Machine Learning: Decision Trees

Chapter 19.3

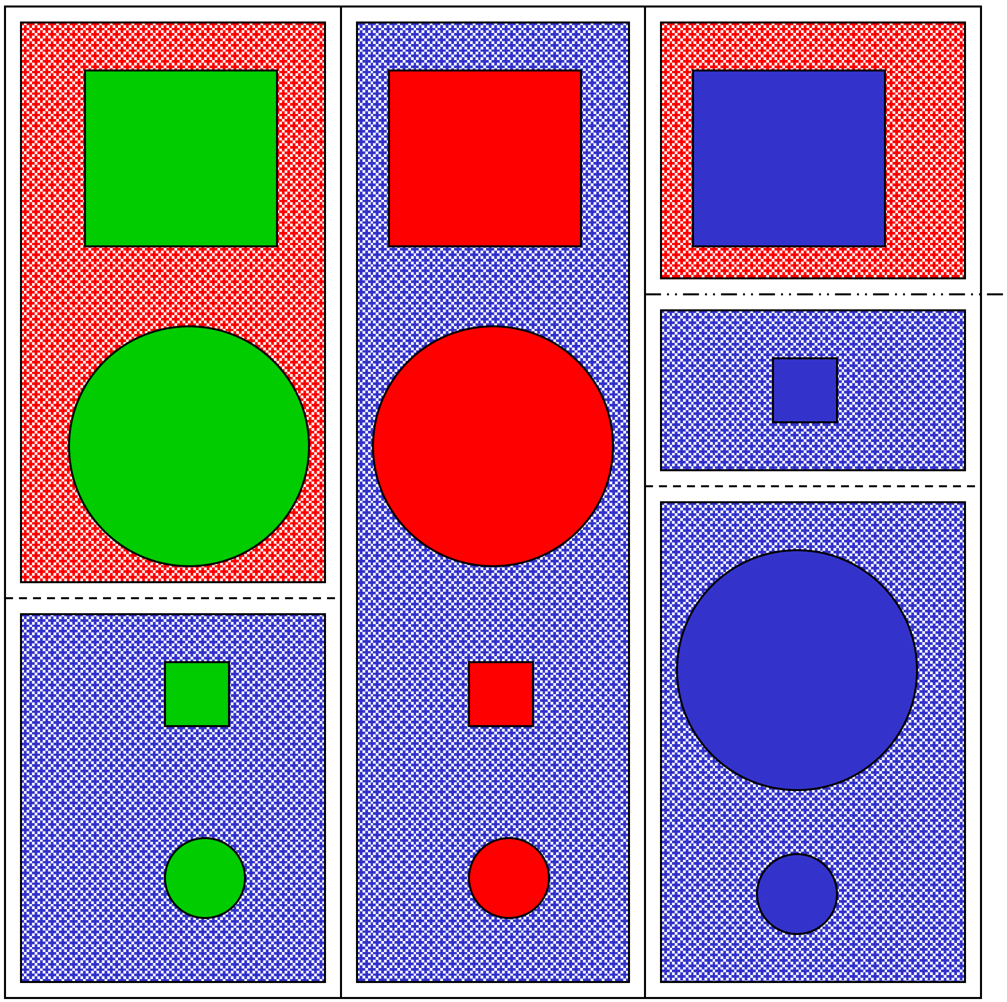
Some material adopted from notes by Chuck Dyer

Decision Trees (DTs)

- A **supervised** learning method used for **classification** and **regression**
- Given a set of training tuples, learn model to predict one value from the others
  - Learned value typically a class (e.g., goodRisk)
- Resulting model is simple to understand, interpret, visualize, and apply

Learning a Concept

The red groups are **negative** examples, blue **positive**



Attributes

- **Size**: large, small
- **Color**: red, green, blue
- **Shape**: square, circle

Task

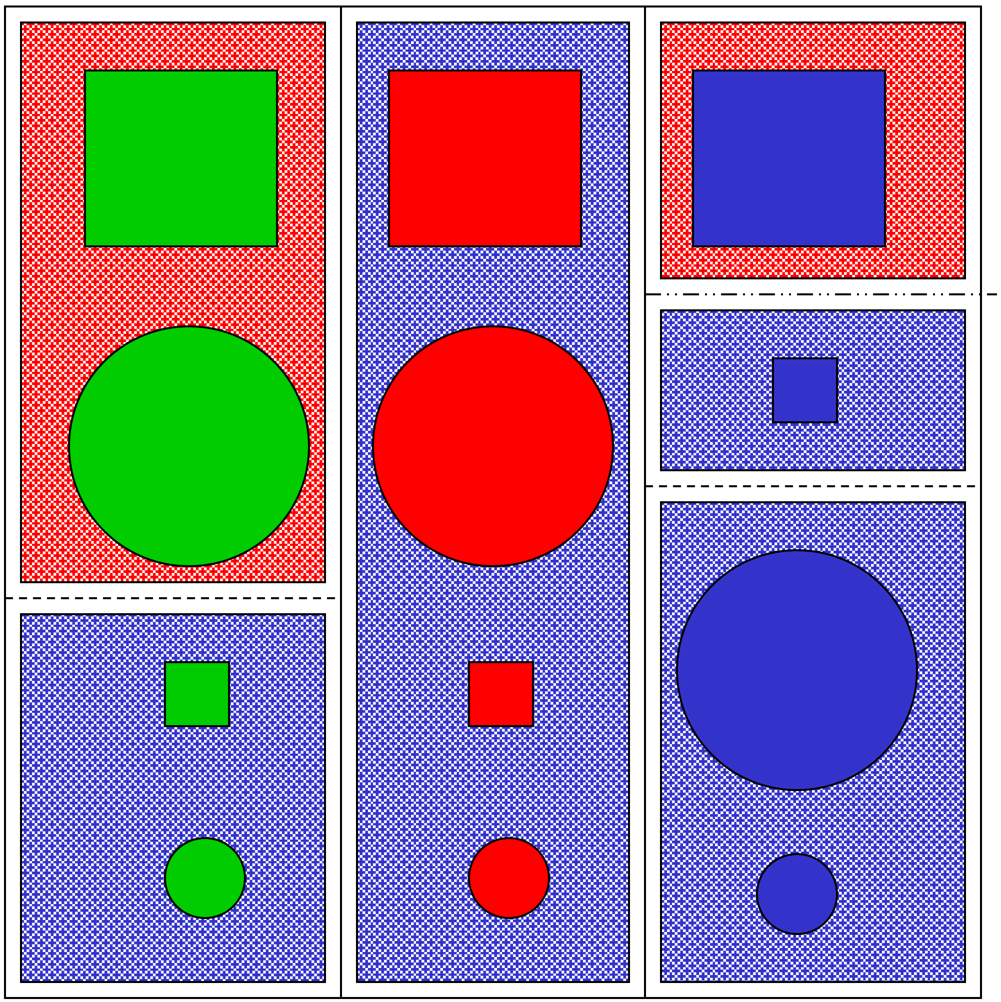
Classify new object with a size, color & shape as positive or negative

