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

Henry Chai

5/17/23

### Front Matter

- Announcements:
	- · PA0 released 5/15, due 5,
		- You must complete all

this Piazza post for de

- · PA1 released 5/18 (tomor
- Recitation tomorrow will
	- Programming tips to h
	- Practice problems for
	- **Recitations are option recorded**; solutions w
- Recommended Readings:
	- **Daumé III, Chapter 1: Dec**

Recall: Decision Stumps Questions

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

2. Why stop at just one feature?

# From **Decision** Stump to **Decision** Tree







Decision Tree Prediction: Pseudocode

 $\int \frac{1}{\sqrt{2}} dx$  $\n *while* (true)$  $\mathcal{L}$  $i\int_{0}^{1}$  internal non-leaful is internal teature  $x_1$  as down the branch  $\frac{1}{2}$  ding to  $\frac{1}{2}$ if current nodes is a leaf nodes in  $\mathcal{C}$  $relint$  the label stored at  $H_{n,s}$  leaf node

# Background: **Recursion**



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#### 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

**6** def contains\_iterative(node, key):  $current$  mode = node  $\frac{1}{\sqrt{1-\delta}}$  $int (true).$  $\Gamma$   $\Gamma$  $\sum_{i=1}^{n}$  $curent$   $r$ else: break  $r = \frac{1}{2}$ 

# Background: Recursion



#### A **binary search tree** (BST) consists of nodes, where each node:

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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):  
\nif key < node. value & node. left != null  
\ncontains - recursive(node. left, key)  
\n
$$
elff
$$
 kry > node. value & node. right != null  
\ncontains - recursive (node. right, key)  
\n $elex$    
\nreturn key == node. value

**7**

Decision Tree Learning: **Pseudocode** 

def train $(D)$ :  $root = free\_recure(D)$ def tree\_recurse $(D')$ :  $\bigstar q$  = new node() base case – if (SOME CONDITION): recursion – else: find best attabute to split on,  $x_d$  $q.$ split =  $x_d$  $f$  or  $v$  in  $V(x)$ , all possible values for  $x$  $V$  =  $\sum_{i=1}^{n}$   $\left(X_{(i)}, \lambda_{(i)}\right) \in \mathcal{V}$  $\binom{1}{r}$  children  $\binom{v}{r}$  =  $\frac{1}{r}$ 

Decision Tree: Pseudocode def train $(D)$ :  $rot = true$ -recurse $(D)$ def tree\_recurse $(D')$ :  $q = new node()$ base case – if  $(D'$  is empty all features in  $D'$  are identice all features in  $D'$  are the sem some stopping criterion):  $\mu^{\lambda}$  and  $\mu$ recursion – else: return q and **9** 

**Decision** Tree: Example – How is Henry getting to work?

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

# Data



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



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

 $H(Y)$ 



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

$$
H(Y) = -\frac{3}{\sqrt{6}} \log_2 \left(\frac{3}{\sqrt{6}}\right)
$$
  

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

$$
-\frac{7}{\sqrt{6}} \log_2 \left(\frac{7}{\sqrt{6}}\right)
$$
  

$$
\approx 1.5052
$$



Recall: 
$$
I(x_d; Y) = H(Y)
$$
  
\n
$$
- \sum_{v \in V(x_d)} (f_v) (H(Y_{x_d=v}))
$$

 $I(x_1, Y) =$ 



Recall: 
$$
I(x_d; Y) = H(Y)
$$
  
\n
$$
- \sum_{v \in V(x_d)} (f_v) (H(Y_{x_d=v}))
$$

$$
(x_1, Y) \approx 1.5052
$$
  
-
$$
\frac{G}{16} \left(-\frac{3}{6} \log_2 \left(\frac{3}{6}\right) - \frac{3}{6} \log_2 \left(\frac{3}{6}\right)\right)
$$



 $\overline{l}$ 

Recall: 
$$
I(x_d; Y) = H(Y)
$$
  
\n
$$
- \sum_{v \in V(x_d)} (f_v) (H(Y_{x_d=v}))
$$

 $I(x_1, Y) \approx 1.5052$ 

6 16 1



Recall: 
$$
I(x_d; Y) = H(Y)
$$
  
\n
$$
- \sum_{v \in V(x_d)} (f_v) (H(Y_{x_d=v}))
$$
\n
$$
I(x_1, Y) \approx 1.5052
$$
\n
$$
- \frac{6}{16}(1)
$$
\n
$$
- \frac{10}{16} \left(-\frac{3}{10} \log_2(\frac{3}{10}) - \frac{3}{10} \log_2(\frac{3}{10}) - \frac{4}{10} \log_2(\frac{3}{10}) - \frac{4}{10} \log_2(\frac{3}{10})\right)
$$



Recall: 
$$
I(x_d; Y) = H(Y - \sum_{v \in V(x_d)} (f_v) (H(Y_{x_d=v}))
$$
  
\n $I(x_1, Y) \approx 1.5052$   
\n $- \frac{6}{16}(1)$   
\n $- \frac{10}{16}(1.5710)$   
\n $\approx 0.1482$ 



Recall: 
$$
I(x_d; Y) = H(Y)
$$
  
\n
$$
- \sum_{v \in V(x_d)} (f_v) (H(Y_{x_d=v}))
$$



![](_page_19_Picture_313.jpeg)

Recall: 
$$
I(x_d; Y) = H(Y)
$$
  
\n
$$
- \sum_{v \in V(x_d)} (f_v) (H(Y_{x_d=v}))
$$

![](_page_20_Picture_322.jpeg)

![](_page_20_Picture_323.jpeg)

Recall:  $I(x_d; Y) = H(Y)$ − M  $v \in V(x_d)$  $f_{\nu}$ )  $\left(H(Y_{x_d=v})\right)$ 

