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

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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 http://poll.mlcourse.org
- 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:

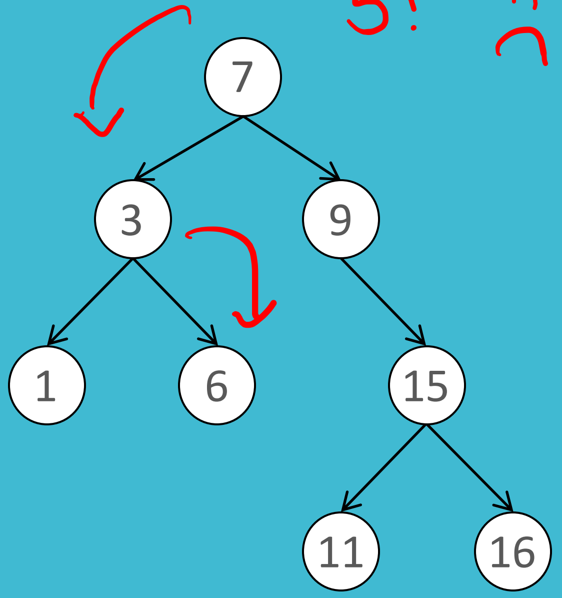
Which of the following did you bring to class today? Select all that apply

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

Background: Recursion

5?

11?

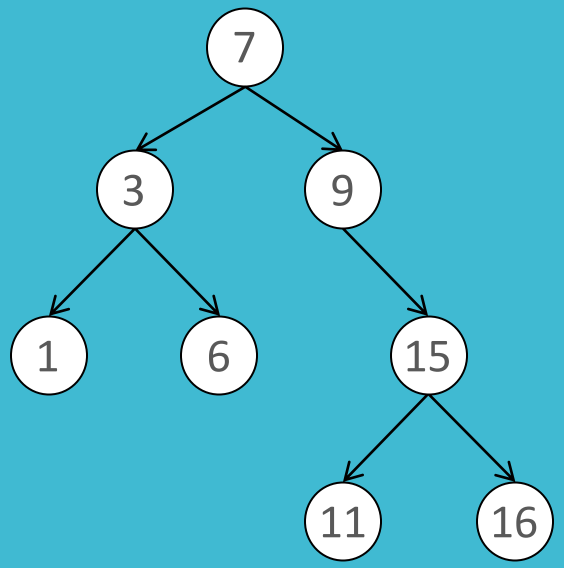


- A **binary search tree** (BST) consists of nodes, where each node:
  - has a value, v
  - up to 2 children, a left descendant and a right descendant
  - all its left descendants have values less than v and its right descendants have values greater than v
- We like BSTs because they permit search in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

root

```
def contains_iterative(node, key):
    curr = node
    while (true):
        if key < curr.val & curr.left ≠ none
            curr = curr.left
        else if key > curr.val & curr.right ≠ none
            curr = curr.right
        else: key == curr.val
```

Background: Recursion



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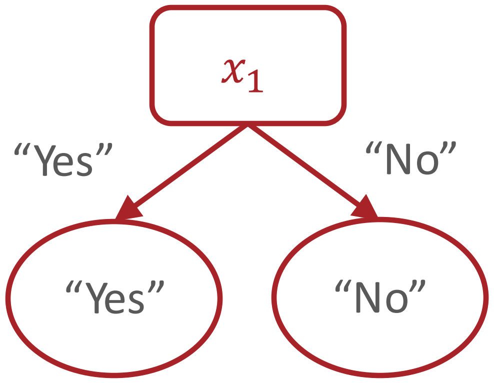
- We like BSTs because they permit search in O(log(n)) time, assuming n nodes in the tree

```
def contains_recursive(node, key):
    if key < node.val & node.left ≠ none:
        contains_recursive(node.left, key)
    else if key > node.val & node.right ≠ none:
        contains_recursive(node.right, key)
    else: key == node.val
      return
```

