# 10-701: Introduction to Machine Learning Lecture 2 – Decision Trees

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8/30/23

#### Front Matter

- Announcements:
  - Recitations will be held on Fridays, at the same time and place as lecture
    - No recitation Friday, September 1st
  - Office hours will start next week
- Recommended Readings:
  - Mitchell, <u>Chapter 3: Decision Tree Learning</u>
  - Daumé III, <u>Chapter 1: Decision Trees</u>

Recall: Our second Machine Learning Classifier • Alright, let's actually (try to) extract a pattern from the data

x <sub>1</sub> Family History	x <sub>2</sub> Resting Blood Pressure	x <sub>3</sub> 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  $x_1$ :

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

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No	Low	Abnormal	Yes
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*
- Insight: use the feature that optimizes the splitting criterion for our decision stump.

Training error rate as a Splitting Criterion



Training error rate as a Splitting Criterion?



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

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  - Training error rate (minimize)
  - Gini impurity (minimize)  $\rightarrow$  CART algorithm
  - <u>Mutual information</u> (maximize)  $\rightarrow$  ID3 algorithm

#### Entropy

 Entropy describes the purity or uniformity of a collection of values: the lower the entropy, the more pure

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

Size of

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

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

• If all the elements in *S* are the same, then

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where S is a collection of values,

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 $S_{\nu}$  is the collection of elements in S with value  $\nu$ 

 $-\frac{(7z)}{N}\log_2\left(\frac{N/z}{N}\right) - \frac{(N/z)}{N}|_{\alpha}$ 

 $\frac{1052}{N} - \frac{1052}{N} - \frac{1052}{N} = \frac{1$ 

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

#### Mutual Information

• Mutual information describes how much information or clarity a particular feature provides about the label

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

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



Mutual Information: Example



### **Mutual** Information as a Splitting Criterion



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



Decision Stumps: Questions

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

2. Why stop at just one feature?

#### From Decision Stump

•••

				"/
x <sub>1</sub> Family History	x <sub>2</sub> Resting Blood Pressure	x <sub>3</sub> 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<sub>3</sub> 'Abnormal" "Normal" "Yes" "No"

$x_1$ Family History	x <sub>2</sub> Resting Blood Pressure	x <sub>3</sub> Cholesterol	y Heart Disease?
Yes	Low	Normal	No
No	Medium	Normal	No
No	Low	Abnormal	Yes
Yes	Medium	Normal	Yes
Yes	High	Abnormal	Yes



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No	High	Normal	No
----	------	--------	----



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Decision Tree Prediction: Pseudocode

[x', x', ..., x'] def predict(x'): It walk from the root node to a leaf while (true): if current\_node =/= leaf check associated feature, Xi go down branch corresponding to Xi if current node == leaf return label stored in the node

Decision Tree Learning: Pseudocode def train( $\mathcal{D}$ ): store root = tree\_recurse (D) def tree\_recurse( $\mathcal{D}'$ ): q = new node()base case - if (SOME CONDITION): recursion – else: find best fecture to split on X1  $q. split = x_{d}$ for  $V = V(X_1)$  (all possible values of  $D_V = \mathcal{E}(x^{(n)}, y^{(n)}) \in D' [X_1^{(n)}, X_2]$   $Q. child(v) = tree - recurse(D_1)$  Decision Tree: Pseudocode def tree recurse( $\mathcal{D}'$ ): q = new node()base case - if (all labels in D'are the sme OR all features have been split on (all feature vectors in D'are identical) OR D' is empty (or just very small)) 9. label = majority\_vote(D') recursion - else: return q

Decision Tree: Example

- How is Henry getting to work?
- Label: mode of transportation
  - $y \in \mathcal{Y} = \{Bike, Drive, Bus\}$
- Features: 4 categorial features
  - Is it raining?  $x_1 \in \{\text{Rain}, \text{No Rain}\}$
  - 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?  $x_4 \in \{\text{Tired}, \text{Not Tired}\}$

## Data

$x_1$	<i>x</i> <sub>2</sub>	<i>x</i> <sub>3</sub>	<i>x</i> <sub>4</sub>	у
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?

