CMSC 471
Fall 2012

Class #22

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Machine Learning I

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Today's Class

- Go over HW4 (quickly)
- HW5 Clarifications
- Machine learning
  - What is ML?
  - Inductive learning
    - Supervised
    - Unsupervised
  - Decision trees
- Later we'll also cover:
  - Other classification methods (k-nearest neighbor, naïve Bayes, BN learning)
  - Clustering (k-means)

Machine Learning

Chapter 18.1-18.3

Some material adopted from notes
by Chuck Dyer

What is Learning?

- "Learning denotes changes in a system that ... enable a system to do the same task more efficiently the next time." –Herbert Simon
- "Learning is constructing or modifying representations of what is being experienced." –Ryszard Michalski
- "Learning is making useful changes in our minds." –Marvin Minsky

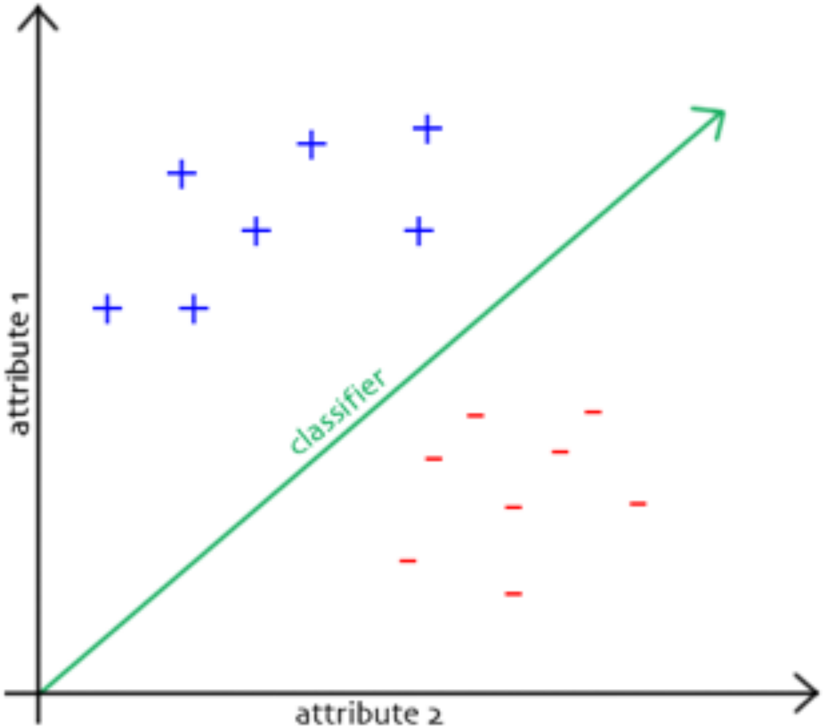
Why Learn?

- Understand and improve efficiency of human learning
  - Use to improve methods for teaching and tutoring people (e.g., better computer-aided instruction)
- Discover new things or structure that were previously unknown to humans
  - Examples: data mining, scientific discovery
- Fill in skeletal or incomplete specifications about a domain
  - Large, complex AI systems cannot be completely derived by hand and require dynamic updating to incorporate new information.
  - Learning new characteristics expands the domain or expertise and lessens the “brittleness” of the system
- Build software agents that can adapt to their users or to other software agents

Major Paradigms of Machine Learning

- **Rote learning** – One-to-one mapping from inputs to stored representation. "Learning by memorization." Association-based storage and retrieval.
- **Induction** – Use specific examples to reach general conclusions
- **Clustering** – Unsupervised identification of natural groups in data
- **Analogy** – Determine correspondence between two different representations
- **Discovery** – Unsupervised, specific goal not given
- **Genetic algorithms** – "Evolutionary" search techniques, based on an analogy to "survival of the fittest"
- **Reinforcement** – Feedback (positive or negative reward) given at the end of a sequence of steps

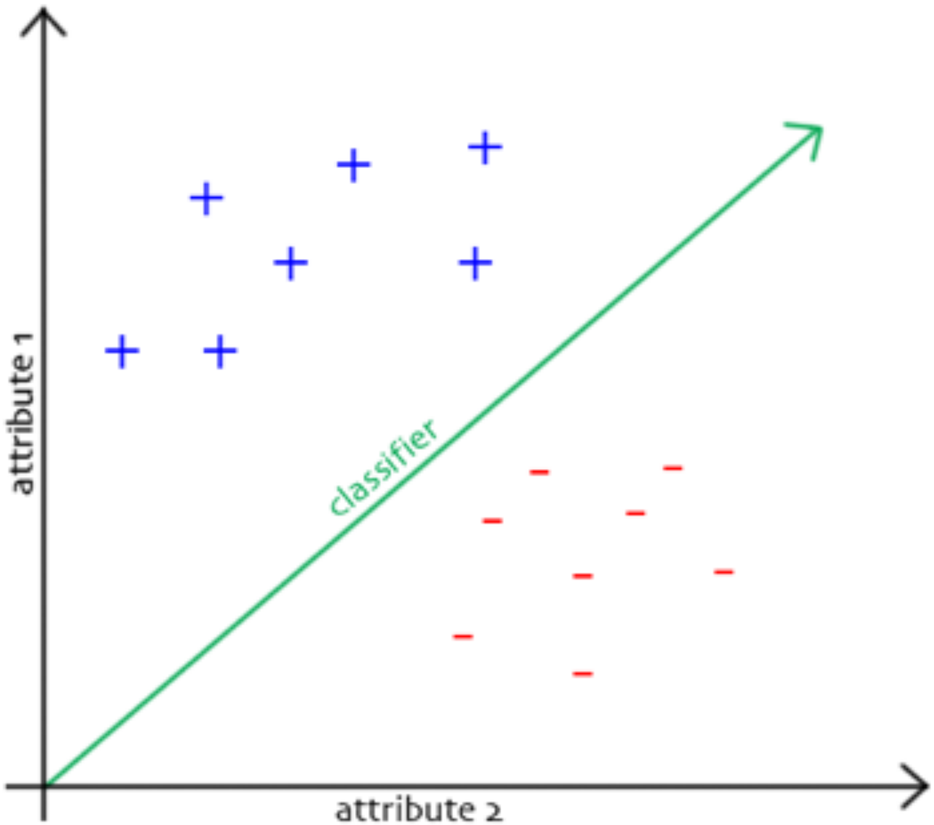
The Classification Problem



- Extrapolate from a given set of examples to make accurate predictions about future examples
- Supervised versus unsupervised learning
  - Learn an unknown function f(X) = Y, where X is an input example and Y is the desired output.
  - **Supervised learning** implies we are given a **training set** of (X, Y) pairs by a "teacher"
  - **Unsupervised learning** means we are only given the Xs and some (ultimate) feedback function on our performance.

