

# Decision Trees

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Nipun Batra and teaching staff

January 14, 2024

IIT Gandhinagar

**Discrete Input Discrete Output**

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# The need for interpretability

## How to maintain trust in AI

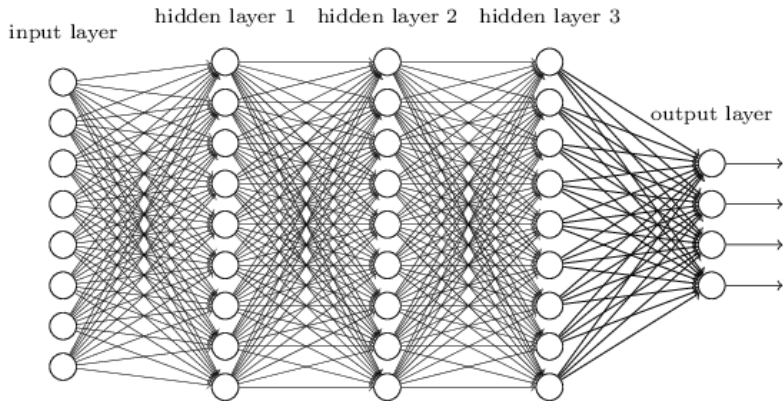
Beyond developing initial trust, however, creators of AI also must work to maintain that trust. Siau and Wang suggest seven ways of "developing continuous trust" beyond the initial phases of product development:

- Usability and reliability. AI "should be designed to operate easily and intuitively," Siau and Wang write. "There should be no unexpected downtime or crashes."
- Collaboration and communication. AI developers want to create systems that perform autonomously, without human involvement. Developers must focus on creating AI 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. AI 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.

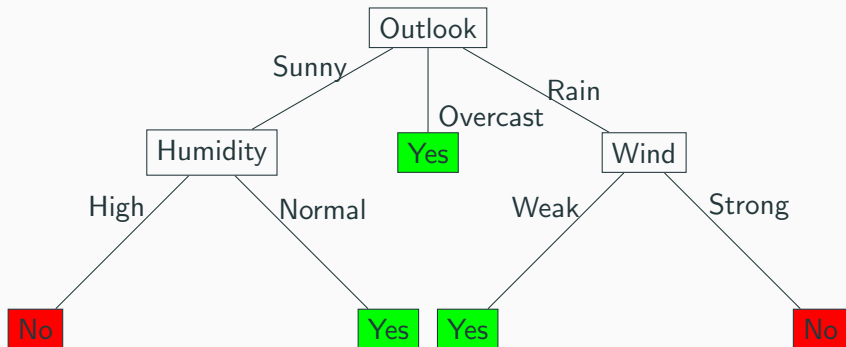
## Training Data

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
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D10	Rain	Mild	Normal	Weak	Yes
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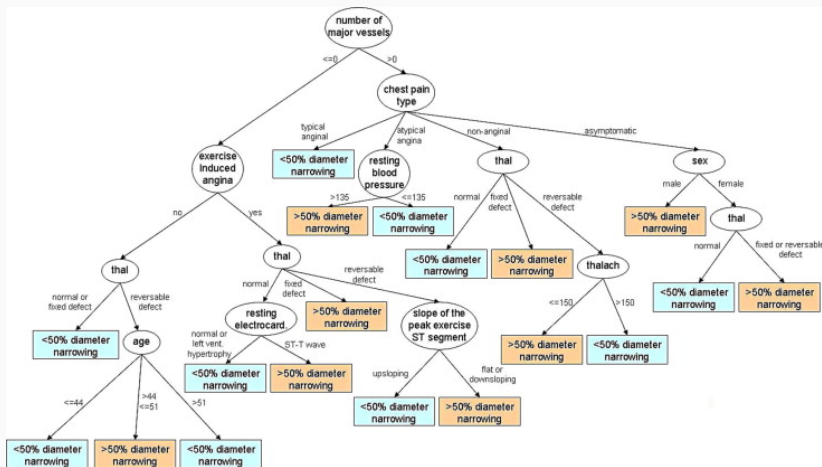
# Learning a Complicated Neural Network



# Learnt Decision Tree



# Medical Diagnosis using Decision Trees



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



## Leo Breiman 1928-2005

Professor of Statistics, [UC Berkeley](#)  
Verified email at [stat.berkeley.edu](mailto:stat.berkeley.edu) - [Homepage](#)  
[Data Analysis](#) [Statistics](#) [Machine Learning](#)

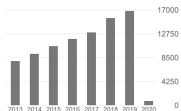
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Volume 5, number 1

INFORMATION PROCESSING LETTERS

May 1976

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

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and

Ronald L. RIVEST

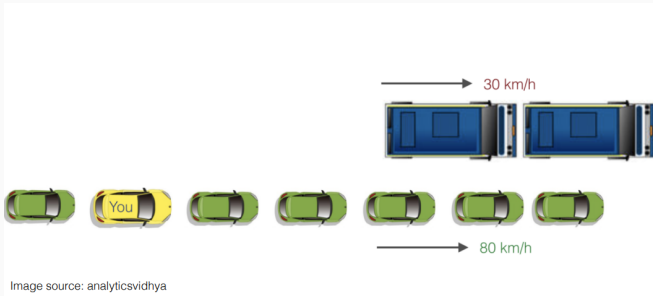
*Dept. of Electrical Engineering and Computer Science, M.I.T., Cambridge, Massachusetts 02139, USA*

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!



Greedy!≠Optimal

## Towards biggest estimated performance gain

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
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## Towards biggest estimated performance gain

Day	Outlook	Temp	Humidity	Windy	Play
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- For examples, we have 9 Yes, 5 No

## Towards biggest estimated performance gain

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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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- For examples, we have 9 Yes, 5 No
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- Yes!
- Key insights: Problem is “easier” when there is lesser disagreement

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D13	Overcast	Hot	Normal	Weak	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?
- Yes!
- Key insights: Problem is “easier” when there is lesser disagreement
- Need some statistical measure of “disagreement”



# Entropy

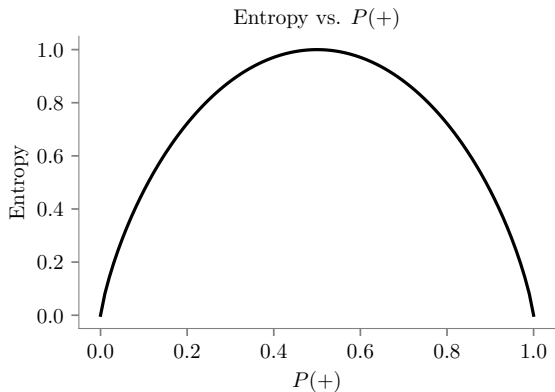
Statistical measure to characterize the (im)purity of examples

# Entropy

Statistical measure to characterize the (im)purity of examples

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

Notebook: entropy.html



## Towards biggest estimated performance gain

Day	Outlook	Temp	Humidity	Windy	Play
D1	Sunny	Hot	High	Weak	No
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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?