Recall: 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



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
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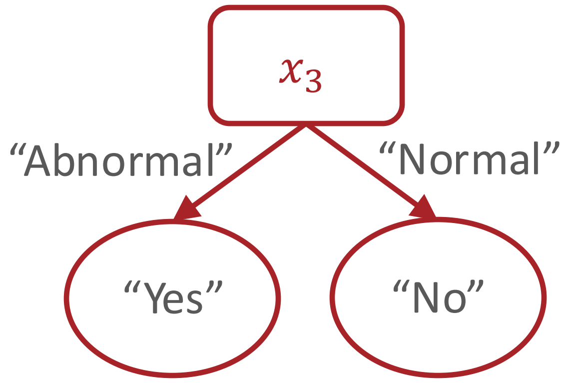

From Decision Stump to Decision Tree

x_1 Family History	x_2 Resting Blood Pressure	x_3 Cholesterol	y Heart Disease?
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No	Medium	Normal	No
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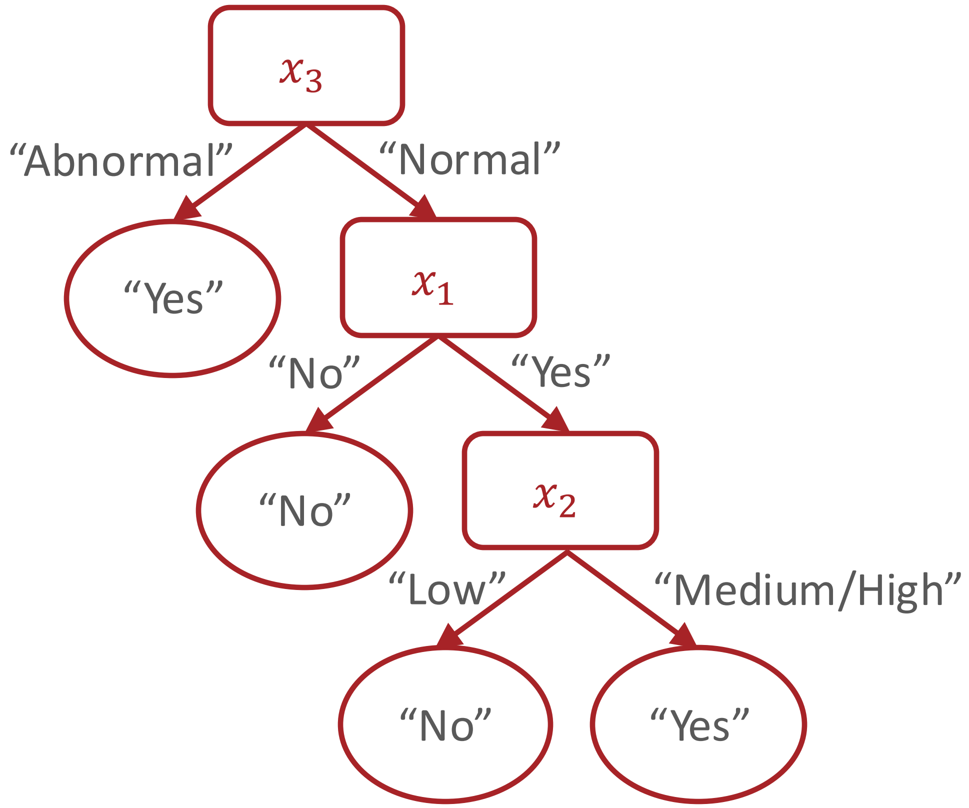

