# 10-301/601: Introduction to Machine Learning Lecture 3 – Decision Trees

Matt Gormley & Henry Chai 9/4/24

#### **Front Matter**

- Announcements:
  - HW1 released 8/26, due 9/4 (today!) at 11:59 PM
    - Reminder: we will grant (basically) any extension requests for this assignment!
  - HW2 released 9/4 (today!), due 9/16 at 11:59 PM
    - Unlike HW1, you will only have:
      - 1 (graded) submission for the written portion
      - 10 submissions of the programming portion to our autograder

#### Q & A:

# How do these in-class polls work?

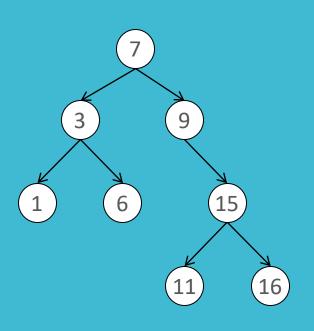
- Open the poll, either by clicking the [Poll] link on the schedule page of our course website or going to <a href="http://poll.mlcourse.org">http://poll.mlcourse.org</a>
- Sign into Google Forms using your Andrew email
- Answer all poll questions during lecture for full credit or within 24 hours for half credit
- Avoid the toxic option (will be clearly specified in lecture) which gives negative poll points
- You have 8 free "poll points" for the semester that will excuse you from all polls from a single lecture; you cannot use more than 3 poll points consecutively.

### Poll Question 1:

Which of the following did you bring to class today? Select all that apply

- A. A smartphone
- B. A flip phone
- C. A payphone
- D. No phone

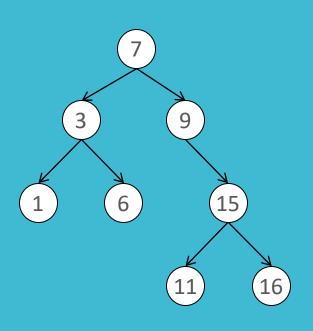
### Background: Recursion



- A binary search tree (BST) consists of nodes, where each node:
  - · has a value, v
  - up to 2 children, a left descendant and a right descendant
  - 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

```
def contains_iterative(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</pre>
```

### Background: Recursion

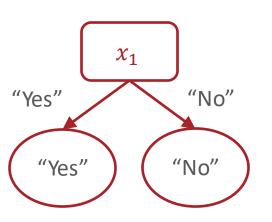


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  - has a value, v
  - up to 2 children, a left descendant and a right descendant
  - all its left descendants have values less than v and its right descendants have values greater than v
- We like BSTs because they permit search in O(log(n)) time, assuming n nodes in the tree

```
def contains_recursive(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</pre>
```

### Recall: Decision Stump

$x_1$ Family History	$x_2$ Resting Blood Pressure	$x_3$ Cholesterol	<i>y</i> Heart Disease?
Yes	Low	Normal	No
No	Medium	Normal	No
No	Low	Abnormal	Yes
Yes	Medium	Normal	Yes
Yes	High	Abnormal	Yes



# Recall: Decision Stump Questions

1. How can we pick which feature to split on?

2. Why stop at just one feature? Don't!

a) If we split on more than one feature, how do we decide the order to spilt on?

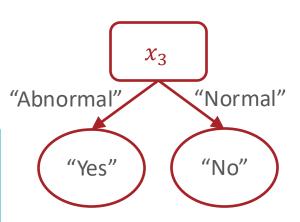
# Decision Tree: In-class Activity

- 1. Group 1: Answer the questions to determine which leaf node corresponds to your feature values
- 2. Group 2:
  - a) Take a blue sticky note if you prefer dogs to cats; otherwise, take a red sticky note
  - b) Answer the questions to determine which leaf node corresponds to your feature values and place your sticky note there
  - c) Answer the new question to determine which new leaf node to move your sticky note to
- 3. Group 3: Answer the questions to determine which leaf node corresponds to your feature values