## Towards biggest estimated performance gain

Day	Outlook	Temp	Humidity	Windy	Play
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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

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

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

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

## ID3 (Examples, Target Attribute, Attributes)

- Create a root node for tree

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## ID3 (Examples, Target Attribute, Attributes)

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- If attributes = empty, return root with most common value of Target Attribute in Examples

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- Create a root node for tree
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- Begin

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- Create a root node for tree
- If all examples are +/-, return root with label = +/-
- If attributes = empty, return root with most common value of Target Attribute in Examples
- Begin
  - $A \leftarrow$  attribute from Attributes which best classifies Examples

## ID3 (Examples, Target Attribute, Attributes)

- Create a root node for tree
- If all examples are +/-, return root with label = +/-
- If attributes = empty, return root with most common value of Target Attribute in Examples
- Begin
  - $A \leftarrow$  attribute from Attributes which best classifies Examples
  - Root  $\leftarrow$  A

## ID3 (Examples, Target Attribute, Attributes)

- Create a root node for tree
- If all examples are +/-, return root with label = +/-
- If attributes = empty, return root with most common value of Target Attribute in Examples
- Begin
  - $A \leftarrow$  attribute from Attributes which best classifies Examples
  - Root  $\leftarrow A$
  - For each value ( $v$ ) of  $A$

## ID3 (Examples, Target Attribute, Attributes)

- Create a root node for tree
- If all examples are  $+/-$ , return root with label =  $+/-$
- If attributes = empty, return root with most common value of Target Attribute in Examples
- Begin
  - $A \leftarrow$  attribute from Attributes which best classifies Examples
  - Root  $\leftarrow A$
  - For each value ( $v$ ) of  $A$ 
    - Add new tree branch :  $A = v$

## ID3 (Examples, Target Attribute, Attributes)

- Create a root node for tree
- If all examples are  $+/-$ , return root with label =  $+/-$
- If attributes = empty, return root with most common value of Target Attribute in Examples
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  - $A \leftarrow$  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  $A = v$

## ID3 (Examples, Target Attribute, Attributes)

- Create a root node for tree
- If all examples are  $+/-$ , return root with label =  $+/-$
- If attributes = empty, return root with most common value of Target Attribute in Examples
- Begin
  - $A \leftarrow$  attribute from Attributes which best classifies Examples
  - Root  $\leftarrow A$
  - For each value ( $v$ ) of  $A$ 
    - Add new tree branch :  $A = v$
    - $Examples_v$ : subset of examples that  $A = v$
    - If  $Examples_v$  is empty: add leaf with label = most common value of Target Attribute



## ID3 (Examples, Target Attribute, Attributes)

- Create a root node for tree
- If all examples are +/-, return root with label = +/-
- If attributes = empty, return root with most common value of Target Attribute in Examples
- Begin
  - $A \leftarrow$  attribute from Attributes which best classifies Examples
  - Root  $\leftarrow A$
  - For each value ( $v$ ) of  $A$ 
    - Add new tree branch :  $A = v$
    - $Examples_v$ : subset of examples that  $A = v$
    - If  $Examples_v$  is empty: add leaf with label = most common value of Target Attribute
    - Else: ID3 ( $Examples_v$ , Target attribute, Attributes -  $A$ )

# Learnt Decision Tree

Root Node (empty)

## 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

## Entropy calculated

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

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

## Information Gain for Outlook

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

## Information Gain for Outlook

Outlook	Play
Sunny	No
Sunny	No
Sunny	No
Sunny	Yes
Sunny	Yes

We have 2 Yes, 3 No

$$\begin{aligned}\text{Entropy} &= \\ &= -3/5 \log_2(3/5) - \\ &= 2/5 \log_2(2/5) = \\ &= 0.971\end{aligned}$$

## Information Gain for Outlook

Outlook	Play
Sunny	No
Sunny	No
Sunny	No
Sunny	Yes
Sunny	Yes

We have 2 Yes, 3 No

$$\begin{aligned}\text{Entropy} &= \\ &= -3/5 \log_2(3/5) - \\ &= 2/5 \log_2(2/5) = \\ &= 0.971\end{aligned}$$

Outlook	Play
Overcast	Yes
Overcast	Yes
Overcast	Yes
Overcast	Yes

We have 4 Yes, 0 No

$$\text{Entropy} = 0$$

## Information Gain for Outlook

Outlook	Play
Sunny	No
Sunny	No
Sunny	No
Sunny	Yes
Sunny	Yes

We have 2 Yes, 3 No

$$\begin{aligned}\text{Entropy} &= \\ &= -3/5 \log_2(3/5) - \\ &= 2/5 \log_2(2/5) = \\ &= 0.971\end{aligned}$$

Outlook	Play
Overcast	Yes
Overcast	Yes
Overcast	Yes
Overcast	Yes

We have 4 Yes, 0 No

$$\text{Entropy} = 0$$

Outlook	Play
Rain	Yes
Rain	Yes
Rain	No
Rain	Yes
Rain	No

We have 3 Yes, 2 No

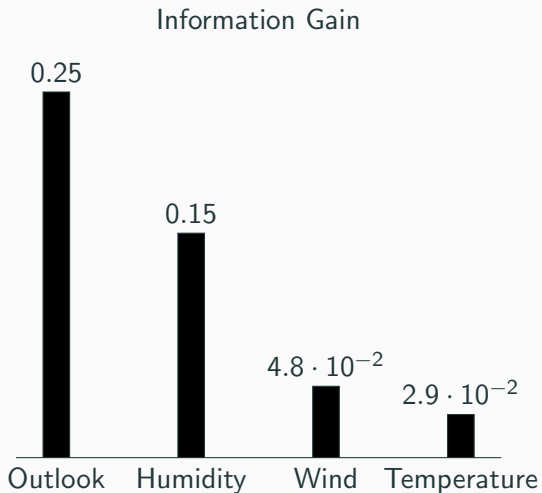
$$\begin{aligned}\text{Entropy} &= \\ &= -3/5 \log_2(3/5) - \\ &= 2/5 \log_2(2/5) = \\ &= 0.971\end{aligned}$$



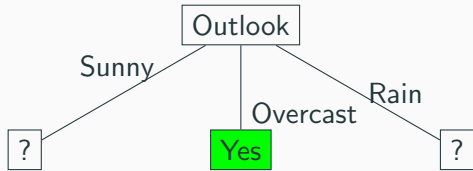
$$\text{Gain}(S, \text{Outlook}) = \text{Entropy}(S) - \sum_{v \in \{\text{Rain}, \text{Sunny}, \text{Windy}\}} \frac{|S_v|}{|S|} \text{Entropy}(S_v)$$

$$\begin{aligned} \text{Gain}(S, \text{Outlook}) &= \text{Entropy}(S) - (5/14) * \text{Entropy}(S_{\text{Sunny}}) - \\ & (4/14) * \text{Entropy}(S_{\text{Overcast}}) - (5/14) * \text{Entropy}(S_{\text{Rain}}) \\ &= 0.940 - 0.347 - 0.347 \\ &= 0.246 \end{aligned}$$

# Information Gain



# Learnt Decision Tree



## Calling ID3 on Outlook=Sunny

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

## Calling ID3 on Outlook=Sunny

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

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

## Calling ID3 on Outlook=Sunny

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
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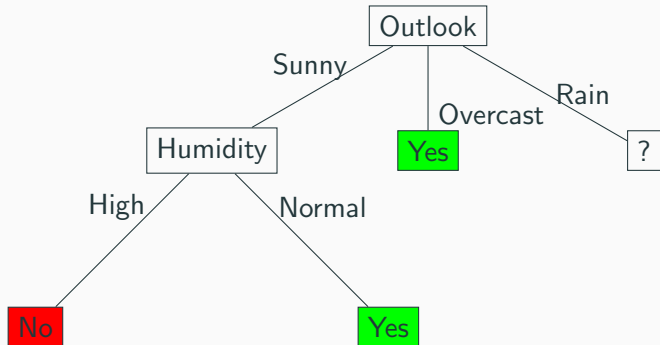
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## Calling ID3 on Outlook=Sunny