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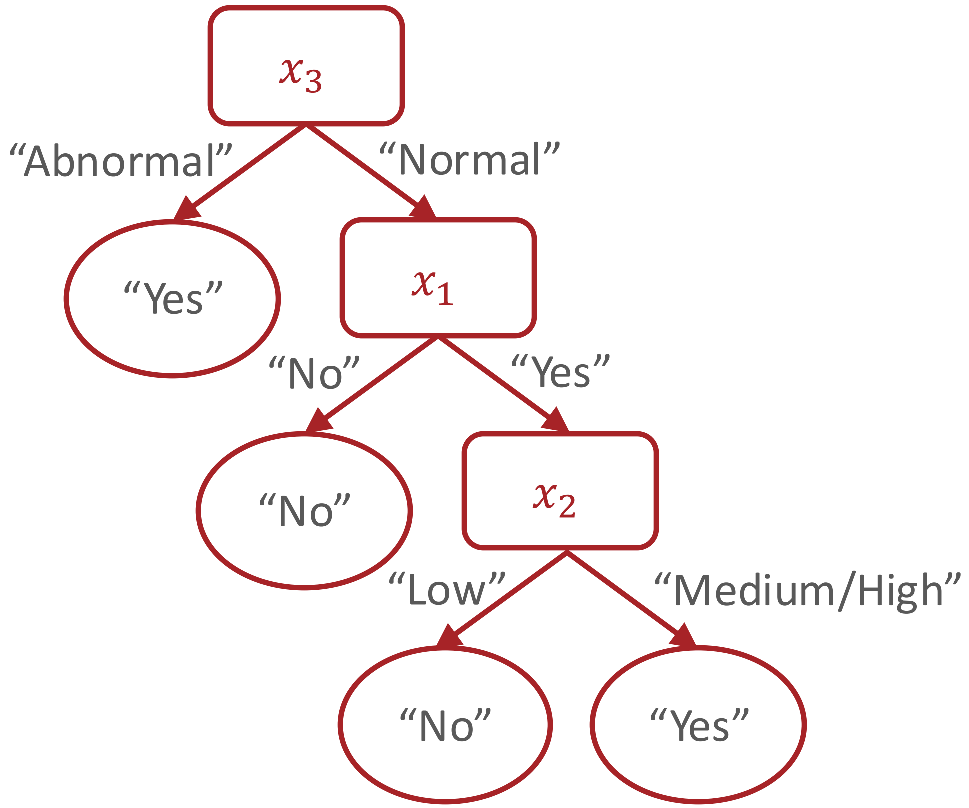

From Decision Stump to Decision Tree

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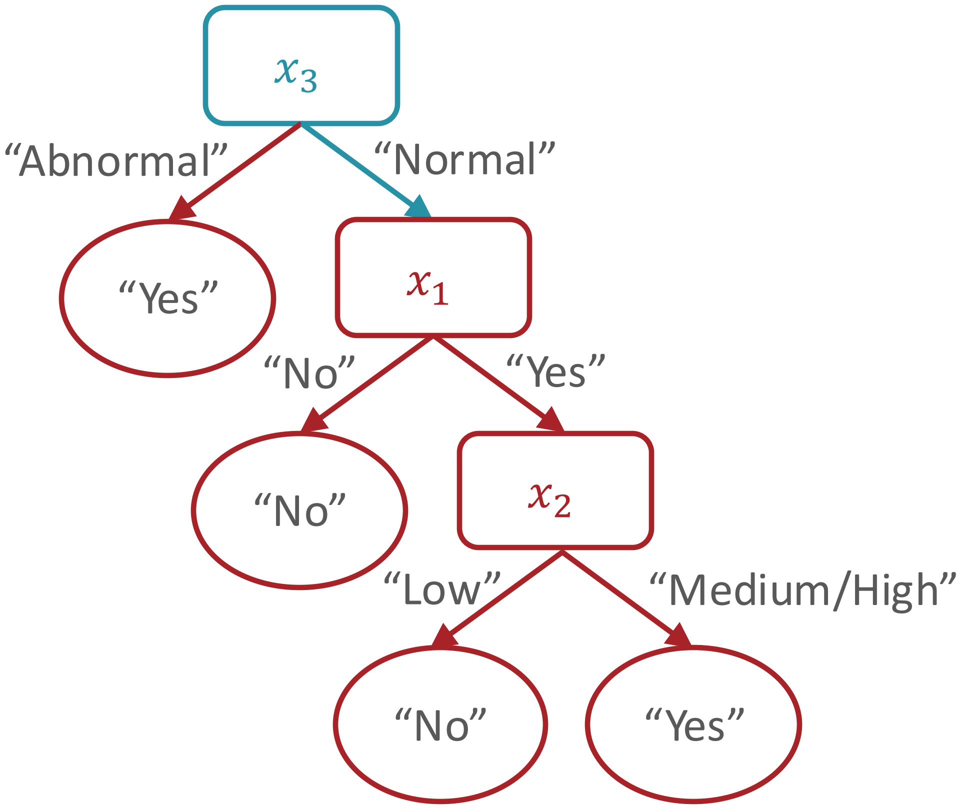