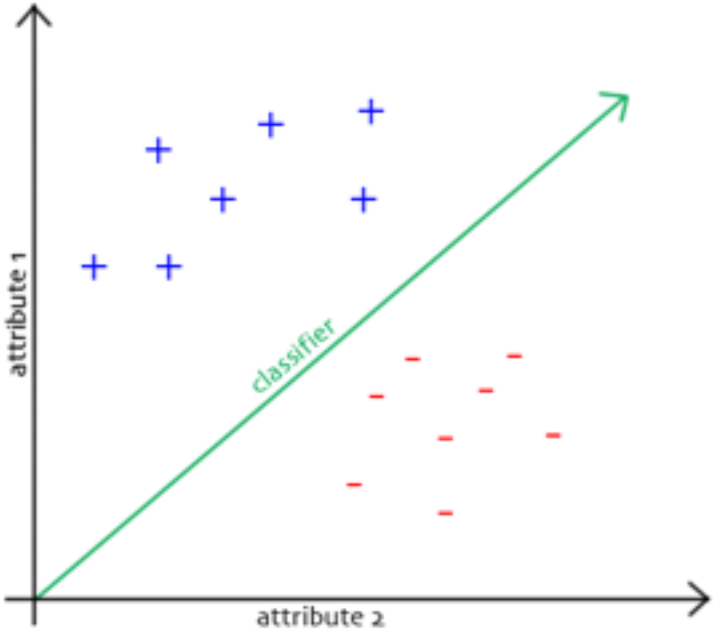
- Concept learning or classification (aka "induction")
  - –Given a set of examples of some concept/class/category, determine if a given example is an instance of the concept or not
  - –If it is an instance, we call it a positive example
  - –If it is not, it is called a negative example
  - –Or we can make a probabilistic prediction (e.g., using a Bayes net)

Supervised Concept Learning



- Given a training set of positive and negative examples of a concept
- Construct a description that will accurately classify whether future examples are positive or negative
- That is, learn some good estimate of function f given a training set $\{(x_1, y_1), (x_2, y_2), ..., (x_n, y_n)\}$, where each y_i is either + (positive) or - (negative), or a probability distribution over +/-

Inductive Learning Framework



- Raw input data from sensors are typically preprocessed to obtain a **feature vector**, X, that adequately describes all of the relevant features for classifying examples
- Each X is a list of (attribute, value) pairs. For example,

  X = [Person:Sue, EyeColor:Brown, Age:Young, Sex:Female]
- The number of attributes (a.k.a. features) is fixed (positive, finite)
- Each attribute has a fixed, finite number of possible values (or could be continuous)

• Each example can be interpreted as a point in an n-dimensional **feature space**, where n is the number of attributes

Measuring Model Quality

- How good is a model?
  - Predictive accuracy
  - False positives / false negatives for a given cutoff threshold
    - Loss function (accounts for cost of different types of errors)
  - Area under the (ROC) curve
  - Minimizing loss can lead to problems with overfitting
- Training error
  - Train on all data; measure error on all data
  - Subject to overfitting (of course we'll make good predictions on the data on which we trained!)
- Regularization
  - Attempt to avoid overfitting
  - Explicitly minimize the complexity of the function while minimizing loss. Tradeoff is modeled with a *regularization parameter*

Cross-Validation

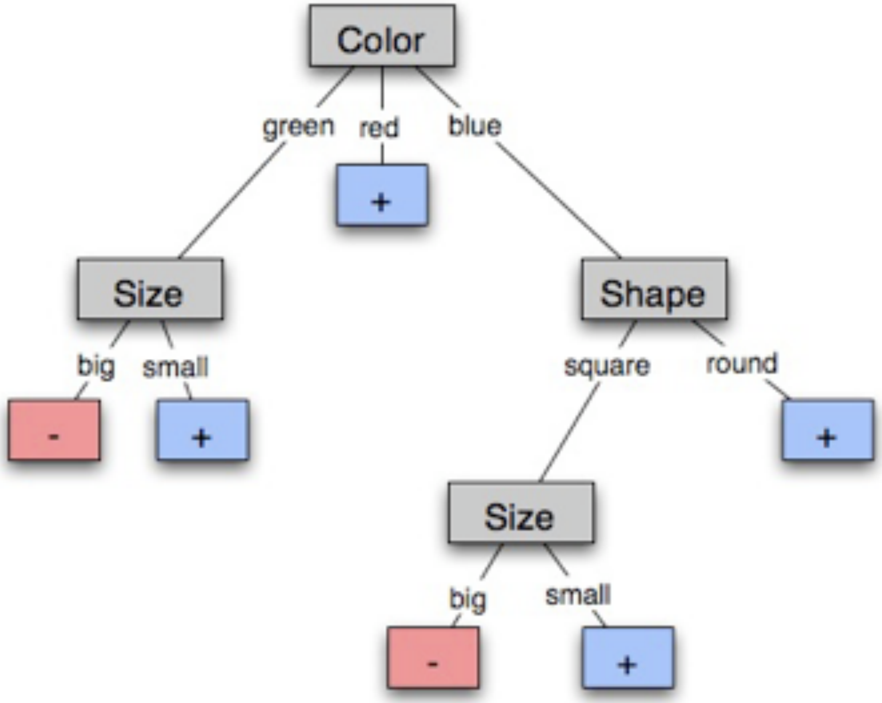
- Holdout cross-validation:
  - Divide data into training set and test set
  - Train on training set; measure error on test set
  - Better than training error, since we are measuring *generalization to new data*
  - To get a good estimate, we need a reasonably large test set
  - But this gives less data to train on, reducing our model quality!

Cross-Validation, cont.

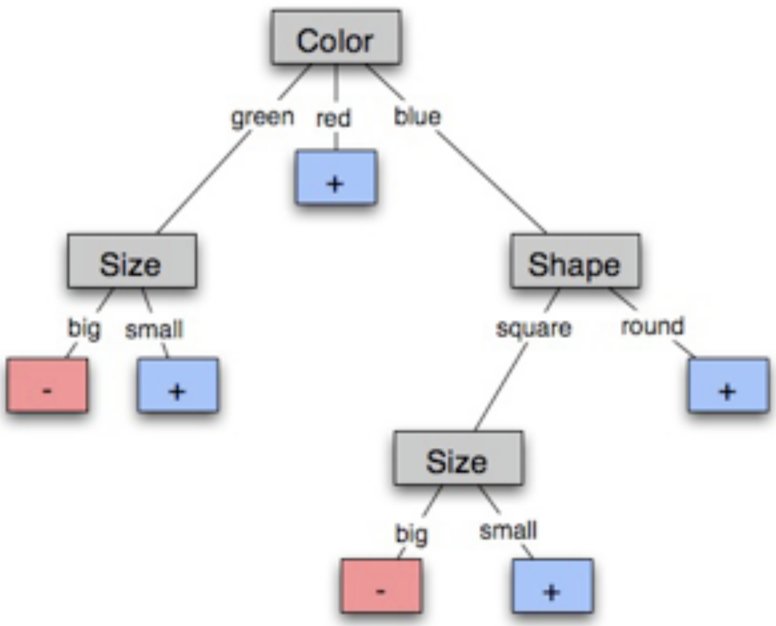
- k-fold cross-validation:
  - Divide data into *k* folds
  - Train on *k-1* folds, use the *k*th fold to measure error
  - Repeat *k* times; use average error to measure generalization accuracy
  - Statistically valid and gives good accuracy estimates
- Leave-one-out cross-validation (LOOCV)
  - *k*-fold cross validation where $k=N$ (test data = 1 instance!)
  - Quite accurate, but also quite expensive, since it requires building N models