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

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

# Learnt Decision Tree



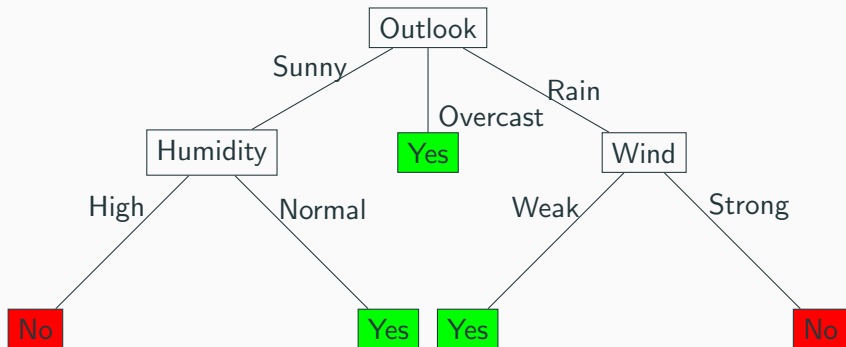


## Calling ID3 on (Outlook=Rain)

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

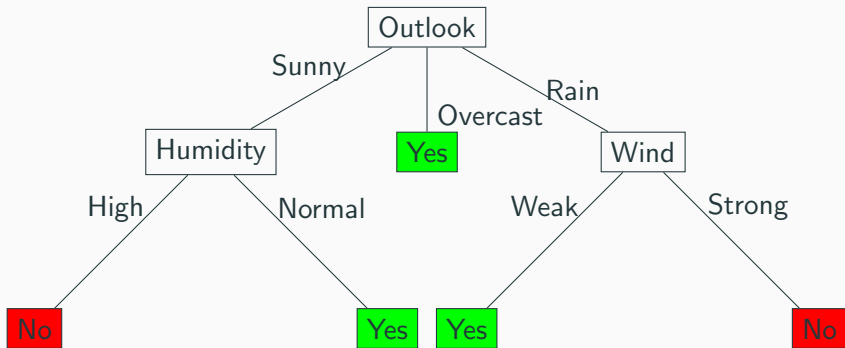
- The attribute Windy gives the highest information gain

# Learnt Decision Tree



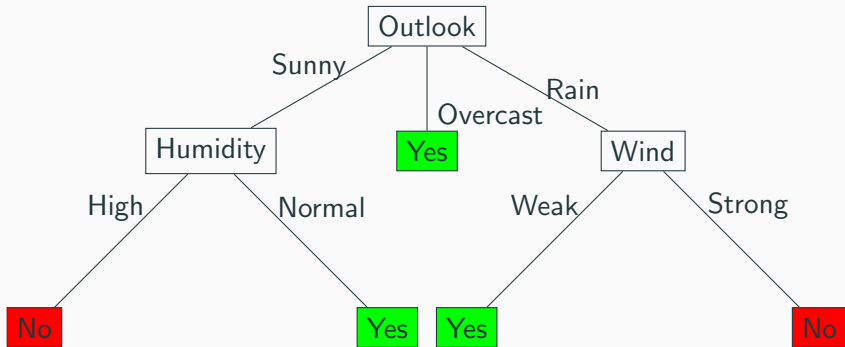
# Prediction for Decision Tree

Just walk down the tree!



## Prediction for Decision Tree

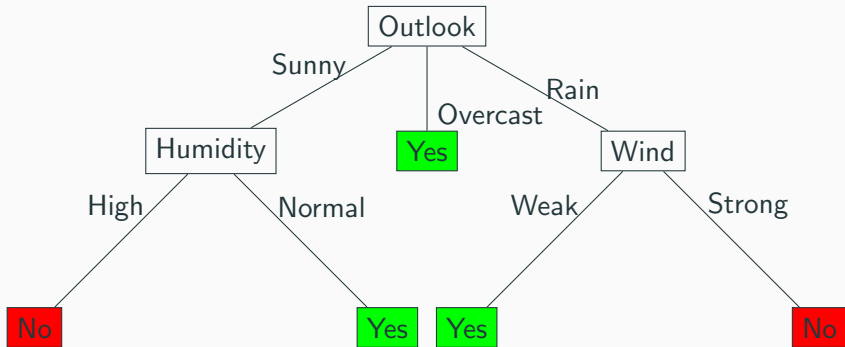
Just walk down the tree!



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 ?

No

## Limiting Depth of Tree

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

## Limiting Depth of Tree

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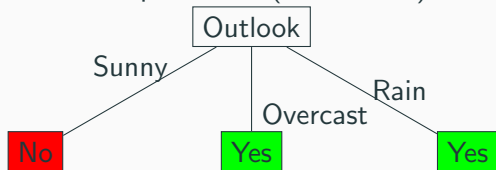
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Always predicting Yes

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## 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

## Measure of Impurity for Regression?

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- Any guesses?

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- $MSE(S) = 311.34$
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- 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

$$\text{MSE}(S) = 311.34$$

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

Weighted

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

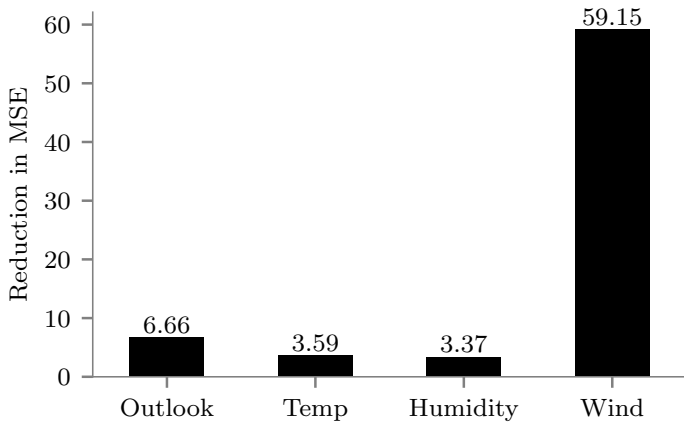
Wind	Minutes Played
Strong	24
Strong	10
Strong	4
Strong	45
Strong	40
Strong	20

Weighted

$$\text{MSE}(S_{\text{Wind}=\text{Strong}}) = (6/14) * 218 = 93$$

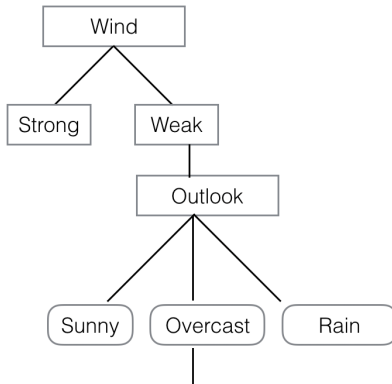
# Information Gain

Notebook: decision-tree-real-output.html



# Learnt Tree

Assume a tree like this is learnt ...



