Decision Trees

Nipun Batra and teaching staff

January 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. 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
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D8	Sunny	Mild	High	Weak	No
D9	Sunny	Cool	Normal	Weak	Yes
D10	Rain	Mild	Normal	Weak	Yes
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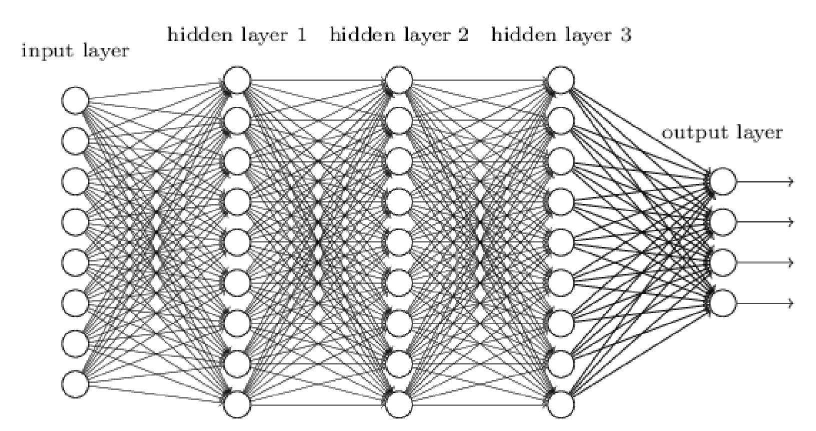
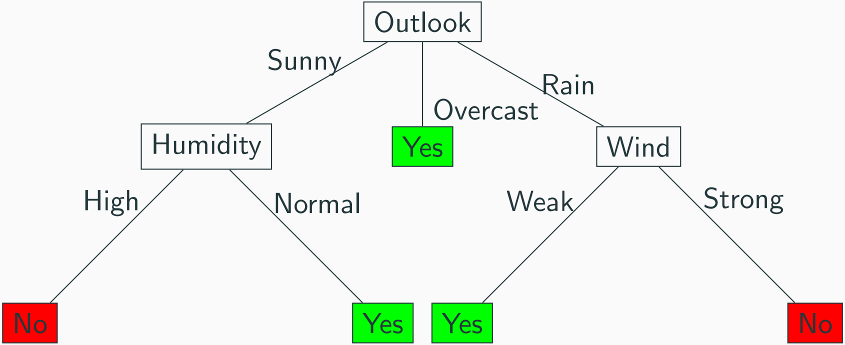
D13	Overcast	Hot	Normal	Weak	Yes
D14	Rain	Mild	High	Strong	No

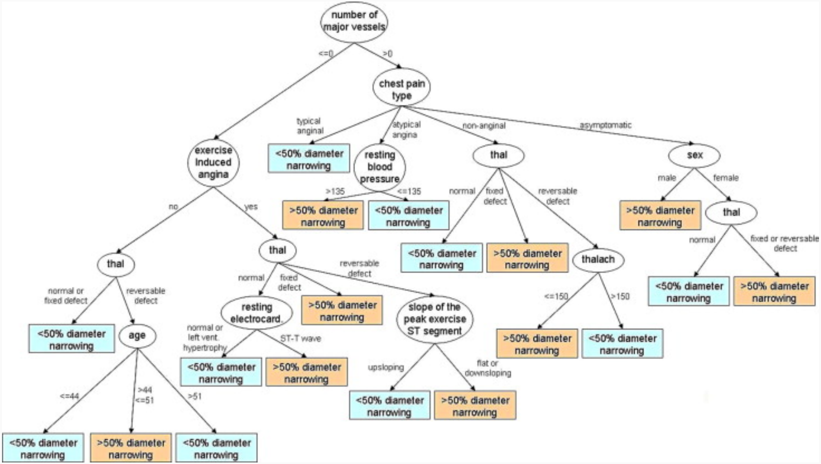
Learning a Complicated Neural Network



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

FOLLOW

Professor of Statistics, UC Berkeley
Verified email at stat.berkeley.edu - Homepage

Data Analysis Statistics Machine Learning

TITLE	CITED BY	YEAR
Random forests L Breiman Machine learning 45 (1), 5-32	53816	2001
Classification and Regression Trees L Breiman, JH Friedman, RA Olshen, CJ Stone CRC Press, New York	~~43992~~ *	1999
Classification and regression trees L Breiman Chapman & Hall/CRC	43992 *	1984
Bagging predictors L Breiman Machine learning 24 (2), 123-140	22742	1996
Statistical Modeling: The Two Cutures L Breiman	2788 *	2003
Statistical modeling: The two cultures (with comments and a rejoinder by the author) L Breiman Statistical Science 16 (3), 199-231	~~2772~~	2001
Estimating optimal transformations for multiple regression and correlation	2096	1985

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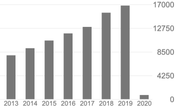


Optimal Decision Tree

Volume 5, number 1 INFORMATION PROCESSING LETTERS May 1976

CONSTRUCTING OPTIMAL BINARY DECISION TREES IS NP-COMPLETE*

Laurent HYAFIL
IRIA – Laboria, 78150 Rocquencourt, France

and

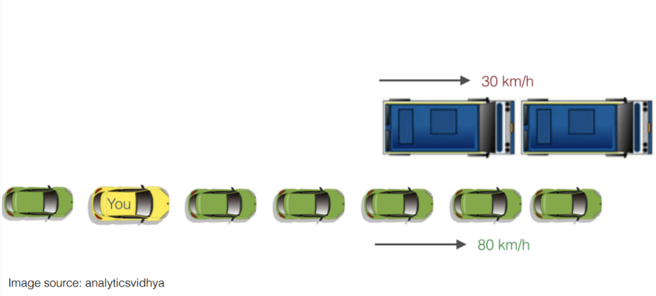
Ronald L. RIVEST
Dept. of Electrical Engineering and Computer Science, M.I.T., Cambridge, Massachusetts 02139, USA

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!