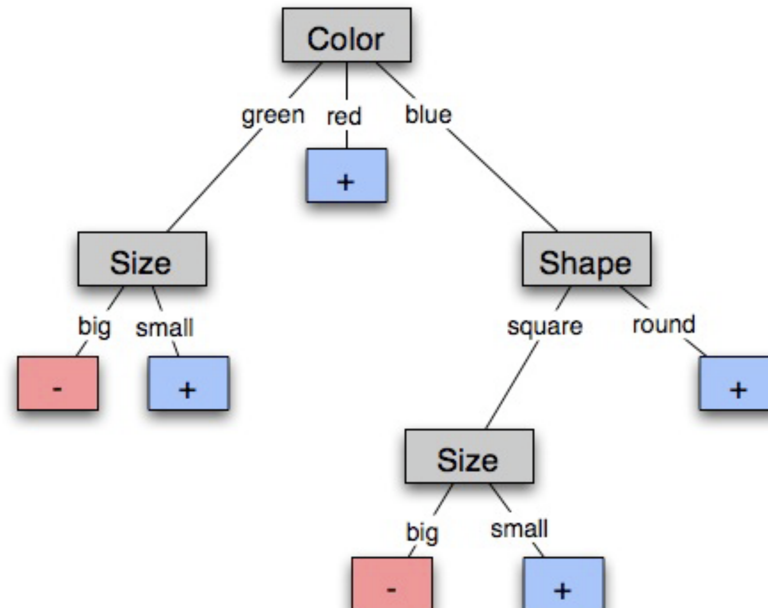
Training data

Size	Color	Shape	class
Large	Green	Square	Negative
Large	Green	Circle	Negative
Small	Green	Square	Positive
Small	Green	Circle	positive
Large	Red	Square	Positive
Large	Red	Circle	Positive
Small	Red	Square	Positive
Small	Red	Circle	Positive
Large	Blue	Square	Negative
Small	Blue	Square	Positive
Large	Blue	Circle	Positive
Small	Blue	Circle	Positive

A decision tree-induced partition

The red groups are negative examples, blue positive

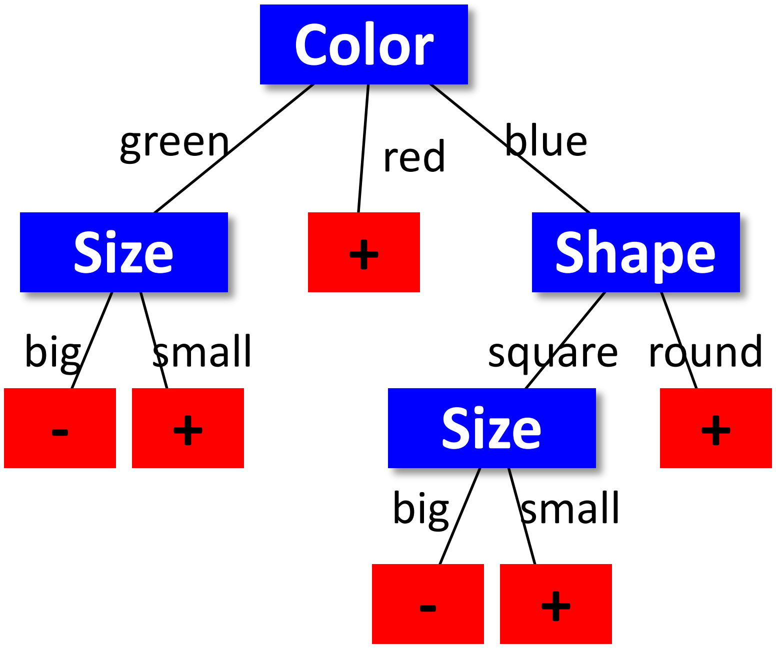




Negative things are big, green shapes and big, blue squares

Learning decision trees

- Goal: Build **decision tree** to classify examples as positive or negative instances of concept using supervised learning from training data
- A **decision tree** is a tree where
  - non-leaf nodes have an attribute (feature)
  - leaf nodes have a classification (+ or -)
  - each arc has a possible value of its attribute

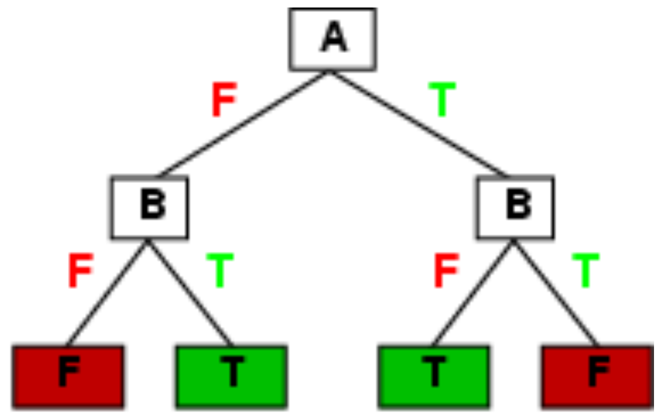


- Generalization: allow for >2 classes
  - e.g., classify stocks as {sell, hold, buy}

Expressiveness of Decision Trees

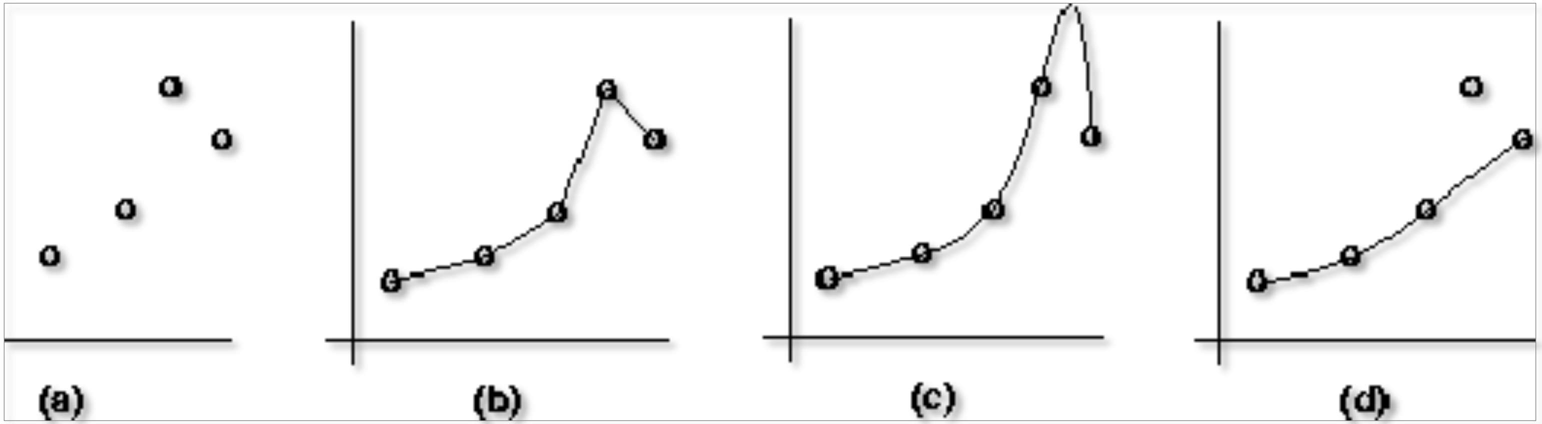
- Can express any function of input attributes, e.g., for Boolean functions, truth table row → path to leaf:

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



- There's a consistent decision tree for any training set with one path to leaf for each example, but it probably won't generalize to new examples
- Prefer more compact decision trees

Inductive learning and bias



- Suppose that we want to learn a function **f(x) = y** and we're given sample (x,y) pairs, as in figure (a)
- Can make several hypotheses about f, e.g.: (b), (c) & (d)
- Preference reveals learning technique **bias**, e.g.:
  - prefer piece-wise functions (b)
  - prefer a smooth function (c)
  - prefer a simple function and treat outliers as noise (d)

Preference bias: Occam's Razor

- William of Ockham (1285-1347)
  - "*non sunt multiplicanda entia praeter necessitatem* "
  - entities are not to be multiplied beyond necessity
- **Simplest** consistent explanation is the best
- **Smaller** decision trees correctly classifying training examples preferred over larger ones
- Finding **the** smallest decision tree is NP-hard, so we use algorithms that find reasonably small ones