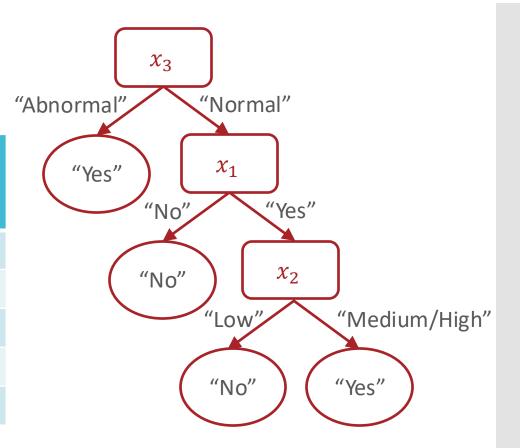
# From Decision Stump

• • •

$x_1$ Family History	$x_2$ Resting Blood Pressure	$x_3$ Cholesterol	y Heart Disease?
Yes	Low	Normal	No
No	Medium	Normal	No
No	Low	Abnormal	Yes
Yes	Medium	Normal	Yes
Yes	High	Abnormal	Yes



$x_1$ Family History	$x_2$ Resting Blood Pressure	$x_3$ Cholesterol	y Heart Disease?
Yes	Low	Normal	No
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No	Low	Abnormal	Yes
Yes	Medium	Normal	Yes
Yes	High	Abnormal	Yes



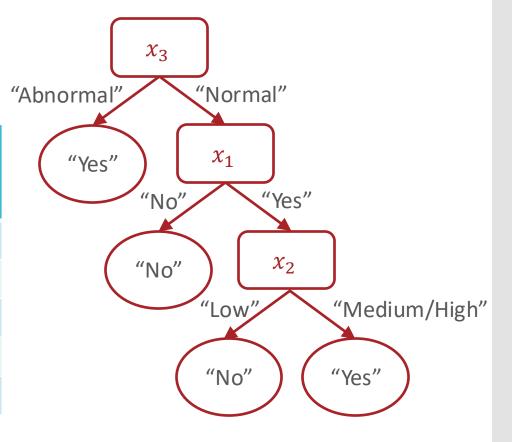
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$x_1$ Family History	$x_2$ Resting Blood Pressure	$x_3$ Cholesterol	<i>y</i> Heart Disease?
Yes	Low	Normal	No
No	Medium	Normal	No
No	Low	Abnormal	Yes
Yes	Medium	Normal	Yes
Yes	High	Abnormal	Yes

Normal

High

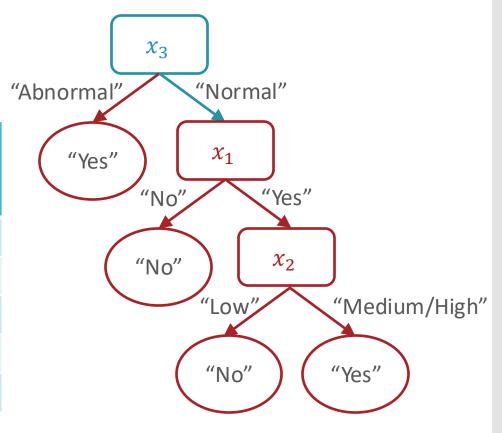
No



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No

$x_1$ Family History	$x_2$ Resting Blood Pressure	$x_3$ Cholesterol	<i>y</i> Heart Disease?
Yes	Low	Normal	No
No	Medium	Normal	No
No	Low	Abnormal	Yes
Yes	Medium	Normal	Yes
Yes	High	Abnormal	Yes



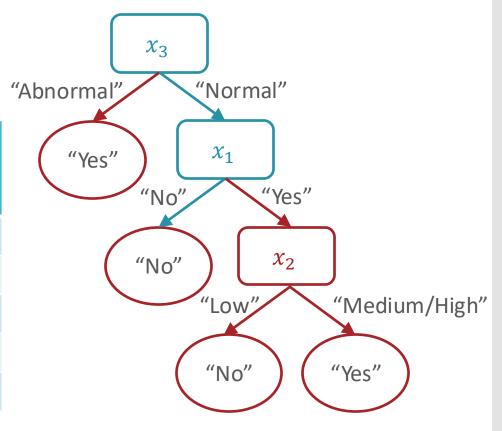
No High Normal No

$x_1$ Family History	$x_2$ Resting Blood Pressure	$x_3$ Cholesterol	y Heart Disease?
Yes	Low	Normal	No
No	Medium	Normal	No
No	Low	Abnormal	Yes
Yes	Medium	Normal	Yes
Yes	High	Abnormal	Yes

