Lecture 4

Decision Trees

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William H. Hsu
Department of Computing and Information Sciences, KSU
http://www.cis.ksu.edu/~bhsu

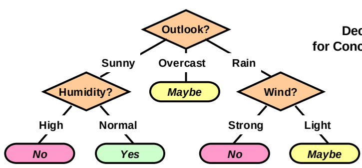
Readings:
Sections 3.1-3.5, Mitchell
Chapter 18, Russell and Norvig
MLC++, Kohavi *et al*

Lecture Outline

- Read 3.1-3.5, Mitchell; Chapter 18, Russell and Norvig; Kohavi *et al* paper
- Handout: "Data Mining with *MLC++*", Kohavi *et al*
- Suggested Exercises: 18.3, Russell and Norvig; 3.1, Mitchell
- Decision Trees (DTs)
  - Examples of decision trees
  - Models: when to use
- Entropy and Information Gain
- *ID3* Algorithm
  - Top-down induction of decision trees
    - Calculating reduction in entropy (information gain)
    - Using information gain in construction of tree
  - Relation of *ID3* to hypothesis space search
  - Inductive bias in *ID3*
- Using *MLC++* (Machine Learning Library in C++)
- Next: More Biases (Occam's Razor); Managing DT Induction

Decision Trees

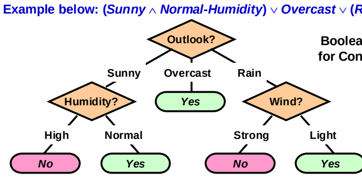
- Classifiers
  - Instances (unlabeled examples): represented as attribute ("feature") vectors
- Internal Nodes: Tests for Attribute Values
  - Typical: equality test (e.g., "Wind = ?")
  - Inequality, other tests possible
- Branches: Attribute Values
  - One-to-one correspondence (e.g., "Wind = Strong", "Wind = Light")
- Leaves: Assigned Classifications (Class Labels)



Decision Tree
for Concept *PlayTennis*

Boolean Decision Trees

- Boolean Functions
  - Representational power: universal set (i.e., can express any boolean function)
  - Q: Why?
    - A: Can be rewritten as rules in Disjunctive Normal Form (DNF)
    - Example below: ($Sunny \wedge Normal\text{-}Humidity$) $\vee$ $Overcast$ $\vee$ ($Rain \wedge Light\text{-}Wind$)



Boolean Decision Tree
for Concept *PlayTennis*

- Other Boolean Concepts (over Boolean Instance Spaces)
  - $\wedge, \vee, \oplus$ (XOR)
  - $(A \wedge B) \vee (C \wedge \neg D \wedge E)$
  - *m-of-n*

A Tree to Predict C-Section Risk

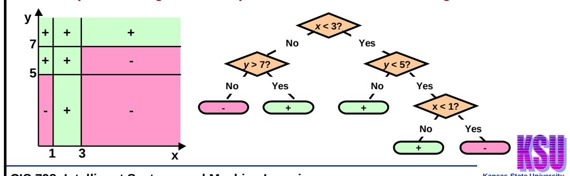
- Learned from Medical Records of 1000 Women
- Negative Examples are Cesarean Sections
  - Prior distribution: [833+, 167-] 0.83+, 0.17-
  - *Fetal-Presentation* = 1: [822+, 167-] 0.88+, 0.12-
    - *Previous-C-Section* = 0: [767+, 81-] 0.90+, 0.10-
      - *Primiparous* = 0: [399+, 13-] 0.97+, 0.03-
      - *Primiparous* = 1: [368+, 68-] 0.84+, 0.16-
        - *Fetal-Distress* = 0: [334+, 47-] 0.88+, 0.12-
          - *Birth-Weight* < 3349 0.95+, 0.05-
          - *Birth-Weight* $\geq$ 3347 0.78+, 0.22-
        - *Fetal-Distress* = 1: [34+, 21-] 0.62+, 0.38-
    - *Previous-C-Section* = 1: [55+, 35-] 0.61+, 0.39-
  - *Fetal-Presentation* = 2: [3+, 29-] 0.11+, 0.89-
  - *Fetal-Presentation* = 3: [8+, 22-] 0.27+, 0.73-

When to Consider Using Decision Trees

- Instances Describable by Attribute-Value Pairs
- Target Function Is Discrete Valued
- Disjunctive Hypothesis May Be Required
- Possibly Noisy Training Data
- Examples
  - Equipment or medical diagnosis
  - Risk analysis
    - Credit, loans
    - Insurance
    - Consumer fraud
    - Employee fraud
  - Modeling calendar scheduling preferences (predicting quality of candidate time)

