#### **Decision Trees**

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August 9, 2024

IIT Gandhinagar

# **Discrete Input Discrete Output**

#### The need for interpretability

#### How to maintain trust in AI

Beyond developing initial trust, however, creators of AI also must work to maintain that trust. Siau and Wang suggest seven ways of "developing continuous trust" beyond the initial phases of product development:

- Usability and reliability. Al "should be designed to operate easily and intuitively,"
   Siau and Wang write. "There should be no unexpected downtime or crashes."
- Collaboration and communication. Al developers want to create systems that
  perform autonomously, without human involvement. Developers must focus on
  creating Al applications that smoothly and easily collaborate and communicate
  with humans.
- Sociability and bonding. Building social activities into AI applications is one way to strengthen trust. A robotic dog that can recognize its owner and show affection is one example, Siau and Wang write.
- Security and privacy protection. Al applications rely on large data sets, so
  ensuring privacy and security will be crucial to establishing trust in the
  applications.
- Interpretability. Just as transparency is instrumental in building initial trust, interpretability – or the ability for a machine to explain its conclusions or actions – will help sustain trust.

# **Training Data**

Day	Outlook	Temp	Humidity	Windy	Play
D1	Sunny	Hot	High	Weak	No
D2	Sunny	Hot	High	Strong	No
D3	Overcast	Hot	High	Weak	Yes
D4	Rain	Mild	High	Weak	Yes
D5	Rain	Cool	Normal	Weak	Yes
D6	Rain	Cool	Normal	Strong	No
D7	Overcast	Cool	Normal	Strong	Yes
D8	Sunny	Mild	High	Weak	No
D9	Sunny	Cool	Normal	Weak	Yes
D10	Rain	Mild	Normal	Weak	Yes
D11	Sunny	Mild	Normal	Strong	Yes
D12	Overcast	Mild	High	Strong	Yes
D13	Overcast	Hot	Normal	Weak	Yes
D14	Rain	Mild	High	Strong	No

# Learning a Complicated Neural Network



#### **Learnt Decision Tree**



#### Medical Diagnosis using Decision Trees



Source: Improving medical decision trees by combining relevant health-care criteria

#### Leo Brieman



#### Leo Breiman 1928-2005

Professor of Statistics, <u>UC Berkeley</u>.

Verified email at stat.berkeley.edu - <u>Homepage</u>

Data Analysis Statistics Machine Learning



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#### **Optimal Decision Tree**

Volume 5, number 1

INFORMATION PROCESSING LETTERS

May 1976

#### CONSTRUCTING OPTIMAL BINARY DECISION TREES IS NP-COMPLETE\*

Laurent HYAFII.

IRIA - Laboria, 78150 Rocquencourt, France

and

Ronald L. RIVEST

Dept. of Electrical Engineering and Computer Science, M.I.T., Cambridge, Massachusetts 02139, USA

Received 7 November 1975, revised version received 26 January 1976

Binary decision trees, computational complexity, NP-complete

# **Greedy Algorithm**

Core idea: At each level, choose an attribute that gives **biggest estimated** performance gain!



 ${\sf Greedy!} {=} {\sf Optimal}$ 

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• For examples, we have 9 Yes, 5 No

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D10	Rain	Mild	Normal	Weak	Yes
D11	Sunny	Mild	Normal	Strong	Yes
D12	Overcast	Mild	High	Strong	Yes
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- For examples, we have 9 Yes, 5 No
- Would it be trivial if we had 14 Yes or 14 No?

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D6	Rain	Cool	Normal	Strong	No
D7	Overcast	Cool	Normal	Strong	Yes
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- Key insights: Problem is "easier" when there is lesser disagreement

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- Would it be trivial if we had 14 Yes or 14 No?
- Yes!
- Key insights: Problem is "easier" when there is lesser disagreement
- Need some statistical measure of "disagreement"

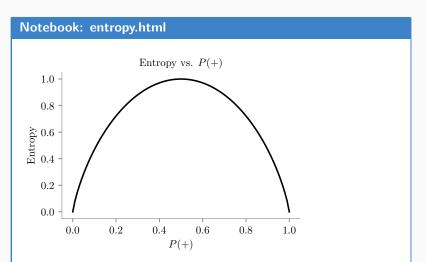
#### **Entropy**

Statistical measure to characterize the (im)purity of examples

#### Entropy

Statistical measure to characterize the (im)purity of examples

$$H(X) = -\sum_{i=1}^{n} p(x_i) \log p(x_i)$$



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 Can we use Outlook as the root node?