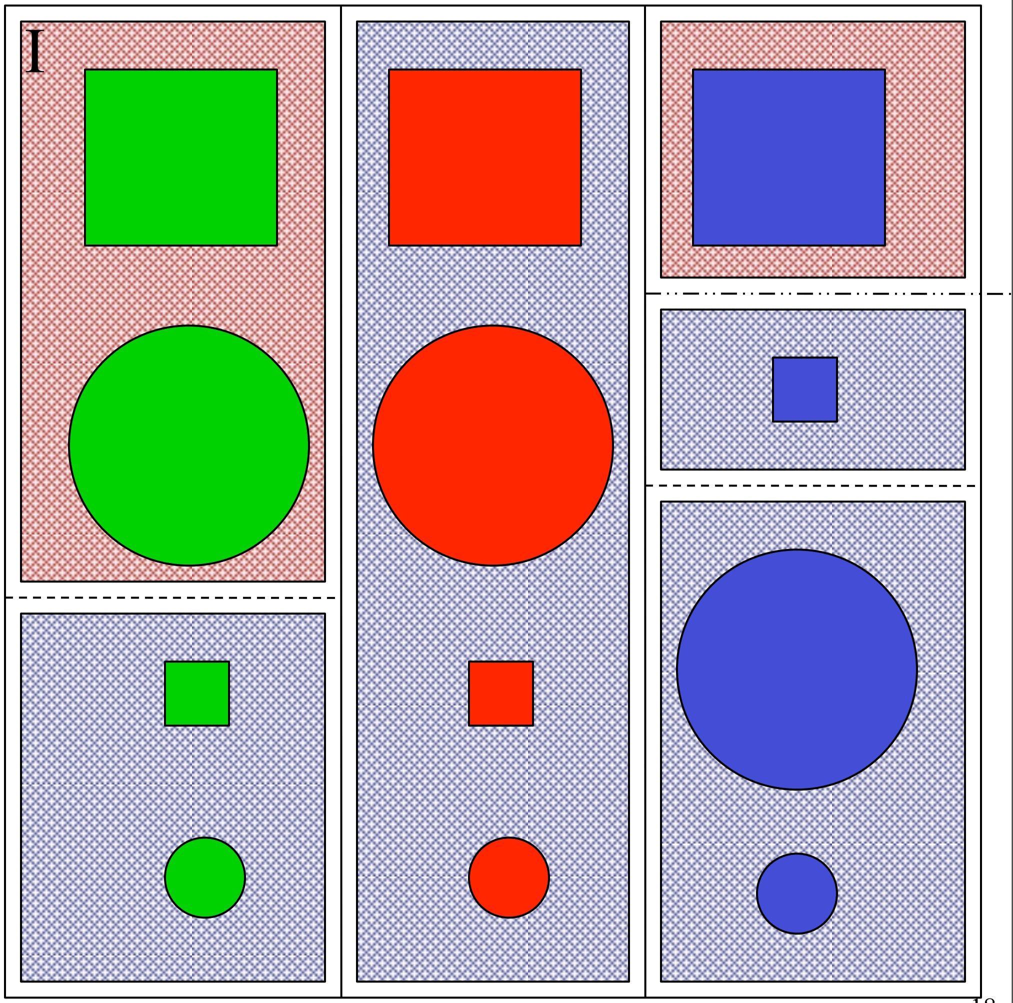
Decision Trees

- Goal: Build a **decision tree** to classify examples as positive or negative instances of a concept using supervised learning from a training set
- A **decision tree** is a tree where
  - each non-leaf node has associated with it an attribute (feature)
  - each leaf node has associated with it a classification (+ or -)
  - each arc has associated with it one of the possible values of the attribute at the node from which the arc is directed
- Generalization: allow for >2 classes
  - e.g., {sell, hold, buy}



Decision Tree-Induced Partition – Example

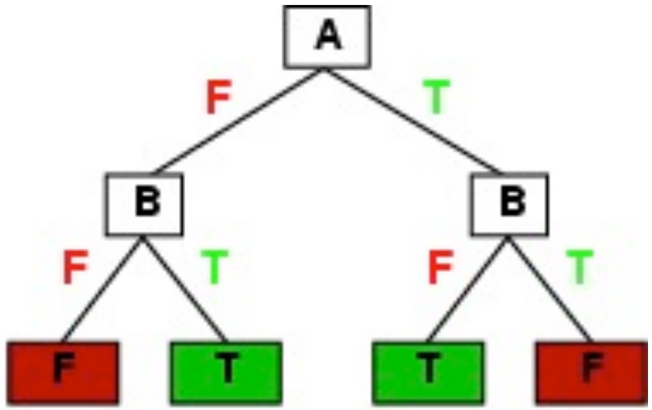




Expressiveness

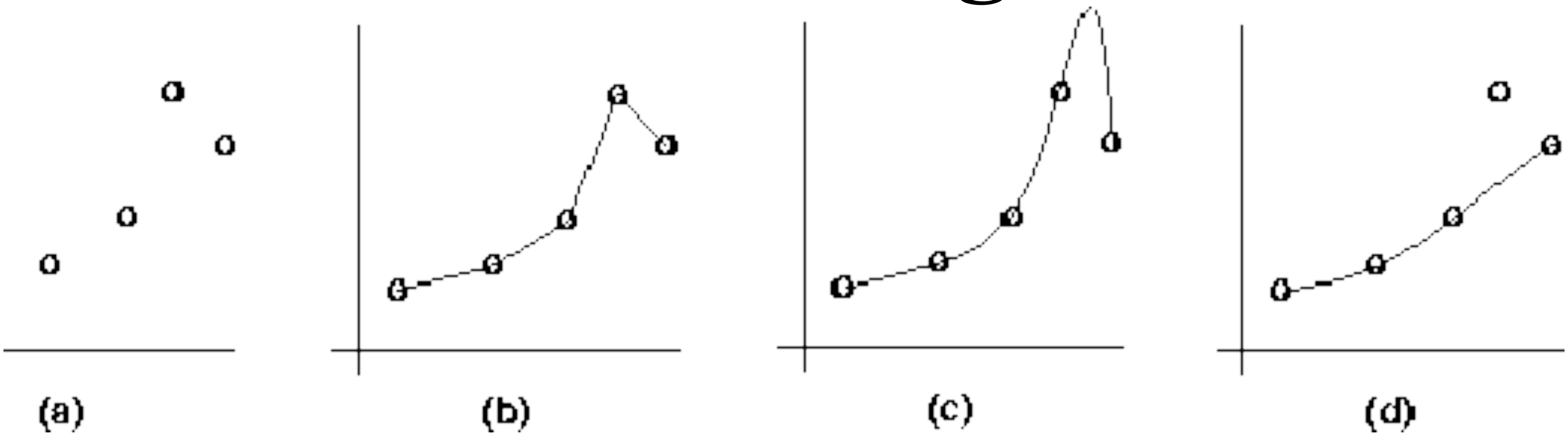
- Decision trees can express any function of the input attributes.
- E.g., for Boolean functions, truth table row → path to leaf:

A	B	A xor B
F	F	F
F	T	T
T	F	T
T	T	F



- Trivially, there is a consistent decision tree for any training set with one path to leaf for each example (unless f nondeterministic in x) but it probably won't generalize to new examples
- We prefer to find more compact decision trees