Greedy!=Optimal

Towards biggest estimated performance gain

Day	Outlook	Temp	Humidity	Windy	Play
D1	Sunny	Hot	High	Weak	No
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- For examples, we have 9 Yes, 5 No

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- Would it be trivial if we had 14 Yes or 14 No?

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- Yes!
- Key insights: Problem is "easier" when there is lesser disagreement

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?
- Yes!
- Key insights: Problem is "easier" when there is lesser disagreement
- Need some statistical measure of "disagreement"

Entropy

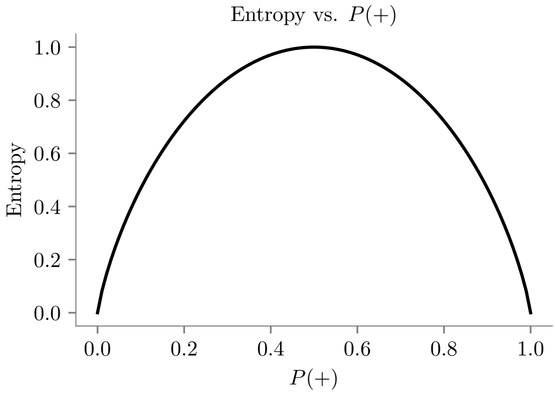
Statistical measure to characterize the (im)purity of examples

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



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- Can we use Outlook as the root node?

Towards biggest estimated performance gain

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D13	Overcast	Hot	Normal	Weak	Yes
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- 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

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

ID3 (Examples, Target Attribute, Attributes)

- Create a root node for tree

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- Create a root node for tree
- If all examples are +/-, return root with label = +/-

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

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

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- 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)

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

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    - Examples_{v}: subset of examples that A = v

ID3 (Examples, Target Attribute, Attributes)

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

$\boxed{\text{Root Node (empty)}}$

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
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D13	Overcast	Hot	Normal	Weak	Yes
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Entropy calculated

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

$$\text{Entropy(S)} = -\,\text{p}_{No} \log_2 \text{p}_{No} - \text{p}_{Yes} \log_2 \text{p}_{Yes}$$

$$= -(5/14)\log_2(5/14) - (9/14)\log_2(9/14) = 0.94$$

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

Entropy =
-3/5$\log_2$(3/5) -
2/5$\log_2$(2/5) =
0.971

Information Gain for Outlook

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

We have 2 Yes, 3 No

Entropy = $-3/5\log_2(3/5) - 2/5\log_2(2/5) = 0.971$

Outlook	**Play**
Overcast	Yes
Overcast	Yes
Overcast	Yes
Overcast	Yes

We have 4 Yes, 0 No

Entropy = 0

Information Gain for Outlook

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

We have 2 Yes, 3 No

Entropy = -3/5$\log_2$(3/5) - 2/5$\log_2$(2/5) = 0.971

Outlook	**Play**
Overcast	Yes
Overcast	Yes
Overcast	Yes
Overcast	Yes

We have 4 Yes, 0 No

Entropy = 0

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

We have 3 Yes, 2 No

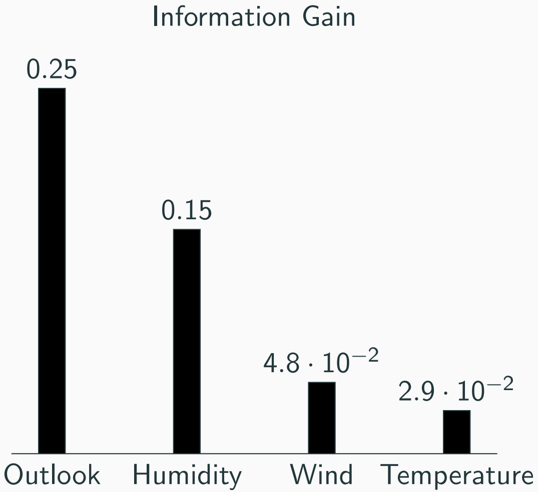
Entropy = -3/5$\log_2$(3/5) - 2/5$\log_2$(2/5) = 0.971

Information Gain

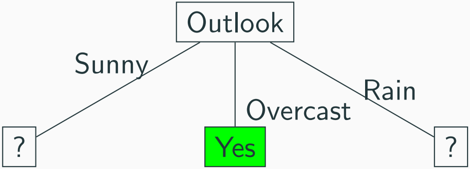
$$\text{Gain}(S, Outlook) = \text{ Entropy } (S) - \sum_{v \in \{Rain, Sunny, Windy\}} \frac{|S_v|}{|S|} \text{Entropy} (S_v)$$

Gain (S, Outlook) $=$ Entropy (S) -(5/14)* Entropy($\mathrm{S}_{\mathrm{Sunny}}$)-
(4/14)* Entropy ($\mathrm{S}_{\mathrm{overcast}}$)$-$(5/14)* Entropy($\mathrm{S}_{\mathrm{Rain}}$)
$=$ 0.940 - 0.347 - 0.347
$=$ 0.246

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

- Gain($S_{\text{Outlook=Sunny}}$, 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)

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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- Gain($S_{\text{Outlook=Sunny}}$, 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($S_{\text{Outlook=Sunny}}$, Humidity) = Entropy(3 Yes, 2 No) - (2/5)*Entropy(2 Yes) -(3/5)*Entropy(3 No) $\implies$ **maximum possible for the set**