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D10	Rain	Mild	Normal	Weak	Yes
D11	Sunny	Mild	Normal	Strong	Yes
D12	Overcast	Mild	High	Strong	Yes
D13	Overcast	Hot	Normal	Weak	Yes
D14	Rain	Mild	High	Strong	No

- Can we use Outlook as the root node?
- When Outlook is overcast, we always Play and thus no "disagreement"

#### **Information Gain**

Reduction in entropy by partitioning examples (S) on attribute A

$$Gain(S, A) \equiv Entropy(S) - \sum_{v \in Values(A)} \frac{|S_v|}{|S|} Entropy(S_v)$$

• Create a root node for tree

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- Begin
  - ullet A  $\leftarrow$  attribute from Attributes which best classifies Examples

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  - Root  $\leftarrow$  A

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  - Root  $\leftarrow$  A
  - For each value (v) of A
    - Add new tree branch : A = v

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- If all examples are +/-, return root with label =+/-
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  - A ← attribute from Attributes which best classifies Examples
  - Root  $\leftarrow$  A
  - For each value (v) of A
    - Add new tree branch : A = v
    - Examples<sub>v</sub>: subset of examples that A = v

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  - For each value (v) of A
    - Add new tree branch : A = v
    - Examples<sub>v</sub>: subset of examples that A = v
    - If Examples<sub>v</sub>is empty: add leaf with label = most common value of Target Attribute

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  - For each value (v) of A
    - Add new tree branch : A = v
    - ullet Examples<sub>v</sub>: subset of examples that A = v
    - If Examples<sub>v</sub>is empty: add leaf with label = most common value of Target Attribute
    - Else: ID3 (Examples<sub>v</sub>, Target attribute, Attributes A)

#### **Learnt Decision Tree**

Root Node (empty)

# **Training Data**

Day	Outlook	Temp	Humidity	Windy	Play
D1	Sunny	Hot	High	Weak	No
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D3	Overcast	Hot	High	Weak	Yes
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D6	Rain	Cool	Normal	Strong	No
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#### **Entropy** calculated

We have 14 examples in S: 5 No, 9 Yes

$$\begin{split} &\text{Entropy(S)} = -\,p_{\textit{No}}\log_2 p_{\textit{No}} - p_{\textit{Yes}}\log_2 p_{\textit{Yes}} \\ &= -(5/14)\log_2(5/14) - (9/14)\log_2(9/14) = 0.94 \end{split}$$

Outlook	Play	
Sunny	No	
Sunny	No	
Overcast	Yes	
Rain	Yes	
Rain	Yes	
Rain	No	
Overcast	Yes	
Sunny	No	
Sunny	Yes	
Rain	Yes	
Sunny	Yes	
Overcast	Yes	
Overcast	Yes	
Rain	No	

Outlook	Play		
Sunny	No		
Sunny	No		
Sunny	No		
Sunny	Yes		
Sunny	Yes		
We have 2 Y	'es, 3 N		
Entropy	/ =		
$-3/5\log_2(3)$	3/5) -		
$2/5\log_2(2)$	/5) =		
0.97	1		

Outlook	Play
Sunny	No
Sunny	No
Sunny	No
Sunny	Yes
Sunny	Yes
We have 2 \	es, 3 N
Entrop	y =
$-3/5\log_2($	3/5) -
$2/5\log_2(2$	(2/5) =
0.97	1

	Outlook	Play
	Overcast	Yes
	Overcast	Yes
Overcast		Yes
	Overcast	Yes
Λ	Ve have 4 Y	es, 0 No
	Entropy	= 0

Outlook	Play			
Sunny	No			
Sunny	No			
Sunny	No			
Sunny	Yes			
Sunny	Yes			
We have 2 Y	es, 3 No			
Entropy	/ =			
$-3/5\log_2(3)$	3/5) -			
$2/5\log_2(2/5) =$				
0.97	1			

Outlook	Play
Overcast	Yes
We have 4 Y	es, 0 No
Entropy	= 0

Outlook	Play			
Rain	Yes			
Rain	Yes			
Rain	No			
Rain	Yes			
Rain	No			
We have 3 Y	és, 2 No			
Entropy	/ =			
$-3/5\log_2(3/5)$ -				
$2/5\log_2(2/5) =$				
0.971	1			

#### **Information Gain**

= 0.246

$$\begin{aligned} & \mathsf{Gain}(S,\mathit{Outlook}) = \; \mathsf{Entropy}\;(S) - \sum_{v \in \{\mathit{Rain},\mathit{Sunny},\mathit{Windy}\}} \frac{|S_v|}{|S|} \mathsf{Entropy}\,(S_v) \\ & \mathsf{Gain}\;(\mathsf{S},\;\mathsf{Outlook}) = \mathsf{Entropy}\;(\mathsf{S})\;\text{-}(5/14)^*\;\mathsf{Entropy}(\mathsf{S}_{\mathsf{Sunny}}) \text{-}\\ & (4/14)^*\;\mathsf{Entropy}\;(\mathsf{S}_{\mathsf{overcast}}) - (5/14)^*\;\mathsf{Entropy}(\mathsf{S}_{\mathsf{Rain}}) \\ & = 0.940\;\text{-}\;0.347\;\text{-}\;0.347 \end{aligned}$$