Inductive Learning and Bias



- Suppose that we want to learn a function f(x) = y and we are given some sample (x,y) pairs, as in figure (a)
- There are several hypotheses we could make about this function, e.g.: (b), (c) and (d)
- A preference for one over the others reveals the **bias** of our learning technique, e.g.:
  - prefer piece-wise functions (b)
  - prefer a smooth function (c)
  - prefer a simple function and treat outliers as noise (d)

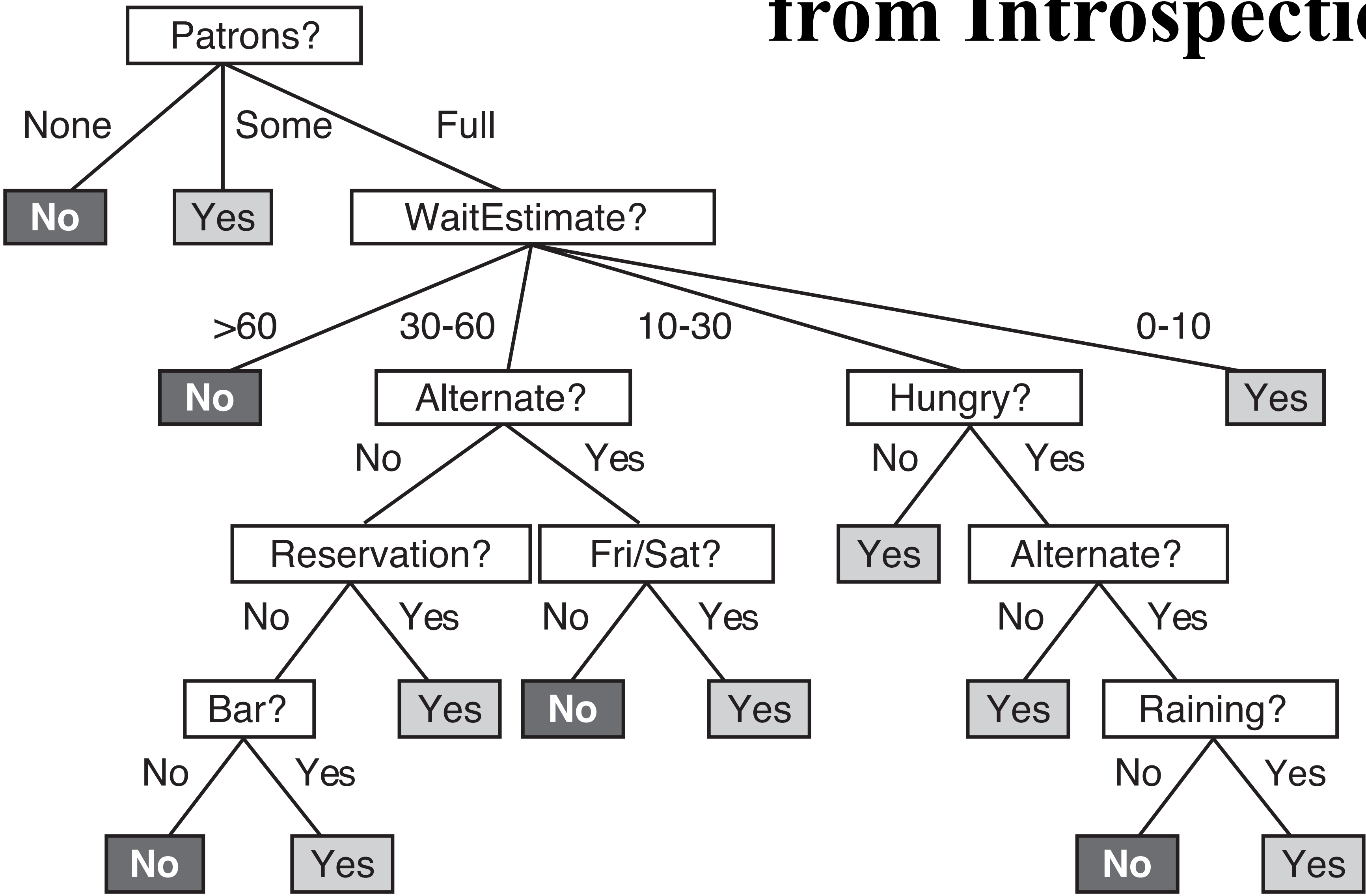
Preference Bias: Ockham's Razor

- A.k.a. Occam's Razor, Law of Economy, or Law of Parsimony
- Principle stated by William of Ockham (1285-1347/49) that
  - "*non sunt multiplicanda entia praeter necessitatem*"
  - or, entities are not to be multiplied beyond necessity
- The simplest consistent explanation is the best
- Therefore, the smallest decision tree that correctly classifies all of the training examples is best
- Finding the provably smallest decision tree is NP-hard, so instead of constructing the absolute smallest tree consistent with the training examples, construct one that is pretty small

R&N's Restaurant Domain

- Develop a decision tree to model the decision a patron makes when deciding whether or not to wait for a table at a restaurant
- Two classes: wait, leave
- Ten attributes: Alternative available? Bar in restaurant? Is it Friday? Are we hungry? How full is the restaurant? How expensive? Is it raining? Do we have a reservation? What type of restaurant is it? What's the purported waiting time?
- Training set of 12 examples
- ~ 7000 possible cases

A Decision Tree from Introspection



A Training Set

Example	Attributes										Goal
	Alt	Bar	Fri	Hun	Pat	Price	Rain	Res	Type	Est	WillWait
X_1	Yes	No	No	Yes	Some	$$$	No	Yes	French	0–10	Yes
X_2	Yes	No	No	Yes	Full	$	No	No	Thai	30–60	No
X_3	No	Yes	No	No	Some	$	No	No	Burger	0–10	Yes
X_4	Yes	No	Yes	Yes	Full	$	No	No	Thai	10–30	Yes
X_5	Yes	No	Yes	No	Full	$$$	No	Yes	French	>60	No
X_6	No	Yes	No	Yes	Some	$$	Yes	Yes	Italian	0–10	Yes
X_7	No	Yes	No	No	None	$	Yes	No	Burger	0–10	No
X_8	No	No	No	Yes	Some	$$	Yes	Yes	Thai	0–10	Yes
X_9	No	Yes	Yes	No	Full	$	Yes	No	Burger	>60	No
X_{10}	Yes	Yes	Yes	Yes	Full	$$$	No	Yes	Italian	10–30	No
X_{11}	No	No	No	No	None	$	No	No	Thai	0–10	No
X_{12}	Yes	Yes	Yes	Yes	Full	$	No	No	Burger	30–60	Yes