Normal

High

No



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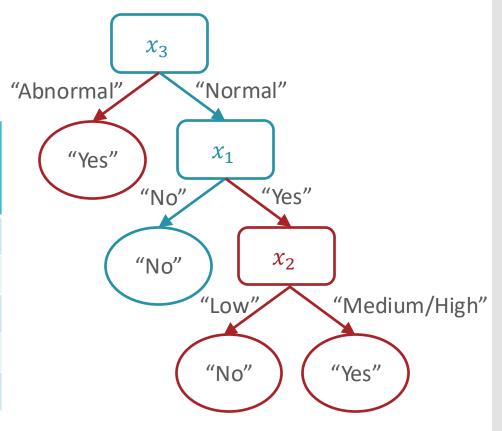
No

$x_1$ Family History	$x_2$ Resting Blood Pressure	$x_3$ Cholesterol	y Heart Disease?
Yes	Low	Normal	No
No	Medium	Normal	No
No	Low	Abnormal	Yes
Yes	Medium	Normal	Yes
Yes	High	Abnormal	Yes

Normal

High

No



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No

# Decision Tree: Pseudocode

```
def h(x'):
 - walk from root node to a leaf node
   while(true):
     if current node is internal (non-leaf):
           check the associated attribute, x_d
           go down branch according to x'_d
     if current node is a leaf node:
           return label stored at that leaf
```