R&N's restaurant domain

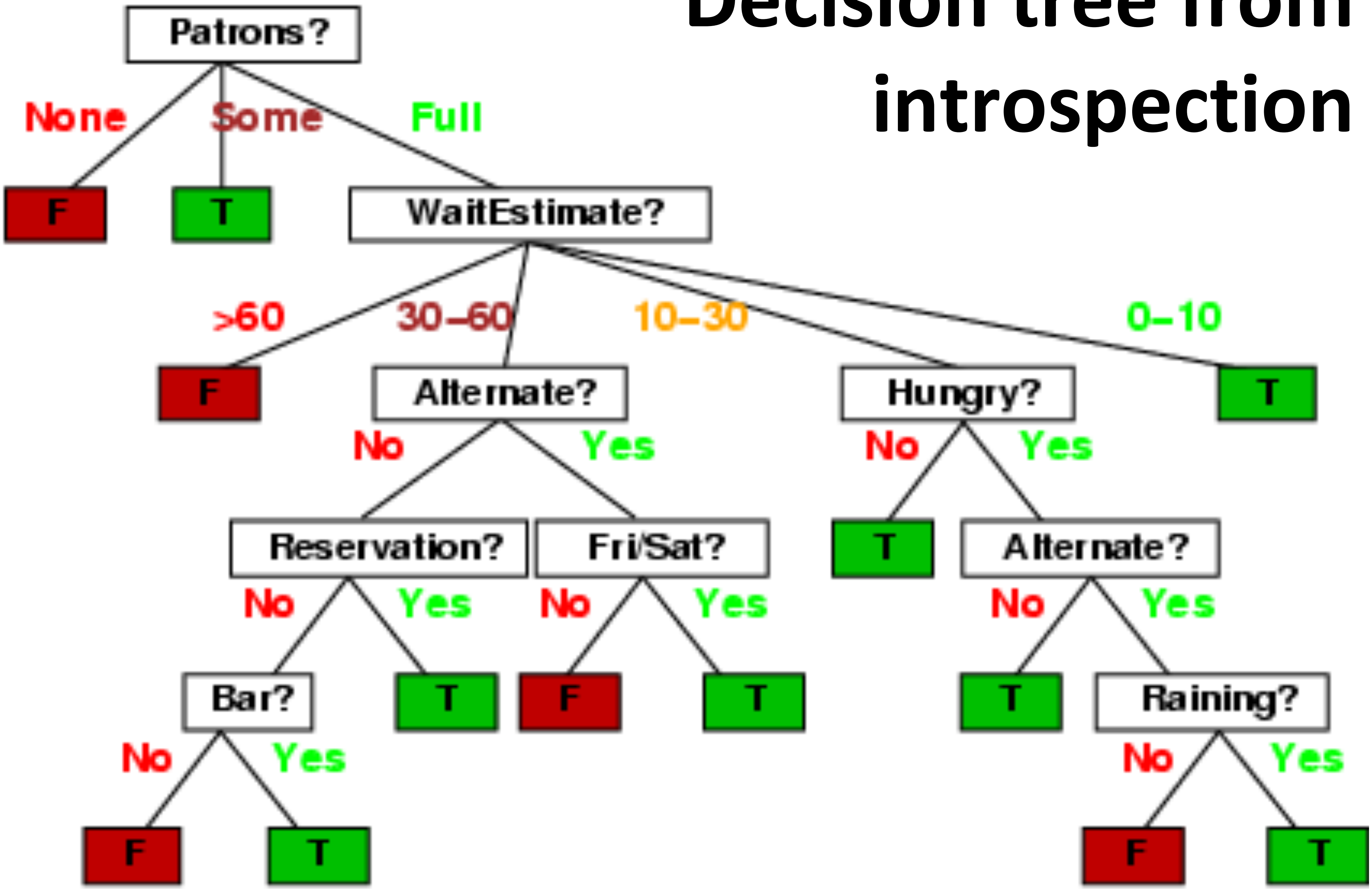
- Develop decision tree that customers make when deciding whether to wait for a table or leave
- **Two classes**: wait, leave
- **Ten attributes**: Alternative available? Bar in restaurant? Is it Friday? Are we hungry? How full is restaurant? How expensive? Is it raining? Do we have reservation? What type of restaurant is it? Estimated waiting time?
- Set of **12 training examples**
- ~7000 possible cases

Attribute-based representations

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

- Examples described by attribute values (Boolean, discrete, continuous), e.g., situations where will/won't wait for a table
- Classification of examples is positive (T) or negative (F)
- Serves as a training set

Decision tree from introspection



Issues

- It's like 20 questions
- We can generate many decision trees depending on what attributes we ask about and in what order
- How do we decide?
- What makes one decision tree better than another: number of nodes? number of leaves? maximum depth?

ID3 / C4.5 / J48 Algorithm

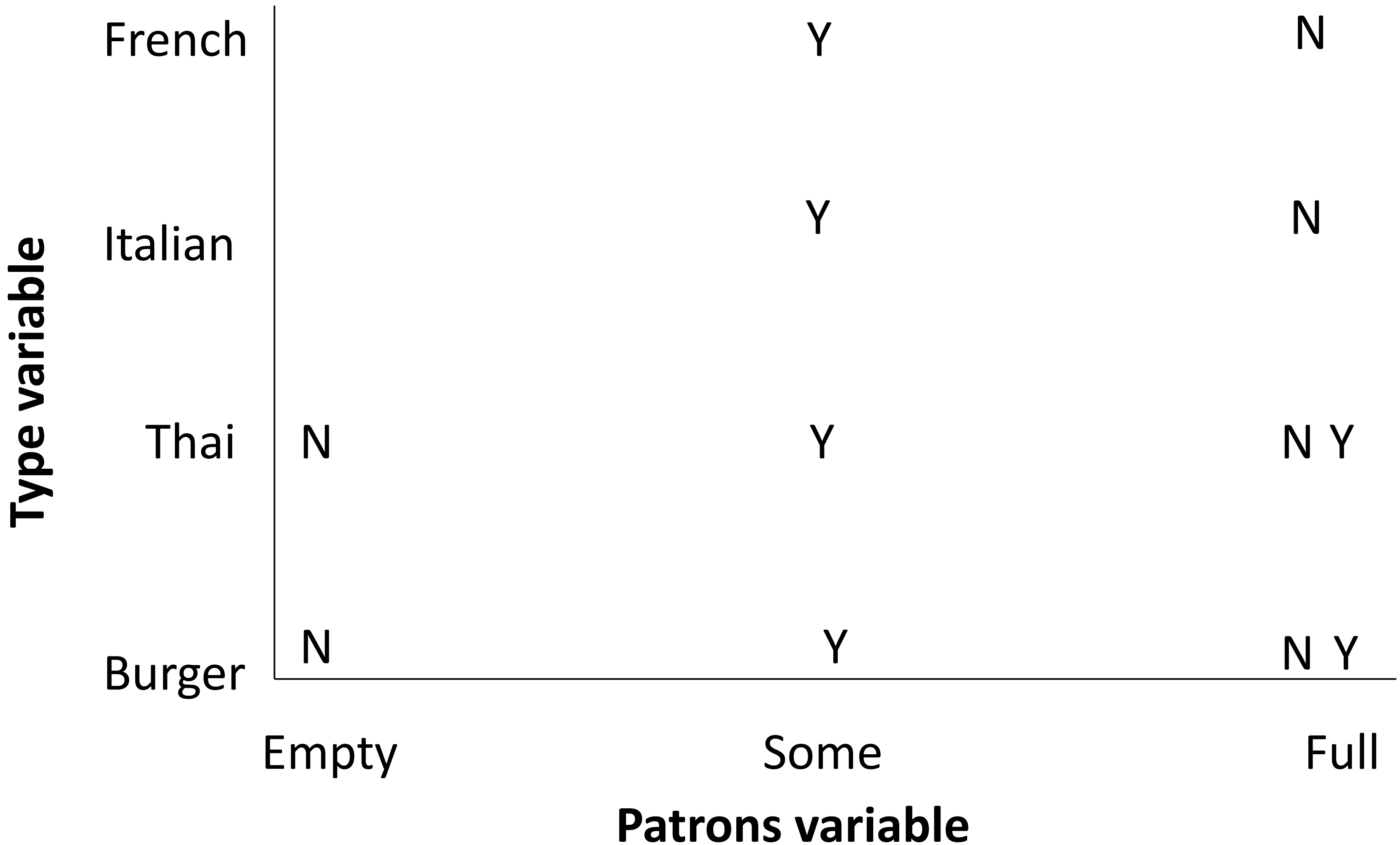
- Greedy algorithm for decision tree construction developed by Ross Quinlan circa 1987
- Top-down construction of tree by recursively selecting ***best attribute*** to use at current node
  - Once attribute selected for current node, generate child nodes, one for each possible attribute value
  - Partition examples using values of attribute, & assign these subsets of examples to the child nodes
  - Repeat for each child node until examples associated with a node are all positive or negative