#### **Information Gain**



#### **Learnt Decision Tree**



Day	Temp	Humidity	Windy	Play
D1	Hot	High	Weak	No
D2	Hot	High	Strong	No
D8	Mild	High	Weak	No
D9	Cool	Normal	Weak	Yes
D11	Mild	Normal	Strong	Yes

Day	Temp	Humidity	Windy	Play
D1	Hot	High	Weak	No
D2	Hot	High	Strong	No
D8	Mild	High	Weak	No
D9	Cool	Normal	Weak	Yes
D11	Mild	Normal	Strong	Yes

•  $Gain(S_{Outlook=Sunny}, Temp) = Entropy(3 Yes, 2 No) - (2/5)*Entropy(2 No, 0 Yes) - (2/5)*Entropy(1 No, 1 Yes) - (1/5)*Entropy(1 Yes)$ 

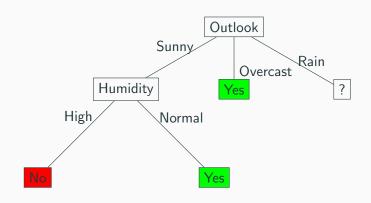
Day	Temp	Humidity	Windy	Play
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- $Gain(S_{Outlook=Sunny}, Temp) = Entropy(3 Yes, 2 No) (2/5)*Entropy(2 No, 0 Yes) (2/5)*Entropy(1 No, 1 Yes) (1/5)*Entropy(1 Yes)$
- Gain( $S_{Outlook=Sunny}$ , Humidity) = Entropy(3 Yes, 2 No) (2/5)\*Entropy(2 Yes) -(3/5)\*Entropy(3 No)  $\Longrightarrow$  maximum possible for the set

Day	Temp	Humidity	Windy	Play
D1	Hot	High	Weak	No
D2	Hot	High	Strong	No
D8	Mild	High	Weak	No
D9	Cool	Normal	Weak	Yes
D11	Mild	Normal	Strong	Yes

- Gain(S<sub>Outlook=Sunny</sub>, Temp) = Entropy(3 Yes, 2 No) -(2/5)\*Entropy(2 No, 0 Yes) -(2/5)\*Entropy(1 No, 1 Yes) -(1/5)\*Entropy(1 Yes)
- $Gain(S_{Outlook=Sunny}, Humidity) = Entropy(3 Yes, 2 No) (2/5)*Entropy(2 Yes) (3/5)*Entropy(3 No) <math>\Longrightarrow$  maximum possible for the set
- Gain(S<sub>Outlook=Sunny</sub>, Windy) = Entropy(3 Yes, 2 No) -(3/5)\*Entropy(2 No, 1 Yes) -(2/5)\*Entropy(1 No, 1 Yes)

#### **Learnt Decision Tree**



# Calling ID3 on (Outlook=Rain)

Day	Temp	Humidity	Windy	Play
D4	Mild	High	Weak	Yes
D5	Cool	Normal	Weak	Yes
D6	Cool	Normal	Strong	No
D10	Mild	Normal	Weak	Yes
D14	Mild	High	Strong	No

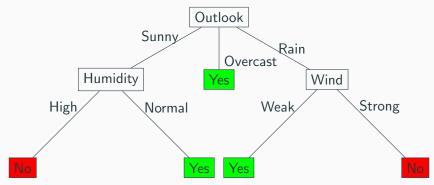
• The attribute Windy gives the highest information gain

#### **Learnt Decision Tree**



#### **Prediction for Decision Tree**

Just walk down the tree!



#### **Prediction for Decision Tree**

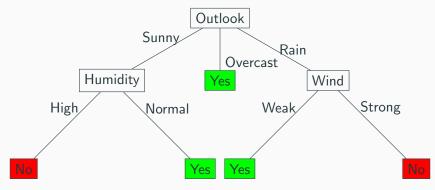
Just walk down the tree!



Prediction for <High Humidity, Strong Wind, Sunny Outlook, Hot Temp> is ?

#### **Prediction for Decision Tree**

Just walk down the tree!



Prediction for <High Humidity, Strong Wind, Sunny Outlook, Hot Temp> is ?

Assuming if you were only allowed depth-1 trees, how would it look for the current dataset?

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Apply the same rules, except when depth limit reached, the leaf node is assigned the "most" common occuring value in that path.

What is depth-0 tree (no decision) for the examples? Always predicting Yes

What is depth-1 tree (no decision) for the examples?



# Discrete Input, Real Output

### **Modified Dataset**

Day	Outlook	Temp	Humidity	Wind	Minutes Played
D1	Sunny	Hot	High	Weak	20
D2	Sunny	Hot	High	Strong	24
D3	Overcast	Hot	High	Weak	40
D4	Rain	Mild	High	Weak	50
D5	Rain	Cool	Normal	Weak	60
D6	Rain	Cool	Normal	Strong	10
D7	Overcast	Cool	Normal	Strong	4
D8	Sunny	Mild	High	Weak	10
D9	Sunny	Cool	Normal	Weak	60
D10	Rain	Mild	Normal	Weak	40
D11	Sunny	Mild	High	Strong	45
D12	Overcast	Mild	High	Strong	40
D13	Overcast	Hot	Normal	Weak	35
D14	Rain	Mild	High	Strong	20

• Any guesses?

