

10-701: Introduction to Machine Learning

# Lecture 2 – Decision Trees

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\* Slides adopted from F24 offering of 10701 by Henry Chai.

# Notation

- Feature space,  $\mathcal{X}$
- Label space,  $\mathcal{Y}$
- (Unknown) Target function,  $c^*: \mathcal{X} \rightarrow \mathcal{Y}$
- Training dataset:  $\mathcal{D} = \{ \langle \mathbf{x}^{(1)}, y^{(1)} \rangle, \dots, \langle \mathbf{x}^{(N)}, y^{(N)} \rangle \}$
- Data point:  
 $\langle \mathbf{x}^{(i)}, y^{(i)} \rangle = \langle x_1^{(i)}, x_2^{(i)}, \dots, x_D^{(i)}, y = c^*(\mathbf{x}) \rangle$
- Classifier,  $h : \mathcal{X} \rightarrow \mathcal{Y}$
- Goal: find a classifier,  $h$ , that best approximates  $c^*$

# Notation

- Loss function,  $\ell : \mathcal{Y} \times \mathcal{Y} \rightarrow \mathbb{R}$ 
  - Defines how “bad” predictions,  $\hat{y} = h(x)$  are
  - compared to the true labels,  $y = c^*(x)$

- Common choices

- Binary or 0-1 loss (for classification):

$$\ell(y, \hat{y}) = \mathbf{1}[y \neq \hat{y}]$$

- Squared loss (for regression):

$$\ell(y, \hat{y}) = (y - \hat{y})^2$$

- Error rate:

$$Err(h, D) = \frac{1}{N} \sum_{i=1} \ell(y^{(i)}, \hat{y}^{(i)})$$

# A Typical (Supervised) Machine Learning Routine

- Step 1 – **training**
  - Input: a labelled training dataset
  - Output: a classifier
- Step 2 – **testing**
  - Inputs: a classifier, a test dataset
  - Output: predictions for each test data point
- Step 3 – **evaluation**
  - Inputs: predictions from step 2, test dataset labels
  - Output: some measure of how good the predictions are;  
usually (but not always) error rate

# Sample Classifiers

- **Majority vote classifier:** always predict the most common label in the dataset
- **Memorizer:** if the input feature vector exists in the **training** dataset, predict its corresponding label; otherwise, predict the majority vote
- **Decision stump** using a specific feature.

## Recall: Our second Machine Learning Classifier

- Alright, let's actually (try to) extract a pattern from the data

$x_1$ 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

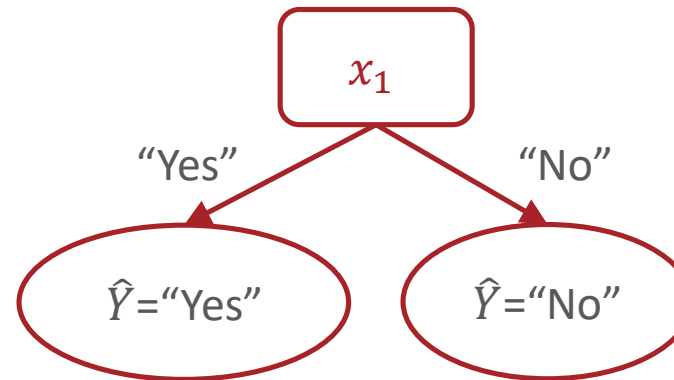
- Decision stump on  $x_1$ :

$$h(\mathbf{x}') = h(x'_1, \dots, x'_D) = \begin{cases} \text{"Yes"} & \text{if } x'_1 = \text{"Yes"} \\ \text{"No"} & \text{otherwise} \end{cases}$$

# Recall: Our second Machine Learning Classifier

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Yes	Medium	Normal	Yes
Yes	High	Abnormal	Yes



# Decision Stumps: Questions

1. How can we pick which feature to split on?
2. Why stop at just one feature?

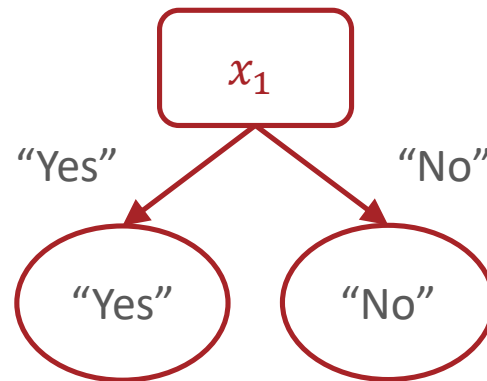


# Splitting Criterion

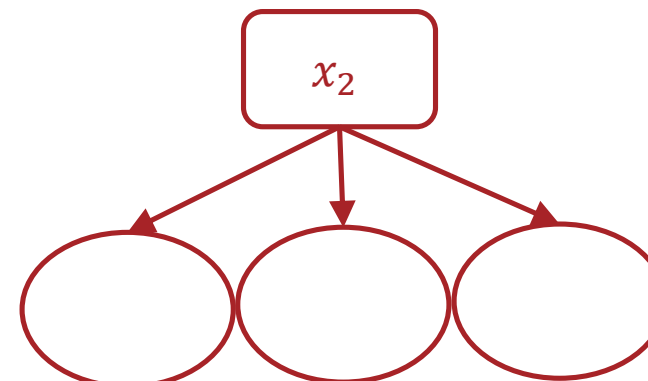
- A **splitting criterion** is a function that measures how good or useful splitting on a particular feature is *for a specified dataset*
- Idea: use the feature that optimizes the splitting criterion for our decision stump.