	<b>Day</b>	<b>Outlook</b>	<b>Temp</b>	<b>Humidity</b>	<b>Wind</b>	<b>Minutes Played</b>	
	<b>2</b>	D3	Overcast	Hot	High	Weak	40
	<b>12</b>	D13	Overcast	Hot	Normal	Weak	35

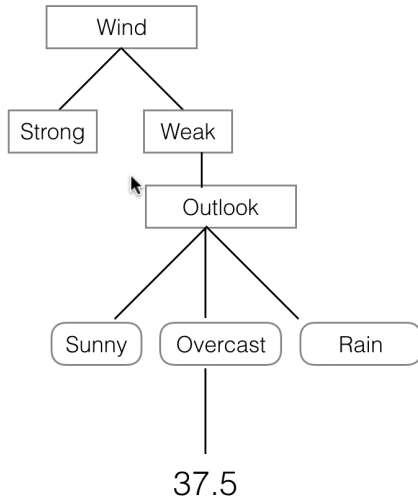
# Learnt Tree

## Method 1

Mins

Played=(40+35)

/2



## Real Input Discrete Output

---



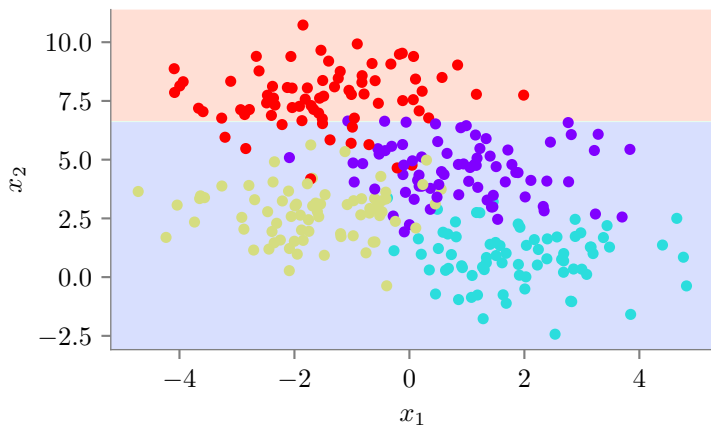
## Finding splits

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
- Find attribute values where changes happen
- For example, splits are:  $\text{Temp} > (48+60)/2$  and  $\text{Temp} > (80+90)/2$

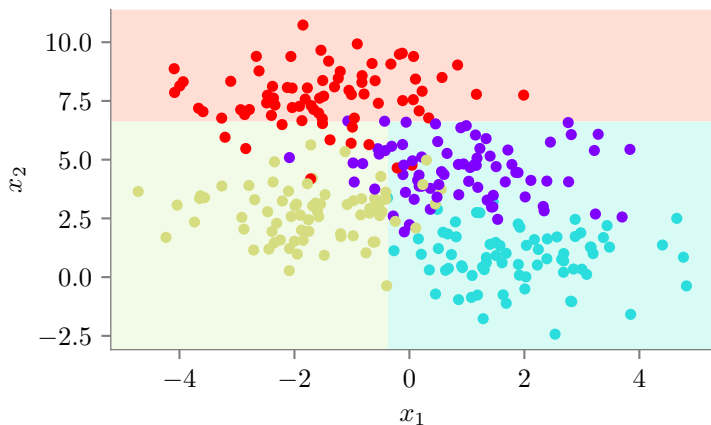
## Example (DT of depth 1)

Notebook: [decision-tree-real-input-discrete-output.html](#)



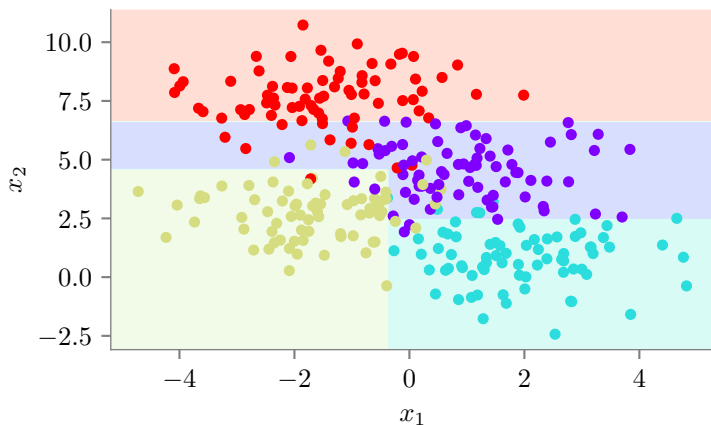
## Example (DT of depth 2)

Notebook: [decision-tree-real-input-discrete-output.html](#)



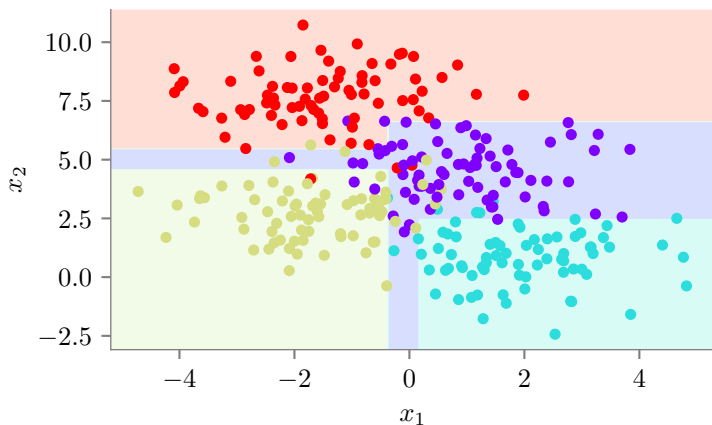
## Example (DT of depth 3)

Notebook: [decision-tree-real-input-discrete-output.html](#)



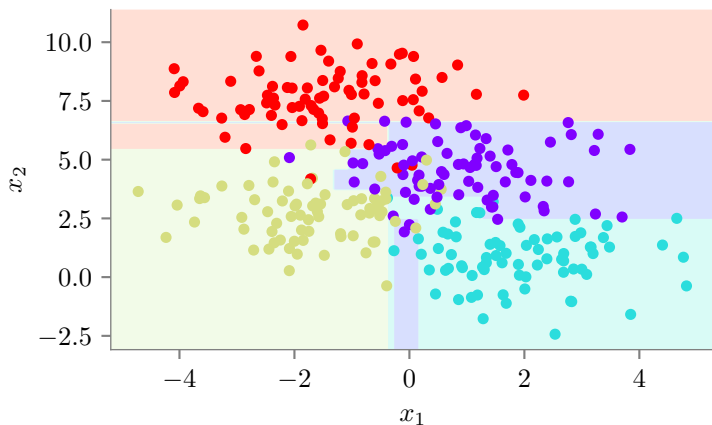
## Example (DT of depth 4)

Notebook: [decision-tree-real-input-discrete-output.html](#)



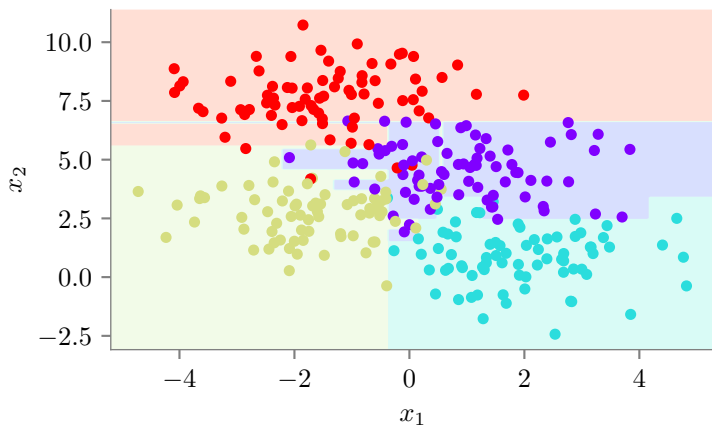
## Example (DT of depth 5)