ID3/C4.5

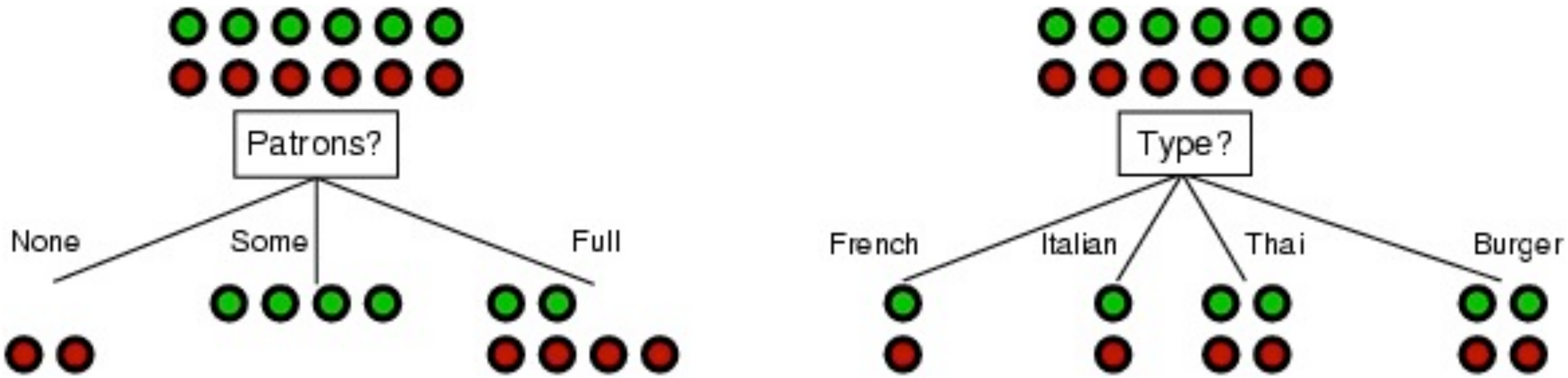
- A greedy algorithm for decision tree construction developed by Ross Quinlan, 1987
- Top-down construction of the decision tree by recursively selecting the “best attribute” to use at the current node in the tree
  - Once the attribute is selected for the current node, generate children nodes, one for each possible value of the selected attribute
  - Partition the examples using the possible values of this attribute, and assign these subsets of the examples to the appropriate child node
  - Repeat for each child node until all examples associated with a node are either all positive or all negative

Choosing the Best Attribute

- The key problem is choosing which attribute to split a given set of examples
- Some possibilities are:
  - **Random:** Select any attribute at random
  - **Least-Values:** Choose the attribute with the smallest number of possible values
  - **Most-Values:** Choose the attribute with the largest number of possible values
  - **Max-Gain:** Choose the attribute that has the largest expected information gain–i.e., the attribute that will result in the smallest expected size of the subtrees rooted at its children
- The ID3 algorithm uses the Max-Gain method of selecting the best attribute

Choosing an Attribute

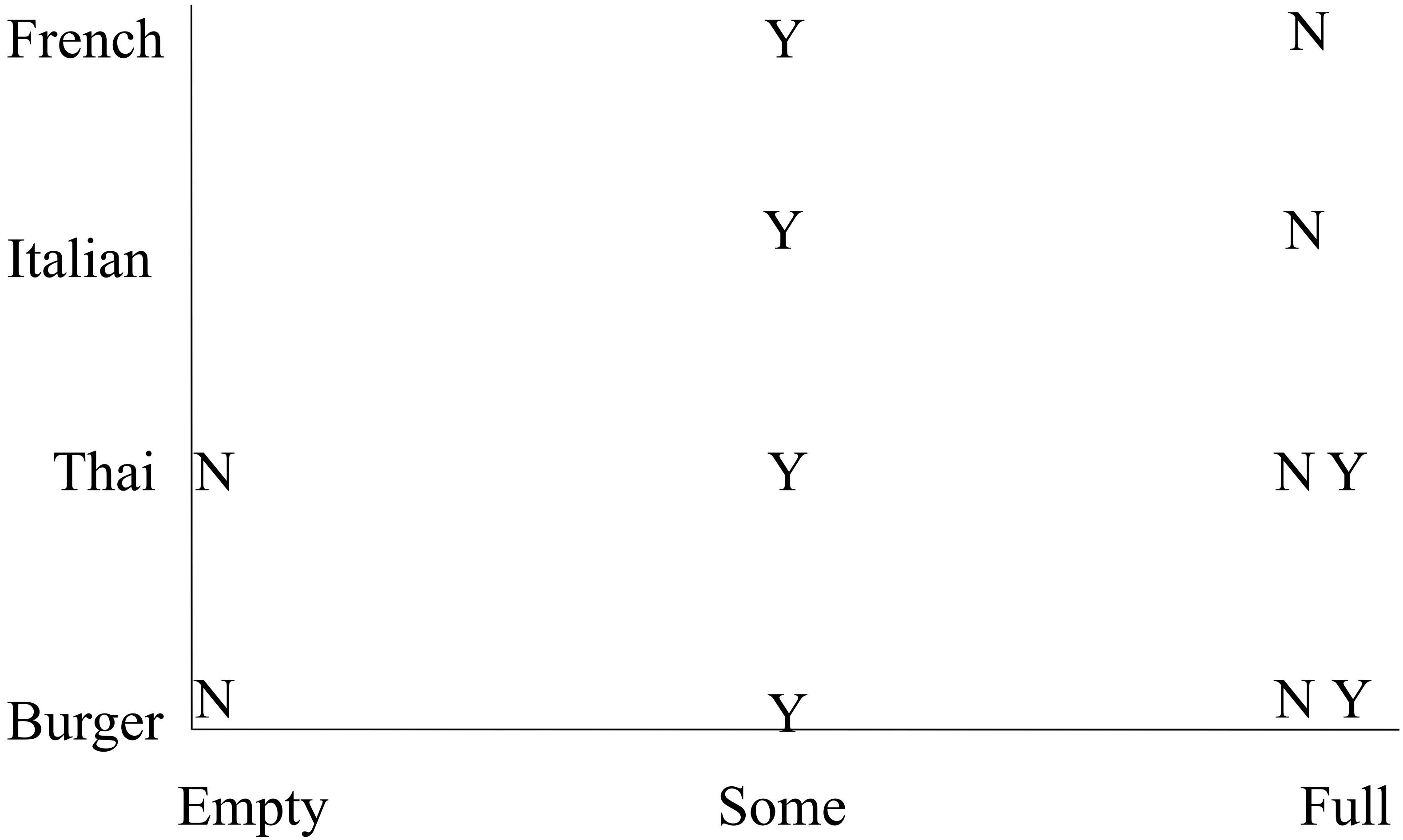
Idea: a good attribute splits the examples into subsets that are (ideally) “all positive” or “all negative”