# Training error rate as a Splitting Criterion

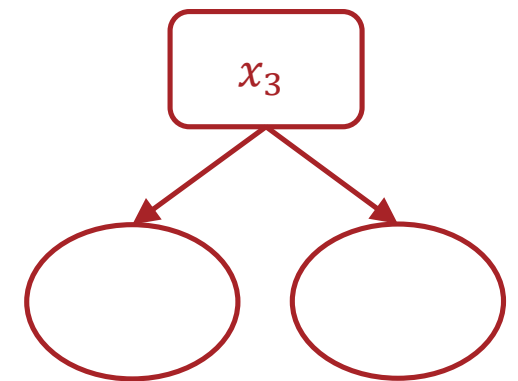
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Yes	Low	Normal	No
No	Medium	Normal	No
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Yes	Medium	Normal	Yes
Yes	High	Abnormal	Yes



Training error rate: 2/5



Training error rate:

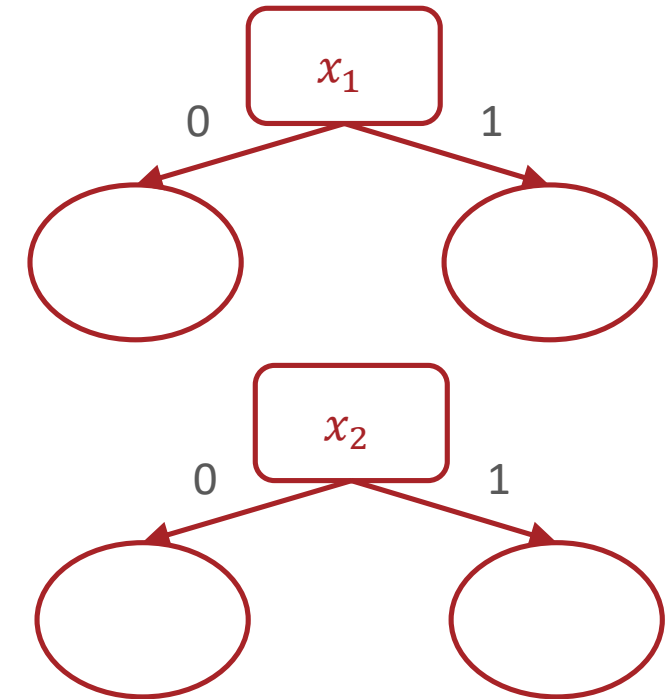


Training error rate:

# Training error rate as a 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

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



# 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: use the feature that optimizes the splitting criterion for our decision stump.
- Potential splitting criteria:
  - Training error rate (minimize)
  - Gini impurity (minimize) → CART algorithm
  - Mutual information (maximize) → ID3 algorithm

# 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: use the feature that optimizes the splitting criterion for our decision stump.
- Potential splitting criteria:
  - Training error rate (minimize)
  - Gini impurity (minimize) → CART algorithm
  - Mutual information (maximize) → ID3 algorithm

# Entropy

- Entropy of a (discrete) random variable  $X$  that takes on values in  $\mathcal{X}$ :

$$H(X) = - \sum_{x \in \mathcal{X}} p(x) \log_2(p(x))$$

Entropy is a measure of randomness, uncertainty, disorder.

Example: biased vs. fair coin

# Entropy

- Entropy of a collection of values  $S$ :

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

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

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

- Example: If all the elements in  $S$  are the same, then

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

# Entropy

- Entropy of a collection of values  $S$ :

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

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

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

- Example: 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

- Mutual information between two random variables  $X$  and  $Y$  describes how much clarity about the value of one variable is gained by observing the other

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

Where  $H(Y|X) = \sum_x p(x) H(Y|X = x)$

$$= -\sum_x p(x) \sum_y \frac{p(x,y)}{p(x)} \log_2 \left( \frac{p(x,y)}{p(x)} \right)$$

$$= -\sum_{x,y} p(x,y) \log_2 \left( \frac{p(x,y)}{p(x)} \right)$$

# Mutual Information

- Mutual information can be used to compute how much information or clarity a particular feature provides about the label

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

where  $x_d$  is a feature

$Y$  is the collection of all labels

$V(x_d)$  is the set of unique values of  $x_d$

$f_v$  is the fraction of inputs where  $x_d = v$

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

## Mutual Information: Example

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

$$\begin{aligned} I(x_d, Y) &= H(Y) - \sum_{v \in V(x_d)} (f_v) \left( H(Y_{x_d=v}) \right) \\ &= 1 - \frac{1}{2} H(Y_{x_d=0}) - \frac{1}{2} H(Y_{x_d=1}) \\ &= 1 - \frac{1}{2} (0) - \frac{1}{2} (0) = 1 \end{aligned}$$

## Mutual Information: Example

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

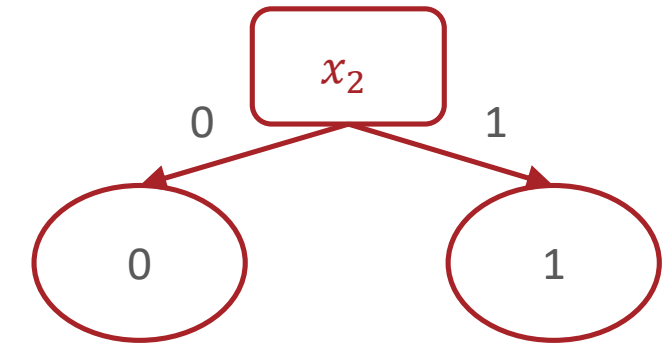
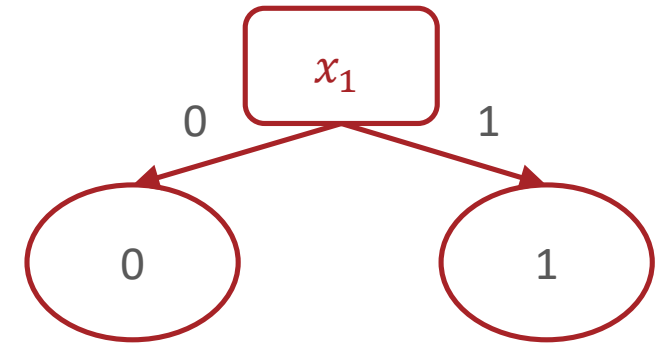
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Poll 1:



$x_1$	$x_2$	$y$
1	0	0
1	0	0
1	0	1
1	0	1
1	1	1
1	1	1
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- Which feature would you split on using mutual information as the splitting criterion?