Notebook: [decision-tree-real-input-discrete-output.html](#)



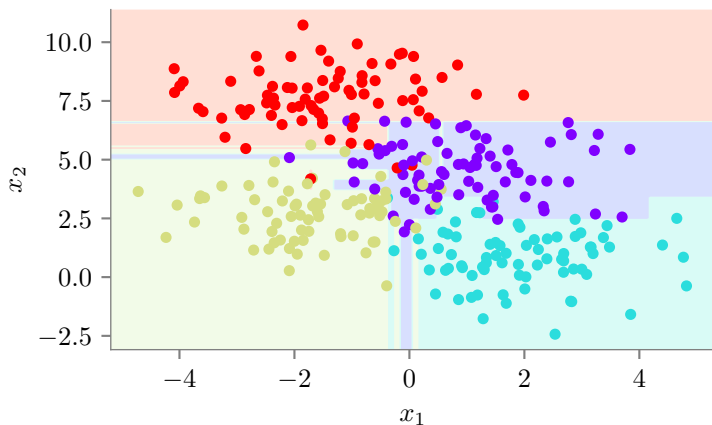
## Example (DT of depth 6)

Notebook: [decision-tree-real-input-discrete-output.html](#)



## Example (DT of depth 7)

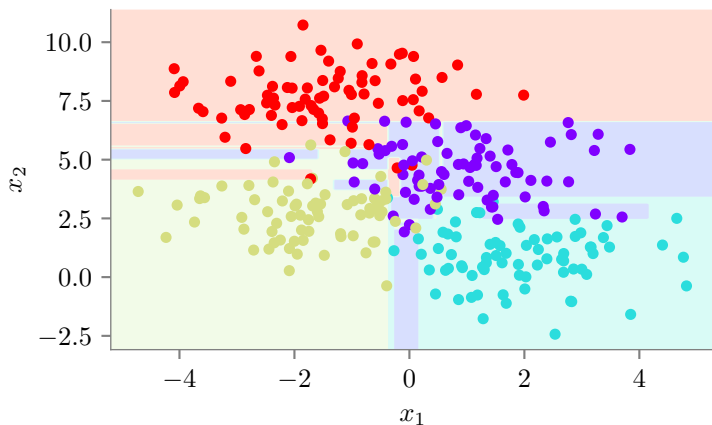
Notebook: [decision-tree-real-input-discrete-output.html](#)





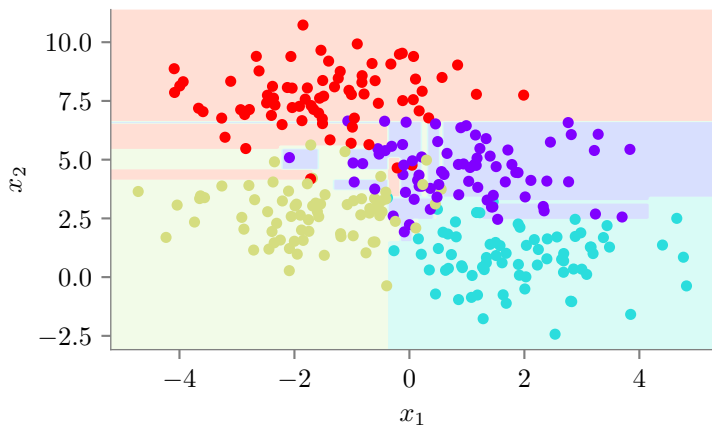
## Example (DT of depth 8)

Notebook: [decision-tree-real-input-discrete-output.html](#)



## Example (DT of depth 9)

Notebook: [decision-tree-real-input-discrete-output.html](#)

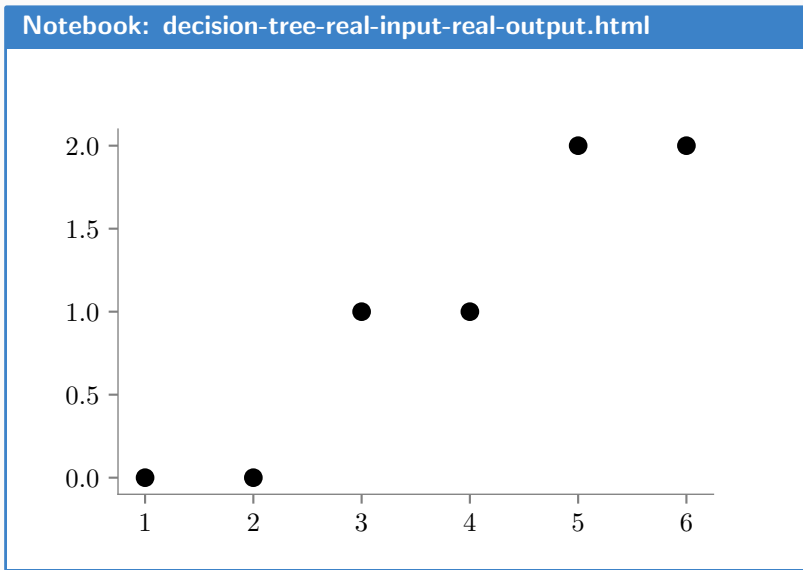


**Real Input Real Output**

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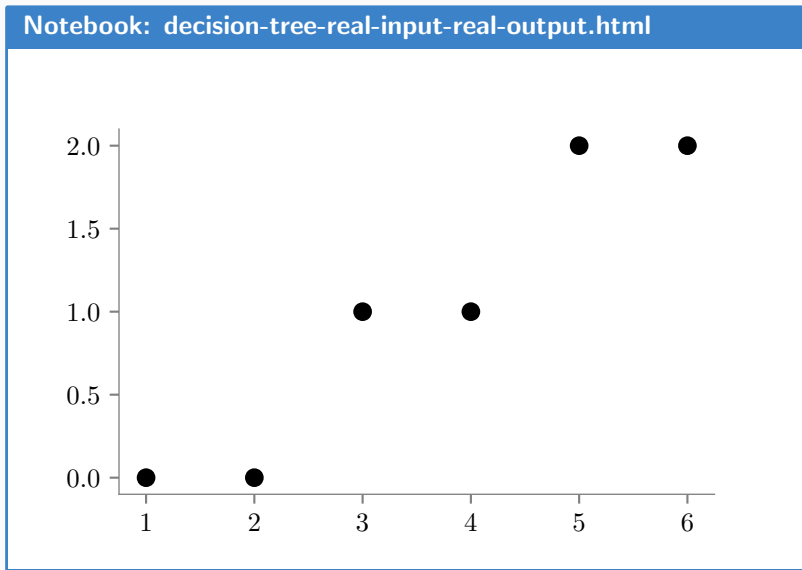
## Example 1