![](_page_21_Picture_301.jpeg)

![](_page_21_Picture_302.jpeg)

Recall: 
$$
I(x_d; Y) = H(Y)
$$
  
\n
$$
- \sum_{v \in V(x_d)} (f_v) (H(Y_{x_d=v}))
$$

![](_page_22_Picture_312.jpeg)

![](_page_22_Picture_313.jpeg)

![](_page_23_Picture_208.jpeg)

# Decision Tree: Example

![](_page_24_Picture_205.jpeg)

No Rain After Both Tired Drive

![](_page_25_Picture_217.jpeg)

No Rain After Both Tired Drive

 $H(Y_{x_4} = \text{Tired}) =$ 

![](_page_26_Picture_232.jpeg)

$$
I(x_1, Y_{x_4} = \text{Tired}) = H(Y_{x_4} = \text{Tired}) - \frac{4}{9}H(Y_{x_4} = \text{Tired}, x_1 = \text{Rain}) - \frac{5}{9}H(Y_{x_4} = \text{Tired}, x_1 = \text{No Rain})
$$

![](_page_27_Picture_235.jpeg)

$$
I(x_1, Y_{x_4} =
$$
Tired)  $\approx 1.2244 - \frac{4}{9}(0.8113) - \frac{5}{9}(0.9710) \approx 0.3244$ 

![](_page_28_Picture_245.jpeg)

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

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

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

**Drive** 

**Drive** 

**Bus** 

**Drive** 

**Bike** 

Drive

Drive

No Rain After Both Tired Drive

![](_page_29_Picture_232.jpeg)

No Rain Before Lunchbox Tired Drive

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

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

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

![](_page_30_Figure_0.jpeg)

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

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

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

![](_page_31_Figure_0.jpeg)

![](_page_32_Picture_0.jpeg)

#### **Untitled survey**

#### 0 done

Counderway

Start the presentation to see live content. For screen share software, share the entire screen. Get help at pollev.com/app

# True or False: if we use mutual information maximization as the splitting criterion, we will always learn the shortest possible decision tree with zero training error.

True

False

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# True or False: if we use training error minimization as the splitting criterion, we will always learn the shortest possible decision tree with zero training error.

![](_page_34_Figure_2.jpeg)

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Given this dataset, if you used training error rate as the splitting criterion, you would learn this tree…

![](_page_35_Figure_1.jpeg)

![](_page_35_Figure_2.jpeg)

… but there actually exists a shorter decision tree with zero training error!

![](_page_36_Figure_1.jpeg)

![](_page_36_Figure_2.jpeg)

**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 shortest tree that achieves taining error with

Criterion features at the top information) Occam's razor: try to find the "simplest" (e.g., smallest

decision tree) classifier that explains the training dataset

**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

Real -Valued Features: Example  $x =$  Outside Temperature (°F)

![](_page_39_Figure_1.jpeg)

Real -Valued Features: Example  $x =$  Outside Temperature (°F)

![](_page_40_Figure_1.jpeg)

Real -Valued Features: Example  $x =$  Outside Temperature (°F)

![](_page_41_Figure_1.jpeg)

Real-Valued Features: Example  $x =$ Outside Temperature (℉)

![](_page_42_Figure_1.jpeg)

**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 =  $err(h, D_{test})$
- 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  $err(h)$   $\geq$   $err(h, D_{train})$ •  $err(h) - err(h, D_{train})$  can be thought of as a measure of overfitting

![](_page_46_Figure_0.jpeg)

![](_page_47_Figure_0.jpeg)

![](_page_48_Figure_0.jpeg)

This tree only misclassifies one training data point!

## Overfitting in Decision Trees

![](_page_49_Figure_1.jpeg)

**Combatting** Overfitting in Decision Trees · Heuristics:

- $\cdot$  Do not split leaves past a fixed depth,  $\delta$
- $\cdot$  Do not split leaves with fewer than  $c$  data points
- Do not split leaves where the maximal information gain is less than  $\tau$
- Take a majority vote in impure leaves

**Combatting** Overfitting in Decision Trees

- Pruning:
	- 1. First, learn a decision tree
	- 2. Then, evaluate each split using a "validation" dataset by comparing the validation error rate with and without that split
	- 3. Greedily remove the split that most decreases the validation error rate
		- Break ties in favor of smaller trees
	- 4. Stop if no split is removed

## Pruning Decision Trees

![](_page_52_Figure_1.jpeg)

![](_page_53_Figure_0.jpeg)

![](_page_54_Figure_0.jpeg)

![](_page_55_Figure_0.jpeg)

![](_page_56_Picture_0.jpeg)

$x_1$	$x_2$	$x_3$	$x_4$	$y$	
Rain	During	Backpack	Tired	Bus	
1	Rain	After	Both	NotTired	Bus
2	No Rain	Before	Backpack	NotTired	Bus
2	No Rain	During	Lunchbox	Tired	Brive
2	No Rain	During	Lunchbox	Tired	Drive

![](_page_57_Picture_0.jpeg)

$x_1$	$x_2$	$x_3$	$x_4$	$y$	
Rain	During	Backpack	Tired	Bus	
$D_{val}$	Rain	After	Both	NotTired	Bus
$err(h - S_1, D_{val}) = 0.4$	No Rain	During	Lunchbox	Tired	Dirive
No Rain	After	Lunchbox	Tired	Dirive	

![](_page_58_Figure_0.jpeg)

![](_page_59_Figure_0.jpeg)

![](_page_60_Figure_0.jpeg)

![](_page_61_Figure_0.jpeg)

![](_page_62_Figure_0.jpeg)

![](_page_63_Figure_0.jpeg)

![](_page_64_Figure_0.jpeg)

![](_page_65_Figure_0.jpeg)

## 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