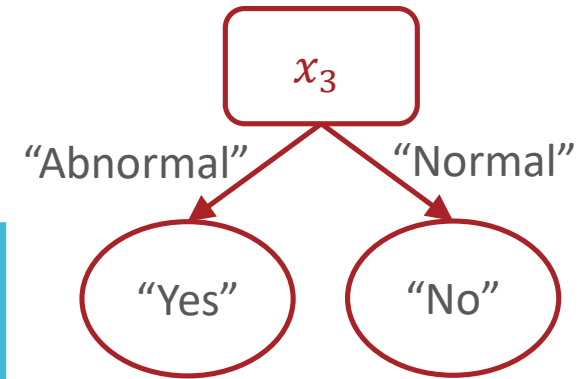


# Decision Stumps: Questions

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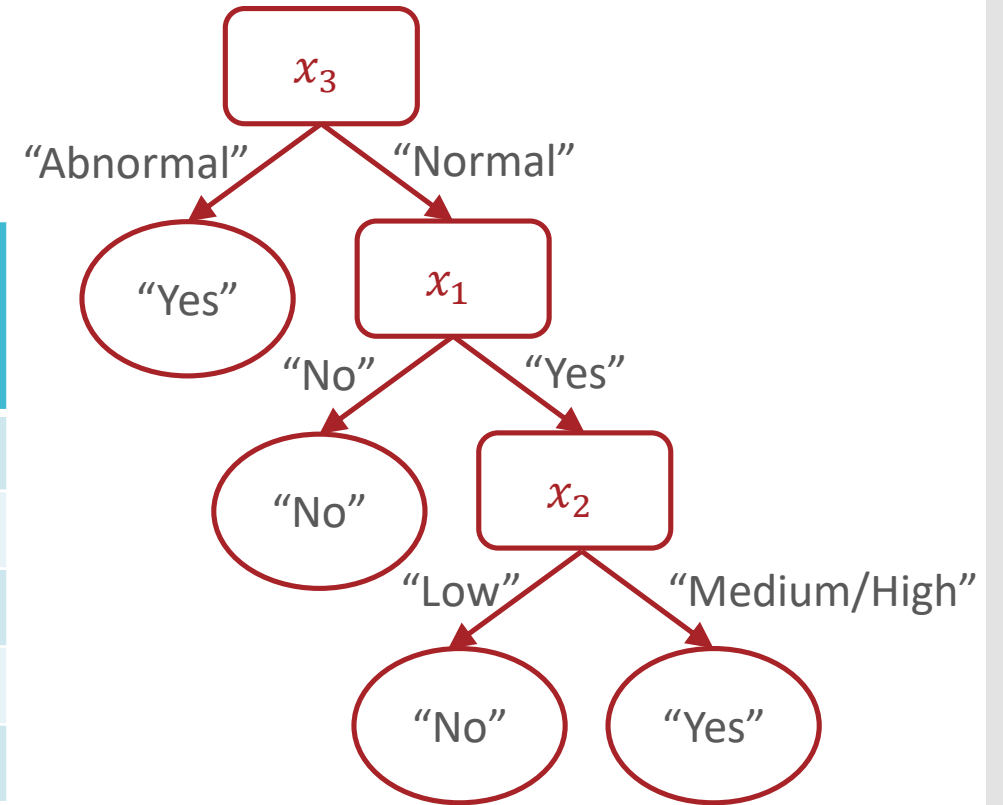
# From Decision Stump ...

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# From Decision Stump to Decision Tree

