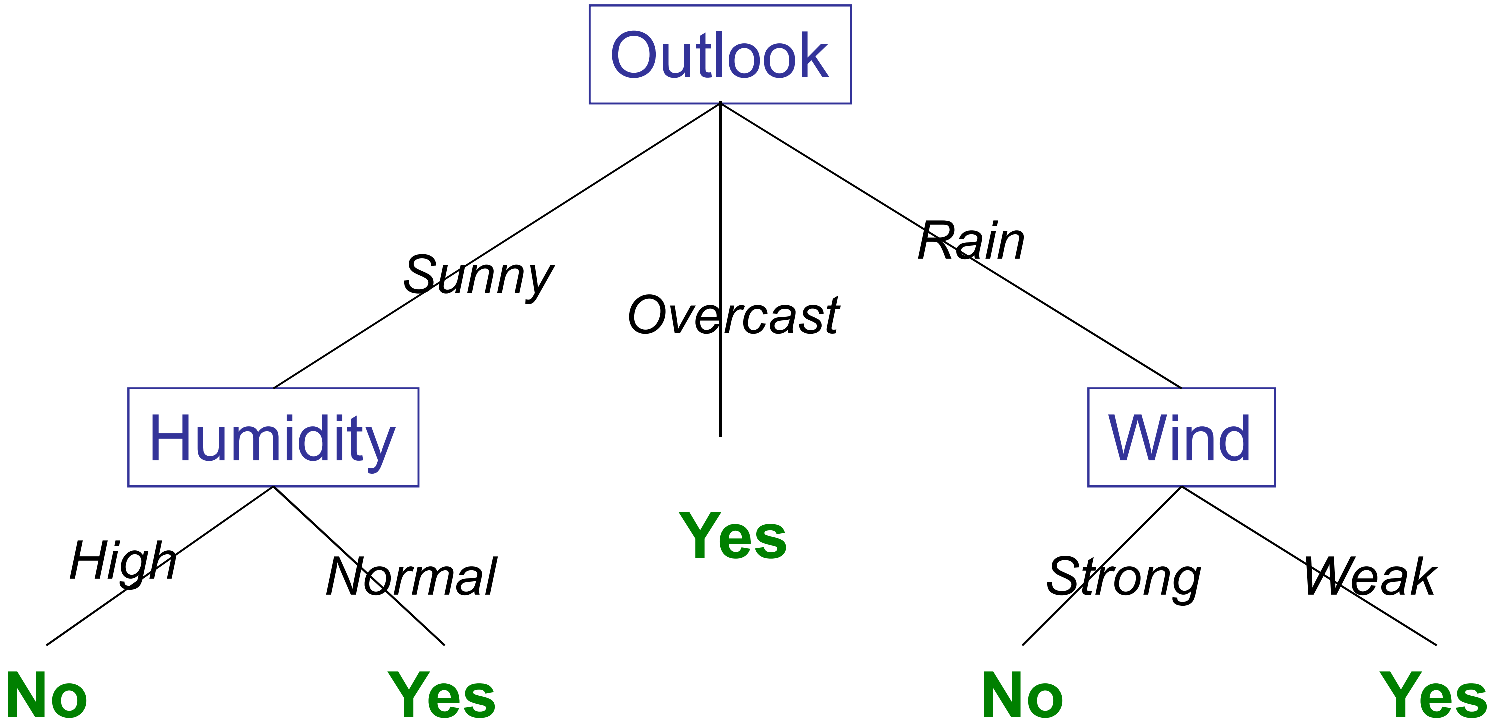
- But there is a tradeoff between expressiveness of a hypothesis class and complexity of finding simple, consistent hypothesis within the space
  - Fitting straight lines is easy, fitting high degree polynomials is hard, fitting Turing machines is very hard!

