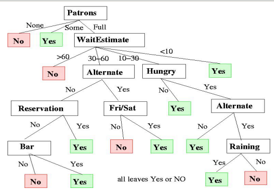
Machine Learning I: Decision Trees

AI Class 14 (Ch. 18.1–18.3)



Bookkeeping (Lots)

- Schedule mostly finalized
- HW4 due 11/8 @ 11:59
- No HW6
- Final date and time posted
- Full project description posted

<table>
<tr><td>Teams</td><td>now</td><td>Link on Piazza</td></tr>
<tr><td>Project Design</td><td>11/5</td><td rowspan="6">11:59 pm</td></tr>
<tr><td>HW 4</td><td>11/8</td></tr>
<tr><td>Phase 1</td><td>11/15</td></tr>
<tr><td>HW 5</td><td>11/20</td></tr>
<tr><td>Phase II</td><td>11/29</td></tr>
<tr><td>Final Writeup</td><td>12/11</td></tr>
<tr><td>Final Exam</td><td>12/19</td><td>1:00-3:00</td></tr>
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Today's Class

- Machine learning
  - What is ML?
  - Inductive learning ← Review: What is induction?
    - Supervised
    - Unsupervised
  - Decision trees
- Later: Bayesian learning, naïve Bayes, and BN learning

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?

- Discover previously-unknown new things or structure
  - Data mining, scientific discovery
- Fill in skeletal or incomplete domain knowledge
  - 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 agents that can adapt to users or other agents
- Understand and improve efficiency of human learning
  - Use to improve methods for teaching and tutoring people (e.g., better computer-aided instruction)

Pre-Reading Quiz

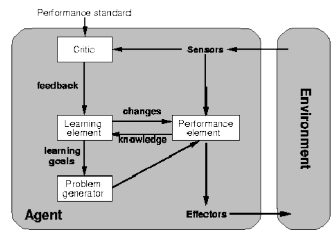
- What's supervised learning?
  - What's classification? What's regression?
  - What's a hypothesis? What's a hypothesis space?
  - What are the training set and test set?
  - What is Ockham's razor?
- What's unsupervised learning?

Some Terminology

The Big Idea: given some data, you learn a model of how the world works that lets you predict new data.

- **Training Set:** Data from which you learn initially.
- **Model:** What you learn. A "model" of how inputs are associated with outputs.
- **Test set:** New data you test tour model against.
- **Corpus:** A body of data. (pl.: corpora)
- **Representation:** The computational expression of data

A General Model of Learning Agents



Major Paradigms of Machine Learning

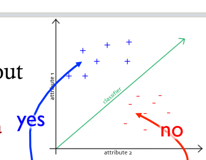
- **Rote learning:** 1:1 mapping from **inputs** to stored representation
  - You've seen a problem before
  - Learning by memorization
  - Association-based storage and retrieval
- **Induction:** Specific examples → general conclusions
- **Clustering:** Unsupervised grouping of data

Major Paradigms of Machine Learning

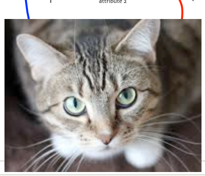
- **Analogy:** Model is **correspondence** between two different **representations**
- **Discovery:** Unsupervised, specific goal not given
- **Genetic algorithms:** "Evolutionary" search techniques
  - Based on an analogy to "survival of the fittest"
  - Surprisingly hard to get right/working
- **Reinforcement:** Feedback (positive or negative reward) given at the end of a sequence of steps

The Classification Problem

- Extrapolate from **examples** to make accurate **predictions** about future data points
  - Examples are called **training data**

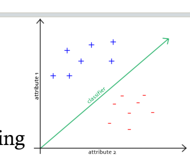


- Predict into **classes**, based on attributes ("**features**")
  - Example: it has tomato sauce, cheese, and no bread. Is it pizza?
  - Example: does this image contain a cat?