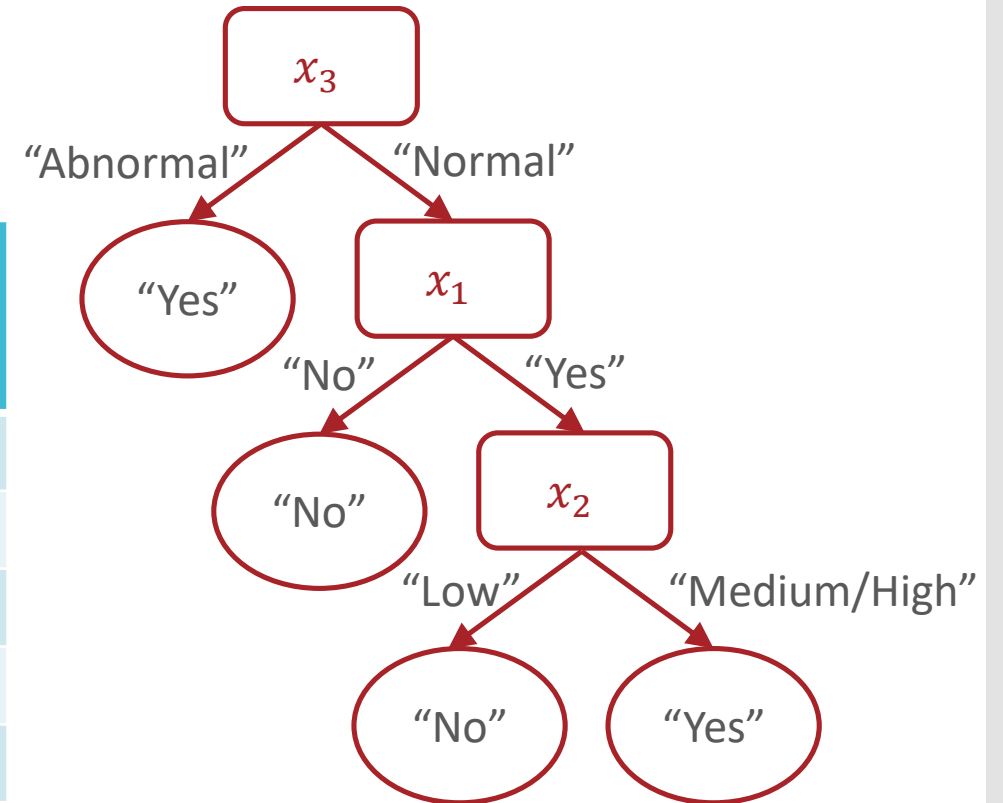
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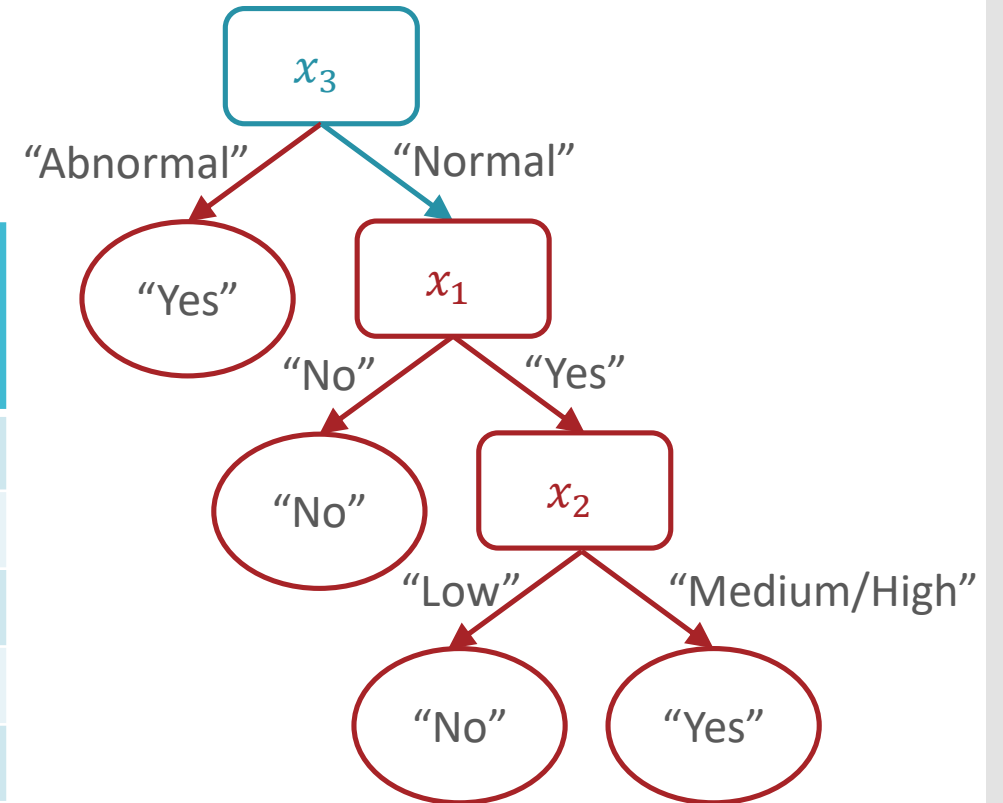
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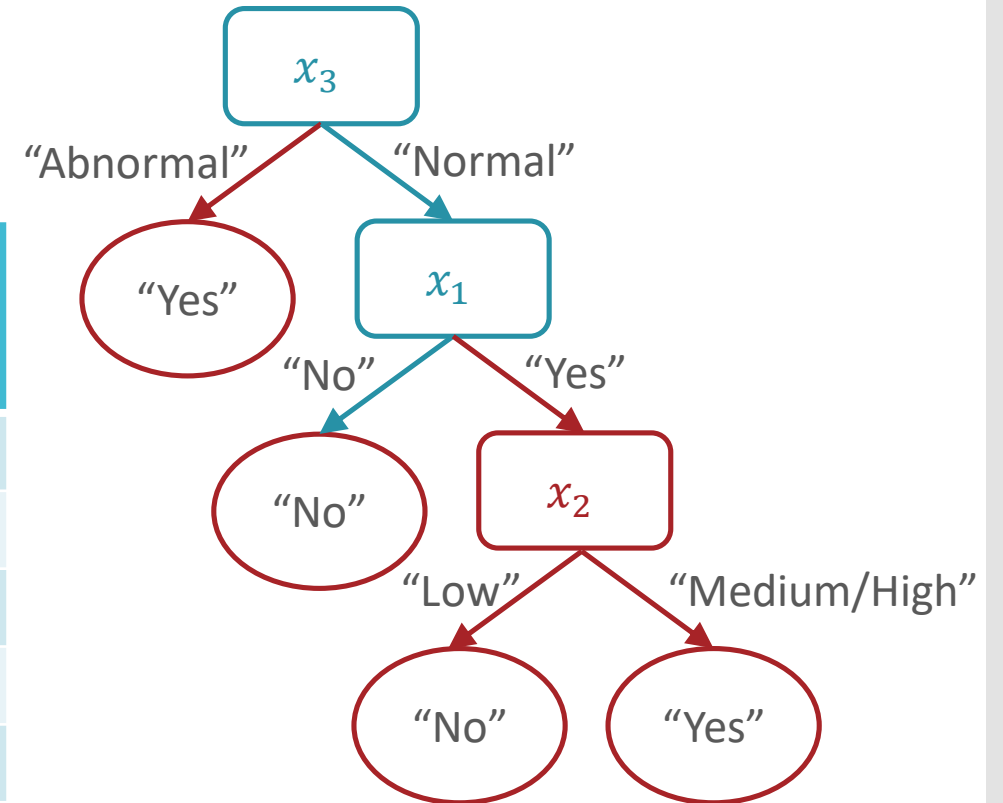
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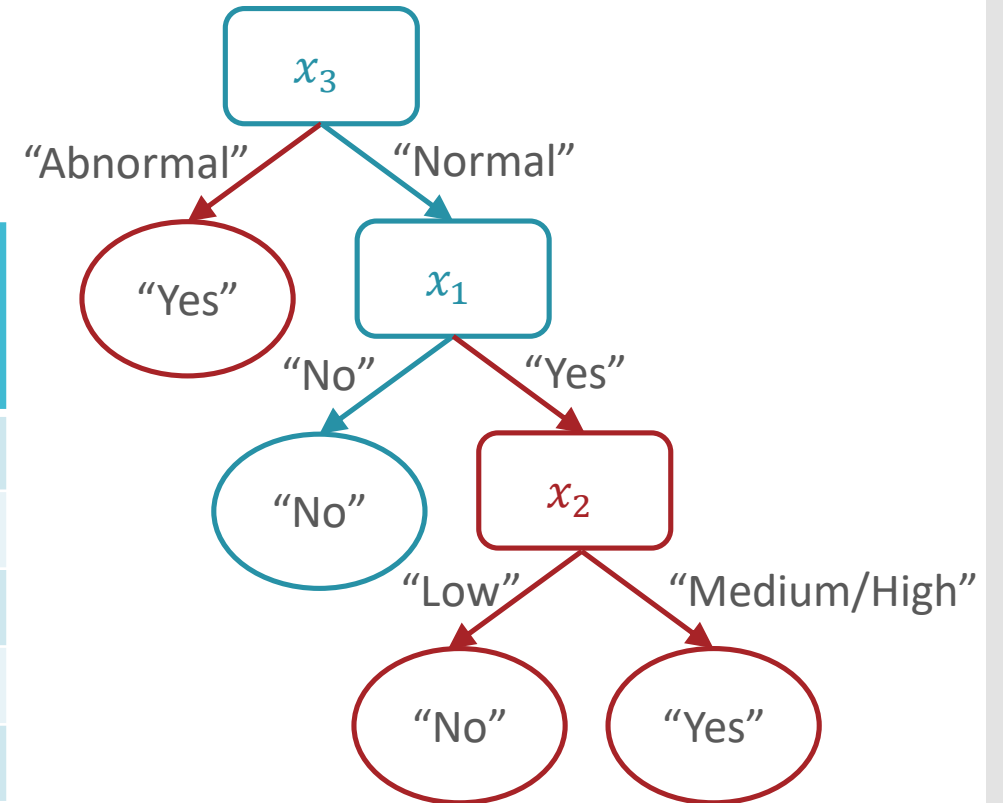
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## Decision Tree Prediction: Pseudocode

```
def predict( $x'$ ):  
    - 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 Learning: ID3 Algorithm

1. Start with the entire training dataset,  $\mathcal{D}$ .
2. For each attribute,  $x_d$ , calculate the information gain if the dataset were split using that attribute.
3. Select the attribute with the highest information gain as the splitting attribute for the current node.
4. Create a new node in the decision tree with this attribute.
5. For each possible value of the chosen attribute, create a new branch and a corresponding subset of the data.
6. Recursively apply steps 2-6 to each subset until a stopping criteria is met:
  - All examples in the subset have the same label.
  - There are no more attributes to split on.
  - There are no more examples in the subset.
  - ...

# Decision Tree Learning: 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  $x_d$ :  
             $\mathcal{D}_v = \{(x^{(n)}, y^{(n)}) \in \mathcal{D} \mid x_d^{(n)} = v\}$   
            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
```