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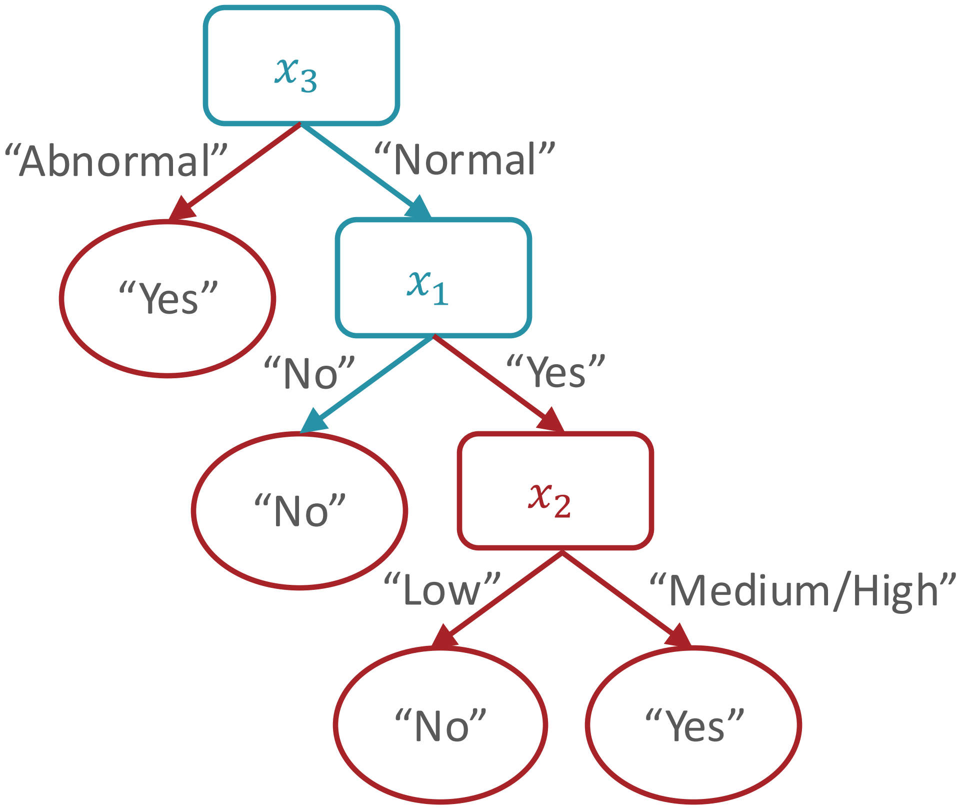