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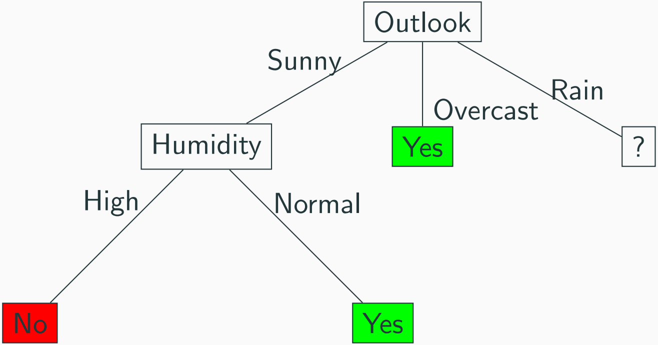
- Gain($S_{\text{Outlook=Sunny}}$, Temp) = Entropy(3 Yes, 2 No) - (2/5)*Entropy(2 No, 0 Yes) -(2/5)*Entropy(1 No, 1 Yes) - (1/5)*Entropy(1 Yes)
- Gain($S_{\text{Outlook=Sunny}}$, Humidity) = Entropy(3 Yes, 2 No) - (2/5)*Entropy(2 Yes) -(3/5)*Entropy(3 No) $\Longrightarrow$ **maximum possible for the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

Learnt Decision Tree

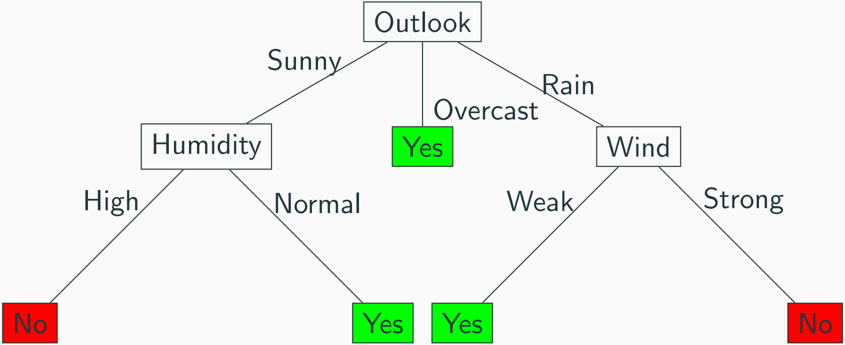


Calling ID3 on (Outlook=Rain)

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

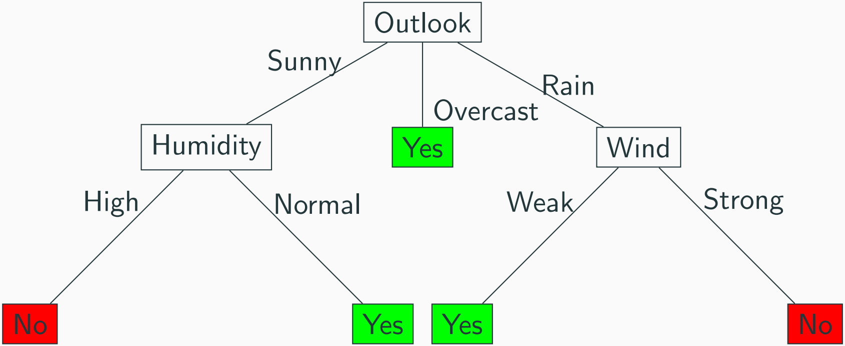
- The attribute Windy gives the highest information gain

Learnt Decision Tree



Prediction for Decision Tree

Just walk down the tree!



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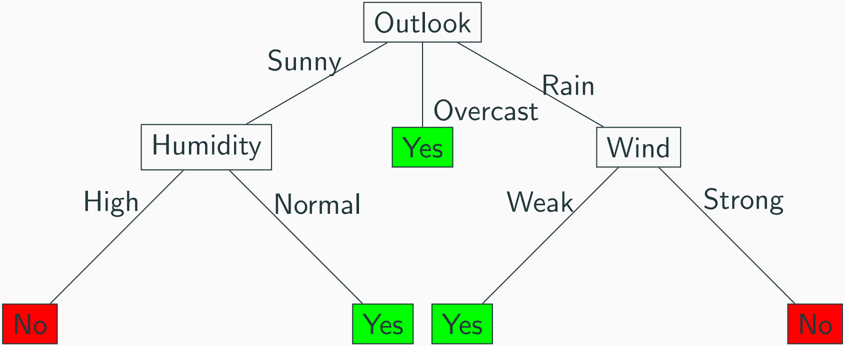

Prediction for <High Humidity, Strong Wind, Sunny Outlook, Hot Temp> is ?

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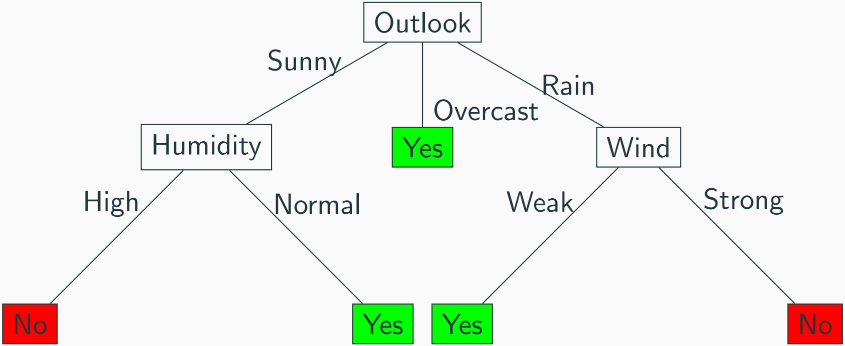

Prediction for <High Humidity, Strong Wind, Sunny Outlook, Hot Temp> is ?

