



10-301/10-601 Introduction to Machine Learning

Machine Learning Department School of Computer Science Carnegie Mellon University

Decision Trees

Matt Gormley Lecture 3 Jan. 25, 2023

Q&A

- Q: In our medical diagnosis example, suppose two of our doctors (i.e. experts) disagree about whether (+) or not (-) the patient is sick. How would the decision tree represent this situation?
- A: Today we will define decision trees that predict a single class by a majority vote at the leaf. More generally, the leaf could provide a probability distribution over output classes p(y|x)

Q&A

Q: How do these In-Class Polls work?

- Sign into Google Form (click [Poll] link on Schedule page http://mlcourse.org/schedule.html) using Andrew Email
 - Answer during lecture for full credit, or within 24 hours for half credit
 - Avoid the toxic option which gives negative points!
 - 8 "free poll points" but can't use more than 3 free polls consecutively. All the questions for one lecture are worth 1 point total.

Latest Poll link: http://poll.mlcourse.org

First In-Class Poll

Question 1 **Question: Answer:** Which of the following did you bring to class today? A. Smartphone B. Flip phone C. Pay phone D. No phone

Reminders

- Homework 1: Background
 - Out: Fri, Jan 20
 - Due: Wed, Jan 25 at 11:59pm
 - unique policy for this assignment: we will grant (essentially) any and all extension requests
- Homework 2: Decision Trees
 - Out: Wed, Jan. 25
 - Due: Fri, Feb. 3 at 11:59pm

MAKING PREDICTIONS WITH A DECISION TREES

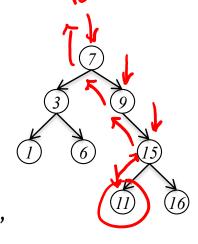
Background: Recursion

- Def: a binary search tree (BST) consists of nodes, where each node:
 - has a value, v
 - up to 2 children
 - all its left descendants have values less than v, and its right descendants have values greater than v
- We like BSTs because they permit search in O(log(n)) time, assuming n nodes in the tree

Node Data Structure

class Node:

int value Node left Node right



```
Recursive Search
def contains(node, key):
      if key < node.value & node.left != null:
            return contains (node.left, key)
      else if node.value < key & node.right != null:
            return contains(node.right, key)
      else:
            return key == node.value
```

Iterative Search

```
def contains(node, key):
      cur = node
      while true:
            if key < cur.value & cur.left != null:
                   cur = cur.left
            else if cur.value < key & cur.right != null:
                   cur = cur.right
            else:
                   break
      return key == cur.value
```

In-Class Exercise: Let's evaluate our (already learned) decision tree's error rate on a real test dataset.

Features:

- $-x_1$: which is better? {green, orange}
- x₂: which is better? {consistency, challenge}
- x₃: which is better? {sandals, sneakers}
- x₄: which is better? {winter, summer}

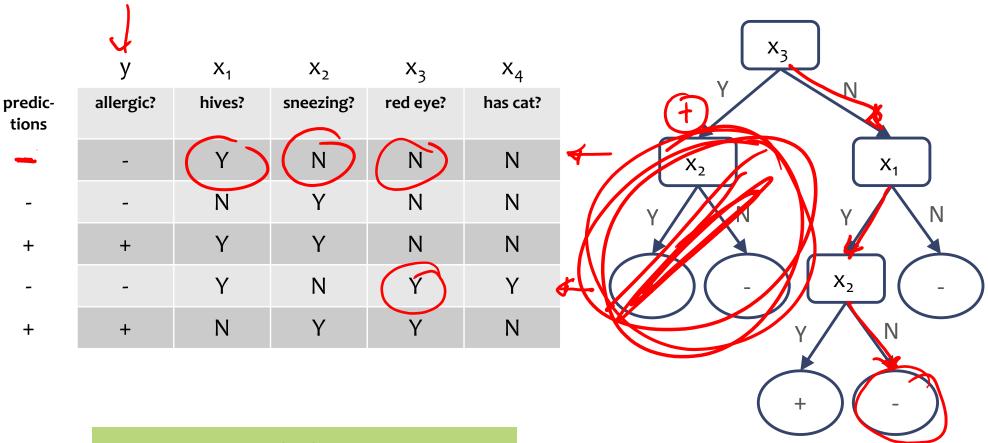
Label:

– y : are you a beach-person or a mountainsperson?

def h(x'):

- Let current node = root
- while(true):
 - if current node is internal (non-leaf):
 - Let m = attribute associated with current node
 - Go down branch labeled with value x'_m
 - if current node is a leaf:
 - return label y stored at that leaf

Algorithm 3 decision tree: recursively walk from root to a leaf, following the attribute values labeled on the branches, and return the label at the leaf



Zero training error!

def h(x'):

- Let current node = root
- while(true):
 - if current node is internal (non-leaf):
 - Let m = attribute associated with current node
 - Go down branch labeled with value x'_m
 - if current node is a leaf:
 - return label y stored at that leaf

Question: The above pseudocode is implementing prediction with a while-loop.