Decision trees

- Decision tree classification
  - Nodes: labeled with attributes
  - Edges: labeled with attribute values
  - Leaves: labeled with classes

- Classify an instance by starting at the root, testing the attribute specified by the root, then moving down the branch corresponding to the value of the attribute
  - Continue until you reach a leaf
  - Return the class

Decision tree (playing tennis)

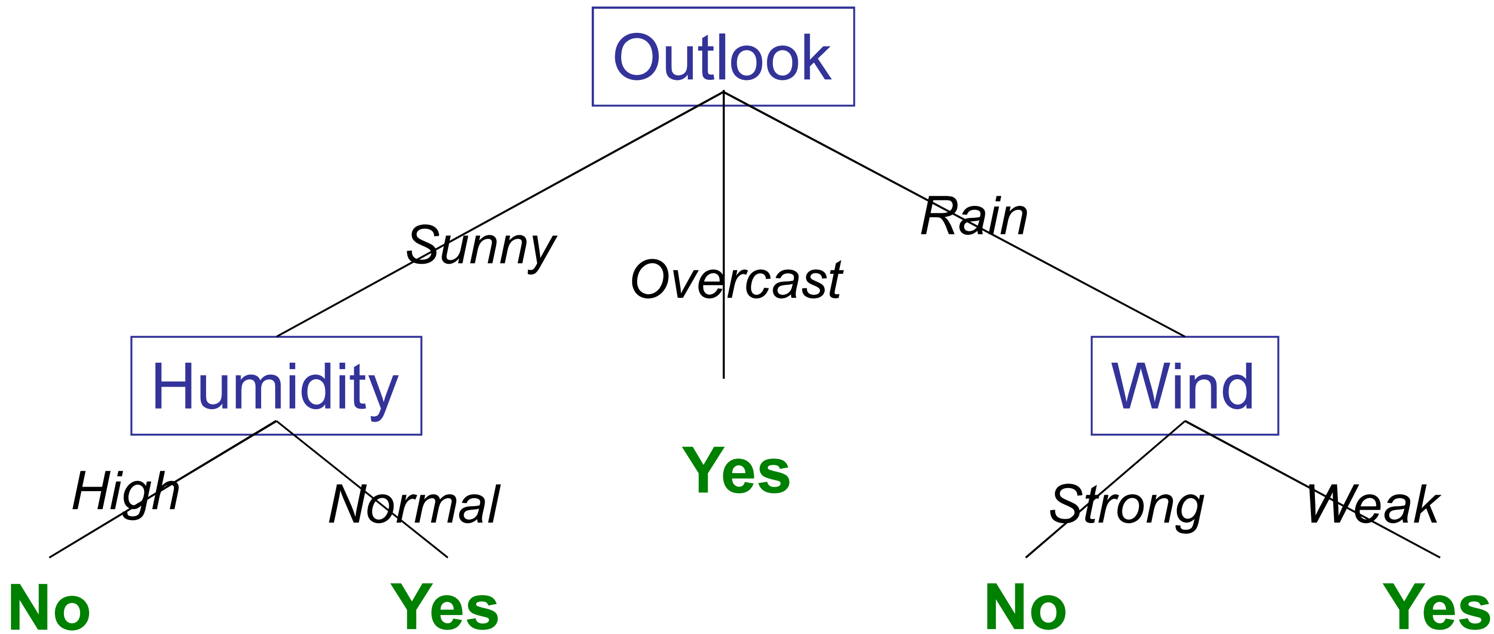


An instance
<Outlook=Sunny, Temp=Hot, Humidity=High, Wind=Strong>

Classification: No

Decision tree representation

- Decision trees can represent disjunctions of conjunctions of constraints on attribute values



(Outlook=Sunny $\wedge$ Humidity=Normal)
$\vee$ (Outlook=Overcast)
$\vee$ (Outlook=Rain $\wedge$ Wind=Weak)

Decision tree representation

- Decision trees are fully expressive within the class of propositional languages
  - Any Boolean function can be written as a decision tree
    - Trivially by allowing each row in a truth table correspond to a path in the tree
    - Can often use small trees
    - Some functions require exponentially large trees (majority function, parity function)
  - However, there is no representation that is efficient for all functions