Choosing best attribute

- Key problem: choose attribute to split given set of examples
- Possibilities for choosing attribute:
  - **Random:** Select one at random
  - **Least-values:** one with smallest # of possible values
  - **Most-values:** one with largest # of possible values
  - **Max-gain:** one with largest expected ***information gain***
  - **Gini impurity:** one with smallest gini impurity value
- The last two measure the **homogeneity** of the target variable within the subsets
- The ID3 algorithm uses **max-gain**

Restaurant: type vs patrons?

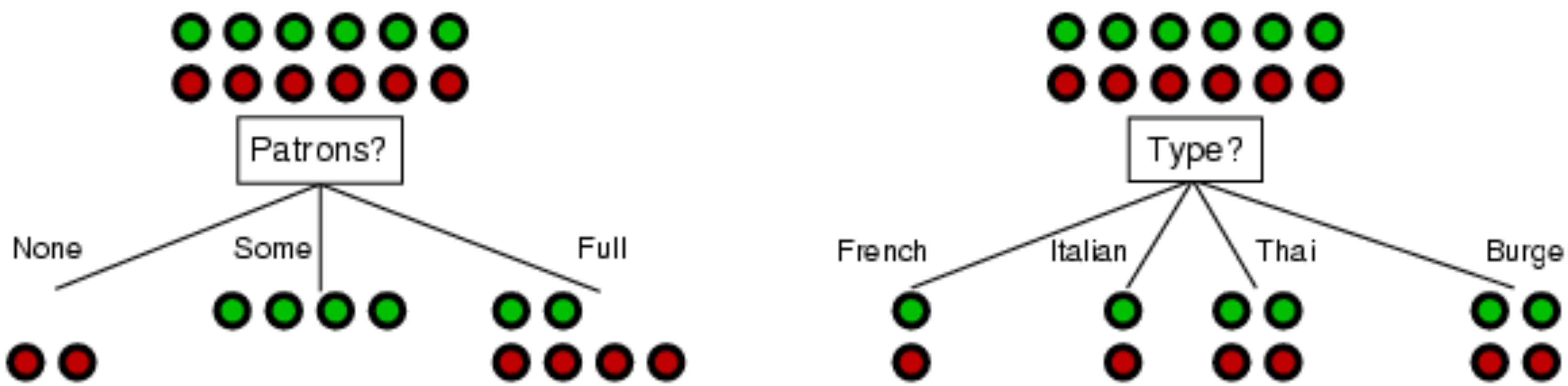
Random: Patrons or Wait-time; **Least-values**: Patrons; **Most-values**: Type; **Max-gain**: ???



Choosing an attribute

stay
leave

Idea: good attribute splits examples into subsets that are (ideally) *all positive* or *all negative*