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- Mean Squared Error

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- Mean Squared Error
- MSE(S) = 311.34
- Information Gain analogoue?
- Reduction in MSE (weighted)

### Gain by splitting on Wind

Wind	Minutes Played
Weak	20
Strong	24
Weak	40
Weak	50
Weak	60
Strong	10
Strong	4
Weak	10
Weak	60
Weak	40
Strong	45
Strong	40
Weak	35
Strong	20

$$MSE(S)=311.34$$

Wind	Minutes Played
Weak	20
Weak	40
Weak	50
Weak	60
Weak	10
Weak	60
Weak	40
Weak	35

Weighted

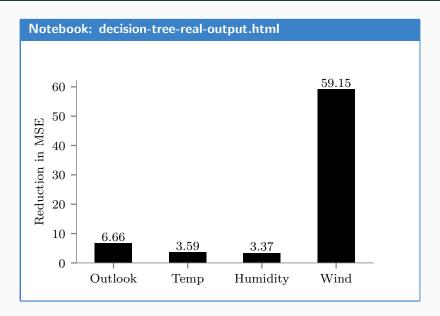
$$MSE(S_{Wind=Weak} = (8/14)*277 = 159)$$

Wind	Minutes Played
Strong	24
Strong	10
Strong	4
Strong	45
Strong	40
Strong	20

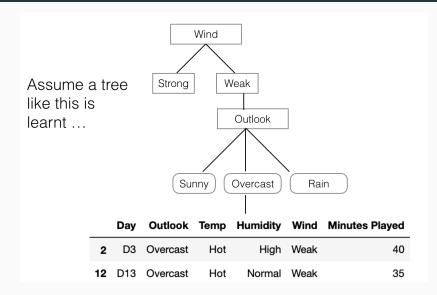
Weighted

$$\mathsf{MSE}(\mathsf{S}_{\mathsf{Wind}=\mathsf{Strong}}{=}(6/14)^*218{=}93)$$

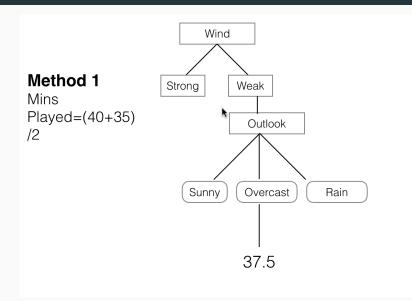
#### **Information Gain**



#### **Learnt Tree**



#### **Learnt Tree**



# **Real Input Discrete Output**

Day	Temperature	PlayTennis
D1	40	No
D2	48	No
D3	60	Yes
D4	72	Yes
D5	80	Yes
D6	90	No

• How do you find splits?

Day	Temperature	PlayTennis
D1	40	No
D2	48	No
D3	60	Yes
D4	72	Yes
D5	80	Yes
D6	90	No

- How do you find splits?
- Sort by attribute

Day	Temperature	PlayTennis
D1	40	No
D2	48	No
D3	60	Yes
D4	72	Yes
D5	80	Yes
D6	90	No

- How do you find splits?
- Sort by attribute
- Find potential split points (midpoints).

Day	Temperature	PlayTennis
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D3	60	Yes
D4	72	Yes
D5	80	Yes
D6	90	No

- How do you find splits?
- Sort by attribute
- Find potential split points (midpoints).
- For the above example, we have 5 potential splits: 44, 54, 66, 76, 85

Day	Temperature	PlayTennis
D1	40	No
D2	48	No
D3	60	Yes
D4	72	Yes
D5	80	Yes
D6	90	No

- How do you find splits?
- Sort by attribute
- Find potential split points (midpoints).
- For the above example, we have 5 potential splits: 44, 54, 66, 76, 85
- Calculate the weighted impurity for each split

Day	Temperature	PlayTennis
D1	40	No
D2	48	No
D3	60	Yes
D4	72	Yes
D5	80	Yes
D6	90	No

- How do you find splits?
- Sort by attribute
- Find potential split points (midpoints).
- For the above example, we have 5 potential splits: 44, 54, 66, 76, 85
- Calculate the weighted impurity for each split
- Choose the split with the lowest impurity

Day	Temperature	PlayTennis
D1	40	No
D2	48	No
D3	60	Yes
D4	72	Yes
D5	80	Yes
D6	90	No

- Consider split at 44
- LHS has 1 No and 0 Yes; RHS has 3 Yes and 2 No
- $\bullet$  Entropy for LHS = 0, Entropy for RHS = 0.971
- Weighted Entropy = 0.971\*5/6 = 0.808