Inducing a decision tree

- Aim: find a small tree consistent with the training examples
- Idea: (recursively) choose "most significant" attribute as root of (sub)tree

Decision Tree Learning

```
function DTL(examples, attributes, default) returns a decision tree
    if examples is empty then return default
    else if all examples have the same classification then return the classification
    else if attributes is empty then return MODE(examples)
    else
        best ← CHOOSE-ATTRIBUTE(attributes, examples)
        tree ← a new decision tree with root test best
        for each value v_i of best do
            examples_i ← {elements of examples with best = v_i}
            subtree ← DTL(examples_i, attributes − best, MODE(examples))
            add a branch to tree with label v_i and subtree subtree
        return tree
```

Choosing attribute tests

- The central choice is deciding which attribute to test at each node

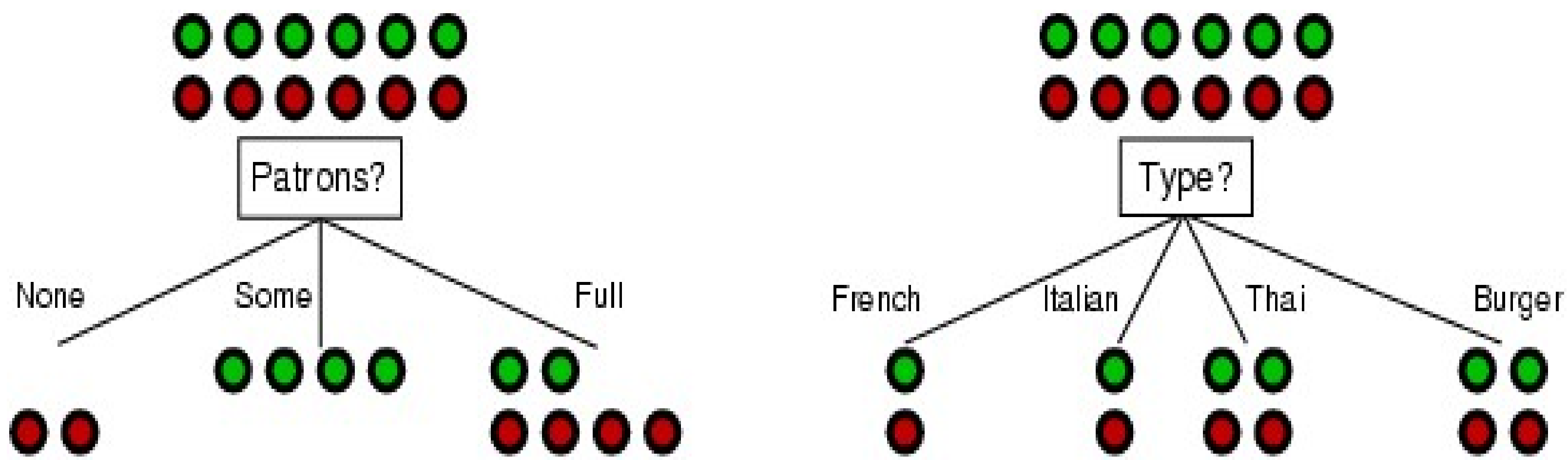
- We want to choose an attribute that is most useful for classifying examples

Example -- Restaurant

Example	Attributes										Target
	Alt	*Bar*	*Fri*	*Hun*	*Pat*	*Price*	*Rain*	*Res*	*Type*	*Est*	*Wait*
X_1	T	F	F	T	Some	$$$	F	T	French	0–10	T
X_2	T	F	F	T	Full	$	F	F	Thai	30–60	F
X_3	F	T	F	F	Some	$	F	F	Burger	0–10	T
X_4	T	F	T	T	Full	$	F	F	Thai	10–30	T
X_5	T	F	T	F	Full	$$$	F	T	French	>60	F
X_6	F	T	F	T	Some	$$	T	T	Italian	0–10	T
X_7	F	T	F	F	None	$	T	F	Burger	0–10	F
X_8	F	F	F	T	Some	$$	T	T	Thai	0–10	T
X_9	F	T	T	F	Full	$	T	F	Burger	>60	F
X_{10}	T	T	T	T	Full	$$$	F	T	Italian	10–30	F
X_{11}	F	F	F	F	None	$	F	F	Thai	0–10	F
X_{12}	T	T	T	T	Full	$	F	F	Burger	30–60	T