Decision Trees and Decision Boundaries

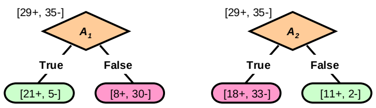
- Instances Usually Represented Using Discrete Valued Attributes
  - Typical types
    - Nominal ({red, yellow, green})
    - Quantized ({low, medium, high})
  - Handling numerical values
    - Discretization, a form of vector quantization (e.g., histogramming)
    - Using thresholds for splitting nodes
- Example: Dividing Instance Space into Axis-Parallel Rectangles



Decision Tree Learning: Top-Down Induction (*ID3*)

- Algorithm *Build-DT* (*Examples*, *Attributes*)

  IF all examples have the same label THEN RETURN (leaf node with *label*)
  ELSE
  IF set of attributes is empty THEN RETURN (leaf with *majority label*)
  ELSE
  Choose best attribute *A* as root
  FOR each value *v* of *A*
  Create a branch out of the root for the condition *A* = *v*
  IF $\{x \in Examples: x.A = v\} = Ø$ THEN RETURN (leaf with *majority label*)
  ELSE *Build-DT* ($\{x \in Examples: x.A = v\}$, Attributes ~ {A})
- But Which Attribute Is Best?



Broadening the Applicability of Decision Trees

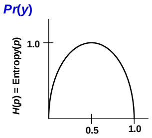
- Assumptions in Previous Algorithm
  - Discrete *output*
    - Real-valued outputs are possible
    - Regression trees [Breiman *et al*, 1984]
  - Discrete *input*
    - Quantization methods
    - *Inequalities* at nodes instead of equality tests (see rectangle example)
- Scaling Up
  - Critical in knowledge discovery and database mining (KDD) from very large databases (VLDB)
  - Good news: efficient algorithms exist for processing many *examples*
  - Bad news: much harder when there are too many *attributes*
- Other Desired Tolerances
  - Noisy data (classification noise ≡ incorrect labels; attribute noise ≡ inaccurate or imprecise data)
  - Missing attribute values

Choosing the "Best" Root Attribute

- Objective
  - Construct a decision tree that is a small as possible (Occam's Razor)
  - Subject to: consistency with labels on training data
- Obstacles
  - Finding the *minimal* consistent hypothesis (i.e., decision tree) is $\mathcal{NP}$-hard (D'oh!)
  - Recursive algorithm (*Build-DT*)
    - A greedy heuristic search for a simple tree
    - Cannot guarantee optimality (D'oh!)
- Main Decision: Next Attribute to Condition On
  - Want: attributes that split examples into sets that are relatively pure in one label
  - Result: closer to a leaf node
  - Most popular heuristic
    - Developed by J. R. Quinlan
    - Based on information gain
    - Used in *ID3* algorithm

Entropy: Intuitive Notion

- A Measure of Uncertainty
  - The Quantity
    - Purity: how close a set of instances is to having just one label
    - Impurity (disorder): how close it is to total uncertainty over labels
  - The Measure: Entropy
    - Directly proportional to impurity, uncertainty, irregularity, surprise
    - Inversely proportional to purity, certainty, regularity, redundancy
- Example
  - For simplicity, assume $\mathcal{H} = \{0, 1\}$, distributed according to $Pr(y)$
    - Can have (more than 2) discrete class labels
    - Continuous random variables: differential entropy
  - Optimal purity for *y*: either
    - $Pr(y = 0) = 1$, $Pr(y = 1) = 0$
    - $Pr(y = 1) = 1$, $Pr(y = 0) = 0$
  - What is the least pure probability distribution?
    - $Pr(y = 0) = 0.5$, $Pr(y = 1) = 0.5$
    - Corresponds to maximum impurity/uncertainty/irregularity/surprise
    - Property of entropy: concave function ("concave downward")