Supervised vs. Unsupervised

- Goal: Learn an unknown function $f(X) = Y$, where
  - X is an input example
  - Y is the desired output. (f is the..?)
- **Supervised learning:** given a training set of (X, Y) pairs by a "teacher"

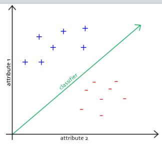


X			*Y*
bread	cheese	tomato sauce	**pizza**
¬ bread	¬ cheese	tomato sauce	**¬ not pizza**
bread	cheese	¬ tomato sauce	gross pizza but still **pizza**
lots more rows…			

"class labels" provided

Supervised vs. Unsupervised

- Goal: Learn an unknown function $f(X) = Y$, where
  - X is an input example
  - Y is the desired output. (f is the..?)
- **Unsupervised learning:** only given Xs and some (eventual) feedback



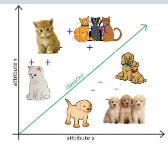
	X	
bread	cheese	tomato sauce
¬ bread	¬ cheese	tomato sauce
bread	cheese	¬ tomato sauce
	lots more rows…	

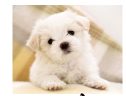
I think:
pizza,
¬ pizza,
¬ pizza

67% right

Concept Learning

- Concept learning or classification (aka "induction")
  - Given a set of examples of some concept/class/category:
    1. Determine if a given example is an instance of the concept (class member) or not
    2. If it **is**: **positive example**
    3. If it **is not**: **negative example**
    4. Or we can make a probabilistic prediction (e.g., using a Bayes net)

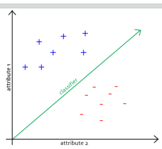




cat?

Supervised Concept Learning

- Given a training set of positive and negative examples of a concept
- Construct a description (model) that will accurately classify whether future examples are positive or negative



- I.e., learn estimate of function f given a training set:
  $\{(x_1, y_1), (x_2, y_2), \ldots, (x_n, y_n)\}$
  where each y_i is either + (positive) or - (negative), or a probability distribution over +/-

Inductive Learning Framework

- Raw input data from sensors preprocessed to obtain **feature vector**, **X**
- **Relevant** features for classifying examples
- Each **X** is a list of (attribute, value) pairs
- ***n*** attributes (a.k.a. features): fixed, positive, and finite
- Features have fixed, finite number # of possible values
  - Or continuous within some well-defined space, e.g., "age"
- Each example is a point in an *n*-dimensional feature space
  - X = [Person:Sue, EyeColor:Brown, Age:Young, Sex:Female]
  - X = [Cheese:*f*, Sauce:*t*, Bread:*t*]
  - X = [Texture:Fuzzy, Ears:Pointy, Purrs:Yes, Legs:4]

Inductive Learning as Search

- **Instance space, I,** is set of all possible examples
  - Defines the **language** for the training and test instances
  - Usually each instance i ∈ I is a **feature vector**
  - Features are also sometimes called *attributes* or *variables*

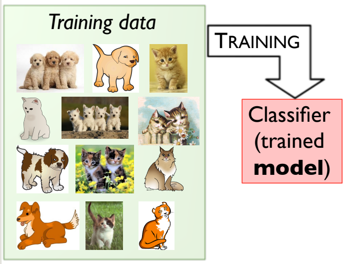
$$I: V_1 \times V_2 \times \ldots \times V_k,\ i = (v_1, v_2, \ldots, v_k)$$

- Class variable C gives an instance's class (to be predicted)

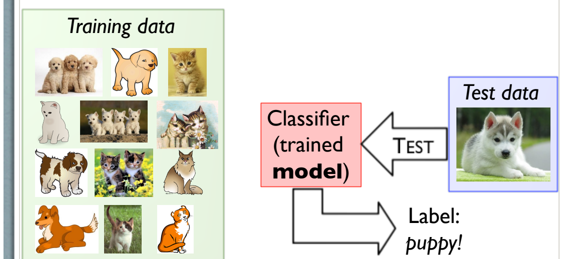
Inductive Learning as Search

- C gives an instance's class
- Model space M defines the possible **classifiers**
  - $M: I \rightarrow C$, $M = \{m_1, \ldots m_n\}$ (possibly infinite)
  - Model space is sometimes defined using same features as instance space (not always)
- Training data lets us search for a good (consistent, complete, simple) hypothesis in the model space
- The learned model is a classifier