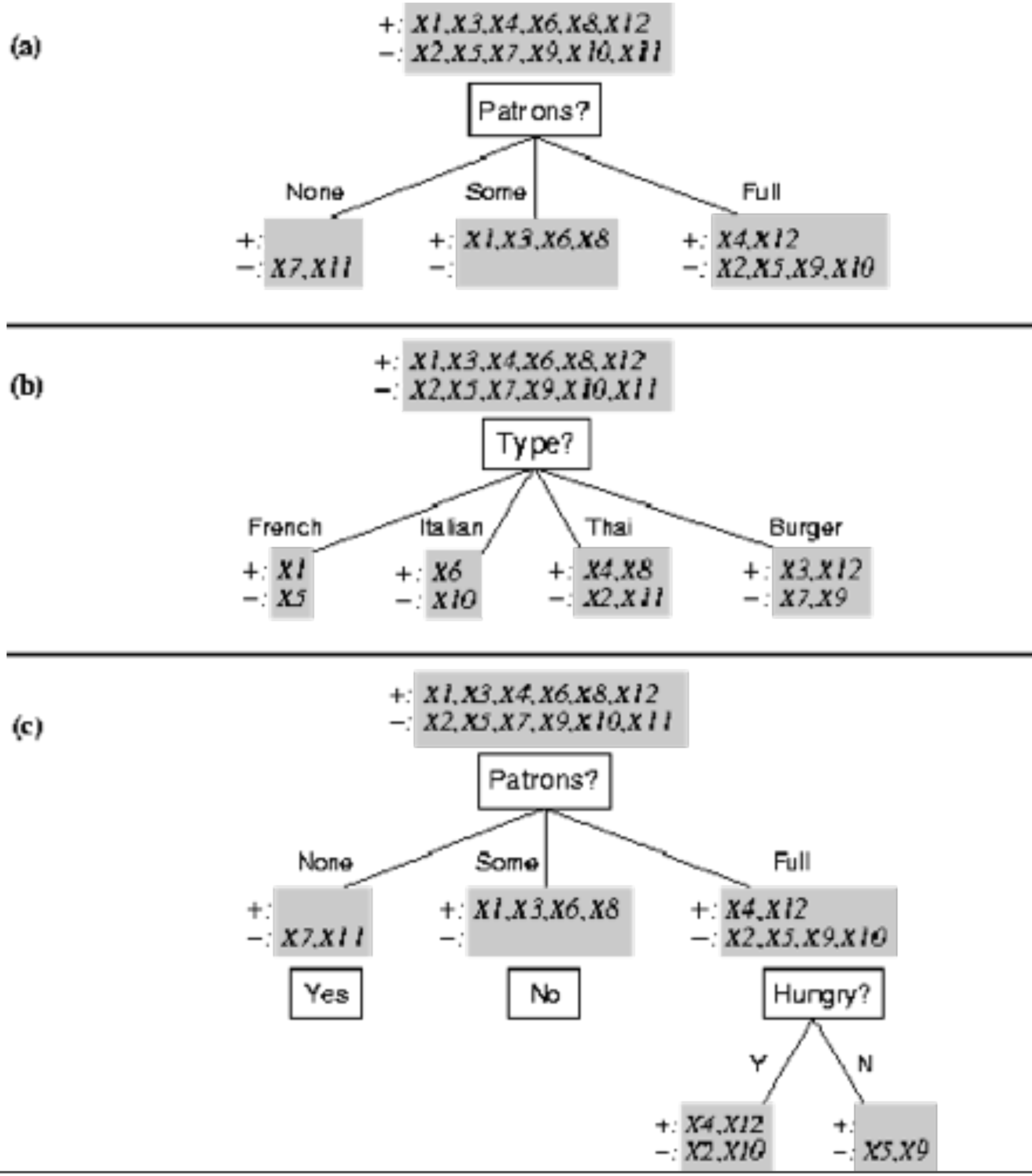
Which is better: *Patrons?* or *Type?*

Restaurant Example

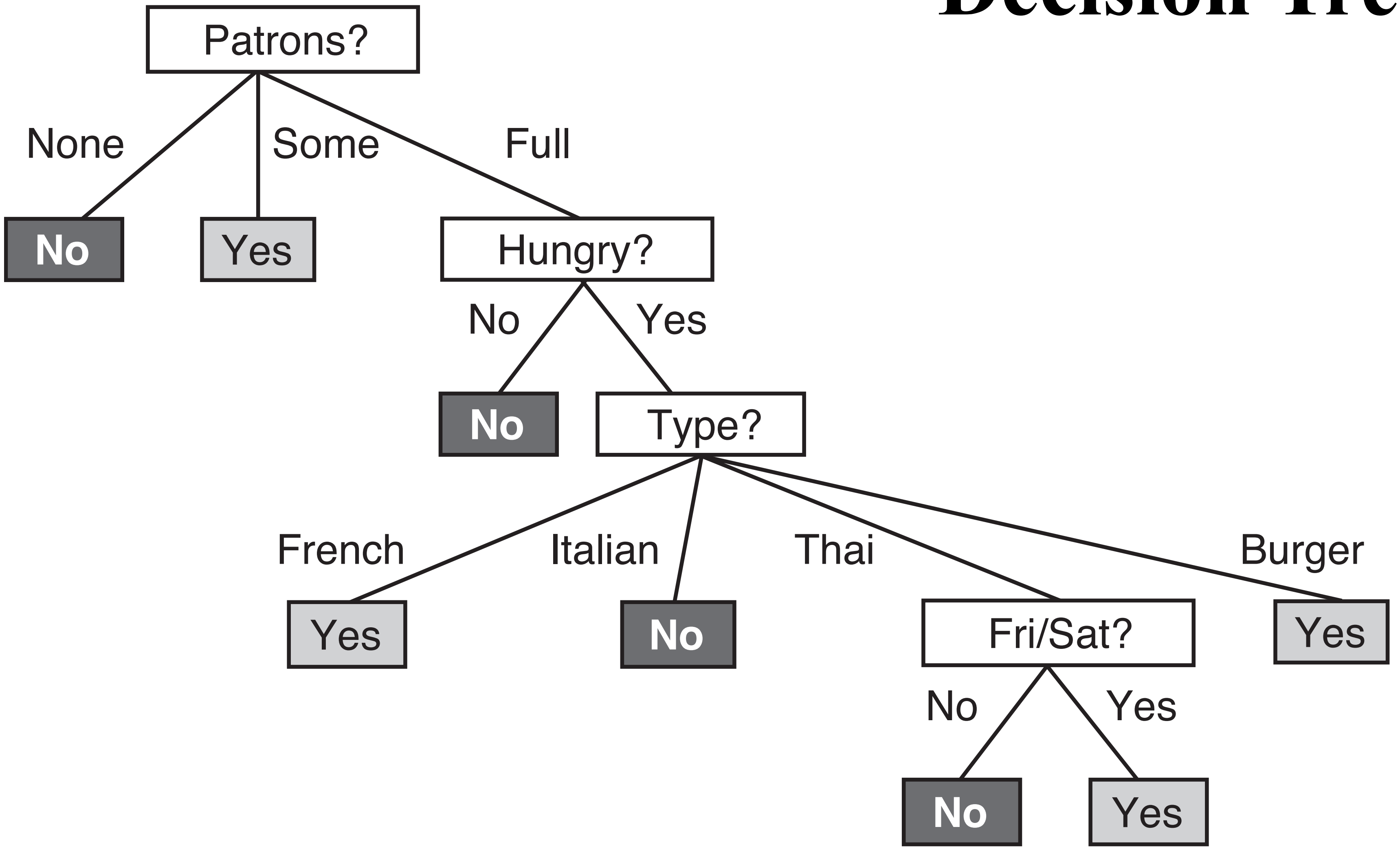
Random: Patrons or Wait-time; **Least-values**: Patrons; **Most-values**: Type; **Max-gain**: ???