Entropy: Information Theoretic Definition

- Components
  - *D*: a set of examples $\{<x_1, c(x_1)>, <x_2, c(x_2)>, \ldots, <x_m, c(x_m)>\}$
  - $p_+ = Pr(c(x) = +)$, $p_- = Pr(c(x) = -)$
- Definition
  - *H* is defined over a probability density function *p*
  - *D* contains examples whose frequency of + and - labels indicates p_+ and p_- *for the observed data*
  - The entropy of *D* relative to *c* is:

$$H(D) \equiv -p_+ \log_b (p_+) - p_- \log_b (p_-)$$

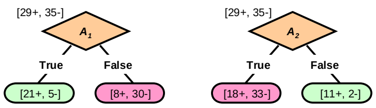
- What Units is H Measured In?
  - Depends on the base *b* of the log (bits for *b* = 2, nats for *b* = e, etc.)
  - A single bit is required to encode each example in the worst case ($p_+ = 0.5$)
  - If there is less uncertainty (e.g., $p_+ = 0.8$), we can use less than 1 bit each

Information Gain: Information Theoretic Definition

- Partitioning on Attribute Values
  - Recall: a partition of *D* is a collection of disjoint subsets whose union is *D*
  - Goal: *measure the uncertainty removed* by splitting on the value of attribute *A*
- Definition
  - The information gain of *D* relative to attribute *A* is the expected reduction in entropy due to splitting ("sorting") on A:

$$Gain(D,A) \equiv - H(D) - \sum_{v \in values(A)} \left[\frac{|D_v|}{|D|} \bullet H(D_v) \right]$$

  where D_v is $\{x \in D: x.A = v\}$, the set of examples in *D* where attribute *A* has value *v*
  - Idea: partition on *A*; scale entropy to the size of each subset D_v
- Which Attribute Is Best?



An Illustrative Example

- Training Examples for Concept *PlayTennis*

Day	Outlook	Temperature	Humidity	Wind	*PlayTennis*?
1	Sunny	Hot	High	Light	No
2	Sunny	Hot	High	Strong	No
3	Overcast	Hot	High	Light	Yes
4	Rain	Mild	High	Light	Yes
5	Rain	Cool	Normal	Light	Yes
6	Rain	Cool	Normal	Strong	No
7	Overcast	Cool	Normal	Strong	Yes
8	Sunny	Mild	High	Light	No
9	Sunny	Cool	Normal	Light	Yes
10	Rain	Mild	Normal	Light	Yes
11	Sunny	Mild	Normal	Strong	Yes
12	Overcast	Mild	High	Strong	Yes
13	Overcast	Hot	Normal	Light	Yes
14	Rain	Mild	High	Strong	No

- *ID3* ≡ *Build-DT* using *Gain*(•)
- How Will *ID3* Construct A Decision Tree?

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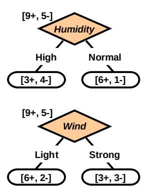
Constructing A Decision Tree for *PlayTennis* using *ID3* [1]

- Selecting The Root Attribute

Day	Outlook	Temperature	Humidity	Wind	*PlayTennis*?
1	Sunny	Hot	High	Light	No
2	Sunny	Hot	High	Strong	No
3	Overcast	Hot	High	Light	Yes
4	Rain	Mild	High	Light	Yes
5	Rain	Cool	Normal	Light	Yes
6	Rain	Cool	Normal	Strong	No
7	Overcast	Cool	Normal	Strong	Yes
8	Sunny	Mild	High	Light	No
9	Sunny	Cool	Normal	Light	Yes
10	Rain	Mild	Normal	Light	Yes
11	Sunny	Mild	Normal	Strong	Yes
12	Overcast	Mild	High	Strong	Yes
13	Overcast	Hot	Normal	Light	Yes
14	Rain	Mild	High	Strong	No



- Prior (unconditioned) distribution: 9+, 5-
  - *H*(*D*) = -(9/14) lg (9/14) - (5/14) lg (5/14) *bits* = 0.94 bits
  - *H*(*D*, *Humidity* = High) = -(3/7) lg (3/7) - (4/7) lg (4/7) = 0.985 bits
  - *H*(*D*, *Humidity* = Normal) = -(6/7) lg (6/7) - (1/7) lg (1/7) = 0.592 bits
  - *Gain*(*D*, *Humidity*) = 0.94 - (7/14) * 0.985 + (7/14) * 0.592 = 0.151 bits
  - Similarly, *Gain* (*D*, *Wind*) = 0.94 - (8/14) * 0.811 + (6/14) * 1.0 = 0.048 bits

$$Gain(D,A) \equiv - H(D) - \sum_{v \in values(A)} \left[\frac{|D_v|}{|D|} \bullet H(D_v) \right]$$

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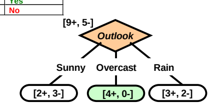
Constructing A Decision Tree for *PlayTennis* using *ID3* [2]