Can you convert it to a recursive implementation?

Decision Trees

Whiteboard

- Example Decision Tree as a hypothesis
- Defining h(x) for a decision tree

Tree to Predict C-Section Risk

Learned from medical records of 1000 women (Sims et al., 2000)

Negative examples are C-sections [833+,167] .83+ .17-Fetal_Presentation = 1: [822+,116-] .88+ .12-Previous_Csection = 0: [767+,81-] .90+ .10-Primiparous = 0: [399+,13-] .97+ .03-| Primiparous = 1: [368+,68-] .84+ .16- $| Fetal_Distress = 0: [334+,47-] .88+ .12-$ | | Birth_Weight < 3349: [201+,10.6-] .95+ . Birth_Weight >= 3349: [133+,36.4-] .78+ $| \text{Fetal_Distress} = 1: [34+,21-] .62+ .38-$ Previous_Csection = 1: [55+,35-] .61+ .39-Fetal_Presentation = 2: [3+,29-] .11+ .89-Fetal_Presentation = 3: [8+,22-] .27+ .73-

LEARNING A DECISION TREE

Decision Trees

Whiteboard

Decision Tree Learning

Recursive Training for Decision Trees

def train(dataset D'):

- Let p = new Node()
- Base Case: If (1) all labels y⁽ⁱ⁾ in D' are identical (2) D' is empty
 (3) for each attribute, all values are identical

```
    p.type = Leaf // The node p is a leaf node
    p.label = majority_vote(D') // Store the label
    return p
```

- Recursive Step: Otherwise
 - Make an internal node

```
– p.type = Internal // The node p is an internal node
```

• Pick the best attribute X_m according to splitting criterion

```
– p.attr = argmax<sub>m</sub> splitting_criterion(D', X<sub>m</sub>)
// Store the attribute on which to split
```

• For each value v of attribute X_m:

```
- D_{Xm=v} = \{(x,y) \text{ in } D': x_m = v\} // Select a partition of the data

- \text{child}_v = \text{train}(D_{Xm=v}) // Recursively build the child

- \text{p.branches}[v] = \text{child}_v // Create a branch with label v

- \text{return } p
```

Dataset:

Output Y, Attributes A, B, C

Y	А	В	C
-	1	0	0
-	1	0	1
-	1	0	0
+	0	0	1
+	1	1	0
+	1	1	1
+	1	1	0
+	1	1	1

In-Class Exercise

Using error rate as the splitting criterion, what decision tree would be learned?

Decision Trees

Whiteboard

Example of Decision Tree Learning with Error
 Rate as splitting criterion

SPLITTING CRITERION: ERROR RATE

Decision Tree Learning

- Definition: a splitting criterion is a function that measures the effectiveness of splitting on a particular attribute
- Our decision tree learner selects the "best" attribute as the one that maximizes the splitting criterion
- Lots of options for a splitting criterion:
 - error rate (or accuracy if we want to pick the tree that maximizes the criterion)
 - Gini gain
 - Mutual information
 - random

– ...

Dataset:

Output Y, Attributes A and B

Υ	А	В
-	1	0
-	1	0
+	1	0
+	1	0
+	1	1
+	1	1
+	1	1
+	1	1

In-Class Exercise

Questron 2

Which attribute would error rate select for the next split?

- 1. A
- 2. B
- 3. A or B (tie)
- 4. Neither toxic

Dataset:

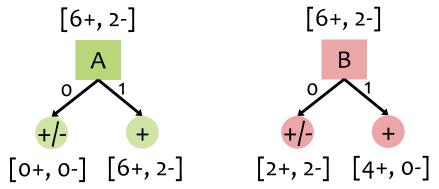
Output Y, Attributes A and B

Y	Α	В
-	1	0
-	1	0
+	1	0
+	1	0
+	1	1
+	1	1
+	1	1
+	1	1

Dataset:

Output Y, Attributes A and B

Y	Α	В
-	1	0
-	1	0
+	1	0
+	1	0
+	1	1
+	1	1
+	1	1
+	1	1



Error Rate

error(
$$h_A$$
, D) = 2/8
error(h_B , D) = 2/8

error rate treats attributes A and B as equally good

SPLITTING CRITERION: MUTUAL INFORMATION

Information Theory & DTs

Whiteboard

- Information Theory primer
 - Entropy
 - (Specific) Conditional Entropy
 - Conditional Entropy
 - Information Gain / Mutual Information
- Information Gain as DT splitting criterion

Mutual Information

Let X be a random variable with $X \in \mathcal{X}$. Let Y be a random variable with $Y \in \mathcal{Y}$.