<i>x</i> <sub>1</sub>	<i>x</i> <sub>2</sub>	<i>x</i> <sub>3</sub>	<i>x</i> <sub>4</sub>	у
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
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Recall:  
$$H(S) = -\sum_{v \in V(S)} \frac{|S_v|}{|S|} \log_2\left(\frac{|S_v|}{|S|}\right)$$

H(Y)

<i>x</i> <sub>1</sub>	<i>x</i> <sub>2</sub>	<i>x</i> <sub>3</sub>	$x_4$	у
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:  

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

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

$$-\frac{6}{16} \log_2 \frac{6}{16}$$

$$-\frac{7}{16} \log_2 \frac{7}{16}$$

$$H(Y) = -\frac{7}{16} \log_2 \frac{7}{16}$$

<i>x</i> <sub>1</sub>	<i>x</i> <sub>2</sub>	<i>x</i> <sub>3</sub>	$x_4$	у
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Recall: 
$$I(x_d; Y) = H(Y)$$
  
$$-\sum_{v \in V(x_d)} (f_v) (H(Y_{x_d=v}))$$

 $I(x_1, Y)$ 

 $IG(x_1, y) = -\frac{7}{16} \log_2\left(\frac{7}{16}\right)$ 

<i>x</i> <sub>1</sub>	<i>x</i> <sub>2</sub>	<i>x</i> <sub>3</sub>	$x_4$	у
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 $I(x_1, Y) \approx 1.5052$ 



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

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

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

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

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$x_1$	<i>x</i> <sub>2</sub>	<i>x</i> <sub>3</sub>	$x_4$	у
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$$I(x_d; Y) = H(Y)$$
  
 $-\sum_{v \in V(x_d)} (f_v) (H(Y_{x_d=v}))$   
 $I(x_1, Y) \approx 1.5052$   
 $-\frac{6}{16}(1)$   
 $-\frac{10}{16}(1.5710)$   
 $\approx 0.1482$ 

<i>x</i> <sub>1</sub>	<i>x</i> <sub>2</sub>	<i>x</i> <sub>3</sub>	$x_4$	у
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Rain	During	Both	Not Tired	Bus
Rain	During	Both	Tired	Drive
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$$I(x_d; Y) = H(Y)$$
  

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

$I(x_d, Y)$		
<i>x</i> <sub>1</sub>	0.1482	
<i>x</i> <sub>2</sub>	0.1302	
<i>x</i> <sub>3</sub>	0.5358	
$x_4$	0.5576	

<i>x</i> <sub>1</sub>	<i>x</i> <sub>2</sub>	<i>x</i> <sub>3</sub>	<i>x</i> <sub>4</sub>	у
Rain	Before	Both	Tired	Drive
Rain	During	Both	Not Tired	Bus
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<i>x</i> <sub>2</sub>	0.1302	
<i>x</i> <sub>3</sub>	0.5358	
<i>x</i> <sub>4</sub>	0.5576	

<i>x</i> <sub>1</sub>	<i>x</i> <sub>2</sub>	<i>x</i> <sub>3</sub>	<i>x</i> <sub>4</sub>	у
Rain	During	Both	Not Tired	Bus
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<i>I(</i> 2	$(x_d, Y)$
<i>x</i> <sub>1</sub>	0.1482
<i>x</i> <sub>2</sub>	0.1302
<i>x</i> <sub>3</sub>	0.5358
<i>x</i> <sub>4</sub>	0.5576

<i>x</i> <sub>1</sub>	<i>x</i> <sub>2</sub>	<i>x</i> <sub>3</sub>	$x_4$	у
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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
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I()	$(x_d, Y)$
<i>x</i> <sub>1</sub>	0.1482
<i>x</i> <sub>2</sub>	0.1302
<i>x</i> <sub>3</sub>	0.5358
$x_4$	0.5576

<i>x</i> <sub>1</sub>	<i>x</i> <sub>2</sub>	<i>x</i> <sub>3</sub>	$x_4$	у
Rain	During	Both	NotTired	Bus
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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

			NotTire	ed	<i>x</i> <sub>4</sub>	Tir	ed			
1	<i>x</i> <sub>2</sub>	<i>x</i> <sub>3</sub>	<i>x</i> <sub>4</sub>	у		<i>x</i> <sub>1</sub>	<i>x</i> <sub>2</sub>	<i>x</i> <sub>3</sub>	<i>x</i> <sub>4</sub>	
Rain	During	Both	Not Tired	Bus		Rain	Before	Both	Tired	D
Rain	After	Backpack	Not Tired	Bus		Rain	During	Both	Tired	D
lo Rain	Before	Lunchbox	Not Tired	Bus		Rain	After	Backpack	Tired	E
lo Rain	During	Backpack	Not Tired	Bus		Rain	After	Lunchbox	Tired	D
lo Rain	After	Backpack	Not Tired	Bike		No Rain	Before	Backpack	Tired	B
lo Rain	After	Both	Not Tired	Bus		No Rain	Before	Lunchbox	Tired	D
lo Rain	After	Lunchbox	Not Tired	Bus		No Rain	During	Both	Tired	D
						No Rain	After	Backpack	Tired	E
						No Rain	After	Both	Tired	D