- Selecting The Root Attribute

Day	Outlook	Temperature	Humidity	Wind	*PlayTennis*?
1	Sunny	Hot	High	Light	No
2	Sunny	Hot	High	Strong	No
3	Overcast	Hot	High	Light	Yes
4	Rain	Mild	High	Light	Yes
5	Rain	Cool	Normal	Light	Yes
6	Rain	Cool	Normal	Strong	No
7	Overcast	Cool	Normal	Strong	Yes
8	Sunny	Mild	High	Light	No
9	Sunny	Cool	Normal	Light	Yes
10	Rain	Mild	Normal	Light	Yes
11	Sunny	Mild	Normal	Strong	Yes
12	Overcast	Mild	High	Strong	Yes
13	Overcast	Hot	Normal	Light	Yes
14	Rain	Mild	High	Strong	No

  - *Gain*(*D*, *Humidity*) = 0.151 bits
  - *Gain*(*D*, *Wind*) = 0.048 bits
  - *Gain*(*D*, *Temperature*) = 0.029 bits
  - *Gain*(*D*, *Outlook*) = 0.246 bits



- Selecting The Next Attribute (Root of Subtree)
  - Continue until every example is included in path or purity = 100%
  - What does purity = 100% mean?
  - Can *Gain*(*D*, *A*) < 0?

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Constructing A Decision Tree for *PlayTennis* using *ID3* [3]

- Selecting The Next Attribute (Root of Subtree)

Day	Outlook	Temperature	Humidity	Wind	*PlayTennis*?
1	Sunny	Hot	High	Light	No
2	Sunny	Hot	High	Strong	No
3	Overcast	Hot	High	Light	Yes
4	Rain	Mild	High	Light	Yes
5	Rain	Cool	Normal	Light	Yes
6	Rain	Cool	Normal	Strong	No
7	Overcast	Cool	Normal	Strong	Yes
8	Sunny	Mild	High	Light	No
9	Sunny	Cool	Normal	Light	Yes
10	Rain	Mild	Normal	Light	Yes
11	Sunny	Mild	Normal	Strong	Yes
12	Overcast	Mild	High	Strong	Yes
13	Overcast	Hot	Normal	Light	Yes
14	Rain	Mild	High	Strong	No

  - Convention: lg (0/a) = 0
  - *Gain*(D_{Sunny}, *Humidity*) = 0.97 - (3/5) * 0 - (2/5) * 0 = 0.97 bits
  - *Gain*(D_{Sunny}, *Wind*) = 0.97 - (2/5) * 1 - (3/5) * 0.92 = 0.02 bits
  - *Gain*(D_{Sunny}, *Temperature*) = 0.57 bits
- Top-Down Induction
  - For discrete-valued attributes, terminates in $O(n)$ splits
  - Makes at most one pass through data set at each level (why?)

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Constructing A Decision Tree for *PlayTennis* using *ID3* [4]

Day	Outlook	Temperature	Humidity	Wind	*PlayTennis*?
1	Sunny	Hot	High	Light	No
2	Sunny	Hot	High	Strong	No
3	Overcast	Hot	High	Light	Yes
4	Rain	Mild	High	Light	Yes
5	Rain	Cool	Normal	Light	Yes
6	Rain	Cool	Normal	Strong	No
7	Overcast	Cool	Normal	Strong	Yes
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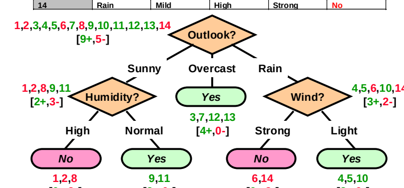

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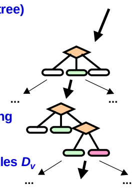
Hypothesis Space Search by *ID3*

- Search Problem
  - Conduct a search of the *space of decision trees*, which can represent all possible discrete functions
    - Pros: expressiveness; flexibility
    - Cons: computational complexity; large, incomprehensible trees (next time)
  - Objective: to find the best decision tree (minimal consistent tree)
  - Obstacle: finding this tree is $\mathcal{NP}$-hard
  - Tradeoff
    - Use heuristic (figure of merit that guides search)
    - Use greedy algorithm
    - *Aka* hill-climbing (gradient "descent") without backtracking
- Statistical Learning
  - Decisions based on statistical descriptors p_+, p_- for subsamples D_v
  - In ID3, *all data used*
  - Robust to noisy data