Entropy:
$$H(Y) = -\sum_{y \in \mathcal{Y}} P(Y = y) \log_2 P(Y = y)$$

Specific Conditional Entropy:
$$H(Y \mid X = x) = -\sum_{y \in \mathcal{Y}} P(Y = y \mid X = x) \log_2 P(Y = y \mid X = x)$$

Conditional Entropy:
$$H(Y \mid X) = \sum_{x \in \mathcal{X}} P(X = x) H(Y \mid X = x)$$

Mutual Information:
$$I(Y;X) = H(Y) - H(Y|X) = H(X) - H(X|Y)$$

- For a decision tree, we can use mutual information of the output class Y and some attribute X on which to split as a splitting criterion
- Given a dataset D of training examples, we can estimate the required probabilities as...

$$P(Y = y) = N_{Y=y}/N$$

$$P(X = x) = N_{X=x}/N$$

$$P(Y = y|X = x) = N_{Y=y,X=x}/N_{X=x}$$

where $N_{Y=y}$ is the number of examples for which Y=y and so on.

Mutual Information

Let X be a random variable with $X \in \mathcal{X}$.

Let Y be a random variable with $Y \in \mathcal{Y}$.



Entropy:
$$H(Y) = -\sum_{y \in \mathcal{Y}} P(Y = y) \log_2 P(Y = y)$$

Specific Conditional Entropy: $H(Y \mid X = x) = -\sum_{y \in \mathcal{Y}} P(Y = y \mid X = x) \log_2 P(Y = y \mid X = x)$



Conditional Entropy:
$$H(Y \mid X) = \sum_{x \in \mathcal{X}} P(X = x) H(Y \mid X = x)$$

Mutual Information: I(Y;X) = H(Y) - H(Y|X) = H(X) - H(X|Y)

- Entropy measures the expected # of bits to code one random draw from X.
- For a decision tree, we want to reduce the entropy of the random variable we are trying to predict!

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Conditional entropy is the expected value of specific conditional entropy $E_{P(X=x)}[H(Y \mid X=x)]$

Informally, we say that **mutual information** is a measure of the following: If we know X, how much does this reduce our uncertainty about Y?

Dataset:

Output Y, Attributes A and B

Y	A B	
-	1	0
-	1	0
+	1	0
+	1	0
+	1	1
+	1	1
+	1	1
+	1	1

In-Class Exercise

Which attribute would mutual information select for the next split?

- 1. A
- 2. B \checkmark
- 3. A or B (tie)
- 4. Neither

Dataset:

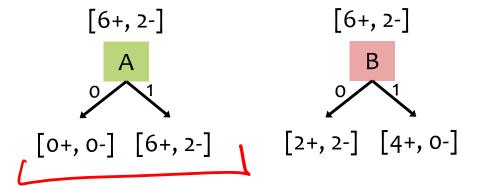
Output Y, Attributes A and B

Υ	Α	В
-	1	0
-	1	0
+	1	0
+	1	0
+	1	1
+	1	1
+	1	1
+	1	1

Dataset:

Output Y, Attributes A and B

Y	А	В
-	1	0
-	1	0
+	1	0
+	1	0
+	1	1
+	1	1
+	1	1
+	1	1



Mutual Information

$$H(Y) = -2/8 \log(2/8) - 6/8 \log(6/8)$$

$$H(Y|A=0) =$$
 "undefined"
 $H(Y|A=1) = -2/8 \log(2/8) - 6/8 \log(6/8)$
 $= H(Y)$
 $H(Y|A) = P(A=0)H(Y|A=0) + P(A=1)H(Y|A=1)$
 $= 0 + H(Y|A=1) = H(Y)$
 $I(Y; A) = H(Y) - H(Y|A=1) = 0$

$$H(Y|B=0) = -2/4 \log(2/4) - 2/4 \log(2/4)$$

 $H(Y|B=1) = -0 \log(0) - 1 \log(1) = 0$
 $H(Y|B) = 4/8(0) + 4/8(H(Y|B=0))$
 $I(Y;B) = H(Y) - 4/8 H(Y|B=0) > 0$

PlayTennis?
No

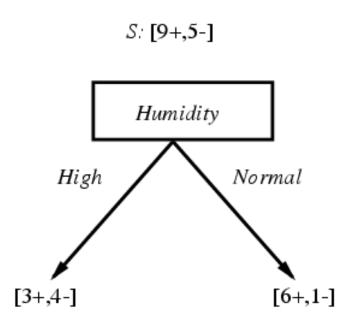
Dataset:

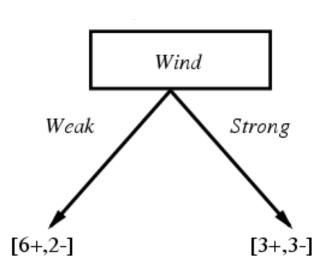
Day Outlook Temperature Humidity Wind PlayTennis?