# Decision Tree: Example (Iteratively)

- How am I getting to work?
- Label: mode of transportation
  - $y \in \mathcal{Y} = \{\text{Bike, Drive, Bus}\}$
- Features: 4 categorical features
  - Is it raining?  $x_1 \in \{\text{Rain, No Rain}\}$
  - When am I leaving (relative to rush hour)?  
 $x_2 \in \{\text{Before, During, After}\}$
  - What am I bringing?  
 $x_3 \in \{\text{Backpack, Lunchbox, Both}\}$
  - Am I tired?  $x_4 \in \{\text{Tired, Not Tired}\}$

# Data

$x_1$	$x_2$	$x_3$	$x_4$	$y$
Rain	Before	Both	Tired	Drive
Rain	During	Both	Not Tired	Bus
Rain	During	Both	Tired	Drive
Rain	After	Backpack	Not Tired	Bus
Rain	After	Backpack	Tired	Bus
Rain	After	Lunchbox	Tired	Drive
No Rain	Before	Backpack	Tired	Bike
No Rain	Before	Lunchbox	Not Tired	Bus
No Rain	Before	Lunchbox	Tired	Drive
No Rain	During	Backpack	Not Tired	Bus
No Rain	During	Both	Tired	Drive
No Rain	After	Backpack	Not Tired	Bike
No Rain	After	Backpack	Tired	Bike
No Rain	After	Both	Not Tired	Bus
No Rain	After	Both	Tired	Drive
No Rain	After	Lunchbox	Not Tired	Bus

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

$x_1$	$x_2$	$x_3$	$x_4$	$y$
Rain	Before	Both	Tired	Drive
Rain	During	Both	Not Tired	Bus
Rain	During	Both	Tired	Drive
Rain	After	Backpack	Not Tired	Bus
Rain	After	Backpack	Tired	Bus
Rain	After	Lunchbox	Tired	Drive
No Rain	Before	Backpack	Tired	Bike
No Rain	Before	Lunchbox	Not Tired	Bus
No Rain	Before	Lunchbox	Tired	Drive
No Rain	During	Backpack	Not Tired	Bus
No Rain	During	Both	Tired	Drive
No Rain	After	Backpack	Not Tired	Bike
No Rain	After	Backpack	Tired	Bike
No Rain	After	Both	Not Tired	Bus
No Rain	After	Both	Tired	Drive
No Rain	After	Lunchbox	Not Tired	Bus

Recall:

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

$H(Y)$

$x_1$	$x_2$	$x_3$	$x_4$	$y$
Rain	Before	Both	Tired	Drive
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Rain	During	Both	Tired	Drive
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Rain	After	Backpack	Tired	Bus
Rain	After	Lunchbox	Tired	Drive
No Rain	Before	Backpack	Tired	Bike
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No Rain	Before	Lunchbox	Tired	Drive
No Rain	During	Backpack	Not Tired	Bus
No Rain	During	Both	Tired	Drive
No Rain	After	Backpack	Not Tired	Bike
No Rain	After	Backpack	Tired	Bike
No Rain	After	Both	Not Tired	Bus
No Rain	After	Both	Tired	Drive
No Rain	After	Lunchbox	Not Tired	Bus

Recall:

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

$$H(Y) = - \frac{3}{16} \log_2 \left( \frac{3}{16} \right)$$

$$- \frac{6}{16} \log_2 \left( \frac{6}{16} \right)$$

$$= - \frac{7}{16} \log_2 \left( \frac{7}{16} \right)$$

$$H(Y) \approx 1.5052$$

$x_1$	$x_2$	$x_3$	$x_4$	$y$
Rain	Before	Both	Tired	Drive
Rain	During	Both	Not Tired	Bus
Rain	During	Both	Tired	Drive
Rain	After	Backpack	Not Tired	Bus
Rain	After	Backpack	Tired	Bus
Rain	After	Lunchbox	Tired	Drive
No Rain	Before	Backpack	Tired	Bike
No Rain	Before	Lunchbox	Not Tired	Bus
No Rain	Before	Lunchbox	Tired	Drive
No Rain	During	Backpack	Not Tired	Bus
No Rain	During	Both	Tired	Drive
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No Rain	After	Backpack	Tired	Bike
No Rain	After	Both	Not Tired	Bus
No Rain	After	Both	Tired	Drive
No Rain	After	Lunchbox	Not Tired	Bus

Recall:  $I(x_d; Y) = H(Y)$

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

$$I(x_1, Y) \approx 1.5052$$

$$- \frac{6}{16} (1)$$

$$- \frac{10}{16} \left( -\frac{3}{10} \log_2 \left( \frac{3}{10} \right) \right)$$

$$- \frac{3}{16} \log_2 \left( \frac{3}{16} \right)$$

$x_1$	$x_2$	$x_3$	$x_4$	$y$
Rain	Before	Both	Tired	Drive
Rain	During	Both	Not Tired	Bus
Rain	During	Both	Tired	Drive
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Recall:  $I(x_d; Y) = H(Y)$