Choosing an attribute

- Idea: a good attribute splits the examples into subsets that are (ideally) "all positive" or "all negative"



- *Patrons?* is a better choice

Using information theory

- To implement **`Choose-Attribute`** in the DTL algorithm
- Measure uncertainty (Entropy):

  $I(P(v_1), \dots , P(v_n)) = \Sigma_{i=1} -P(v_i) \log_2 P(v_i)$
- For a training set containing *p* positive examples and *n* negative examples:

$$I\left(\frac{p}{p+n}, \frac{n}{p+n}\right) = -\frac{p}{p+n}\log_2 \frac{p}{p+n} - \frac{n}{p+n}\log_2 \frac{n}{p+n}$$

Information gain

- A chosen attribute A divides the training set E into subsets $E_1, \dots, E_v$ according to their values for A, where A has v distinct values.

$$remainder(A) = \sum_{i=1}^{v} \frac{p_i + n_i}{p+n} I\left(\frac{p_i}{p_i+n_i}, \frac{n_i}{p_i+n_i}\right)$$

- Information Gain (IG) or reduction in uncertainty from the attribute test:

$$IG(A) = I\left(\frac{p}{p+n}, \frac{n}{p+n}\right) - remainder(A)$$

- Choose the attribute with the largest IG

Information gain

For the training set, $p = n = 6$, $I(6/12, 6/12) = 1$ bit

Consider the attributes *Patrons* and *Type* (and others too):

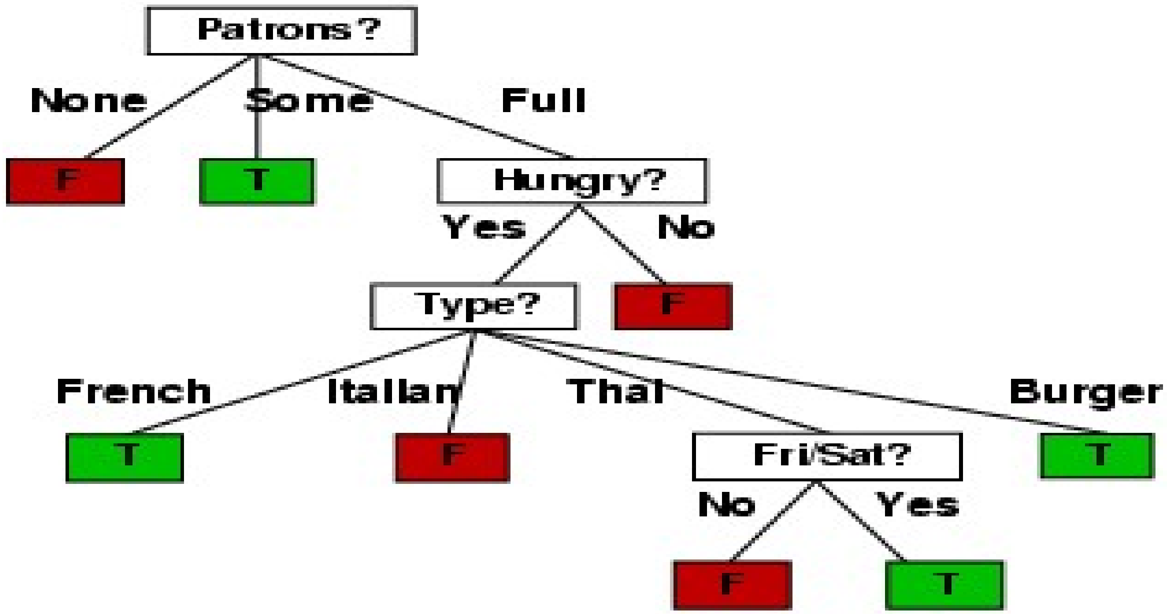
$$IG(Patrons) = 1 - [\frac{2}{12} I(0,1) + \frac{4}{12} I(1,0) + \frac{6}{12} I(\frac{2}{6}, \frac{4}{6})] = .541 \text{ bits}$$