No

Limiting Depth of Tree

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

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Always predicting Yes

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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.

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Always predicting Yes

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

Limiting Depth of Tree

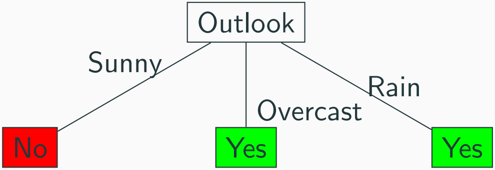
Assuming if you were only allowed depth-1 trees, how would it look for the current dataset?

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

Measure of Impurity for Regression?

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- Any guesses?

Measure of Impurity for Regression?

- Any guesses?
- Mean Squared Error

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

Measure of Impurity for Regression?

- Any guesses?
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- MSE(S) $= 311.34$
- Information Gain analogoue?

Measure of Impurity for Regression?

- Any guesses?
- 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

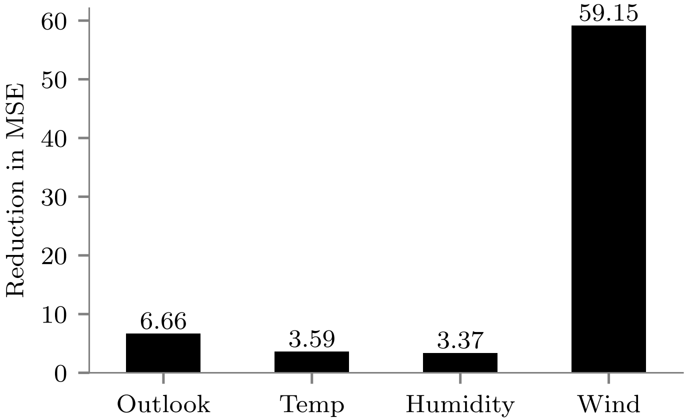
Weighted MSE($S_{Wind=Weak}$=(8/14)*277=159)

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

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

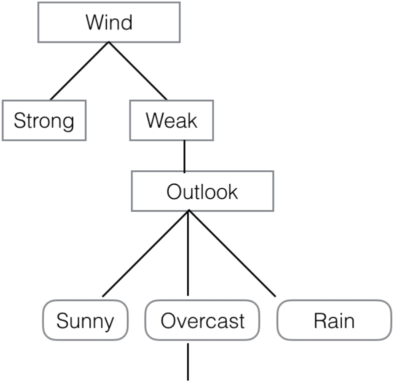
Information Gain

Notebook: decision-tree-real-output.html



Learnt Tree

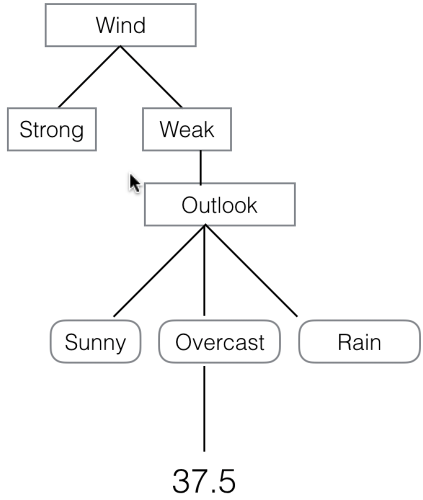
Assume a tree like this is learnt …



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

Learnt Tree

Method 1
Mins Played=(40+35)/2



Real Input Discrete Output

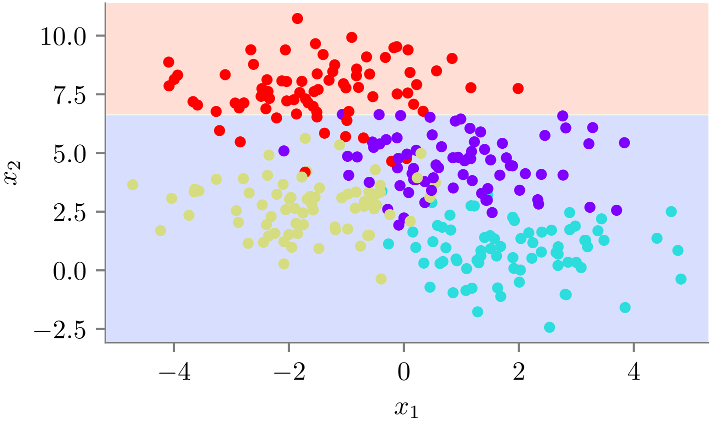
Finding splits

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: Temp $>$ (48+60)/2 and Temp $>$ (80+90)/2

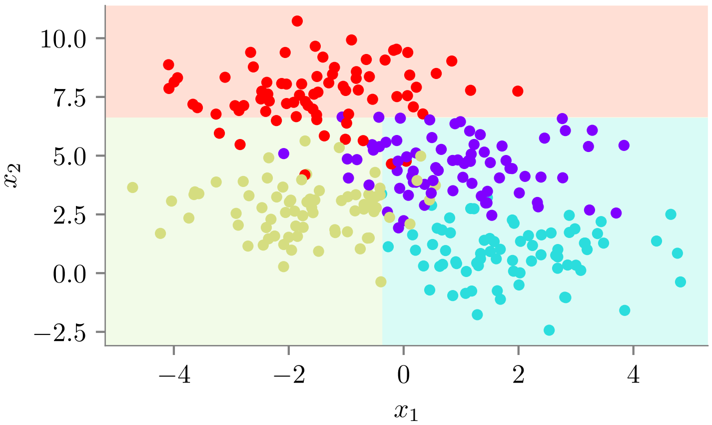
Example (DT of depth 1)