# Decision Tree: Example

Learned from medical records of 1000 women 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-
| | | 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-
```

9/4/24 Figure courtesy of Tom Mitchell

# Decision Tree Questions

1. How can we pick which feature to split on?

2. Why stop at just one feature?

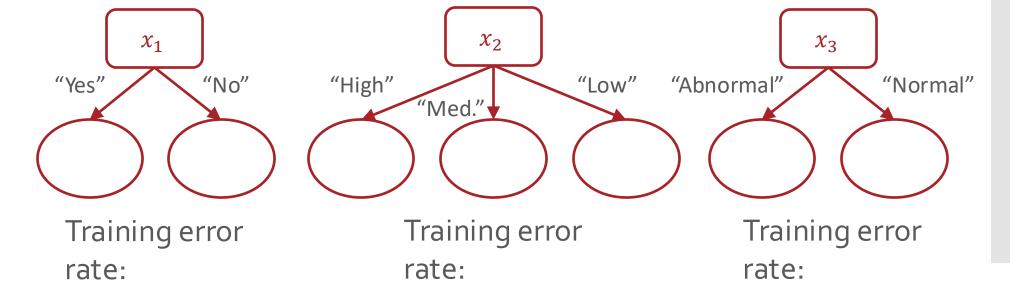
a) If we split on more than one feature, how do we decide the order to spilt on?

# Splitting Criterion

- A **splitting criterion** is a function that measures how good or useful splitting on a particular feature is *for a specified dataset*
- Idea: when deciding which feature to split on, use the one that optimizes the splitting criterion

Training
Error Rate
as a
Splitting
Criterion

$x_1$ Family History	$x_2$ Resting Blood Pressure	$x_3$ Cholesterol	<i>y</i> Heart Disease?
Yes	Low	Normal	No
No	Medium	Normal	No
No	Low	Abnormal	Yes
Yes	Medium	Normal	Yes
Yes	High	Abnormal	Yes



### Poll Question 2:

Which feature would you split on using training error rate as the splitting criterion?

$x_1$	$x_2$	y
1	0	0
1	0	0
1	0	1
1	0	1
1	1	1
1	1	1
1	1	1
1	1	1

A.  $x_1$ 

 $x_2$ 

C. Either  $x_1$  or  $x_2$ 

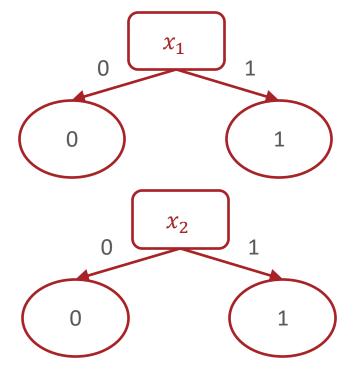
D. Neither  $x_1$  nor  $x_2$ 

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### Poll Question 2:

Which feature would you split on using training error rate as the splitting criterion?

$x_1$	$x_2$	у
1	0	0
1	0	0
1	0	1
1	0	1
1	1	1
1	1	1
1	1	1
1	1	1



Training error rate: 2/8

## Splitting Criterion

- A splitting criterion is a function that measures how good or useful splitting on a particular feature is for a specified dataset
- Idea: when deciding which feature to split on, use the one that optimizes the splitting criterion
- Potential splitting criteria:
  - Training error rate (minimize)
  - Gini impurity (minimize) → CART algorithm
  - Mutual information (maximize) → ID3 algorithm

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## Splitting Criterion

- A **splitting criterion** is a function that measures how good or useful splitting on a particular feature is *for a specified dataset*
- Idea: when deciding which feature to split on, use the one that optimizes the splitting criterion
- Potential splitting criteria:
  - Training error rate (minimize)
  - Gini impurity (minimize) → CART algorithm
  - Mutual information (maximize) → ID3 algorithm

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### Entropy

• The **entropy** of a *random variable* describes the uncertainty of its outcome: the higher the entropy, the less certain we are about what the outcome will be.

$$H(X) = -\sum_{v \in V(X)} P(X = v) \log_2(P(X = v))$$

where *X* is a (discrete) random variable

V(X) is the set of possible values X can take on

### Entropy

 The entropy of a set describes how uniform or pure it is: the higher the entropy, the more impure or "mixed-up" the set is

$$H(S) = -\sum_{v \in V(S)} \frac{|S_v|}{|S|} \log_2 \left(\frac{|S_v|}{|S|}\right)$$

where *S* is a collection of values,

V(S) is the set of unique values in S

 $S_v$  is the collection of elements in S with value v

If all the elements in S are the same, then

$$H(S) = -1 \log_2(1) = 0$$

### Entropy

 The entropy of a set describes how uniform or pure it is: the higher the entropy, the more impure or "mixed-up" the set is

$$H(S) = -\sum_{v \in V(S)} \frac{|S_v|}{|S|} \log_2 \left(\frac{|S_v|}{|S|}\right)$$

where *S* is a collection of values,

V(S) is the set of unique values in S

 $S_v$  is the collection of elements in S with value v

If S is split fifty-fifty between two values, then

$$H(S) = -\frac{1}{2}\log_2\left(\frac{1}{2}\right) - \frac{1}{2}\log_2\left(\frac{1}{2}\right) = -\log_2\left(\frac{1}{2}\right) = 1$$