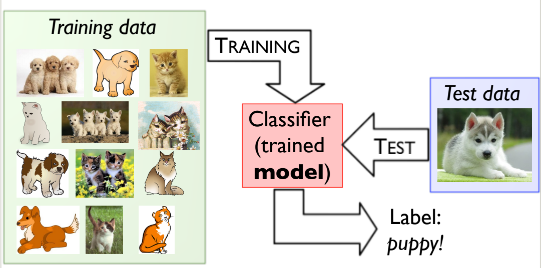
Inductive Learning Pipeline



Inductive Learning Pipeline



Inductive Learning Pipeline



Inductive Learning Pipeline

Training data, X

Text-ure	*Ears*	*Legs*	*Class*
Fuzzy	Round	4	+
Slimy	Missing	8	-
Fuzzy	Pointy	4	-
Fuzzy	Round	4	+
Fuzzy	Pointy	4	+
…			

TRAINING

Classifier (trained **model**)

TEST

Test data

x_1 = <Fuzzy, Pointy, 4>

Label: +

Model Spaces (1)

- Decision trees
  - Partition the instance space **I** into axis-parallel regions
  - Labeled with class value
- Nearest-neighbor classifiers
  - Partition the instance space **I** into regions defined by centroid instances (or cluster of k instances)
- Bayesian networks
  - Probabilistic dependencies of class on attributes
  - Naïve Bayes: special case of BNs where class → each attribute

Model Spaces (2)

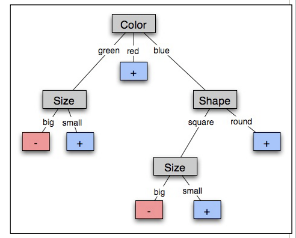
- Neural networks
  - Nonlinear feed-forward functions of attribute values
- Support vector machines
  - Find a separating plane in a high-dimensional feature space
- Associative rules (feature values → class)
- First-order logical rules

Decision Trees

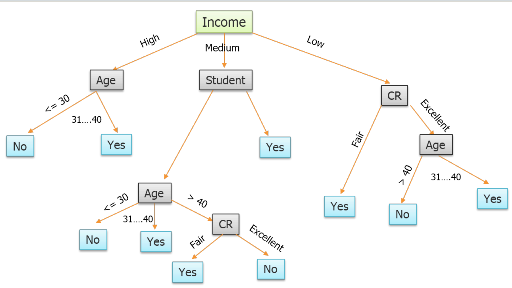
- **Goal:** Build a tree to classify examples as positive or negative instances of a concept using supervised learning from a training set
- A decision tree is a tree where:
  - Each **non-leaf** node is an attribute (feature)
  - Each **leaf** node is a classification (+ or -)
    - Positive and negative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

Learning Decision Trees

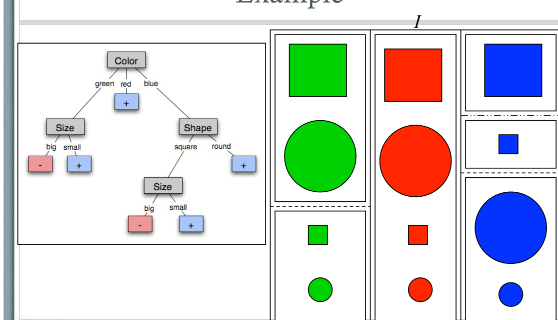
- Each **non-leaf** node is associated with an attribute (feature)
- Each **leaf** node is associated with a classification (+ or -)
- Each **arc** is associated with one possible value of the attribute at the node from which the arc is directed



Will You Buy My Product?