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



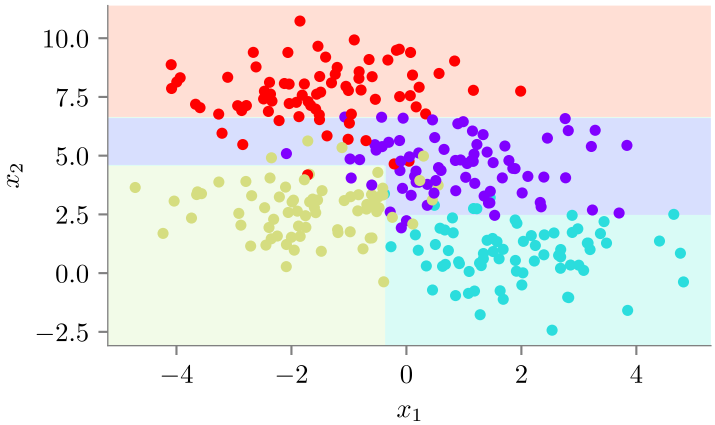
Example (DT of depth 2)

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



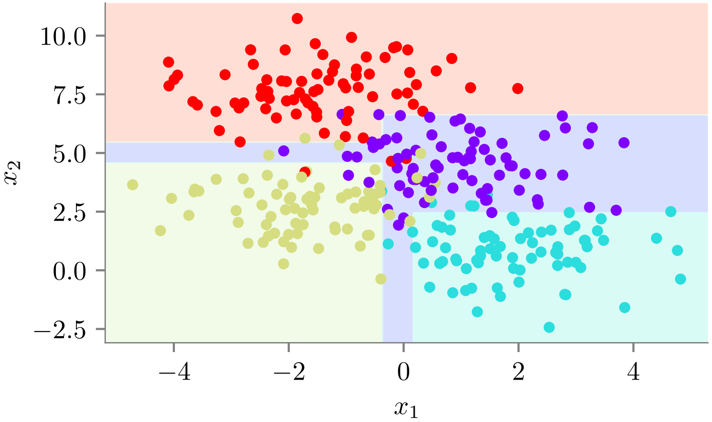
Example (DT of depth 3)

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



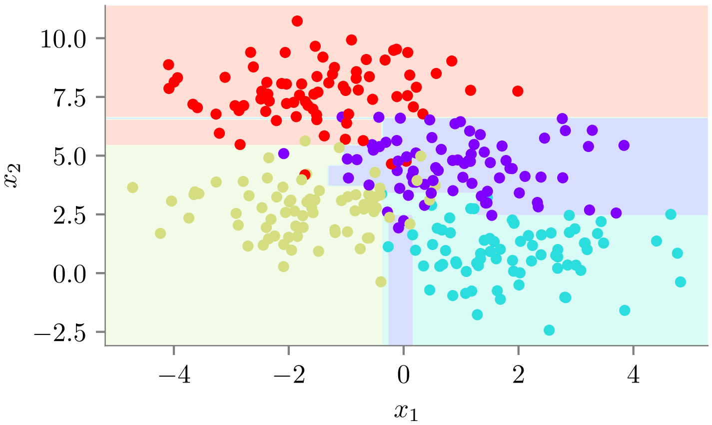
Example (DT of depth 4)

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



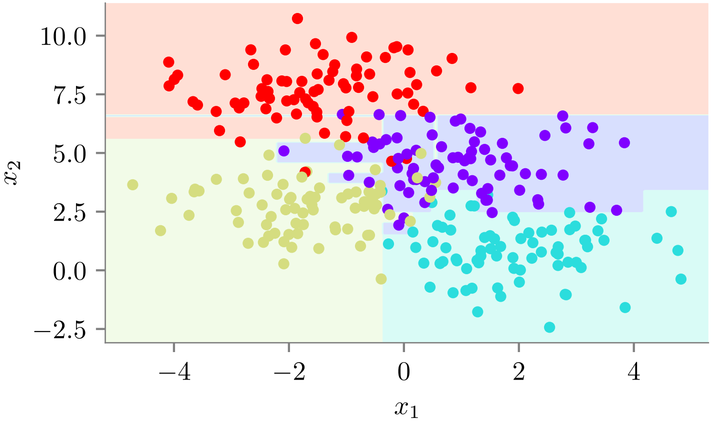
Example (DT of depth 5)

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



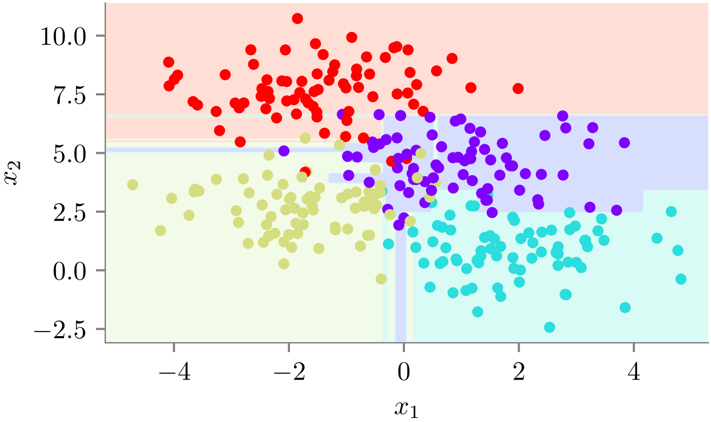
Example (DT of depth 6)