Day	Temperature	PlayTennis
D1	40	No
D2	48	No
D3	60	Yes
D4	72	Yes
D5	80	Yes
D6	90	No

- Consider split at 54
- LHS has 2 No and 0 Yes; RHS has 3 Yes and 1 No
- $\bullet$  Entropy for LHS = 0, Entropy for RHS = 0.811
- Weighted Entropy = 0.811\*4/6 = 0.541

Day	Temperature	PlayTennis
D1	40	No
D2	48	No
D3	60	Yes
D4	72	Yes
D5	80	Yes
D6	90	No

- Consider split at 66
- LHS has 2 No and 1 Yes; RHS has 2 Yes and 1 No
- ullet Entropy for LHS = 0.918, Entropy for RHS = 0.918
- $\bullet$  Weighted Entropy = 0.918\*3/6 + 0.918\*3/6 = 0.918

Day	Temperature	PlayTennis
D1	40	No
D2	48	No
D3	60	Yes
D4	72	Yes
D5	80	Yes
D6	90	No

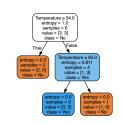
- Consider split at 76
- LHS has 2 No and 2 Yes; RHS has 1 Yes and 1 No
- ullet Entropy for LHS = 1, Entropy for RHS = 1
- $\bullet \ \ \mathsf{Weighted} \ \mathsf{Entropy} = 1 \text{*}4/6 + 1 \text{*}2/6 = 1$

Day	Temperature	PlayTennis
D1	40	No
D2	48	No
D3	60	Yes
D4	72	Yes
D5	80	Yes
D6	90	No

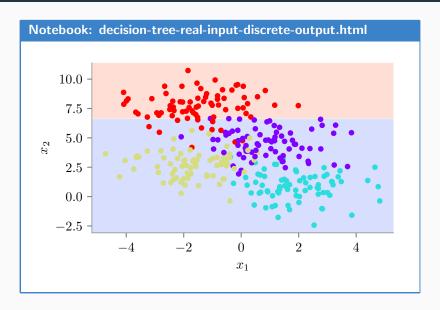
#### Notebook: decision-tree-real-input-discrete-output.html Temperature ≤ 54.0 entropy = 1.0 samples = 6 value = [3, 3] class = No True \False entropy = 0.0 entropy = 0.811 samples = 2 samples = 4 value = [2, 0] value = [1, 3] class = No class = Yes

Day	Temperature	PlayTennis
D1	40	No
D2	48	No
D3	60	Yes
D4	72	Yes
D5	80	Yes
D6	90	No

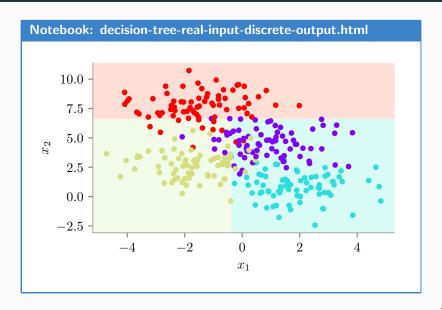
#### Notebook: decision-tree-real-input-discrete-output.html



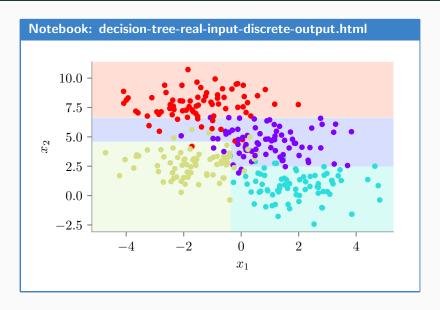
#### Example (DT of depth 1)



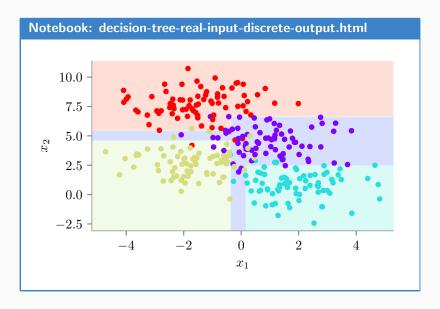
#### Example (DT of depth 2)



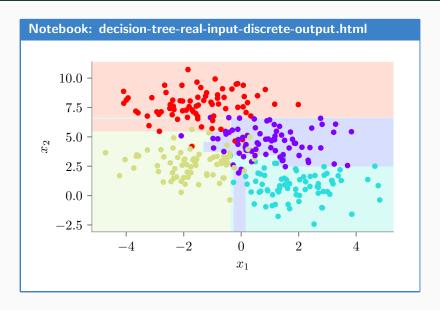
#### Example (DT of depth 3)



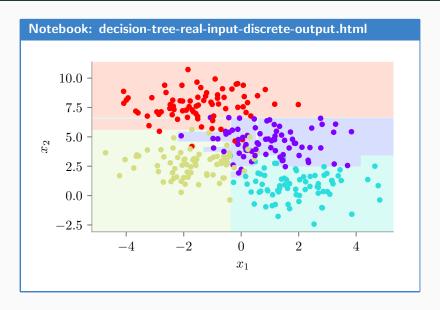
#### Example (DT of depth 4)