Inductive Bias in *ID3*

- Heuristic : Search :: Inductive Bias : Inductive Generalization
  - *H* is the power set of instances in *X*
  - ⇒ Unbiased? Not really…
    - Preference for short trees (termination condition)
    - Preference for trees with high information gain attributes near the root
    - *Gain*(•): a heuristic function that *captures the inductive bias of ID3*
  - Bias in *ID3*
    - Preference for some hypotheses is encoded in heuristic function
    - Compare: a restriction of hypothesis space *H* (previous discussion of propositional normal forms: *k*-CNF, etc.)
- Preference for Shortest Tree
  - Prefer shortest tree that fits the data
  - An Occam's Razor bias: shortest hypothesis that explains the observations

MLC++: A Machine Learning Library

- *MLC++*
  - http://www.sgi.com/Technology/mlc
  - An object-oriented machine learning library
  - Contains a suite of inductive learning algorithms (including *ID3*)
  - Supports incorporation, reuse of other DT algorithms (*C4.5*, etc.)
  - Automation of statistical evaluation, cross-validation
- Wrappers
  - Optimization loops that iterate over inductive learning functions (inducers)
  - Used for performance tuning (finding subset of *relevant* attributes, etc.)
- Combiners
  - Optimization loops that iterate over or interleave inductive learning functions
  - Used for performance tuning (finding subset of *relevant* attributes, etc.)
  - Examples: bagging, boosting (later in this course) of *ID3*, *C4.5*
- Graphical Display of Structures
  - Visualization of DTs (AT&T *dotty*, SGI *MineSet TreeViz*)
  - General logic diagrams (projection visualization)

Using *MLC++*

- Refer to *MLC++* references
  - Data mining paper (Kohavi, Sommerfeld, and Dougherty, 1996)
  - *MLC++* user manual: Utilities 2.0 (Kohavi and Sommerfeld, 1996)
  - *MLC++* tutorial (Kohavi, 1995)
  - Other development guides and tools on SGI *MLC++* web site
- Online Documentation
  - Consult class web page after Homework 2 is handed out
  - *MLC++* (Linux build) to be used for Homework 3
  - Related system: *MineSet* (commercial data mining edition of *MLC++*)
    - http://www.sgi.com/software/mineset
    - Many common algorithms
    - Common DT display format
    - Similar data formats
- Experimental Corpora (Data Sets)
  - UC Irvine Machine Learning Database Repository (MLDBR)
  - See http://www.kdnuggets.com and class "Resources on the Web" page

Terminology

- Decision Trees (DTs)
  - Boolean DTs: target concept is binary-valued (i.e., Boolean-valued)
  - Building DTs
    - Histogramming: a method of vector quantization (encoding input using bins)
    - Discretization: converting continuous input into discrete (e.g.., by histogramming)
- Entropy and Information Gain
  - Entropy *H*(*D*) for a data set *D* relative to an implicit concept *c*
  - Information gain *Gain* (*D*, *A*) for a data set partitioned by attribute *A*
  - Impurity, uncertainty, irregularity, surprise versus purity, certainty, regularity, redundancy
- Heuristic Search
  - Algorithm *Build-DT*: greedy search (hill-climbing without backtracking)
  - *ID3* as *Build-DT* using the heuristic *Gain*(•)
  - Heuristic : Search :: Inductive Bias : Inductive Generalization
- *MLC++* (Machine Learning Library in C++)
  - Data mining libraries (e.g., *MLC++*) and packages (e.g., *MineSet*)
  - Irvine Database: the Machine Learning Database Repository at UCI

Summary Points

- Decision Trees (DTs)
  - Can be boolean ($c(x) \in \{+, -\}$) or range over multiple classes
  - When to use DT-based models
- Generic Algorithm *Build-DT*: Top Down Induction
  - Calculating best attribute upon which to split
  - Recursive partitioning
- Entropy and Information Gain
  - Goal: to measure *uncertainty removed* by splitting on a candidate attribute *A*
    - Calculating information gain (change in entropy)
    - Using information gain in construction of tree
  - *ID3* ≡ *Build-DT* using *Gain*(•)
- ID3 as Hypothesis Space Search (in State Space of Decision Trees)
- Heuristic Search and Inductive Bias
- Data Mining using *MLC++* (Machine Learning Library in C++)
- Next: More Biases (Occam's Razor); Managing DT Induction