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



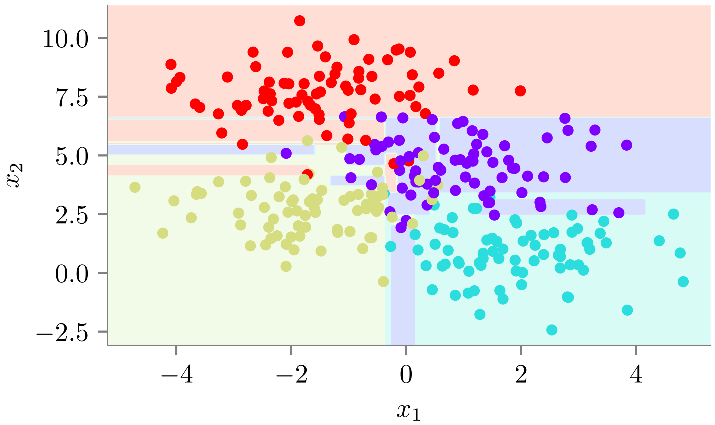
Example (DT of depth 7)

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



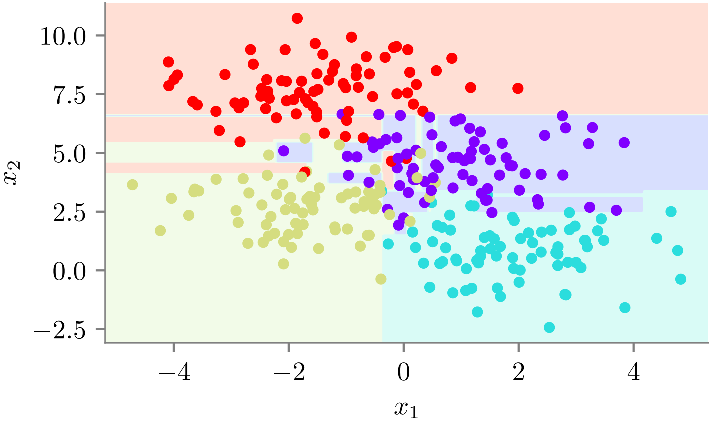
Example (DT of depth 8)

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



Example (DT of depth 9)

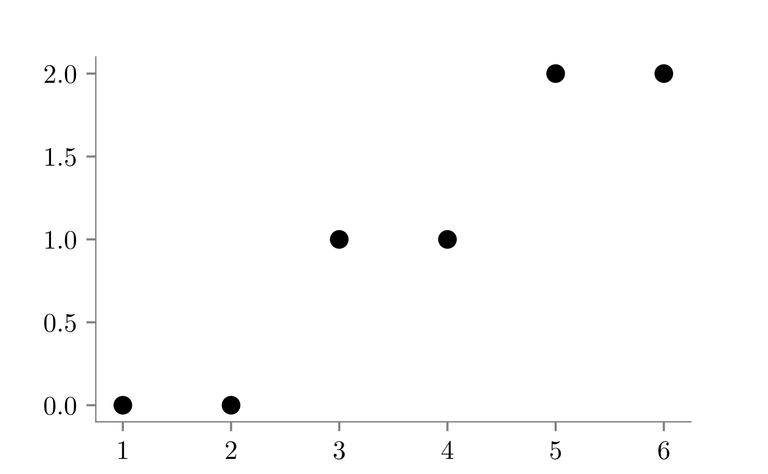
Notebook: decision-tree-real-input-discrete-output.html



Real Input Real Output

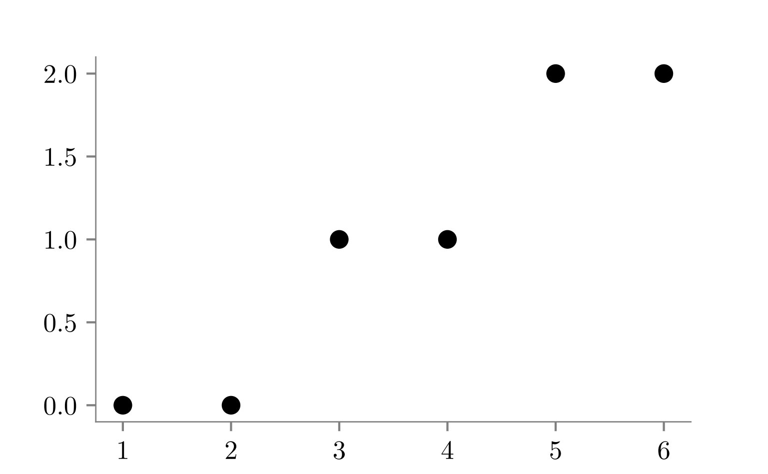
Example 1

Let us consider the dataset given below



Example 1

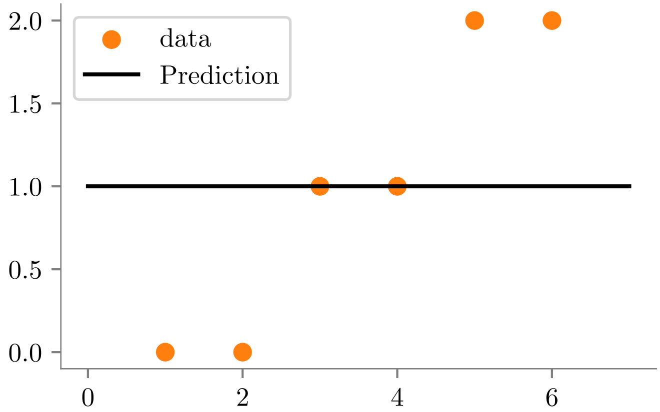
What would be the prediction for decision tree with depth 0?