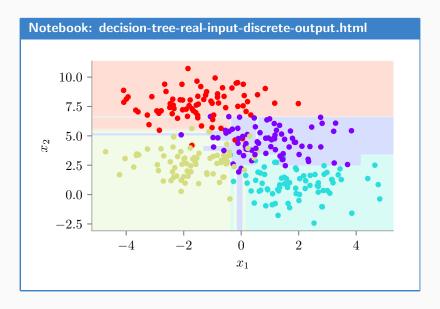
#### Example (DT of depth 5)



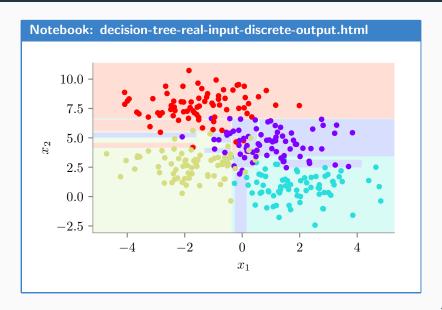
#### Example (DT of depth 6)



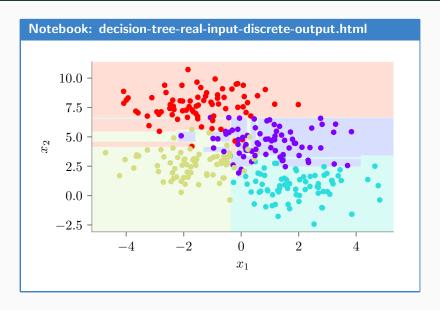
#### Example (DT of depth 7)



#### Example (DT of depth 8)

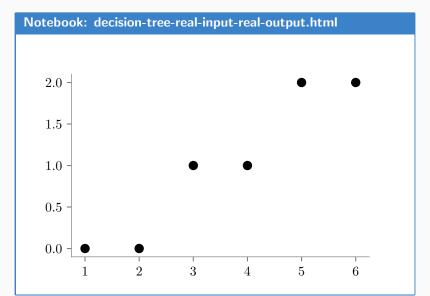


#### Example (DT of depth 9)

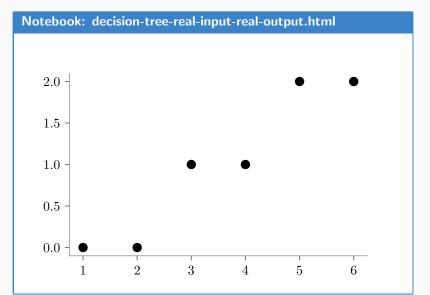


# Real Input Real Output

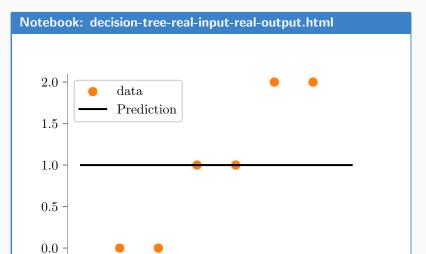
Let us consider the dataset given below



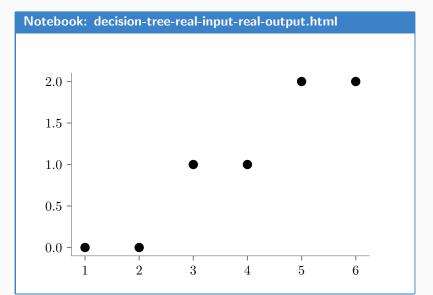
What would be the prediction for decision tree with depth 0?



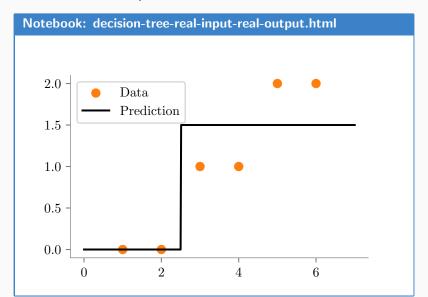
Prediction for decision tree with depth 0. Horizontal dashed line shows the predicted Y value. It is the average of Y values of all datapoints.



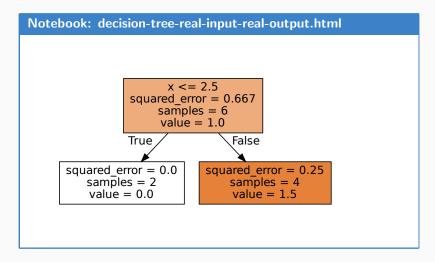
What would be the decision tree with depth 1?