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

$$I(x_1, Y) \approx 1.5052$$

$$- \frac{6}{16} (1)$$

$$- \frac{10}{16} (1.5710)$$

$$\approx 0.1482$$

$x_1$	$x_2$	$x_3$	$x_4$	$y$
Rain	Before	Both	Tired	Drive
Rain	During	Both	Not Tired	Bus
Rain	During	Both	Tired	Drive
Rain	After	Backpack	Not Tired	Bus
Rain	After	Backpack	Tired	Bus
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Recall:  $I(x_d; Y) = H(Y)$   
 $- \sum_{v \in V(x_d)} (f_v) (H(Y_{x_d=v}))$

$I(x_d, Y)$	
$x_1$	0.1482
$x_2$	0.1302
$x_3$	0.5358
$x_4$	0.5576

$x_1$	$x_2$	$x_3$	$x_4$	$y$
Rain	Before	Both	Tired	Drive
Rain	During	Both	Not Tired	Bus
Rain	During	Both	Tired	Drive
Rain	After	Backpack	Not Tired	Bus
Rain	After	Backpack	Tired	Bus
Rain	After	Lunchbox	Tired	Drive
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No Rain	Before	Lunchbox	Tired	Drive
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Recall:  $I(x_d; Y) = H(Y)$

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

$I(x_d, Y)$	
$x_1$	0.1482
$x_2$	0.1302
$x_3$	0.5358
$x_4$	0.5576

$x_1$	$x_2$	$x_3$	$x_4$	$y$
Rain	During	Both	Not Tired	Bus
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Recall:  $I(x_d; Y) = H(Y)$

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$I(x_d, Y)$	
$x_1$	0.1482
$x_2$	0.1302
$x_3$	0.5358
$x_4$	0.5576

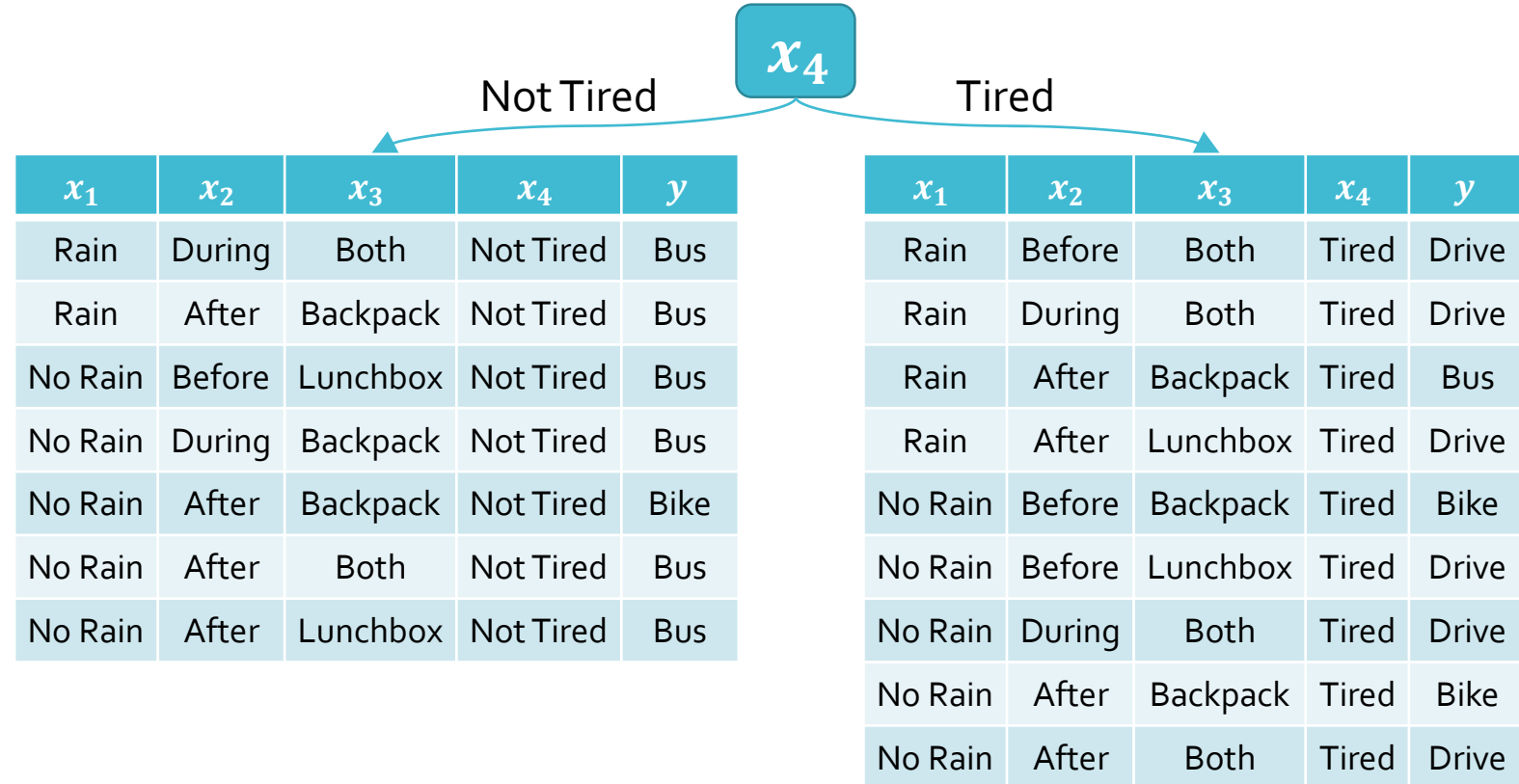
$x_1$	$x_2$	$x_3$	$x_4$	$y$
Rain	During	Both	Not Tired	Bus
Rain	After	Backpack	Not Tired	Bus
No Rain	Before	Lunchbox	Not Tired	Bus
No Rain	During	Backpack	Not Tired	Bus
No Rain	After	Backpack	Not Tired	Bike
No Rain	After	Both	Not Tired	Bus
No Rain	After	Lunchbox	Not Tired	Bus
Rain	Before	Both	Tired	Drive
Rain	During	Both	Tired	Drive
Rain	After	Backpack	Tired	Metro
Rain	After	Lunchbox	Tired	Drive
No Rain	Before	Backpack	Tired	Bike
No Rain	Before	Lunchbox	Tired	Drive
No Rain	During	Both	Tired	Drive
No Rain	After	Backpack	Tired	Bike
No Rain	After	Both	Tired	Drive