From Decision Stump to Decision Tree

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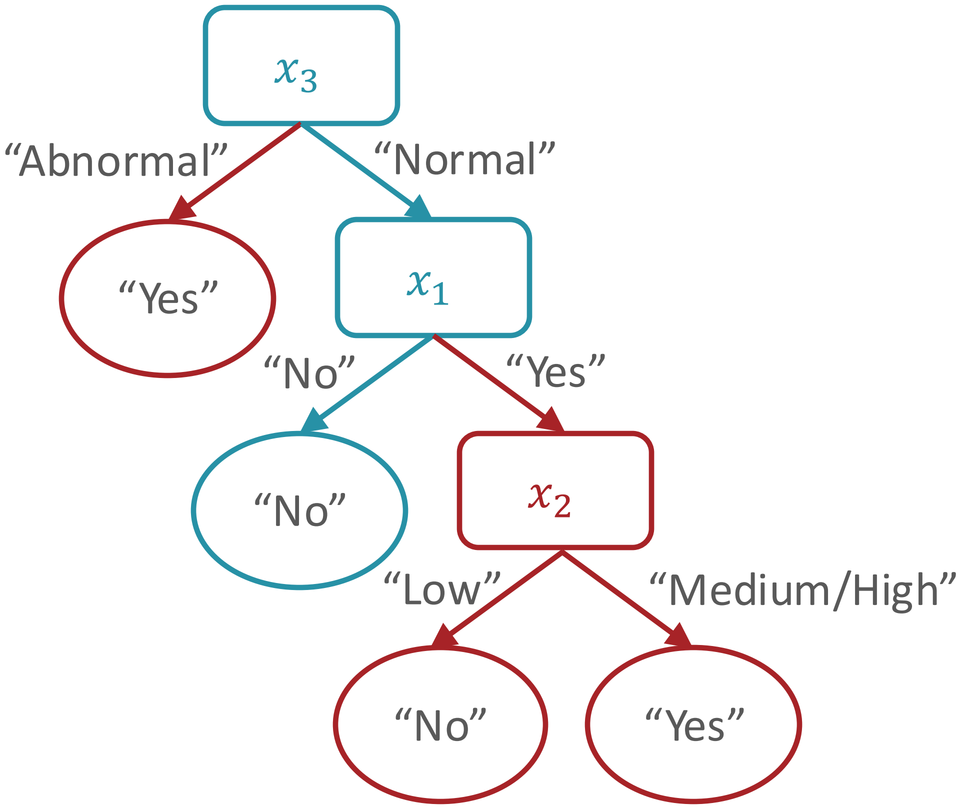
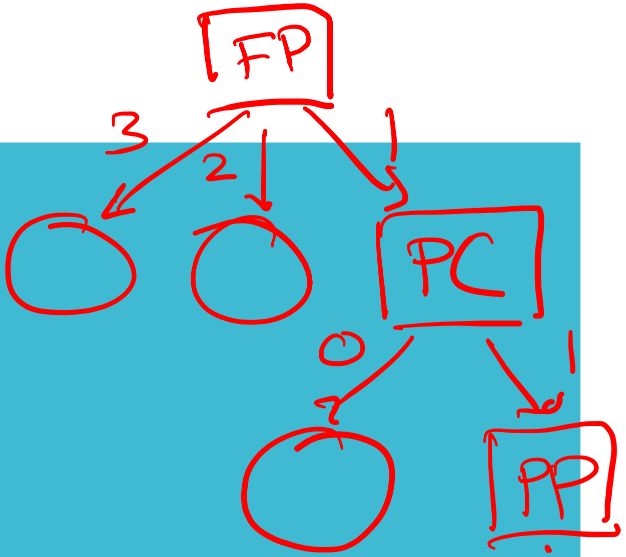


Decision Tree: Pseudocode

$[x'_1, x'_2, \ldots, x'_D]$

```
def h(x⃗'):
    # walk from the root to some
      leaf node and return the stored
      prediction
    while (true):
        if current_node is internal:
            check the stored feature, x_d
            go down the branch corresponding
            to x'_d
        else:
            # current_node is a leaf
            return the stored prediction
```