Decision Tree-Induced Partition – Example



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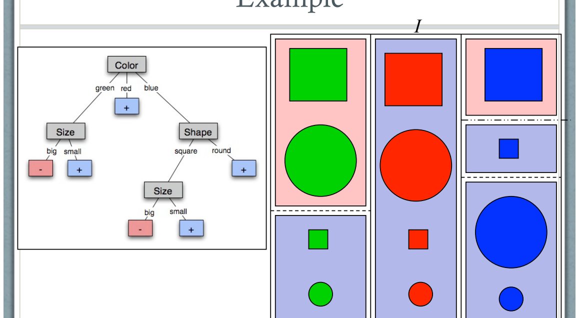
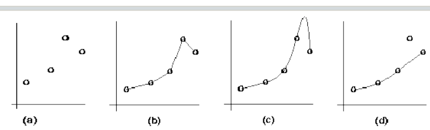


Inductive Learning and Bias



- We want to learn a function f(x) = y
  - We are given sample (x,y) pairs, as in figure (a)
  - Several hypotheses for this function: (b), (c) and (d) (and others)
- A preference here reveals our learning technique's **bias**
  - 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
- Stated by William of Ockham (1285-1347/49):
  - *"Non sunt multiplicanda entia praeter necessitatem"*
  - "Entities are not to be multiplied beyond necessity"
- **"The simplest consistent explanation is the best."**
- Smallest decision tree that correctly classifies all training examples
- 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

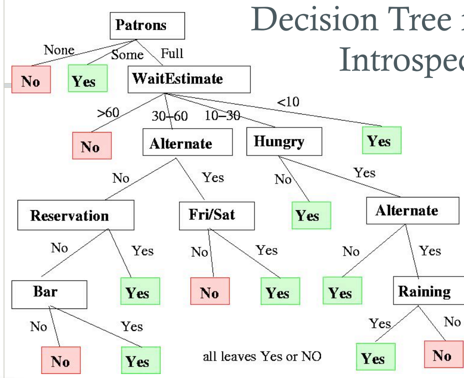
- Model decision a patron makes when deciding whether to wait for a table
  - Two classes (outcomes): wait, leave
  - Ten attributes: Alternative available? ∃ Bar? Is it Friday? Hungry? How full is restaurant? How expensive? Is it raining? Do we have a reservation? What type of restaurant is it? What's purported waiting time?
- Training set of 12 examples
- ~ 7000 possible cases

A Training Set

Datum	Attributes										Outcome
	Alt	Bar	Fri	Hun	Pat	Price	Rain	Res	Type	Est	Wait
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	£	Yes	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

Problem from R&N, table from Dr. Manfred Kerber @ Birmingham, with thanks – www.cs.bham.ac.uk/~mmk/Teaching/AI/l3.html

Decision Tree from Introspection



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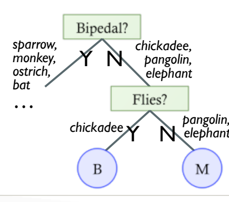
ID3/C4.5

- A **greedy** algorithm for decision tree construction
  - Ross Quinlan, 1987
- Construct decision tree top-down by recursively selecting the "best attribute" to use at current node
  1. Select attribute for current node
  2. Generate child nodes (one for each possible value of attribute)
  3. Partition training data using attribute values
  4. Assign subsets of examples to the appropriate child node
  5. Repeat for each child node until all examples associated with a node are either all positive or all negative

Bird or Mammal?