Example 1

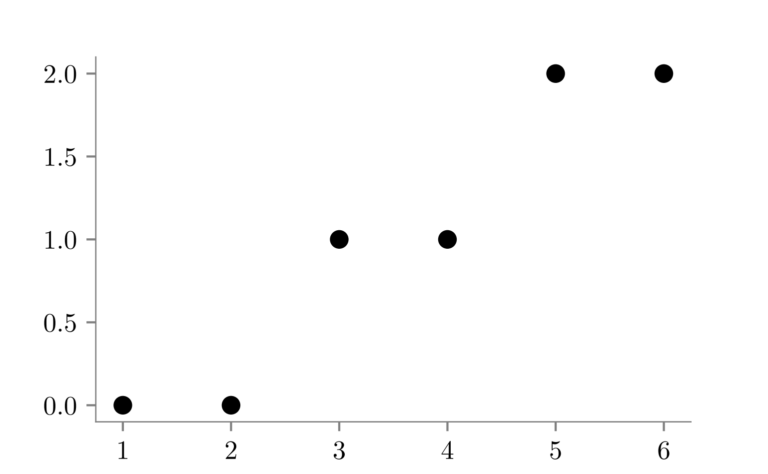
Prediction for decision tree with depth 0.

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



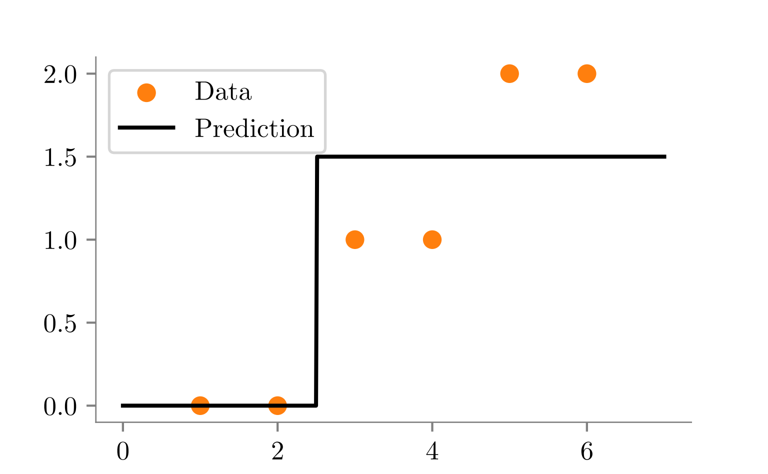
Example 1

What would be the decision tree with depth 1?



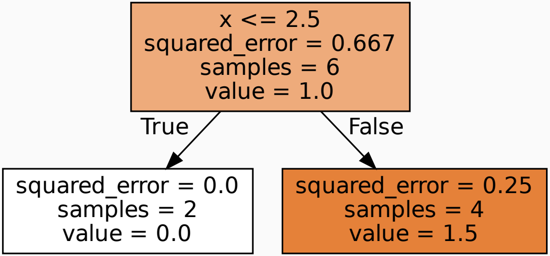
Example 1

Decision tree with depth 1



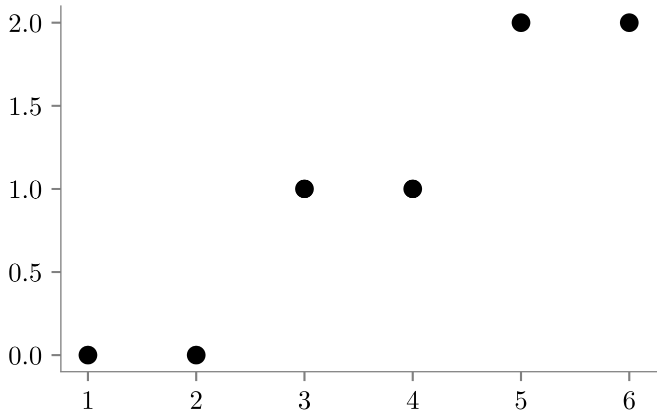
Example 1

The Decision Boundary



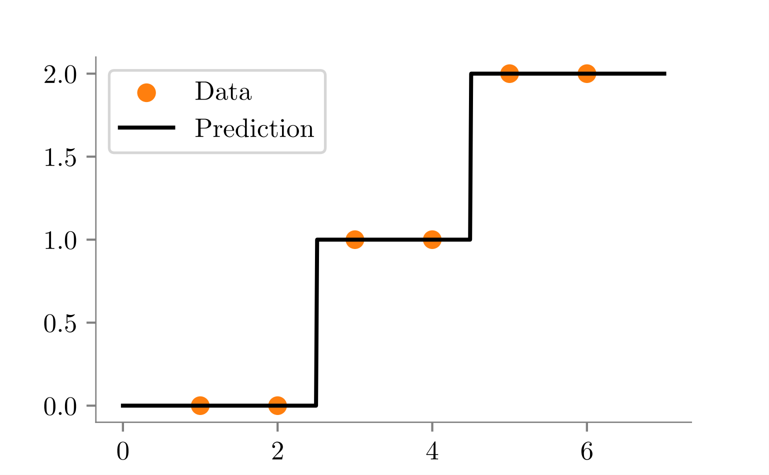
Example 1

What would be the decision tree with depth 2 ?