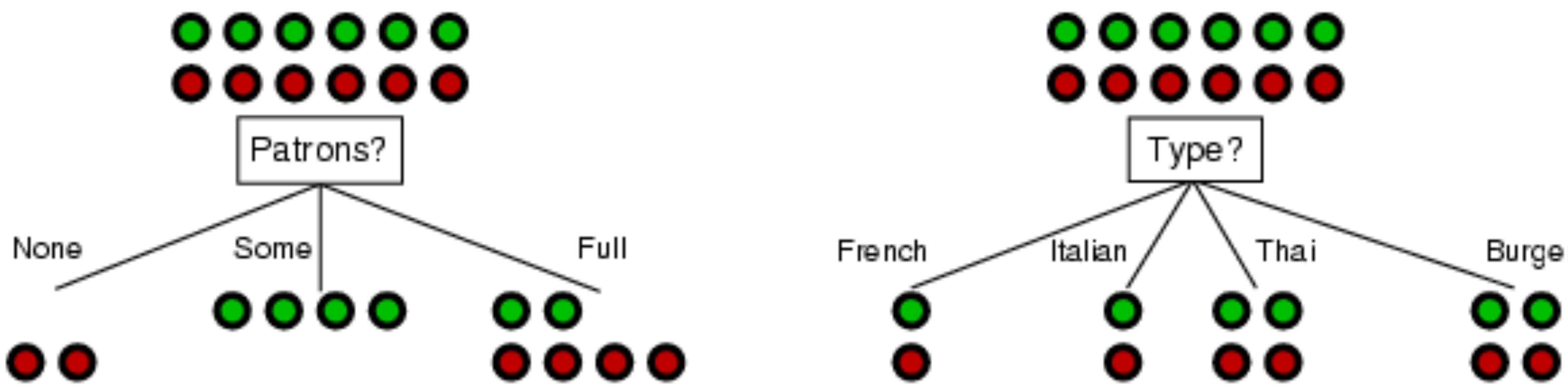


Which is better: *Patrons?* or *Type?*

Choosing an attribute

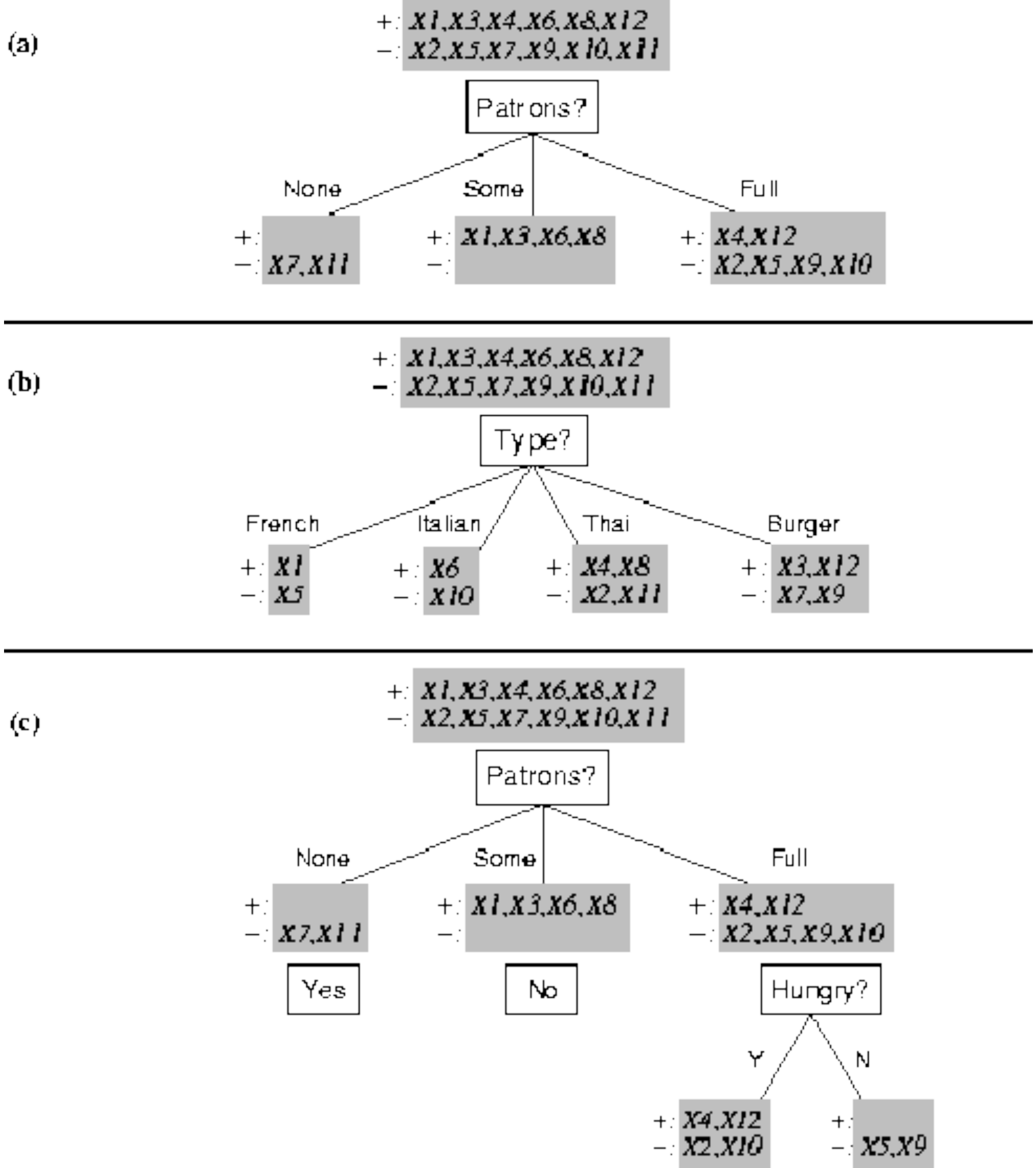
stay
leave

Idea: good attribute splits examples into subsets that are (ideally) *all positive* or *all negative*

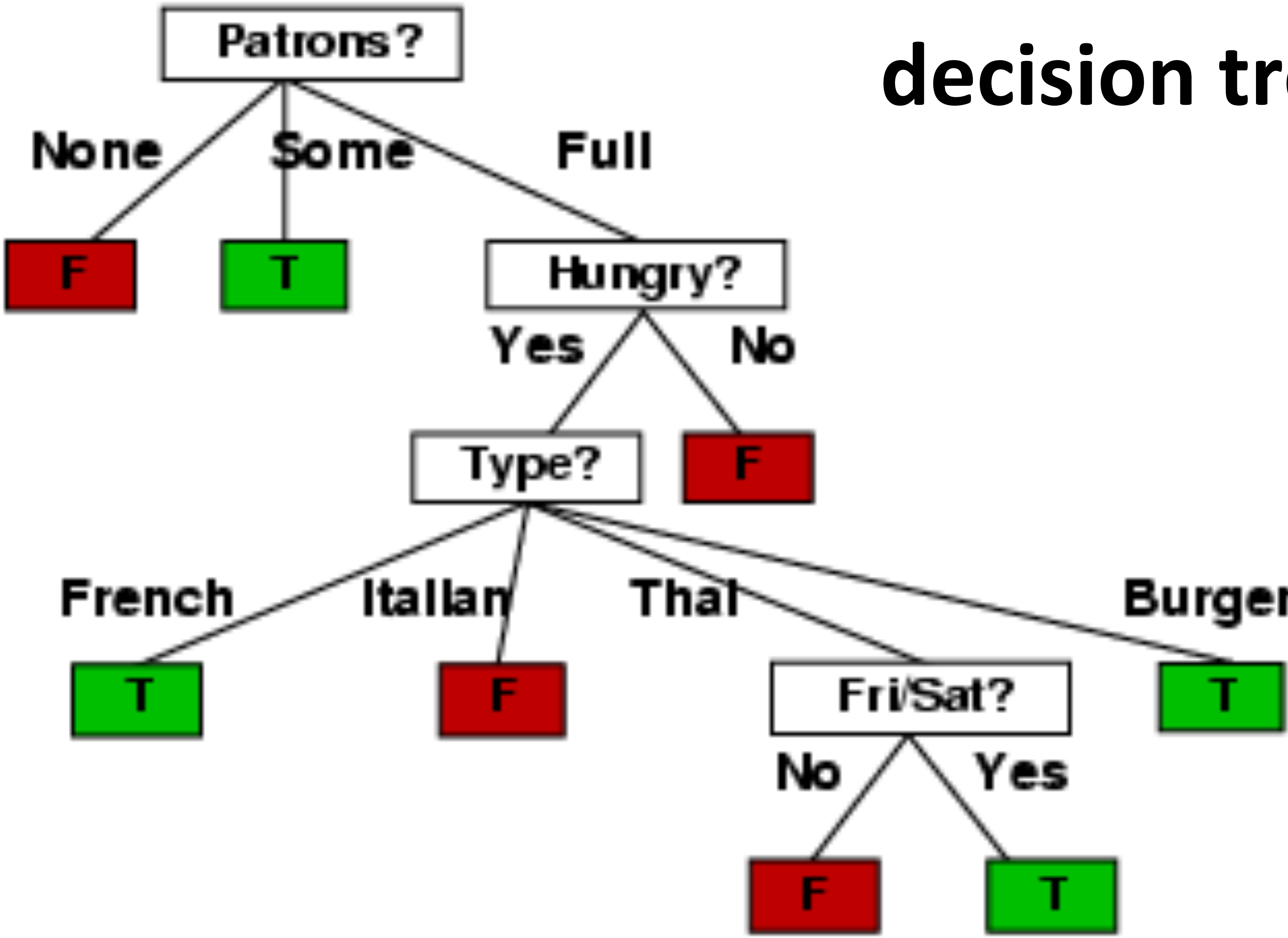


- **Patrons:** for six examples we know the answer and for six we can predict with prob. 0.67
- **Type:** our prediction is no better than chance (0.50)

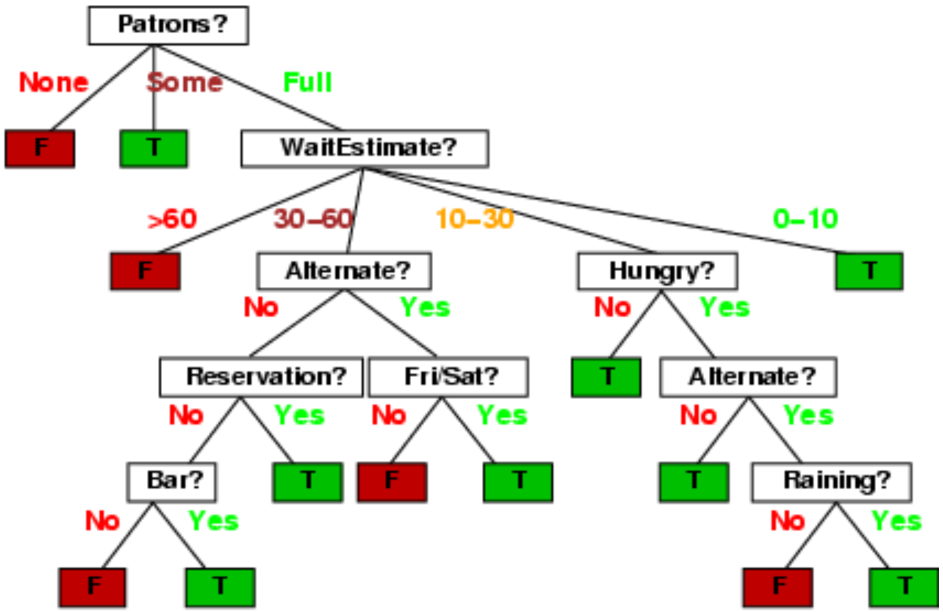
Splitting examples by testing attributes