Recall:  $I(x_d; Y) = H(Y)$

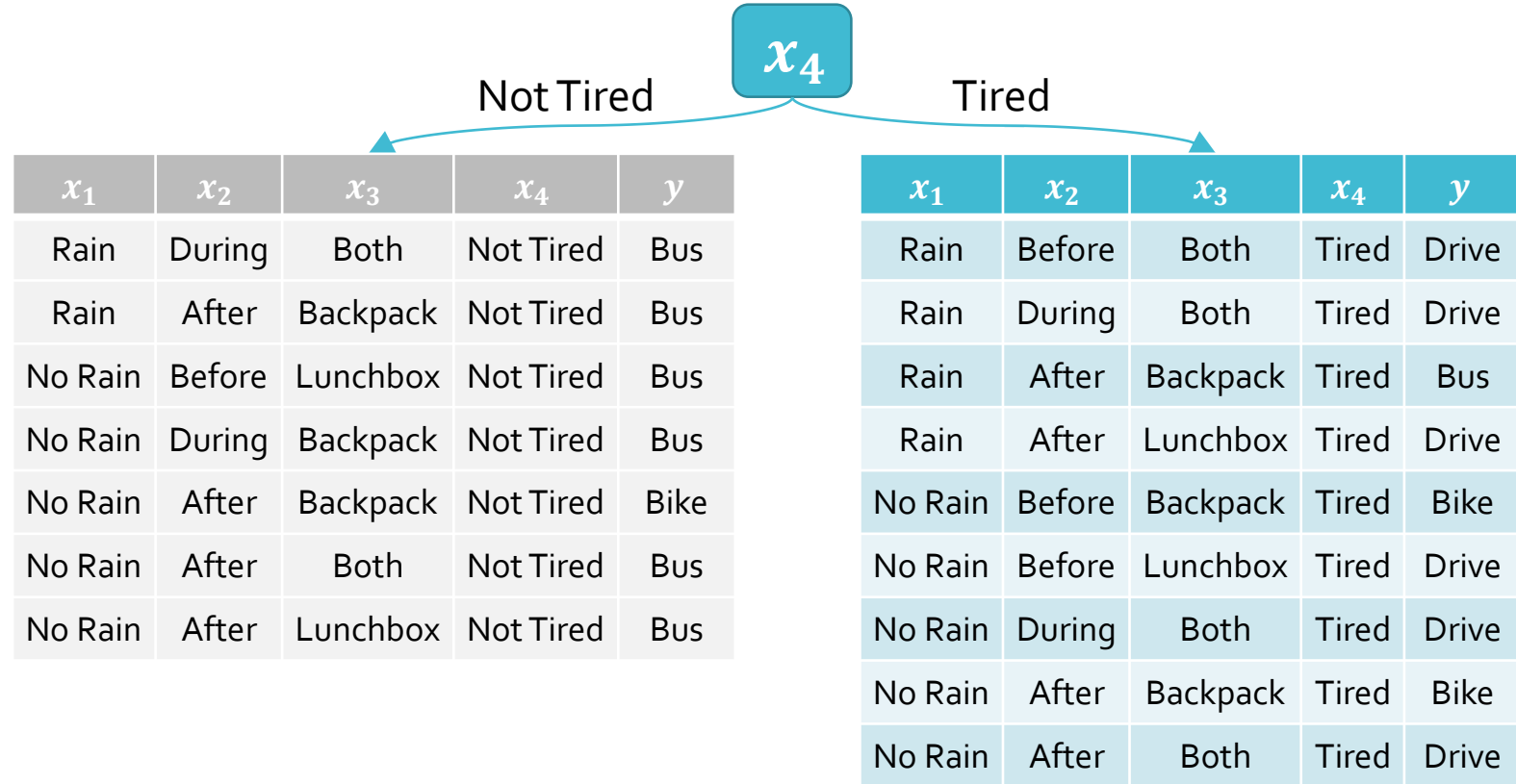
$$- \sum_{v \in V(x_d)} (f_v) \left( H(Y_{x_d=v}) \right)$$

$I(x_d, Y)$	
$x_1$	0.1482
$x_2$	0.1302
$x_3$	0.5358
$x_4$	0.5576

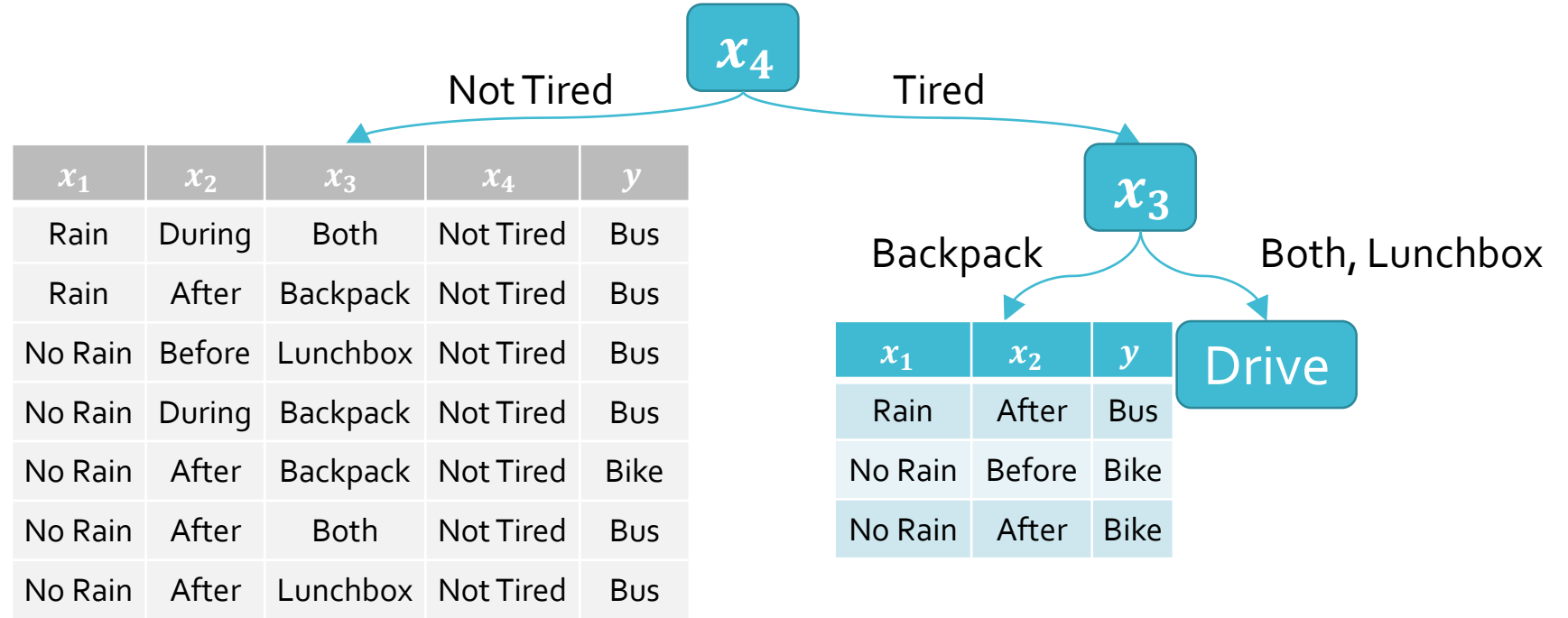
$x_1$	$x_2$	$x_3$	$x_4$	$y$
Rain	During	Both	Not Tired	Bus
Rain	After	Backpack	Not Tired	Bus
No Rain	Before	Lunchbox	Not Tired	Bus
No Rain	During	Backpack	Not Tired	Bus
No Rain	After	Backpack	Not Tired	Bike
No Rain	After	Both	Not Tired	Bus
No Rain	After	Lunchbox	Not Tired	Bus
Rain	Before	Both	Tired	Drive
Rain	During	Both	Tired	Drive
Rain	After	Backpack	Tired	Bus
Rain	After	Lunchbox	Tired	Drive
No Rain	Before	Backpack	Tired	Bike
No Rain	Before	Lunchbox	Tired	Drive
No Rain	During	Both	Tired	Drive
No Rain	After	Backpack	Tired	Bike
No Rain	After	Both	Tired	Drive