1. Select attribute
2. Generate child nodes
3. Partition examples
4. Assign examples to child
5. Repeat until examples are +ve or -ve

Examples (training data)	Attributes			Outcome
	Bi-pedal	Flies	Feath-ers	
Sparrow	Y	Y	Y	B
Monkey	Y	N	N	M
Ostrich	Y	N	Y	B
Pangolin	N	N	N	M
Bat	Y	Y	N	M
Elephant	N	N	N	M
Chickadee	N	Y	Y	B



Test

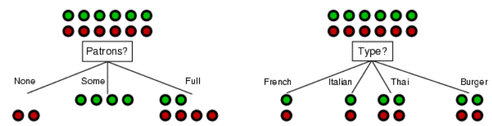
mouse: <B:N, Fl:N, Fe:N>

Choosing the Best Attribute

- **Key problem:** what attribute to split on?
- Some possibilities are:
  - **Random:** Select any attribute at random
  - **Least-Values:** Choose attribute with smallest number of values
  - **Most-Values:** Choose attribute with largest number of values
  - **Max-Gain:** Choose attribute that has the largest expected information gain—the attribute that will result in the smallest expected size of the subtrees rooted at its children
- ID3 uses Max-Gain to select the best attribute

Choosing an Attribute

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



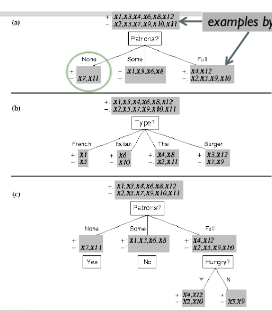
- Which is better: *Patrons?* or *Type?*
- **Why?**

Restaurant Example

- What do these approaches split restaurants on, given the data in the table?
  - **Random:** Patrons or Type
  - **Least-values:** Patrons
  - **Most-values:** Type
  - **Max-gain:** ???

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

Splitting Examples by Testing Attributes



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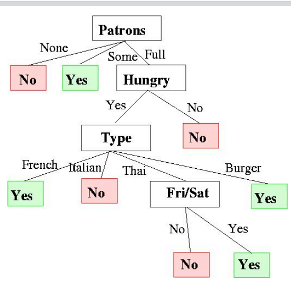
X_8	No	No	No	Yes	Some	££	Yes	Yes	Thai	0-10	Yes
X_9	No	Yes	Yes	No	Full	£	Yes	No	Burger	>60	No
X_{10}	Yes	Yes	Yes	Yes	Full	£££	No	Yes	Italian	10-30	No
X_{11}	No	No	No	No	None	£	No	No	Thai	0-10	No
X_{12}	Yes	Yes	Yes	Yes	Full	£	No	No	Burger	30-60	Yes

ID3-induced Decision Tree



Information Theory 101

- **Information:** 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"
- Intuition: minimize effort to communicate/store
  - Common words (a, the, dog) are shorter than less common ones (parliamentarian, foreshadowing)
  - In Morse code, common (probable) letters have shorter encodings

"A Mathematical Theory of Communication," Bell System Technical Journal, 1948, Claude E. Shannon, Bell Labs

Information Theory 102

- Information is measured in **bits.**
- Information in a message depends on its probability.
- Given *n* equally probable possible messages, what is probability p_n of each one?

  1/n

- Information conveyed by a message is $\log_2(n) = -\log_2(p)$
- Example: with 16 possible messages, $\log_2(16) = 4$, and we need 4 bits to identify/send each message

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Information Theory 102.b

- Information conveyed by a message is $\log_2(n) = -\log_2(p)$
- Given a probability distribution for n messages:

  $P = (p_1,p_2...p_n)$

- The information conveyed by that distribution is:

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

- This is the **entropy** of P.

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Information Theory 103

- Entropy: **average** number of bits (per message) needed to represent a stream of messages

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

- Examples:
  - P = (0.5, 0.5) : I(P) = 1 → entropy of a fair coin flip
  - P = (0.67, 0.33) : I(P) = 0.92
  - P = (0.99, 0.01) : I(P) = 0.08
  - P = (1, 0) : I(P) = 0
- **As the distribution becomes more skewed, the amount of information *decreases.* Why?**
- **Because I can just predict the most likely element, and usually be right**

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Entropy as Measure of **Homogeneity of Examples**

- Entropy can be used to characterize the (im)purity of an arbitrary collection of examples
- **Low entropy** implies **high homogeneity**
  - Given a collection *S* (like the table of 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

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Information Gain

- **Information gain**: how much entropy decreases (homogeneity increases) when a dataset is split on an attribute.
  - High homogeneity → high likelihood samples will have the same class
- Constructing a decision tree is all about finding attribute that returns the highest information gain (i.e., the most homogeneous branches)

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Information Gain, cont.