Let us consider the dataset given below



## Example 1

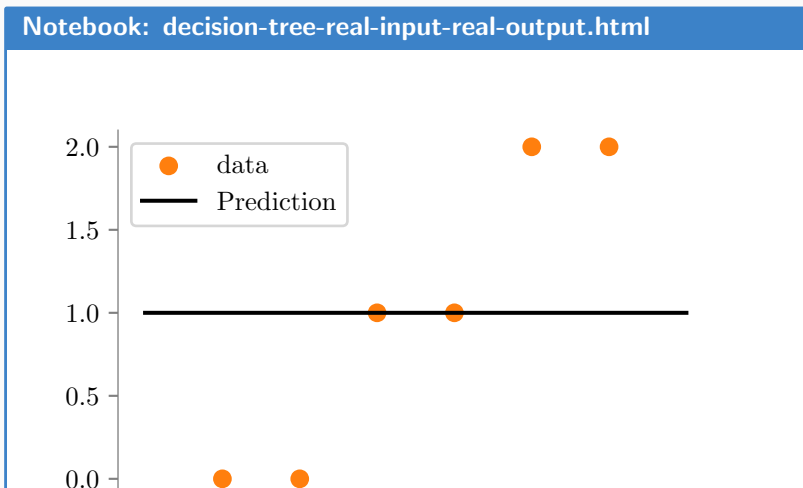
What would be the prediction for decision tree with depth 0?



## Example 1

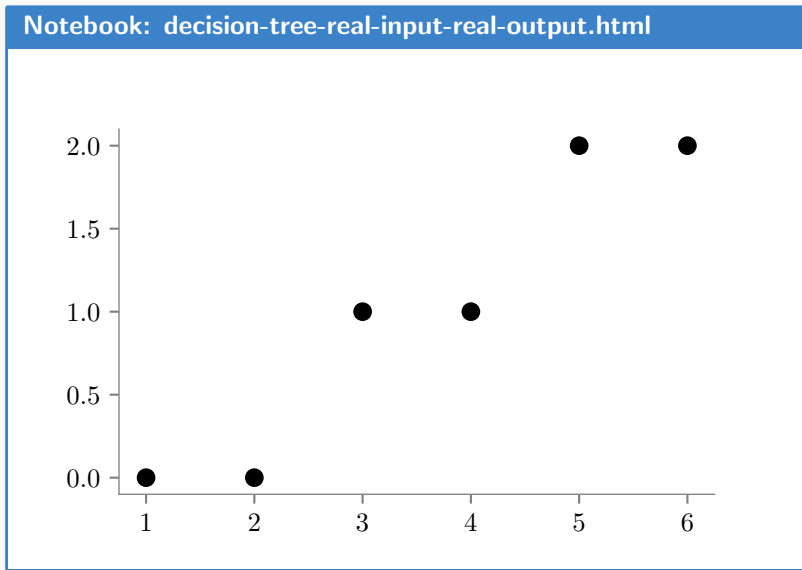
Prediction for decision tree with depth 0.

Horizontal dashed line shows the predicted  $Y$  value. It is the average of  $Y$  values of all datapoints.



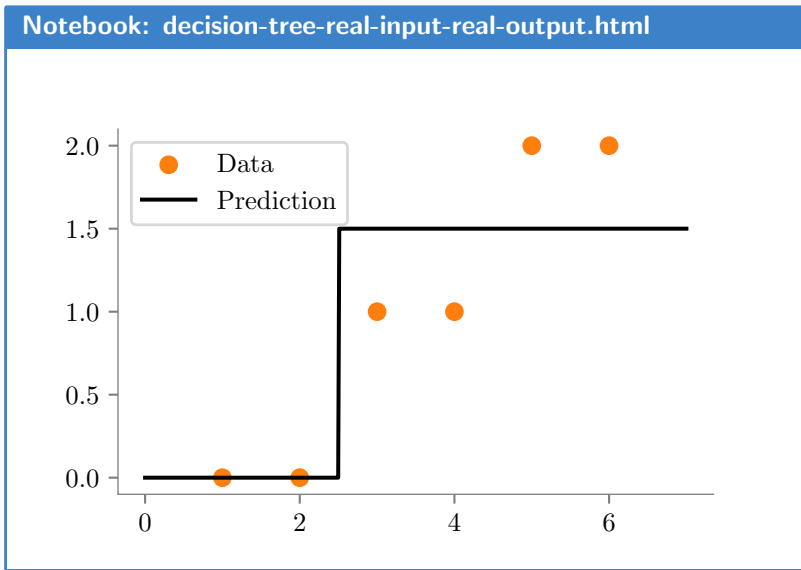
## Example 1

What would be the decision tree with depth 1?



# Example 1

Decision tree with depth 1

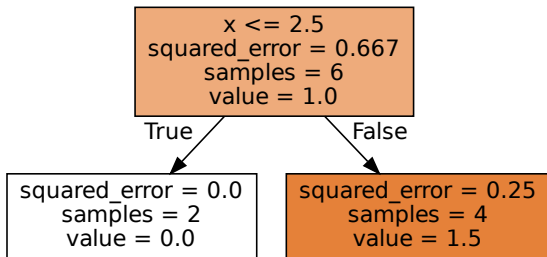




# Example 1

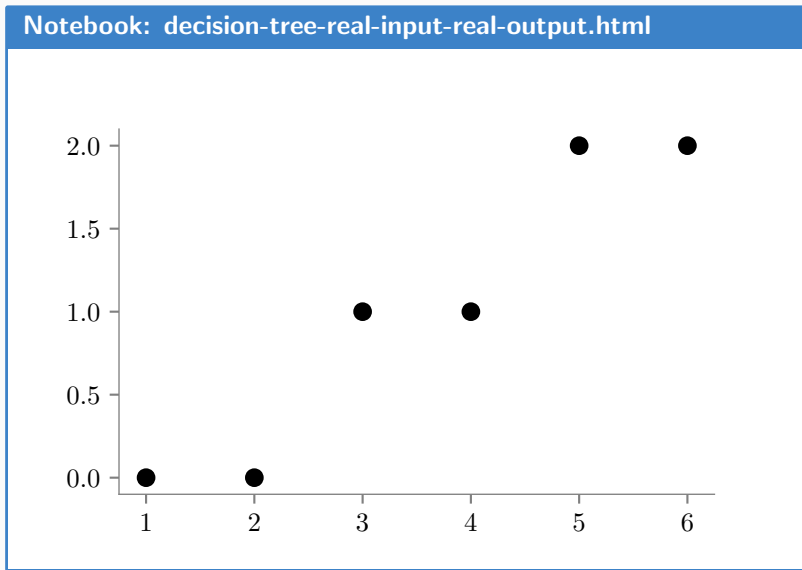
## The Decision Boundary

Notebook: [decision-tree-real-input-real-output.html](#)



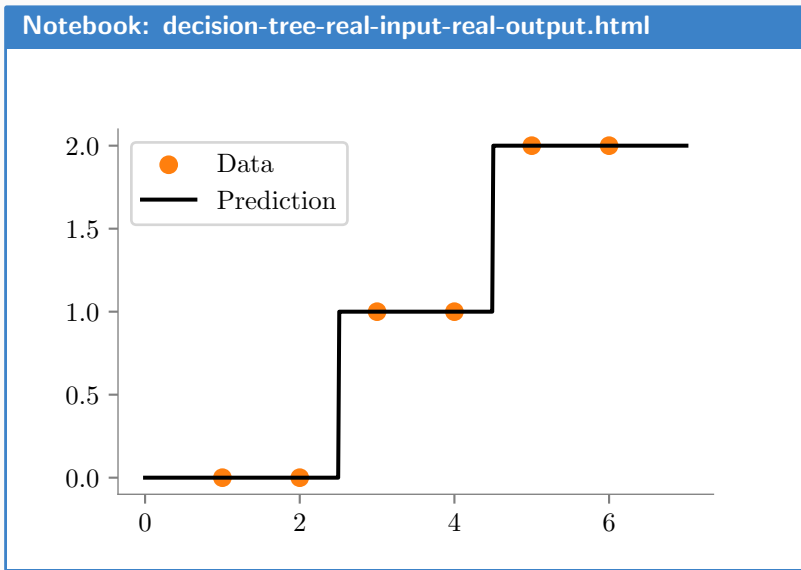
## Example 1

What would be the decision tree with depth 2 ?