### Decision Tree: Example

			NotTire	d	<i>x</i> <sub>4</sub>	Tir	ed			
$x_1$	<i>x</i> <sub>2</sub>	<i>x</i> <sub>3</sub>	$x_4$	y		$x_1$	<i>x</i> <sub>2</sub>	<i>x</i> <sub>3</sub>	<i>x</i> <sub>4</sub>	y
Rain	During	Both	Not Tired	Bus		Rain	Before	Both	Tired	Drive
Rain	After	Backpack	Not Tired	Bus		Rain	During	Both	Tired	Drive
No Rain	Before	Lunchbox	Not Tired	Bus		Rain	After	Backpack	Tired	Bus
No Rain	During	Backpack	Not Tired	Bus		Rain	After	Lunchbox	Tired	Drive
No Rain	After	Backpack	Not Tired	Bike		No Rain	Before	Backpack	Tired	Bike
No Rain	After	Both	Not Tired	Bus		No Rain	Before	Lunchbox	Tired	Drive
No Rain	After	Lunchbox	Not Tired	Bus		No Rain	During	Both	Tired	Drive
						No Rain	After	Backpack	Tired	Bike

No Rain After

Tired Drive

Both

			NotTire	ed	<i>x</i> <sub>4</sub>	Tir	ed			
<i>x</i> <sub>1</sub>	<i>x</i> <sub>2</sub>	<i>x</i> <sub>3</sub>	<i>x</i> <sub>4</sub>	у		<i>x</i> <sub>1</sub>	<i>x</i> <sub>2</sub>	<i>x</i> <sub>3</sub>	<i>x</i> <sub>4</sub>	
Rain	During	Both	Not Tired	Bus		Rain	After	Backpack	Tired	
Rain	After	Backpack	Not Tired	Bus		No Rain	Before	Backpack	Tired	
No Rain	Before	Lunchbox	Not Tired	Bus		No Rain	After	Backpack	Tired	
No Rain	During	Backpack	Not Tired	Bus		Rain	Before	Both	Tired	
No Rain	After	Backpack	Not Tired	Bike		Rain	During	Both	Tired	
No Rain	After	Both	Not Tired	Bus		No Rain	During	Both	Tired	
No Rain	After	Lunchbox	Not Tired	Bus		No Rain	After	Both	Tired	
						Rain	After	Lunchbox	Tired	

No Rain Before Lunchbox Tired Drive

$$I(x_1, Y_{x_4=\text{Tired}}) \approx 0.3244$$
  
 $I(x_2, Y_{x_4=\text{Tired}}) \approx 0.2516$   
 $I(x_3, Y_{x_4=\text{Tired}}) \approx 0.9183$ 

8/30/23



$$I(x_1, Y_{x_4=\text{Tired}}) \approx 0.3244$$
  
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 $I(x_3, Y_{x_4=\text{Tired}}) \approx 0.9183$ 



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 <u>Shortest</u> tree that achieves <u>Zero (or the lovest possible) train</u> with <u>high mutual information</u> 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!

### Overfitting

- Overfitting occurs when the classifier (or model)...
  - is too complex
  - fits noise or "outliers" in the training dataset as opposed to the actual pattern of interest
  - doesn't have enough inductive bias pushing it to generalize
- Underfitting occurs when the classifier (or model)...
  - is too simple
  - can't capture the actual pattern of interest in the training dataset
  - has too much inductive bias

Different Kinds of Error

- Training error rate =  $err(h, D_{train})$
- Test error rate =  $err(h, \mathcal{D}_{test})$
- True error rate = err(h)
  - = the error rate of h on all possible examples
  - In machine learning, this is the quantity that we care about but, in most cases, it is unknowable.
- Overfitting occurs when err(h) > err(h, D<sub>train</sub>)
   err(h) err(h, D<sub>train</sub>) can be thought of as a measure of overfitting







This tree only misclassifies one training data point!

#### Key Takeaways

- Decision tree prediction algorithm
- Decision tree learning algorithm via recursion
- Inductive bias of decision trees
- Overfitting vs. Underfitting
- How to combat overfitting in decision trees