### Mutual Information

The mutual information between two random variables
 describes how much clarity knowing the value of one random
 variables provides about the other

$$I(Y;X) = H(Y) - H(Y|X)$$

$$= H(Y) - \sum_{v \in V(X)} P(X = v)H(Y|X = v)$$

where X and Y are random variables

V(X) is the set of possible values X can take on

H(Y|X=v) is the conditional entropy of Y given X=v

### Mutual Information

• The **mutual information** between *a feature and the label* describes how much clarity knowing the feature provides about the label

$$I(y; x_d) = H(y) - H(y|x_d)$$

$$= H(y) - \sum_{v \in V(x_d)} f_v \left( H(Y_{x_d=v}) \right)$$

where  $x_d$  is a feature and y is the set of all labels

 $V(x_d)$  is the set of possible values  $x_d$  can take on

 $f_v$  is the fraction of data points where  $x_d = v$ 

 $Y_{x_d=v}$  is the set of all labels where  $x_d=v$ 

# Mutual Information: Example

$x_d$	y
1	1
1	1
0	0
0	0

$$I(x_d, Y) = H(Y) - \sum_{v \in V(x_d)} (f_v) \left( H(Y_{x_d=v}) \right)$$

$$= 1 - \frac{1}{2} H(Y_{x_d=0}) - \frac{1}{2} H(Y_{x_d=1})$$

$$= 1 - \frac{1}{2} (0) - \frac{1}{2} (0) = 1$$

# Mutual Information: Example

$x_d$	y
1	1
0	1
1	0
0	0

$$I(x_d, Y) = H(Y) - \sum_{v \in V(x_d)} (f_v) \left( H(Y_{x_d=v}) \right)$$

$$= 1 - \frac{1}{2} H(Y_{x_d=0}) - \frac{1}{2} H(Y_{x_d=1})$$

$$= 1 - \frac{1}{2} (1) - \frac{1}{2} (1) = 0$$

### Poll Question 3:

Which feature would you split on using mutual information as the splitting criterion?

$x_1$	$x_2$	У
1	0	0
1	0	0
1	0	1
1	0	1
1	1	1
1	1	1
1	1	1
1	1	1

A.  $x_1$ 

B.  $\chi_2$ 

C. Either  $x_1$  or  $x_2$ 

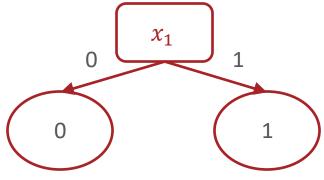
D. Neither  $x_1$  nor  $x_2$ 

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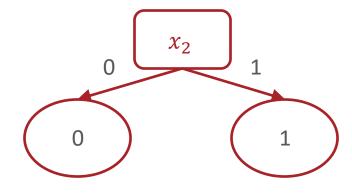
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Which feature would you split on using mutual information as the splitting criterion?

$x_1$	$x_2$	у
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1	0	0
1	0	1
1	0	1
1	1	1
1	1	1
1	1	1
1	1	1



Mutual Information: 0

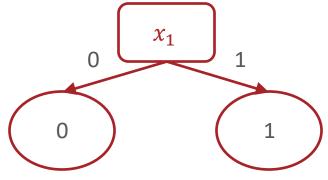


Mutual Information: 
$$H(Y) - \frac{1}{2}H(Y_{x_2=0}) - \frac{1}{2}H(Y_{x_2=1})$$

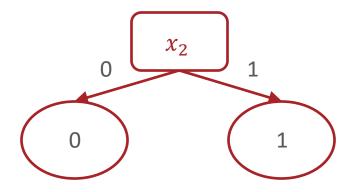
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Which feature would you split on using mutual information as the splitting criterion?

$x_1$	$x_2$	у
1	0	0
1	0	0
1	0	1
1	0	1
1	1	1
1	1	1
1	1	1
1	1	1



Mutual Information: 0



Mutual Information: 
$$-\frac{2}{8}\log_2\frac{2}{8} - \frac{6}{8}\log_2\frac{6}{8} - \frac{1}{2}(1) - \frac{1}{2}(0) \approx 0.31$$

# Decision Tree Questions

1. How can we pick which feature to split on?

2. Why stop at just one feature?

a) If we split on more than one feature, how do we decide the order to spilt on?

# Decision Tree: Pseudocode

```
def train(\mathcal{D}):
    store root = tree recurse(\mathcal{D})
def tree recurse(\mathcal{D}'):
    q = new node()
    base case - if (SOME CONDITION):
    recursion - else:
        find best attribute to split on, x_d
        q.split = x_d
        for v in V(x_d), all possible values of x_d:
               \mathcal{D}_{v} = \left\{ \left( x^{(n)}, y^{(n)} \right) \in \mathcal{D} \mid x_{d}^{(n)} = v \right\}
               q.children(v) = tree_recurse(\mathcal{D}_v)
    return q
```

# Decision Tree: Pseudocode

```
def train(\mathcal{D}):
    store root = tree recurse(\mathcal{D})
def tree recurse(\mathcal{D}'):
   q = new node()
    base case – if (\mathcal{D}') is empty OR
       all labels in \mathcal{D}' are the same OR
       all features in \mathcal{D}' are identical OR
       some other stopping criterion):
           q.label = majority vote(\mathcal{D}')
    recursion - else:
    return q
```