# Example 1

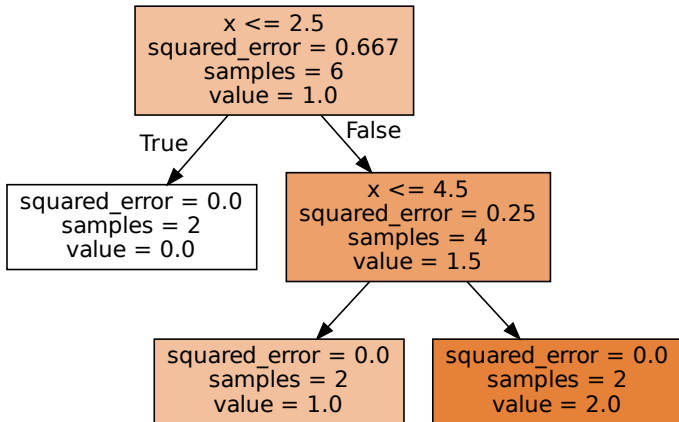
Decision tree with depth 1



# Example 1

## The Decision Boundary

Notebook: [decision-tree-real-input-real-output.html](#)



## Objective function

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  $R_2$ .

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

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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 then select the S with minimum loss.

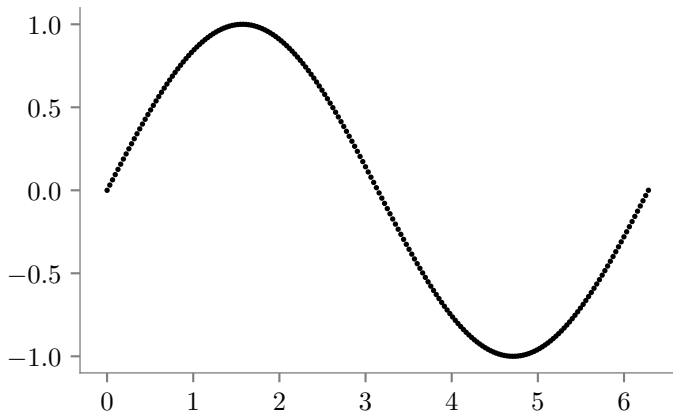
## A Question!

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

## A Question!

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

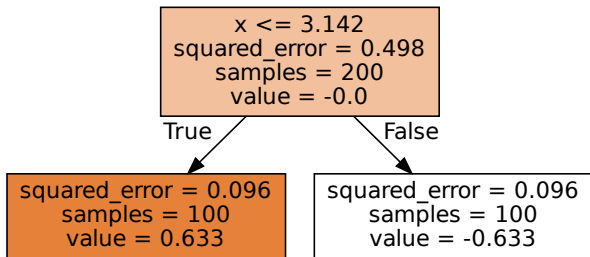
Notebook: [decision-tree-real-input-real-output.html](#)



## A Question!

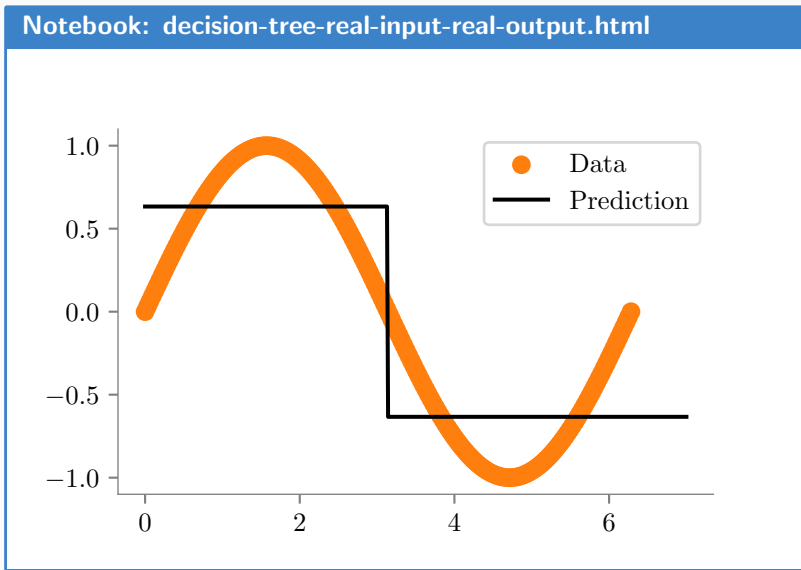
Regression tree of depth 1

Notebook: [decision-tree-real-input-real-output.html](#)



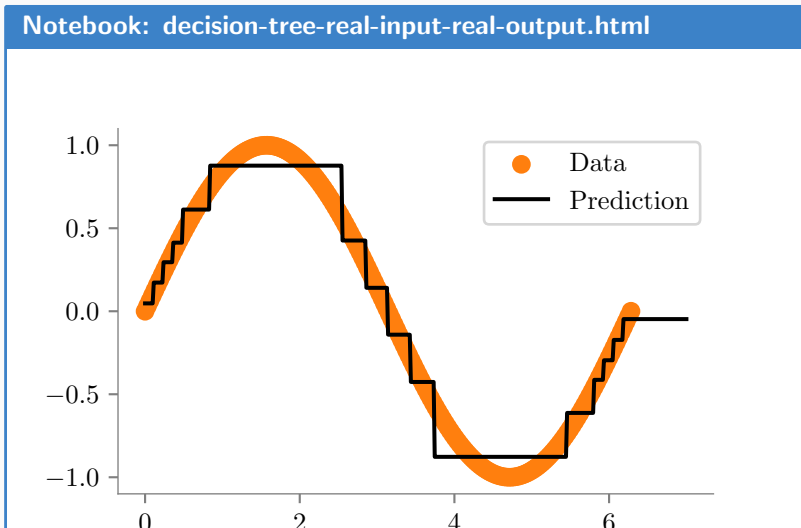
# A Question!

## Decision Boundary



## A Question!

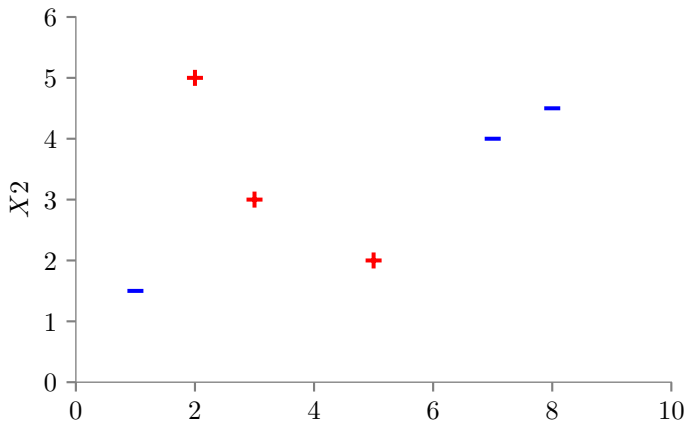
Regression tree with no depth limit is too big to fit in a slide. It has of depth 4. The decision boundaries are in figure below.