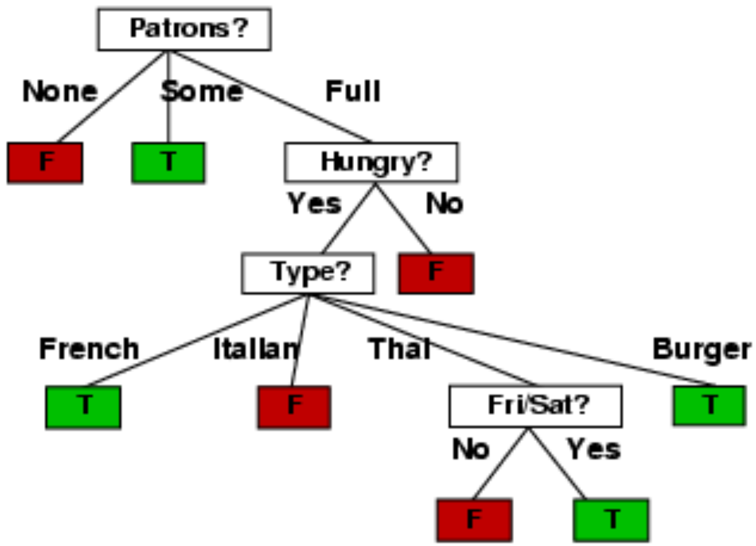
ID3-induced decision tree



Compare the two Decision Trees



Human-generated decision tree



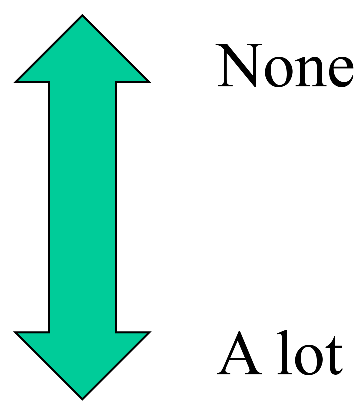
ID3-generated decision tree

Information theory 101

- Sprang fully formed from Claude Shannon's seminal work: Mathematical Theory of Communication in 1948
- Intuitions
  - Common words (a, the, dog) shorter than less common ones (parlimentarian, foreshadowing)
  - Morse code: common letters have shorter encodings
- Information inherent in data/message (inform-ation entropy) measured in minimum number of bits needed to store/send using a good encoding

Information theory 101

- Information entropy ... tells how much information there is in an event. More uncertain an event is, more information it contains
- Receiving a message is an event
- How much information is in these messages
  - The sun rose today!
  - It’s sunny today in Honolulu!
  - The coin toss is heads!
  - It’s sunny today in Seattle!
  - Life discovered on Mars!



Information theory 101

- For **n equally probable** possible messages or data values, each has probability **1/n**
- Information of a message is -log(p) = log(n)

  e.g., with 16 messages, then log(16) = 4 and we need 4 bits to identify/send each message
- For **probability distribution P** $(p_1, p_2 \ldots p_n)$ for n messages, its information (aka H or *entropy*) is:

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

Entropy of a distribution

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

- Examples:
  - If P is (0.5, 0.5) then I(P) = 0.5*1 + 0.5*1 = 1
  - If P is (0.67, 0.33) then I(P) = -(2/3*log(2/3) + 1/3*log(1/3)) = 0.92
  - If P is (1, 0) then I(P) = 1*1 + 0*log(0) = 0
- More **uniform probability** distribution, **greater its information**: more information is conveyed by a message telling you which event actually occurred
- Entropy is the average number of bits/message needed to represent a stream of messages

Example: Huffman code

- In 1952, MIT student David Huffman devised (for a homework assignment!) a coding scheme that's optimal when all data probabilities are powers of 1/2
- A Huffman code can be built as followings:
  - Rank symbols in order of probability of occurrence
  - Successively combine 2 symbols of lowest probability to form new symbol; eventually we get binary tree where each node is probability of nodes below
  - Trace path to each leaf, noting direction at each node

Huffman code example

M	P
A	.125
B	.125
C	.25
D	.5

Huffman code example

M	P
A	.125
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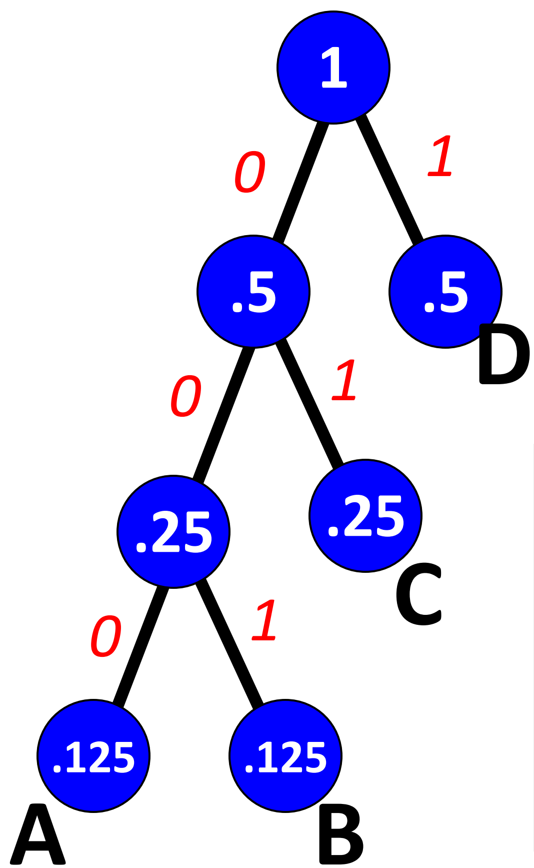
D	.5



M	code	length	prob	
A	000	3	0.125	0.375
B	001	3	0.125	0.375
C	01	2	0.250	0.500
D	1	1	0.500	0.500
average message length				1.750

If we use this code to many messages (A,B,C or D) with this probability distribution, then, over time, the average bits/message should approach 1.75

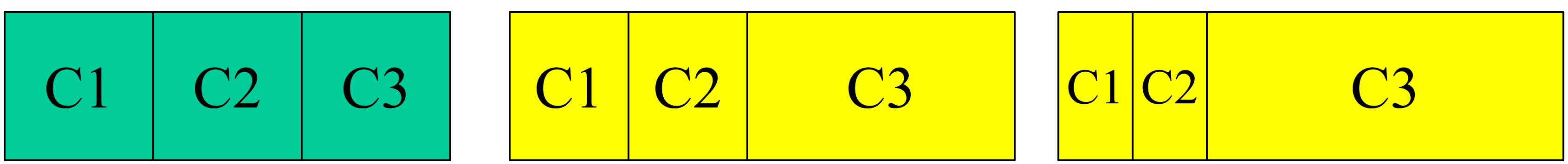
Information for classification

To divide T records is into disjoint "answer" classes ($C_1..C_k$), the information needed to identify class of element of T is:

$$Info(T) = I(P)$$

where P is the probability distribution of partition ($C_1, C_2, .., C_k$):

$$Info(T) = (|C_1|/|T|, |C_2|/|T|, ..., |C_k|/|T|)$$

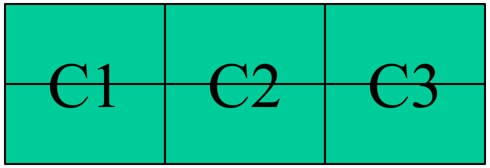


High information　　Lower information　　Still lower

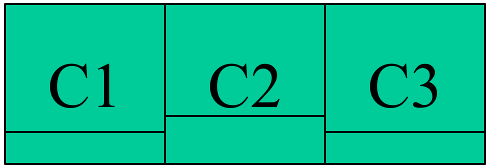
Information for classification II

If we further divide T w.r.t. attribute X into sets $\{T_1, T_2, .., T_n\}$, the information needed to identify class of an element of T is weighted average of information needed to identify class of an element of T_i, i.e., weighted average of $Info(T_i)$:

$$Info(X,T) = \sum |T_i|/|T| * Info(T_i)$$



High information



Low information

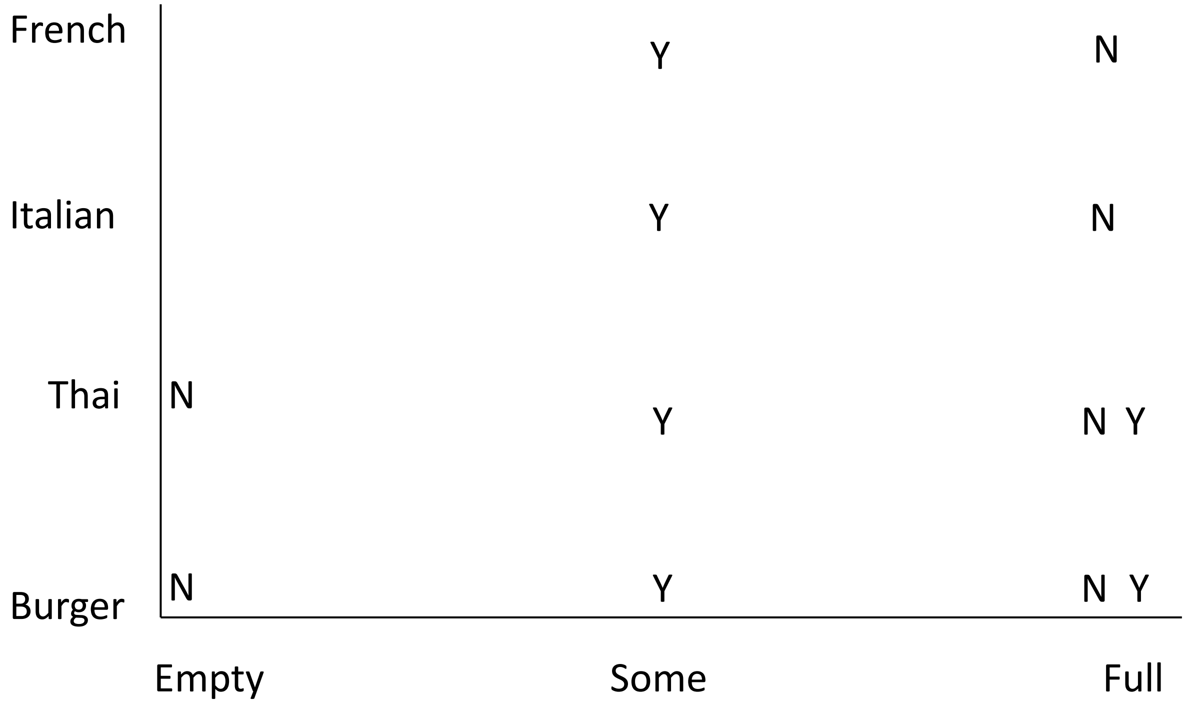
Information gain

- **Gain(X,T) = Info(T) - Info(X,T)** is difference of
  - info needed to identify element of T and
  - info needed to identify element of T after value of attribute X known
- This is gain in information due to attribute X
- Used to rank attributes and build DT where each node uses attribute with greatest gain of those not yet considered in path from root
- goal: **create small DTs** to minimize questions

Computing Information Gain

Should we ask about restaurant type or how many patrons there are?

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



Gain (Patrons, T) = ?

Gain (Type, T) = ?

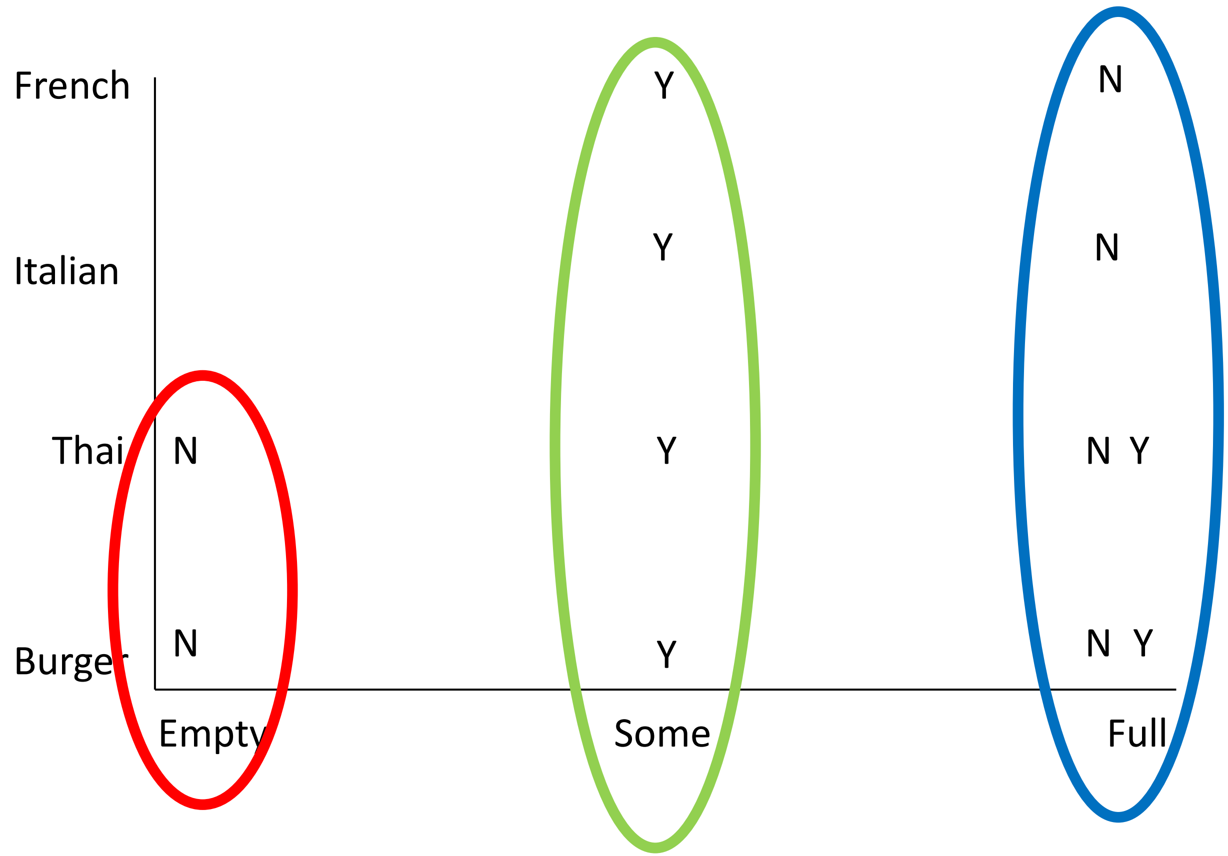
$$I(P) = -(p_1 * \log(p_1) + p_2 * \log(p_2) + .. + p_n * \log(p_n))$$

Computing information gain

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

I (Pat, T) =
2/12 (0) + 4/12 (0) +
6/12 (- (4/6 log 4/6 +
2/6 log 2/6))
= 1/2 (2/3*.6 +
1/3*1.6)
= .47