$$IG(Type) = 1 - [\frac{2}{12} I(\frac{1}{2}, \frac{1}{2}) + \frac{2}{12} I(\frac{1}{2}, \frac{1}{2}) + \frac{4}{12} I(\frac{2}{4}, \frac{2}{4}) + \frac{4}{12} I(\frac{2}{4}, \frac{2}{4})] = 0 \text{ bits}$$

Patrons has the highest IG of all attributes and so is chosen by the DTL algorithm as the root

Example

- Decision tree learned from the 12 examples:



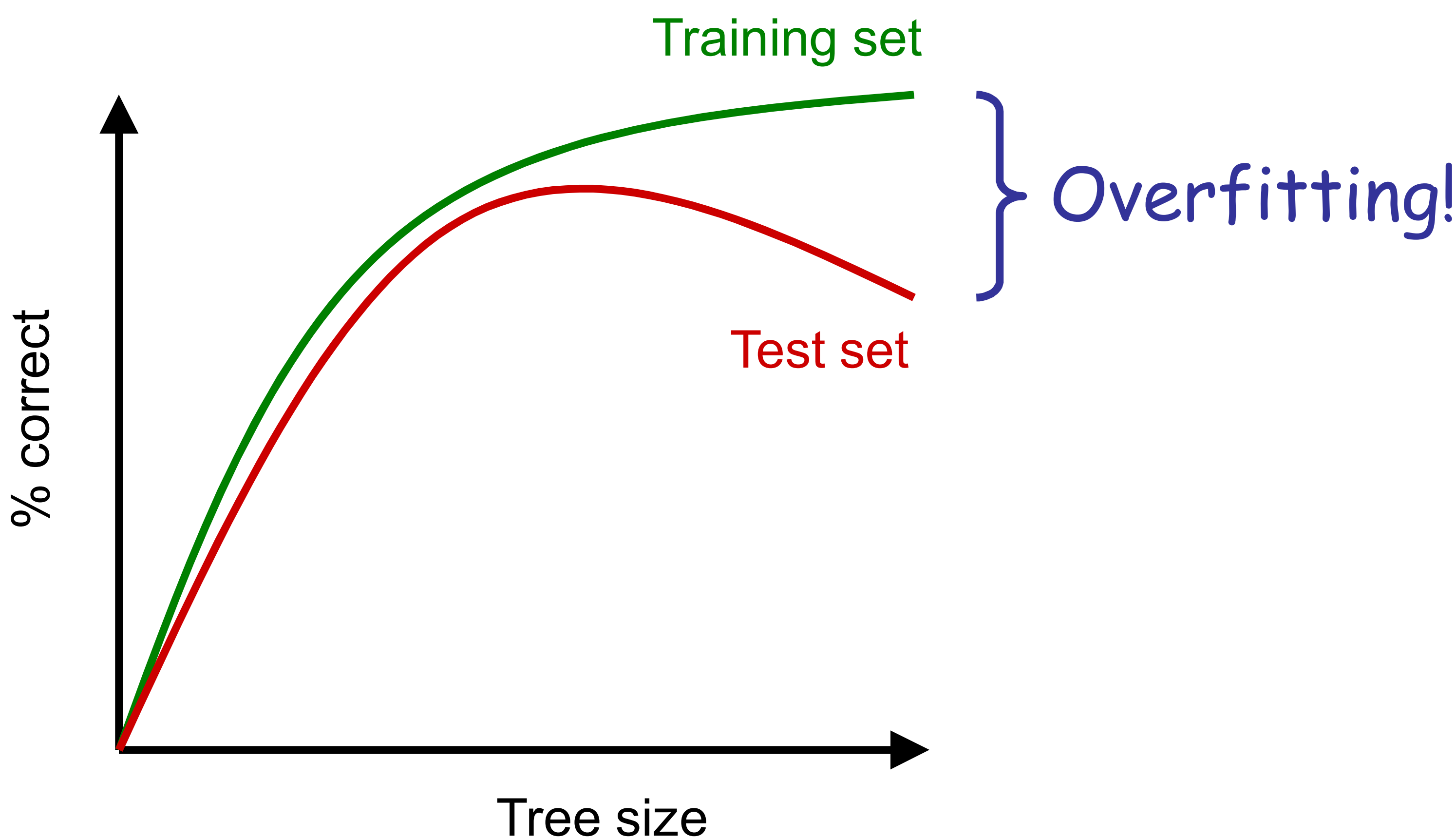
- Substantially simpler than "true" tree---a more complex hypothesis isn't justified by small amount of data