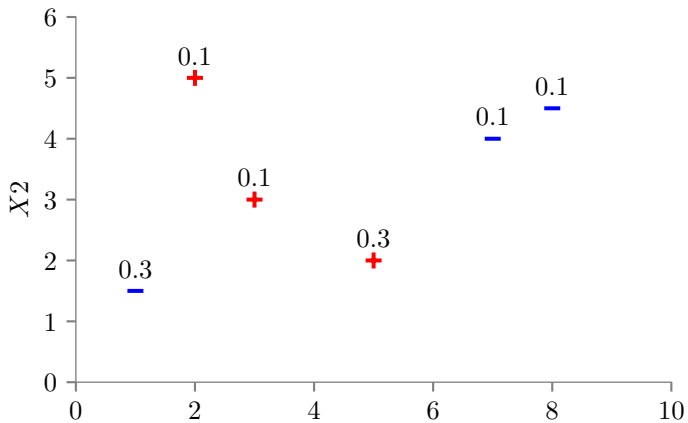


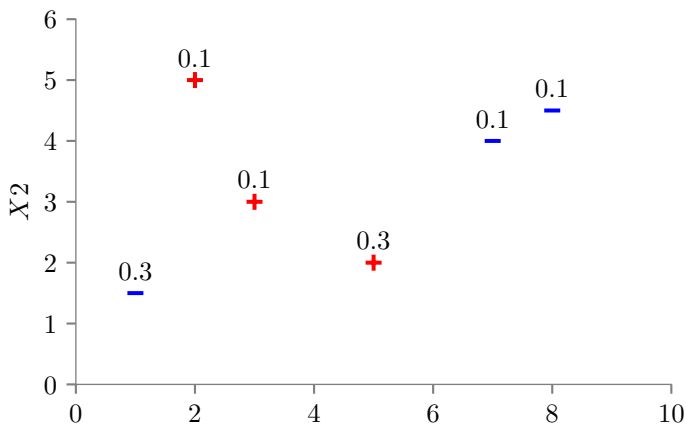


# Summary

- 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







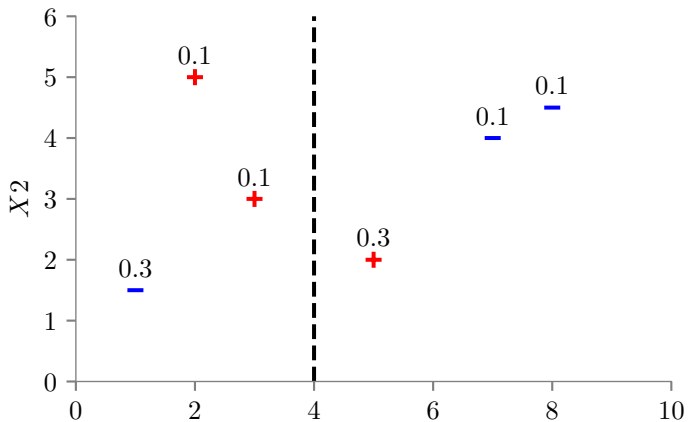
$$ENTROPY = -P(+)\cdot\log_2 P(+)-P(-)\cdot\log_2 P(-)$$

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

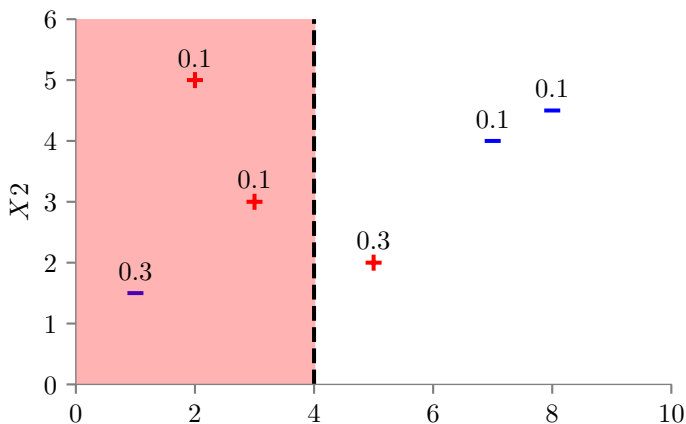
$$ENTROPY = E_s = -\frac{1}{2}\cdot\log_2\frac{1}{2}-\frac{1}{2}\cdot\log_2\frac{1}{2}=1$$

# Weighted Entropy

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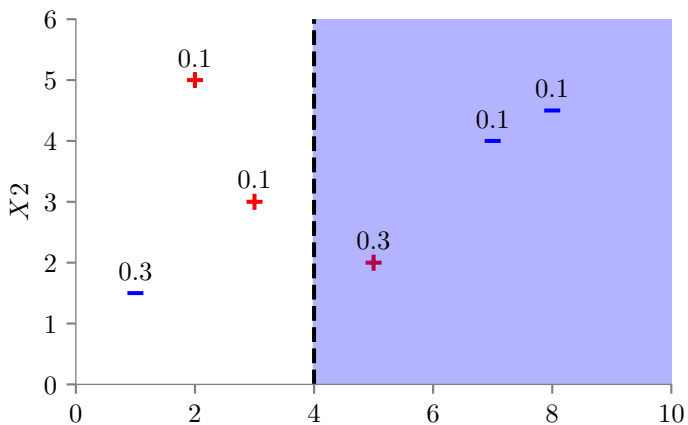
Candidate Line:  $X_1 = 4(X_1^*)$



Entropy of  $X_1 \leq X_1^* = E_{S(X_1 < X_1^*)}$

$$P(+)=\left(\frac{0.1+0.1}{0.1+0.1+0.3}\right)=\frac{2}{5}$$

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

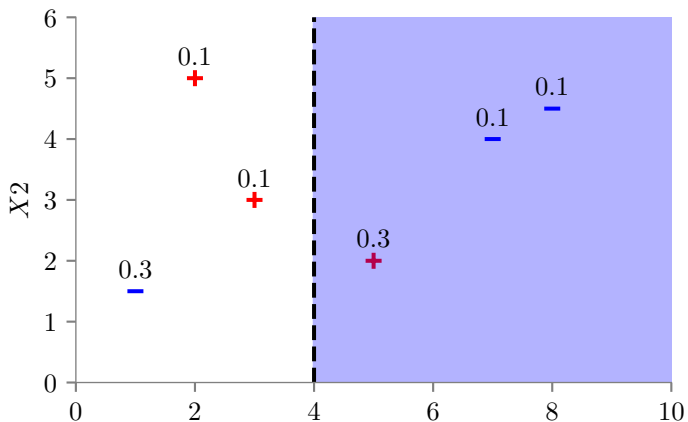


Entropy of  $X_1 > X_1^* = E_{S(X_1 > X_1^*)}$

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

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





$$IG(X_1 = X_1^*) = E_S - \frac{0.5}{1} \cdot E_{S(X_1 < X_1^*)} - \frac{0.5}{1} \cdot E_{S(X_1 > X_1^*)}$$