I (Type, T) =
2/12 (1) + 2/12 (1) +
4/12 (1) + 4/12 (1) = 1



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

Gain (Type, T) = 1 – 1 = 0

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

Computing information gain

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

I (Pat, T) =
2/12 (0) + 4/12 (0) +
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= 1/2 (2/3*.6 +
1/3*1.6)
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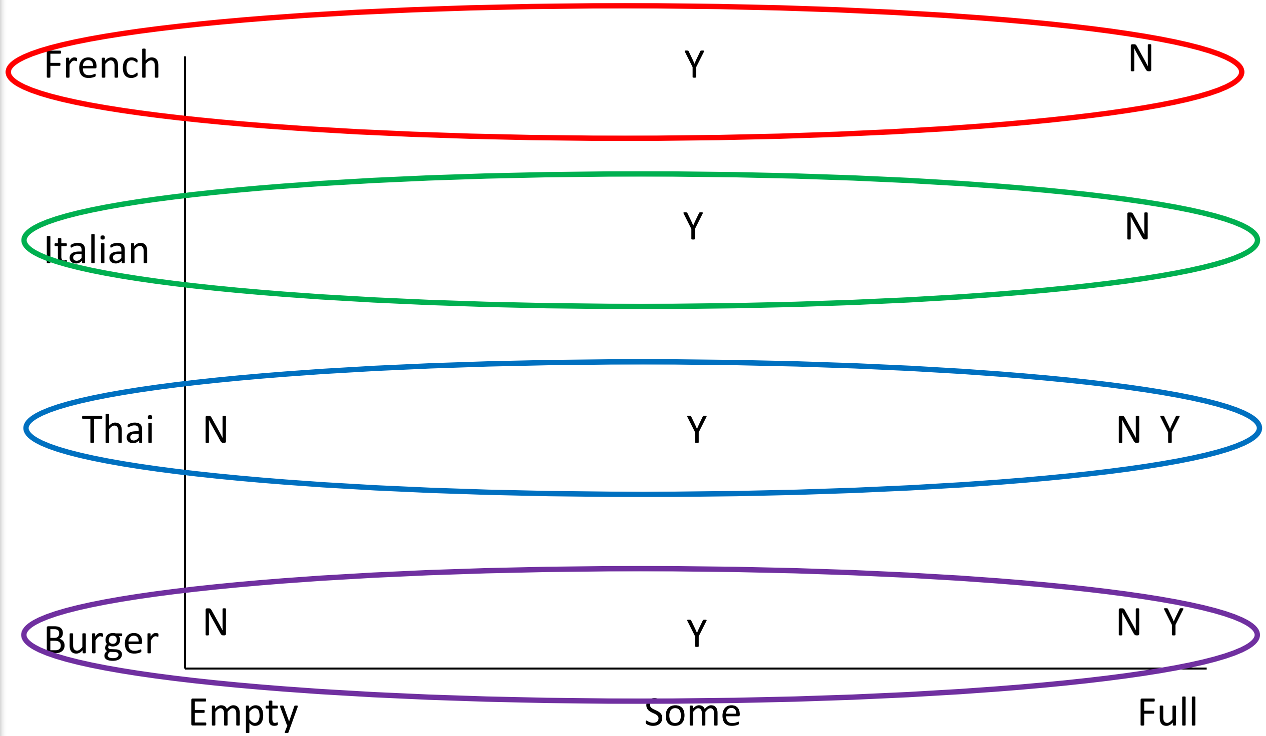


Gain (Patrons, T) = 1 - .47 = .53

Gain (Type, T) = 1 – 1 = 0

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

How well does it work?

Case studies show that decision trees often at least as accurate as human experts

- Study for diagnosing breast cancer had humans correctly classifying examples 65% of the time; DT classified 72% correct
- British Petroleum designed DT 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

Extensions of ID3

- Using alternate selection metric gain ratios, …
- Real-valued data
- Noisy data and overfitting
- Generation of rules
- Setting parameters
- Cross-validation for experimental validation of performance
- **C4.5:** extension of ID3 accounting for unavailable values, continuous attribute value ranges, pruning of decision trees, rule derivation, etc.

Real-valued data?

Many ML systems work only on nominal data

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

Noisy data?

ML systems must deal with *noise* in training data

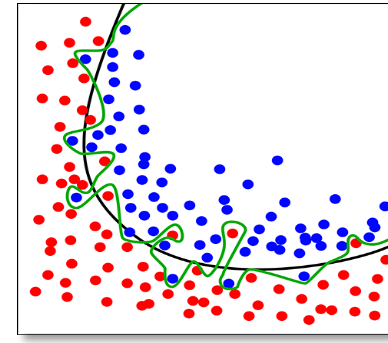
- Two examples have same attribute/value pairs, but different classifications
- Some attribute values wrong due to errors in the data acquisition or preprocessing phase
- Classification is wrong (e.g., + instead of -) because of some error
- Some attributes irrelevant to decision-making, e.g., color of a die is irrelevant to its outcome

Bias in the training data is a related problem

If it's cloudy, that's a tank

- You may hear the story of a machine learning system designed to classify images as those with camouflaged tanks and those without
- It was trained on N images with tanks and M images with no tanks
- But the positive examples were all taken on a cloudy day; the negative on a sunny one
- System worked well, but had learned to detect the weather ☹
- The story is too good to be true; see Neural Net Tank Urban Legend

Overfitting ☹



- *Overfitting* occurs when a statistical model describes random error or noise instead of underlying relationship
- If hypothesis space has many dimensions (many attributes) we may find **meaningless regularity** in data irrelevant to true distinguishing features

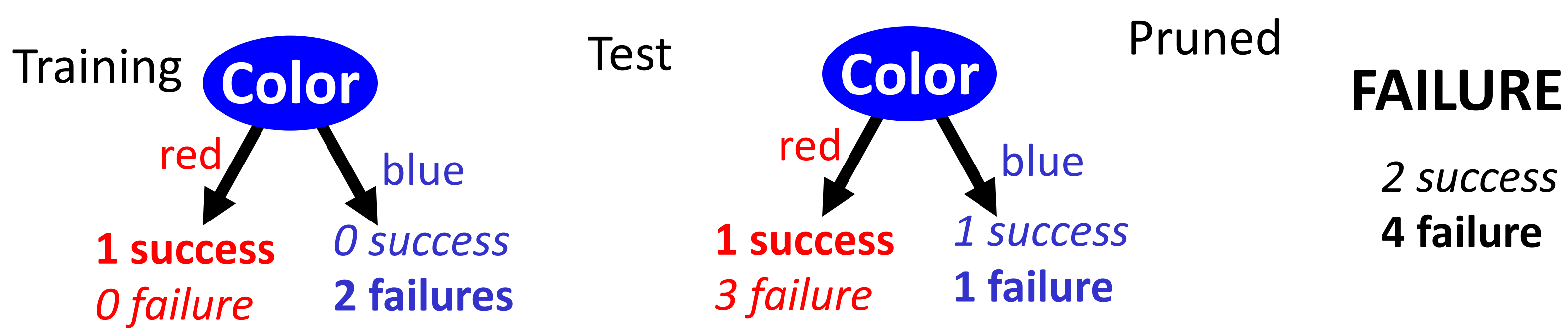
  Students with an *m* in first name, born in July, & whose SSN digits sum to a prime number get better grades in AI
- If we have **too little training data**, even a reasonable hypothesis space can overfit

Avoiding Overfitting

- Remove obviously irrelevant features
  - E.g., remove 'year observed', 'month observed', 'day observed', 'observer name' from feature vector
- Getting more training data
- Pruning lower nodes in a decision tree
  - E.g., if gain of best attribute at a node is below a threshold, stop and make this node a leaf rather than generating children nodes

Pruning decision trees

- Pruning a decision tree is done by replacing a whole subtree by a leaf node
- Replacement takes place if the expected error rate in the subtree is greater than in the single leaf, e.g.,
  - Training: 1 training red success and 2 training blue failures
  - Test: 3 red failures and one blue success
  - Consider replacing this subtree by a single Failure node.
- After replacement, only 2 errors instead of 5



Converting decision trees to rules

- Easy to get rules from decision tree: write rule for each path from the root to leaf
- Rule’s left-hand side built from the label of the nodes & labels of arcs
- Resulting rules set can be simplified:
  - Let LHS be the left hand side of a rule
  - LHS’ obtained from LHS by eliminating some conditions
  - Replace LHS by LHS' in this rule if the subsets of the training set satisfying LHS and LHS' are equal
  - A rule may be eliminated by using meta-conditions such as “if no other rule applies”

Summary: decision tree learning

- Widely used learning methods in practice for problems with relatively **few features**
- Strengths
  - Fast and simple to implement
  - Can convert result to a set of easily interpretable rules
  - Empirically valid in many commercial products
  - Handles noisy data
  - Easy for people to understand
- Weaknesses
  - Large decision trees may be hard to understand
  - Requires fixed-length feature vectors
  - Non-incremental (i.e., batch method)
  - Univariate splits/partitioning using only one attribute at a time so limits types of possible trees