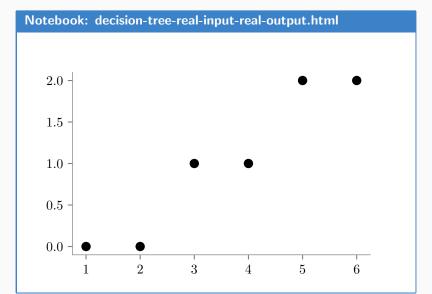
Decision tree with depth 1



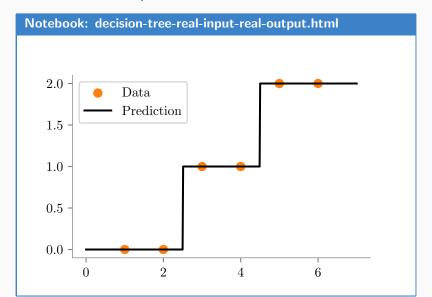
#### The Decision Boundary



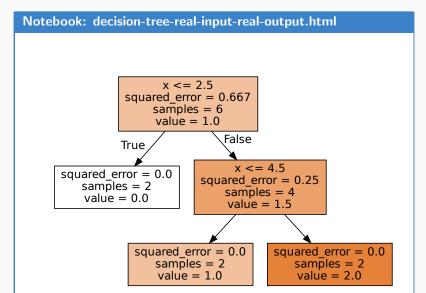
What would be the decision tree with depth 2?



Decision tree with depth 1



#### The Decision Boundary



Here, Feature is denoted by X and Label by Y. Let the "decision boundary" or "split" be at X = S. Let the region X < S, be region  $R_1$ . Let the region X > S, be region  $R_2$ .

Here, Feature is denoted by X and Label by Y.

Let the "decision boundary" or "split" be at X = S.

Let the region X < S, be region  $R_1$ .

Let the region X > S, be region  $R_2$ .

Then, let  $C_1 = \text{Mean } (Y_i | X_i \in R_1)$  $C_2 = \text{Mean } (Y_i | X_i \in R_2)$ 

Here, Feature is denoted by X and Label by Y.

Let the "decision boundary" or "split" be at X = S.

Let the region X < S, be region  $R_1$ .

Let the region X > S, be region  $R_2$ .

Then, let 
$$C_1 = \text{Mean } (Y_i | X_i \in R_1)$$
  
 $C_2 = \text{Mean } (Y_i | X_i \in R_2)$   
 $\text{Loss} = \sum_i ((Y_i - C_1 | X_i \in R_1)^2 + (Y_i - C_2 | X_i \in R_2)^2)$ 

Here, Feature is denoted by X and Label by Y.

Let the "decision boundary" or "split" be at X = S.

Let the region X < S, be region  $R_1$ .

Let the region X > S, be region  $R_2$ .

Then, let 
$$C_1 = \text{Mean } (Y_i | X_i \in R_1)$$
  $C_2 = \text{Mean } (Y_i | X_i \in R_2)$   $\text{Loss} = \sum_i ((Y_i - C_1 | X_i \in R_1)^2 + (Y_i - C_2 | X_i \in R_2)^2)$ 

Our objective is to minimize the loss and find  $min_S \sum_i ((Y_i - C_1 | X_i \in R_1)^2 + (Y_i - C_2 | X_i \in R_2)^2)$ 

# How to find optimal split "S"?

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1. Sort all datapoints (X,Y) in increasing order of X.

## How to find optimal split "S"?

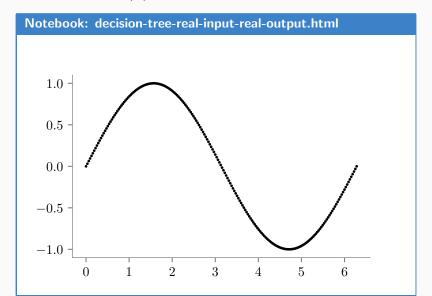
- 1. Sort all datapoints (X,Y) in increasing order of X.
- 2. Evaluate the loss function for all

$$S = \frac{X_i + X_{i+1}}{2}$$

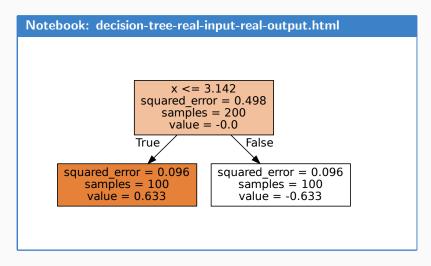
and the select the S with minimum loss.