- Use to rank attributes and build DT (decision tree)!
- Choose nodes using attribute with **greatest gain**
  - → means least information remaining after split
  - I.e., subsets are all as skewed as possible
- Why?
  - Create small decision trees: predictions can be made with few attribute tests
  - Try to find a minimal process that still captures the data (Occam's Razor)

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How Well Does it Work?

At least as accurate as human experts (sometimes)

- Diagnosing breast cancer: humans correct 65% of the time; decision tree classified 72% correct
- BP designed a decision tree for gas-oil separation for offshore oil platforms; 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 DT to classify sky objects **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 a (more applicable) extension of ID3 that accounts for real-world problems: unavailable values, continuous attributes, pruning decision trees, rule derivation, …

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

Converting Decision Trees to Rules

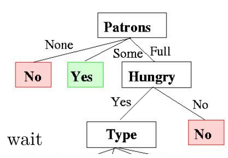
- 1 rule for each **path** in tree (from root to a leaf)
- Left-hand side: labels of nodes and arcs

  Pa.=None → Don't wait

  Pa.=Some → Wait

  Pa.=F ∧ Hu.=No → Don't wait

  etc…



- Resulting rules can be simplified and reasoned over

Simplifying Rules

- Let LHS be the left hand side of a rule
- Let LHS' be obtained from LHS by eliminating some conditions
- We can certainly replace LHS by LHS' in this rule if the subsets of the training set that satisfy respectively LHS and LHS' are equal
- A rule may be eliminated by using metaconditions such as "if no other rule applies"

Noisy Data

- Many kinds of "noise" can occur in the examples:
  - Two examples have same attribute/value pairs, but different classifications
  - Some values of attributes are incorrect because of errors in data acquisition or preprocessing phase
  - The classification is wrong (e.g., + instead of -) because of some error
  - Attributes irrelevant to the decision-making process
    - Color of a die is irrelevant to its outcome
    - Can still be in training data, can be chosen as an attribute

Overfitting

- Sometimes, model fits training data well but doesn't do well on test data
- Can be it "overfit" to the training data
  - Model is too **specific** to training data
  - Doesn't **generalize** to new information well

Examples (training data)	Attributes			Outcome
	Bi-pedal	Flies	Feath-ers	
Sparrow	Y	Y	Y	B
Monkey	Y	N	N	M
Ostrich	Y	N	Y	B
Bat	Y	Y	N	M
Elephant	N	N	N	M

- Learned model: (Y∧Y∧Y→B ∨ Y∧N∧N→M ∨ ...)

Noisy Data and Overfitting

Examples (training data)	Attributes		Class
	Bi-pedal	Feath-ers	
Sparrow	Y	Y	B
Monkey	Y	N	M
Ostrich	Y	Y	B
Bat	Y	N	M
Elephant	N	N	M

- Irrelevant attributes → overfitting
- If hypothesis space has many dimensions (many attributes), may find **meaningless regularity**
  - Ex: Name starts with [A-M] → Mammal
- One fix: prune lower nodes in the decision tree
  - Ex: if Gain of best attribute at a node is below a threshold, stop; make a leaf rather than generating children

Measuring Model Quality

- How good is a model?
  - Predictive accuracy on test data
  - 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
- Overfitting: coming up with a model that is TOO specific to your training data

Measuring Model Quality

- 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 kth 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

Summary: Decision Tree Learning

- 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:
  - Univariate splits/partitioning using only one attribute at a time (limits types of possible trees)
  - Large decision trees may be hard to understand
  - Requires fixed-length feature vectors
  - Non-incremental (i.e., batch method)

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