## Decision Tree: Example



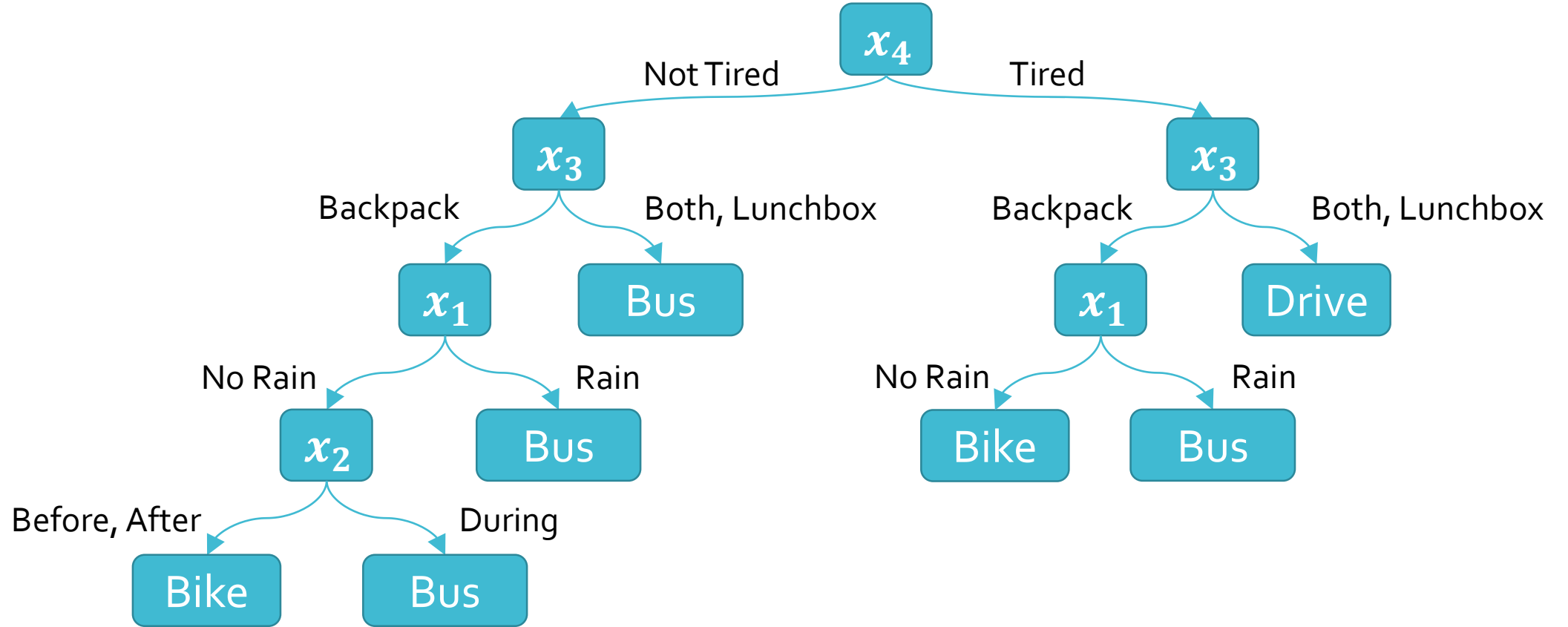




$$I(x_1, Y_{x_4=\text{Tired}}) \approx 0.3244$$

$$I(x_2, Y_{x_4=\text{Tired}}) \approx 0.2516$$

$$I(x_3, Y_{x_4=\text{Tired}}) \approx \mathbf{0.9183}$$





# Decision Trees: Inductive Bias

- The **inductive bias** of a machine learning algorithm is the principal by which it generalizes to unseen examples
- What is the inductive bias of the ID3 algorithm i.e., decision tree learning with mutual information maximization as the splitting criterion?
  - Try to find the \_\_\_\_\_ tree that achieves  
\_\_\_\_\_ with  
\_\_\_\_\_ features at the top

# Decision Trees: Pros & Cons

- Pros
  - Interpretable
  - Efficient (computational cost and storage)
  - Can be used for classification and regression tasks
  - Compatible with categorical and real-valued features
- Cons

# Decision Trees: Pros & Cons

- Pros
  - Interpretable
  - Efficient (computational cost and storage)
  - Can be used for classification and regression tasks
  - Compatible with categorical and real-valued features
- Cons
  - Learned greedily: each split only considers the immediate impact on the splitting criterion
    - Not guaranteed to find the smallest (fewest number of splits) tree that achieves a training error rate of 0.
  - Liable to overfit!