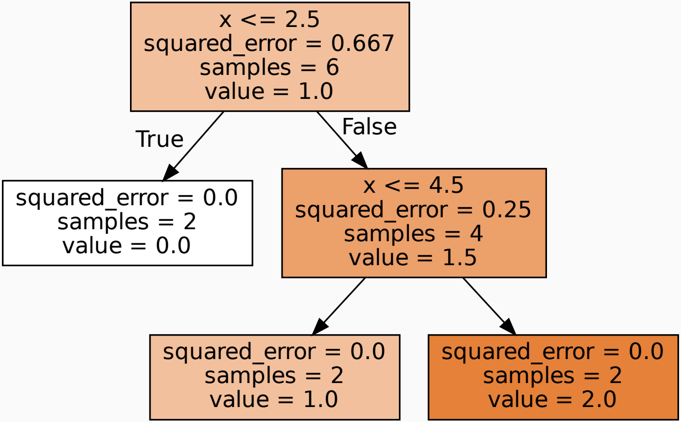
Example 1

Decision tree with depth 1



Example 1

The Decision Boundary



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.

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.

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

Objective function

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Let the "decision boundary" or "split" be at $\mathrm{X} = \mathrm{S}$.
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Then, let

$C_1 = \text{Mean } (Y_i | X_i \in R_1)$

$C_2 = \text{Mean } (Y_i | X_i \in R_2)$

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

Objective function

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

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

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$C_2 = \text{Mean } (Y_i | X_i \in R_2)$

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

Our objective is to minimize the loss and find

$min_S \sum_i \left((Y_i - C_1 | X_i \in R_1)^2 + (Y_i - C_2 | X_i \in R_2)^2\right)$

How to find optimal split "S"?

How to find optimal split “S”?

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

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

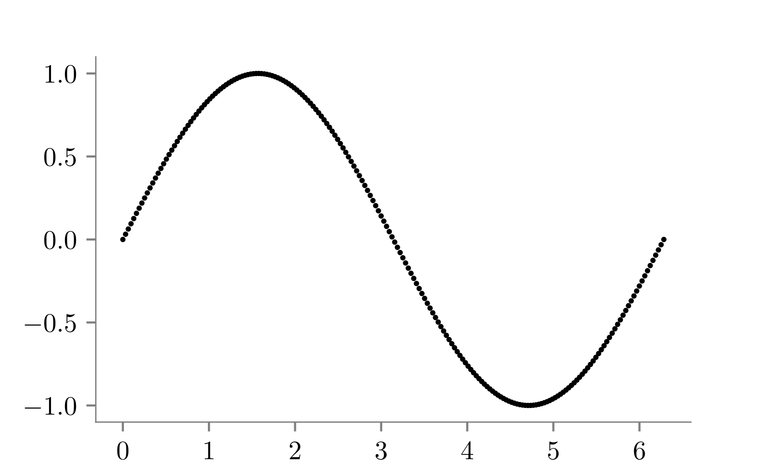
   and the select the S with minimum loss.

A Question!

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

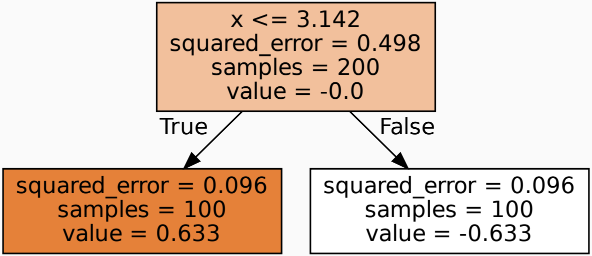
A Question!

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



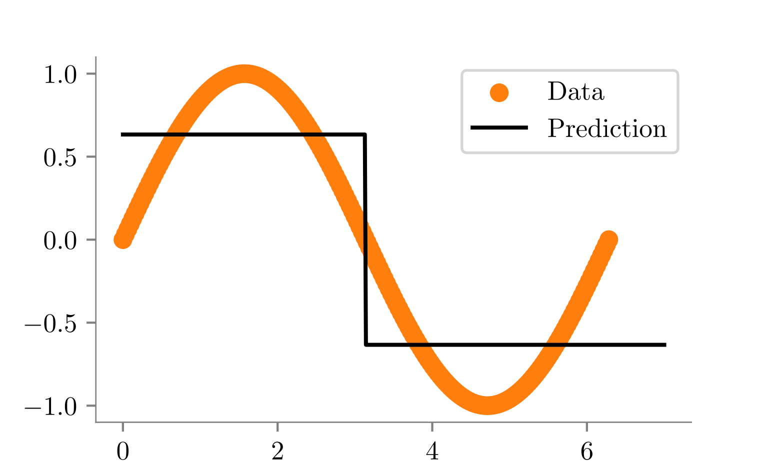
A Question!

Regression tree of depth 1



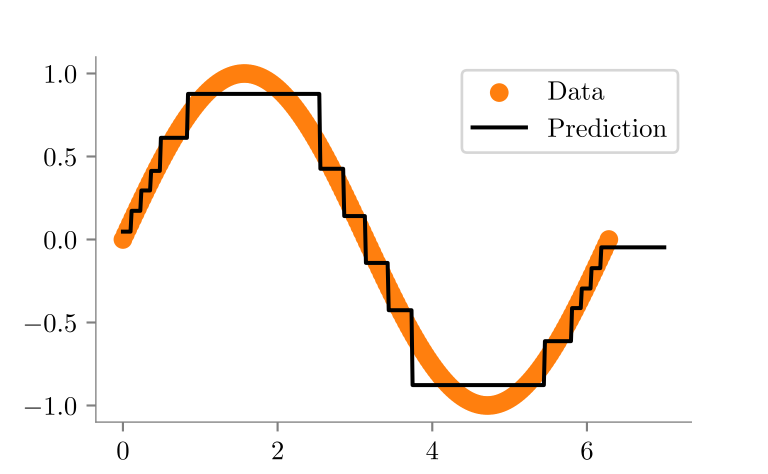
A Question!

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