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-
```


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	y Heart Disease?
Yes	Low	Normal	No
No	Medium	Normal	No
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Yes	Medium	Normal	Yes
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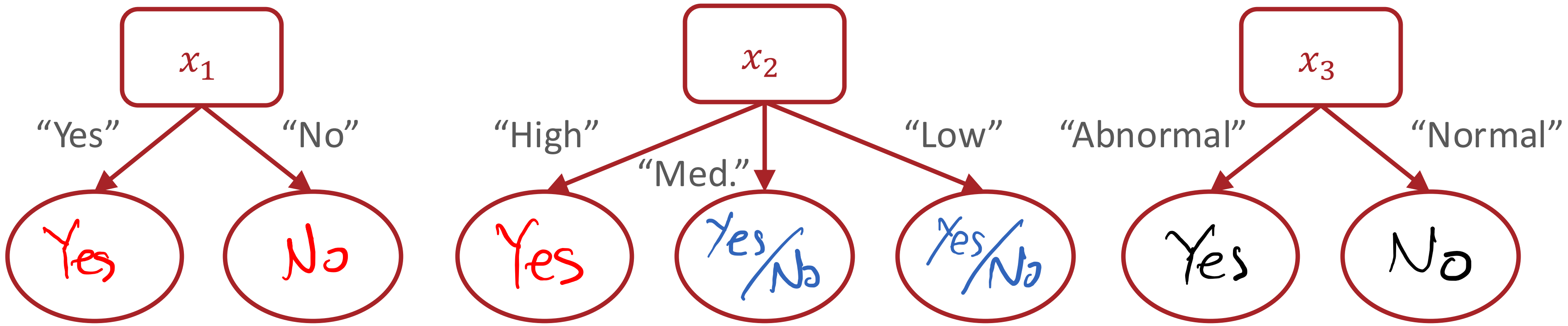


Training error rate: 2/5

Training error rate: 2/5

Training error rate: 1/5

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

B. x_2

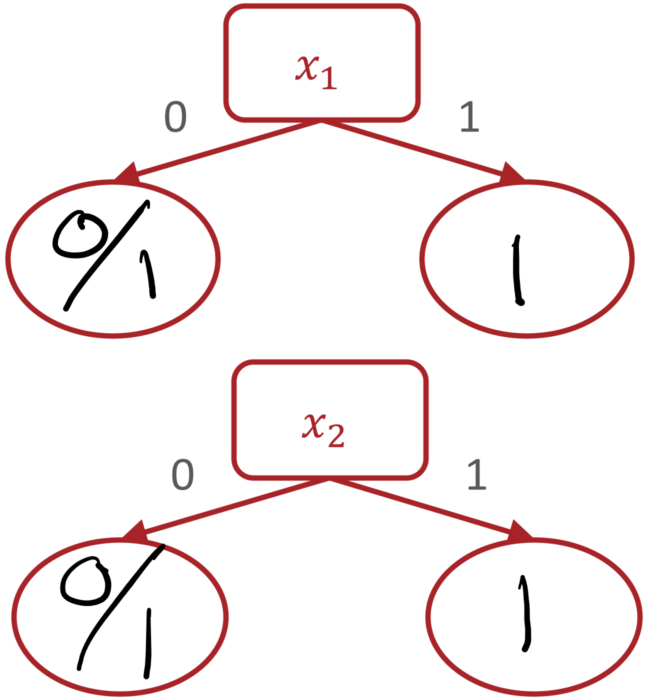
C. Either x_1 or x_2

D. Neither x_1 nor x_2

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



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

Splitting Criterion

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- Potential splitting criteria:
  - Training error rate (minimize)
  - Gini impurity (minimize) → CART algorithm
  - **Mutual information** (maximize) → ID3 algorithm

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.

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

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

$|\cdot|$ = "size of"

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

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

$$H(S) = -\frac{|S|}{|S|} \log_2 \frac{|S|}{|S|} = -1 \log_2 1 = 0$$

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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

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

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

$$I(x_d, y) = H(y) - \left(\frac{2}{4} H(y_{x_d=1}) + \frac{2}{4} H(y_{x_d=0})\right)$$

$$= 1 - 0 = 1$$

Mutual Information: Example

x_d	y
1	1
0	1
1	0
0	0

$$I(x_d, y) = H(y) - \left(\frac{2}{4} H(y_{x_d=1}) + \frac{2}{4} H(y_{x_d=0})\right)$$