D1	Sunny	Hot	High	Weak	No
D2	Sunny	Hot	High	Strong	No
D3	Overcast	Hot	High	Weak	Yes
D4	Rain	Mild	High	Weak	Yes
D5	Rain	Cool	Normal	Weak	Yes
D6	Rain	Cool	Normal	Strong	No
D7	Overcast	Cool	Normal	Strong	Yes
D8	Sunny	Mild	High	Weak	No
D9	Sunny	Cool	Normal	Weak	Yes
D10	Rain	Mild	Normal	Weak	Yes
D11	Sunny	Mild	Normal	Strong	Yes
D12	Overcast	Mild	High	Strong	Yes
D13	Overcast	Hot	Normal	Weak	Yes
D14	Rain	Mild	High	Strong	No

Which attribute yields the best classifier?

Test vour understanding.

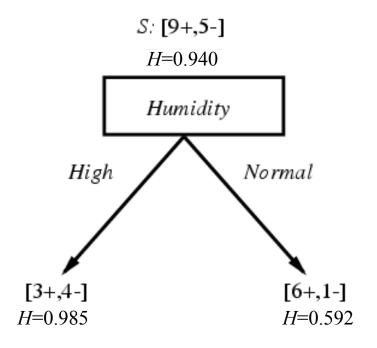


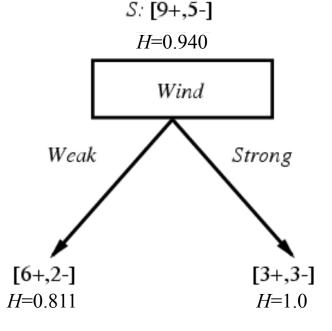


S: [9+,5-]

Which attribute yields the best classifier?

Test Nour understanding.





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Which attribute yields the best classifier?

S: [9+,5-]

H=0.940

Humidity

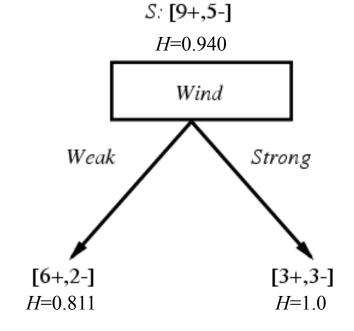
Normal

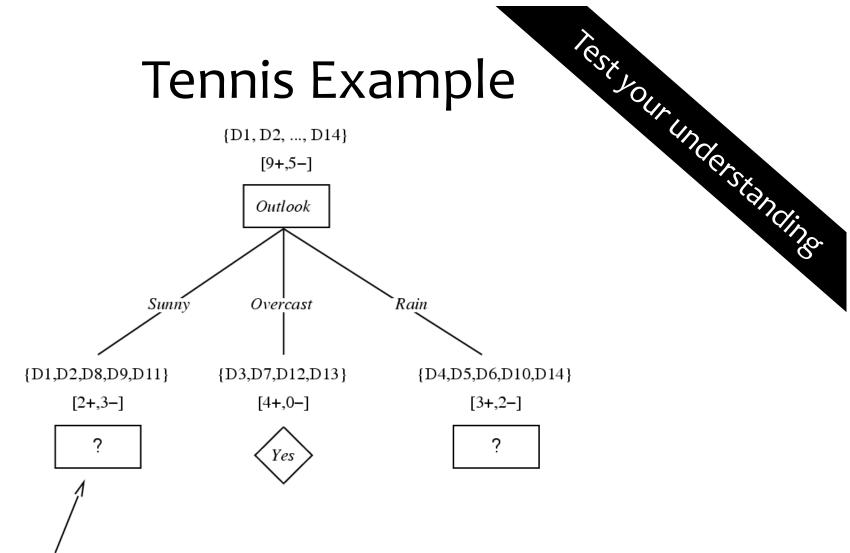
[3+,4-]

H=0.985

[6+,1-]

H=0.592





Which attribute should be tested here?

 $S_{sunnv} = \{D1,D2,D8,D9,D11\}$ $Gain(S_{sunny}, Humidity) = .970 - (3/5) 0.0 - (2/5) 0.0 = .970$ $Gain(S_{sunnv}, Temperature) = .970 - (2/5) 0.0 - (2/5) 1.0 - (1/5) 0.0 = .570$ $Gain(S_{sunny}, Wind) = .970 - (2/5) 1.0 - (3/5) .918 = .019$