Splitting Examples by Testing Attributes



ID3-induced Decision Tree



Information Theory 101

- Information theory sprang almost fully formed from the seminal work of Claude E. Shannon at Bell Labs
  - "A Mathematical Theory of Communication," *Bell System Technical Journal*, 1948
- Intuitions
  - Common words (a, the, dog) are shorter than less common ones (parliamentarian, foreshadowing)
  - In Morse code, common (probable) letters have shorter encodings
- ***Information*** is defined as the ***minimum number of bits*** needed to store or send some information
  - Wikipedia: "The measure of data, known as information entropy, is usually expressed by the average number of bits needed for storage or communication"

Information Theory 102

- Information is measured in bits
- Information conveyed by a message depends on its probability
- With n equally probable possible *messages*, the probability p of each is *1/n*
- Information conveyed by message is $\log_2(n) = -\log_2(p)$
  - e.g., with 16 messages, then $\log_2(16) = 4$ and we need 4 bits to identify/send each message
- Given probability distribution for n messages $P = (p_1, p_2 \ldots p_n)$, the information conveyed by distribution (aka *entropy* of P) is:

$$I(P) = -(p_1 * \log_2(p_1) + p_2 * \log_2(p_2) + .. + p_n * \log_2(p_n))$$

probability of msg 2

info in msg 2

Information Theory 103

- Entropy is the average number of bits/message needed to represent a stream of messages
- Information conveyed by distribution (a.k.a. *entropy* of P):

  $I(P) = -(p_1 * \log_2 (p_1) + p_2 * \log_2 (p_2) + .. + p_n * \log_2 (p_n))$
- Examples:
  - If P is (0.5, 0.5) then I(P) = 1 → entropy of a fair coin flip
  - If P is (0.67, 0.33) then I(P) = 0.92
  - If Pis (0.99, 0.01) then I(P) = 0.08
  - If P is (1, 0) then I(P) = 0
- Note that as the distribution becomes more skewed, the amount of information *decreases*
  - ...because I can just predict the most likely element, and usually be right

Entropy as Measure of Homogeneity of Examples

- Entropy used to characterize the (im)purity of an arbitrary collection of examples.
- Given a collection *S* (e.g., the table with 12 examples for the restaurant domain), containing positive and negative examples of some target concept, the entropy of S relative to its Boolean classification is:

$$I(S) = -(p_+ * \log_2 (p_+) + p_- * \log_2 (p_-))$$

Entropy([6+, 6-]) = 1 → entropy of the restaurant dataset

Entropy([9+, 5-]) = 0.940

Information Gain

- A chosen attribute A divides the training set E into subsets $E_1, \ldots, E_v$ according to their values for A, where A has v distinct values.
- The quantity IG(S,A), the ***information gain*** of an attribute A relative to a collection of examples S, is defined as:

  Gain(S,A) = I(S) – *Remainder*(A)

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

- This represents the difference between
  - I(S) – the entropy of the original collection S
  - *Remainder*(A) - expected value of the entropy after S is partitioned using attribute A
- This is the **gain in information due to attribute A**
  - Expected reduction in entropy
  - IG(S,A) or simply IG(A):

$$IG(S,A) = I(S) - \sum_{v \in Values(A)} \frac{|S_v|}{|S|} \times I(S_v)$$

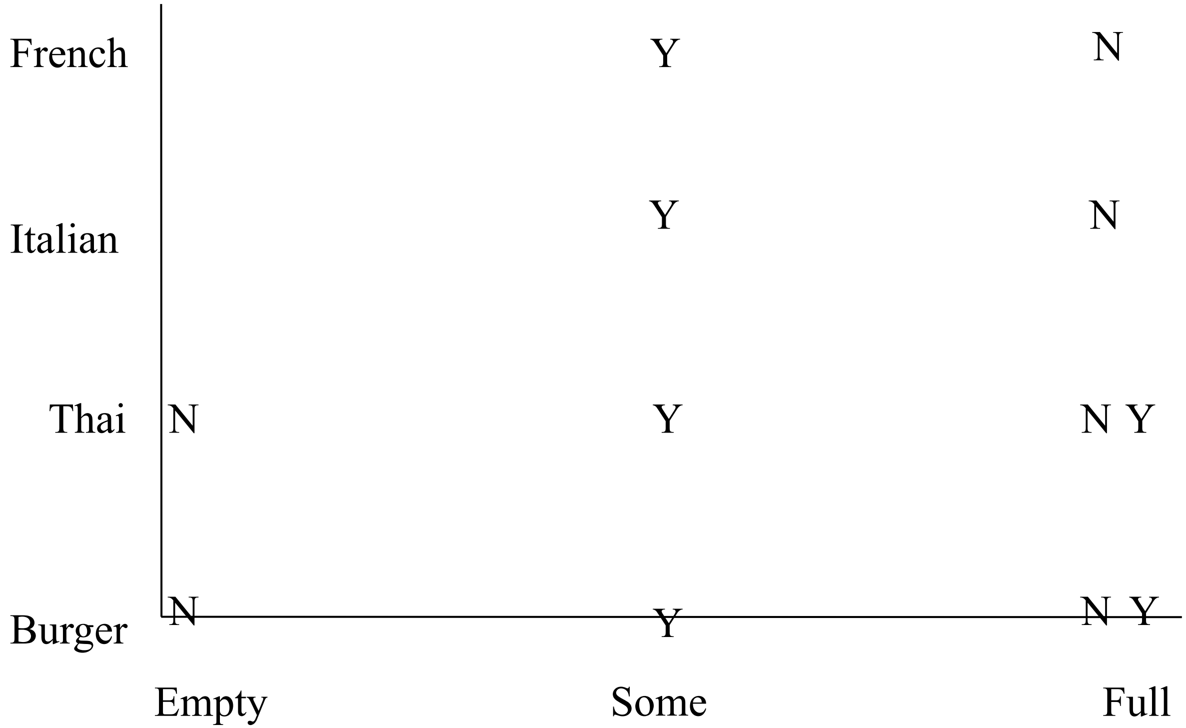
$$IG(A) = I\left(\frac{p}{p+n}, \frac{n}{p+n}\right) - remainder(A)$$

Information Gain, cont.

- Use to rank attributes and build DT (decision tree) where each node uses attribute with **greatest gain** of those not yet considered (in path from root)
  - Greatest gain means least information remaining after split
  - i.e., subsets are all as skewed (towards either positive or negative) as possible
- The intent of this ordering is to:
  - Create small decision trees, so predictions can be made with few attribute tests
  - Match a hoped-for minimality of the process represented by the instances being considered (Occam's Razor)

Computing Information Gain

- I(T) = ?
- I (Pat, T) = ?
- I (Type, T) = ?



Gain (Pat, T) = ?