$$= 1 - \left(\frac{2}{4}(1) + \frac{2}{4}(1)\right) = 0$$

Poll Question 3:

Which feature would you split on using mutual information 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

B. x_2

C. Either x_1 or x_2

D. Neither x_1 nor x_2

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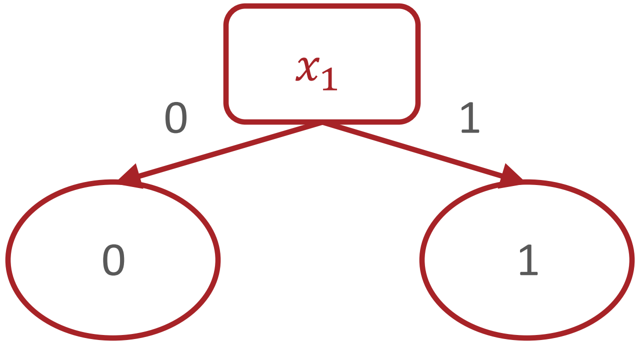
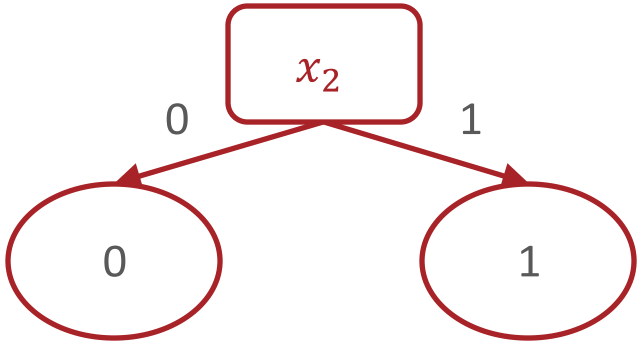


Mutual Information: 0



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

Poll Question 3:

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

x_1	x_2	y
1	0	0
1	0	0
1	0	1
1	0	1
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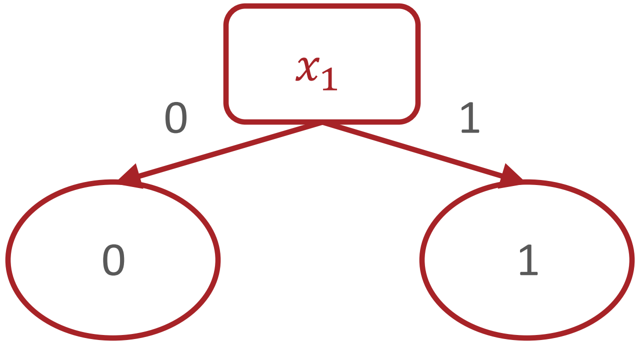
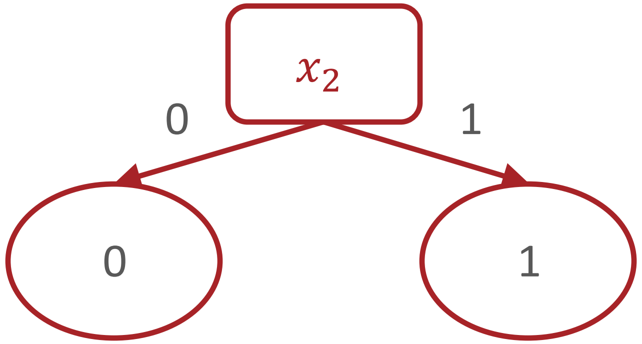
Mutual Information:



Mutual Information: 0



≈ 0.31

Decision Tree Questions

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

   Mutual Information

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?

      Recursion!

Decision Tree: Pseudocode

```
def train(𝒟):
    store root = tree_recurse(𝒟)
def tree_recurse(𝒟′):
    q = new node()
    base case – if (SOME CONDITION):
    recursion – else:
        find the best attribute, X_d
        q.split = X_d
        for v in V(X_d) = {all possible values for X_d}:
            D_v = {(x^(n), y^(n)) ∈ D′ | x_d^(n) = v}
            q.children(v) = tree_recurse(D_v)
    return q
```

Decision Tree: Pseudocode

```
def train(𝒟):
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def tree_recurse(𝒟′):
    q = new node()
    base case – if ( all the labels in D' are
      the same OR all the feature vectors
      in D' are the same OR my tree
      is too big/deep [stopping criterion]
      OR D' is empty):
            q.label = majority_vote(labels in
                                          D')
    recursion – else:
    return q
```