Draw a regression tree for Y =  $\sin(X)$ ,  $0 \le X \le 2\pi$ 

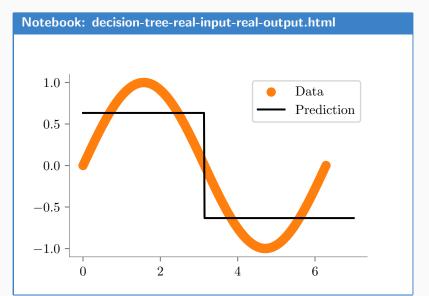
Dataset of Y =  $\sin(X)$ ,  $0 \le X \le 7$  with 10,000 points



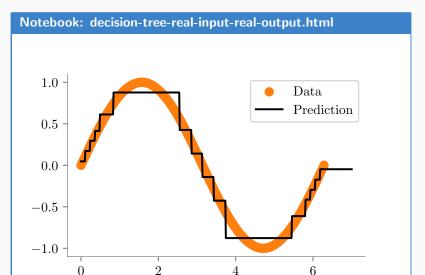
#### Regression tree of depth 1



#### **Decision Boundary**

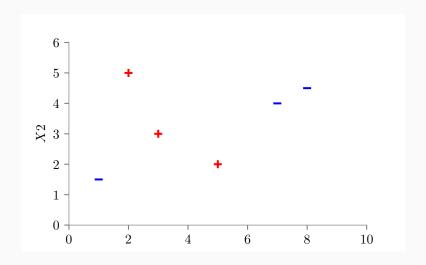


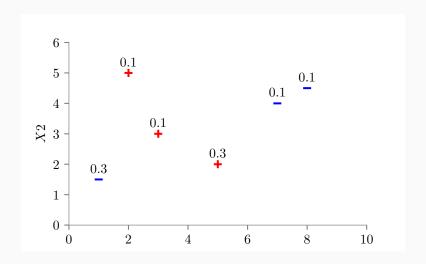
Regression tree with no depth limit is too big to fit in a slide. It has of depth 4. The decision boundaries are in figure below.

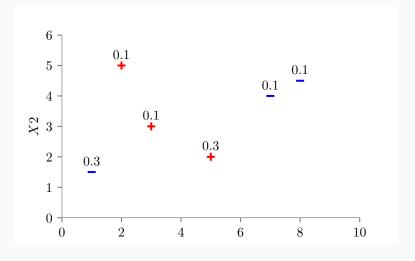


## **Summary**

- Interpretability an important goal
- Decision trees: well known interpretable models
- Learning optimal tree is hard
- Greedy approach:
- Recursively split to maximize "performance gain"
- Issues:
  - · Can overfit easily!
  - Empirically not as powerful as other methods





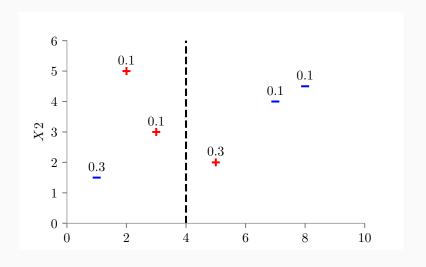


$$ENTROPY = -P(+) \cdot \log_2 P(+) - P(-) \cdot \log_2 P(-)$$

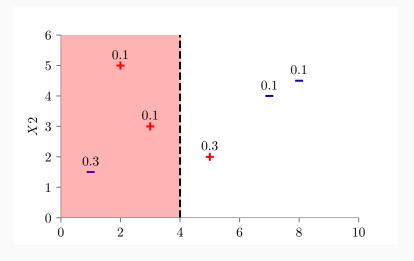
$$P(+) = \left(\frac{0.1 + 0.1 + 0.3}{1}\right) = 0.5, \ P(-) = \left(\frac{0.3 + 0.1 + 0.1}{1}\right) = 0.5$$

$$ENTROPY = E_s = -\frac{1}{2} \cdot \log_2 \frac{1}{2} - \frac{1}{2} \cdot \log_2 \frac{1}{2} = 1$$

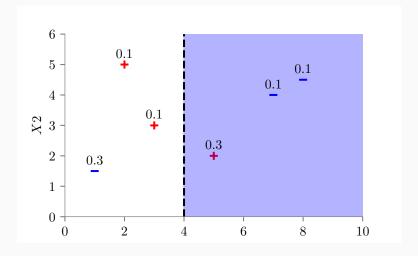
# **Weighted Entropy**



Candidate Line:  $X1 = 4(X1^*)$ 

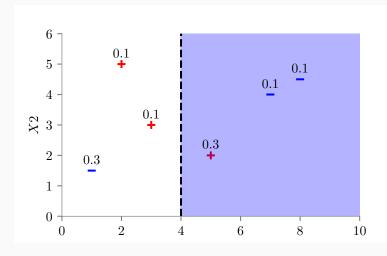


Entropy of 
$$X1 \le X1^* = E_{S(X1 < X1^*)}$$
  
 $P(+) = \left(\frac{0.1 + 0.1}{0.1 + 0.1 + 0.3}\right) = \frac{2}{5}$   
 $P(-) = \frac{3}{5}$ 



Entropy of 
$$X1 > X1^* = E_{S(X1 > X1^*)}$$

$$P(+) = \frac{3}{5}$$
  
 $P(-) = \frac{2}{5}$ 



$$IG(X1 = X1^*) = E_S - \frac{0.5}{1} \cdot E_{S(X1 < X1^*)} - \frac{0.5}{1} \cdot E_{S(X1 > X1^*)}$$