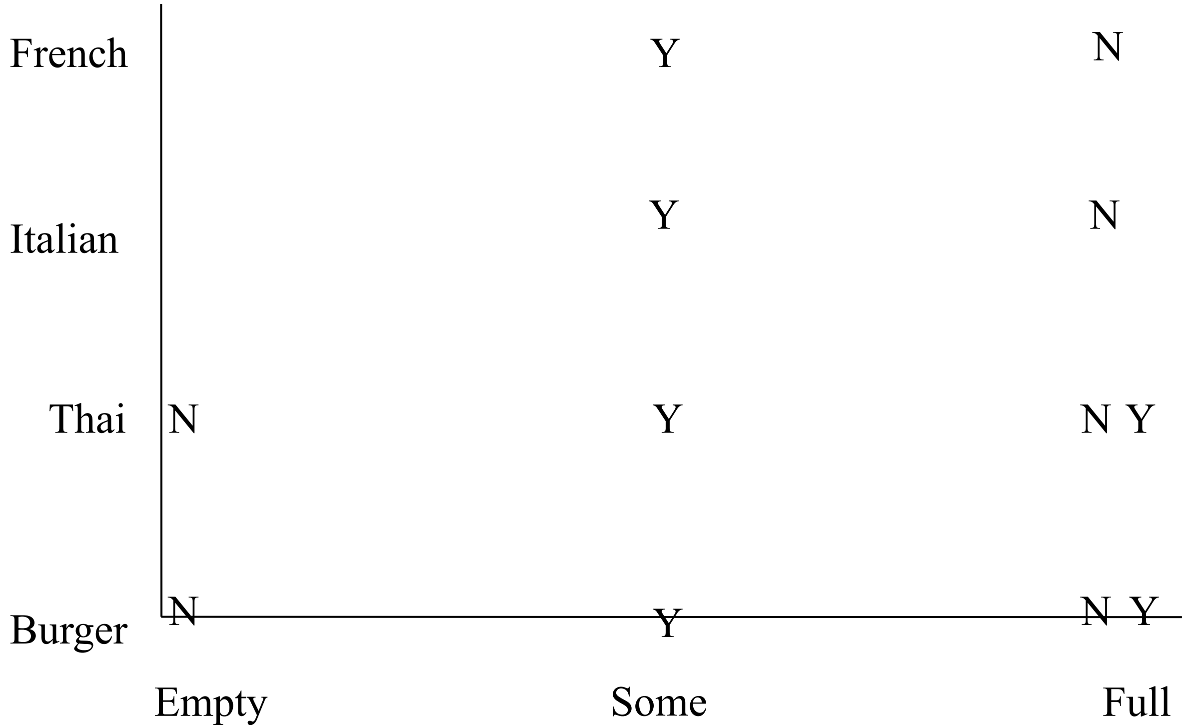
Gain (Type, T) = ?

Computing Information Gain

- I(T) =
  - (.5 log .5 + .5 log .5)
  = .5 + .5 = 1

- I (Pat, T) =
  1/6 (0) + 1/3 (0) +
  1/2 (- (2/3 log 2/3 +
  1/3 log 1/3))
  = 1/2 (2/3*.6 +
  1/3*1.6)
  = .47

- I (Type, T) =
  1/6 (1) + 1/6 (1) +
  1/3 (1) + 1/3 (1) = 1



Gain (Pat, T) = 1 - .47 = .53

Gain (Type, T) = 1 – 1 = 0

The ID3 algorithm is used to build a decision tree, given a set of non-categorical attributes C1, C2, .., Cn, the class attribute C, and a training set T of records.

```
function ID3 (R: a set of input attributes,
                 C: the class attribute,
                 S: a training set) returns a decision tree;
   begin
     If S is empty, return a single node with value Failure;
     If every example in S has the same value for C, return
       single node with that value;
     If R is empty, then return a single node with most
       frequent of the values of C found in examples S;
       [note: there will be errors, i.e., improperly classified
       records];
     Let D be attribute with largest Gain(D,S) among attributes in R;
     Let {dj| j=1,2, .., m} be the values of attribute D;
     Let {Sj| j=1,2, .., m} be the subsets of S consisting
        respectively of records with value dj for attribute D;
     Return a tree with root labeled D and arcs labeled
        d1, d2, .., dm going respectively to the trees
        ID3(R-{D},C,S1), ID3(R-{D},C,S2) ,.., ID3(R-{D},C,Sm);
   end ID3;
```

How Well Does it Work?

Many case studies have shown that decision trees are at least as accurate as human experts.

- A study for diagnosing breast cancer had humans correctly classifying the examples 65% of the time; the decision tree classified 72% correct
- British Petroleum designed a decision tree for gas-oil separation for offshore oil platforms that replaced an earlier rule-based expert system
- Cessna designed an airplane flight controller using 90,000 examples and 20 attributes per example
- SKICAT (Sky Image Cataloging and Analysis Tool) used a decision tree to classify sky objects that were an order of magnitude fainter than was previously possible, with an accuracy of over 90%.

Extensions of the Decision Tree Learning Algorithm

- Using gain ratios
- Real-valued data
- Noisy data and overfitting
- Generation of rules
- Setting parameters
- Cross-validation for experimental validation of performance
- C4.5 is an extension of ID3 that accounts for unavailable values, continuous attribute value ranges, pruning of decision trees, rule derivation, and so on

Using Gain Ratios

- The information gain criterion favors attributes that have a large number of values
  - If we have an attribute D that has a distinct value for each record, then Info(D,T) is 0, thus Gain(D,T) is maximal
- To compensate for this Quinlan suggests using the following ratio instead of Gain:

  GainRatio(D,T) = Gain(D,T) / SplitInfo(D,T)
- SplitInfo(D,T) is the information due to the split of T on the basis of value of categorical attribute D

  SplitInfo(D,T) = I(|T1|/|T|, |T2|/|T|, .., |Tm|/|T|)

where {T1, T2, .. Tm} is the partition of T induced by value of D

Computing Gain Ratio

- I(T) = 1
- I (Pat, T) = .47
- I (Type, T) = 1

Gain (Pat, T) =.53
Gain (Type, T) = 0

	Empty	Some	Full
French		Y	N
Italian		Y	N
Thai	N	Y	N Y
Burger	N	Y	N Y

SplitInfo (Pat, T) = - (1/6 log 1/6 + 1/3 log 1/3 + 1/2 log 1/2) = 1/6*2.6 + 1/3*1.6 + 1/2*1
= 1.47

SplitInfo (Type, T) = 1/6 log 1/6 + 1/6 log 1/6 + 1/3 log 1/3 + 1/3 log 1/3
= 1/6*2.6 + 1/6*2.6 + 1/3*1.6 + 1/3*1.6 = 1.93

GainRatio (Pat, T) = Gain (Pat, T) / SplitInfo(Pat, T) = .53 / 1.47 = .36

GainRatio (Type, T) = Gain (Type, T) / SplitInfo (Type, T) = 0 / 1.93 = 0

Real-Valued Data

- Select a set of thresholds defining intervals
- Each interval becomes a discrete value of the attribute
- Use some simple heuristics…
  - always divide into quartiles
- Use domain knowledge…
  - divide age into infant (0-2), toddler (3 - 5), school-aged (5-8)
- Or treat this as another learning problem
  - Try a range of ways to discretize the continuous variable and see which yield “better results” w.r.t. some metric
  - E.g., try midpoint between every pair of values

Summary: Decision Tree Learning

- Inducing decision trees is one of the most widely used learning methods in practice
- Can out-perform human experts in many problems
- Strengths include
  - Fast
  - Simple to implement
  - Can convert result to a set of easily interpretable rules
  - Empirically valid in many commercial products
  - Handles noisy data
- Weaknesses include:
  - Univariate splits/partitioning using only one attribute at a time so limits types of possible trees
  - Large decision trees may be hard to understand
  - Requires fixed-length feature vectors
  - Non-incremental (i.e., batch method)

Evaluation Methodology

- Standard methodology:
  1. Collect a large set of examples (all with correct classifications)
  2. Randomly divide collection into two disjoint sets: training and test
  3. Apply learning algorithm to training set giving hypothesis H
  4. Measure performance of H w.r.t. test set
- Important: keep the training and test sets disjoint!
- To study the efficiency and robustness of an algorithm, repeat steps 2-4 for different training sets and sizes of training sets
- If you improve your algorithm, start again with step 1 to avoid evolving the algorithm to work well on just this collection