Performance of a learning algorithm

- A learning algorithm is good if it produces a hypothesis that does a good job of predicting classifications of unseen examples

- Verify performance with a **test set**
  1. Collect a large set of examples
  2. Divide into 2 disjoint sets: training set and test set
  3. Learn hypothesis h with training set
  4. Measure percentage of correctly classified examples by h in the test set
  5. Repeat 2-4 for different randomly selected training sets of varying sizes

Learning curves



Overfitting

- Decision-tree grows until all training examples are perfectly classified
- But what if…
  - Data is noisy
  - Training set is too small to give a representative sample of the target function
- May lead to **Overfitting!**
  - Common problem with most learning algo

Overfitting

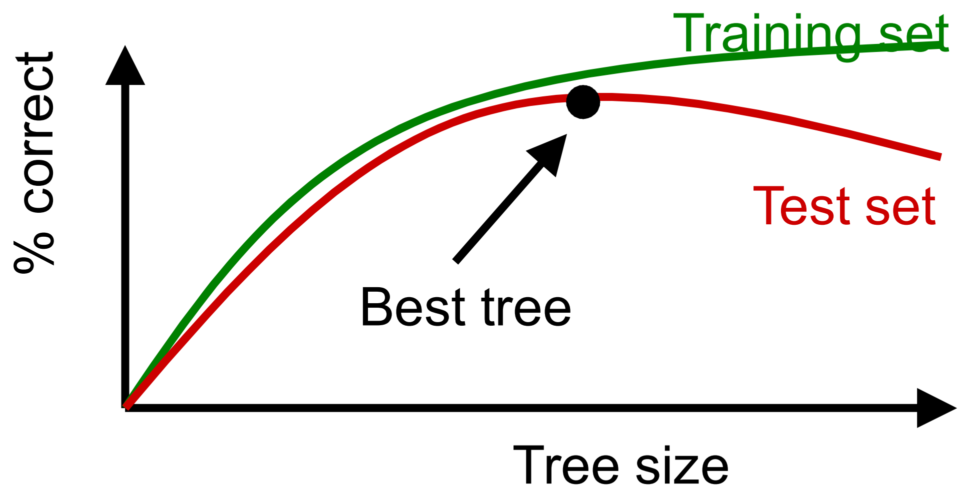
- **Definition**: Given a hypothesis space H, a hypothesis h $\in$ H is said to overfit the training data if there exists some alternative hypothesis h' $\in$ H such that h has smaller error than h' over the training examples but h' has smaller error than h over the entire distribution of instances

- Overfitting has been found to decrease accuracy of decision trees by 10-25%

Avoiding overfitting

Two popular techniques:

1. Prune statistically irrelevant nodes
   - Measure irrelevance with χ^2 test
2. Stop growing tree when test set performance starts decreasing
   - Use cross-validation



Cross-validation

- Split data in two parts, one for training, one for testing the accuracy of a hypothesis

- K-fold cross validation means you run k experiments, each time putting aside 1/k of the data to test on