CSE 6023
Machine Learning

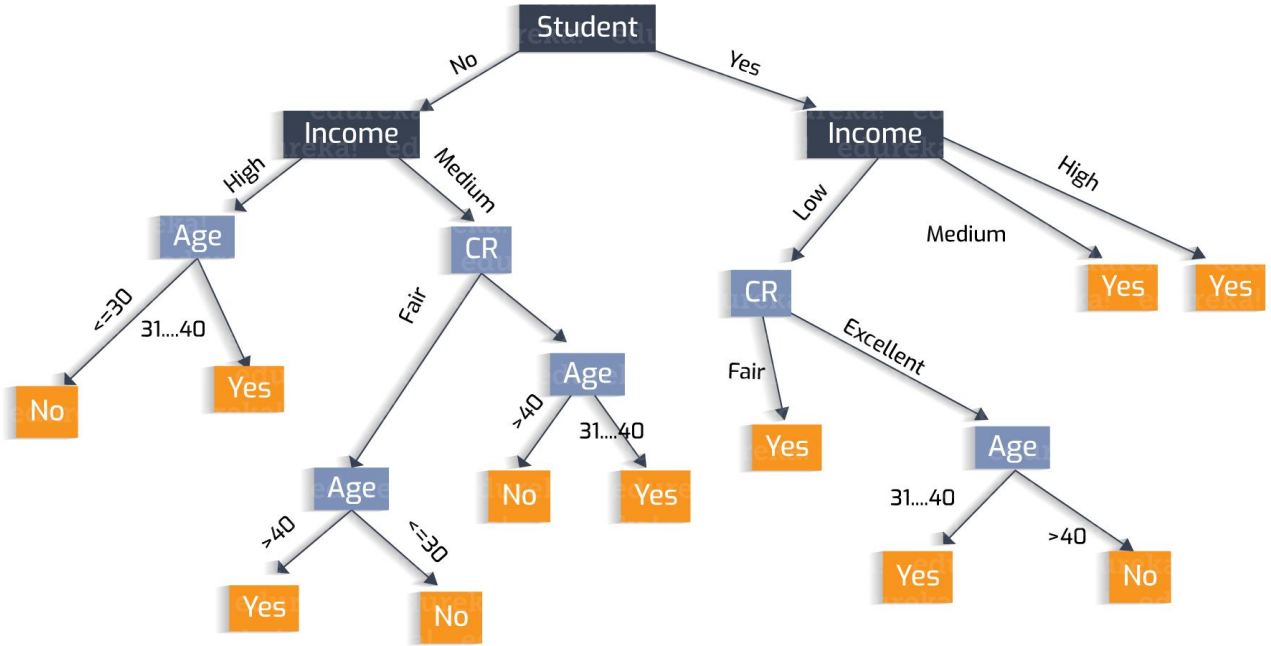
Tree Based Methods
Fall 2020

Contents

- Tree Based Methods
  - ID3, C4.5, CART
  - Mixed of numeric and categorical
  - Missing data
- Pruning
- Visualization
- Rule Generator

https://www.flickr.com/photos/wonderlane/2062184804/

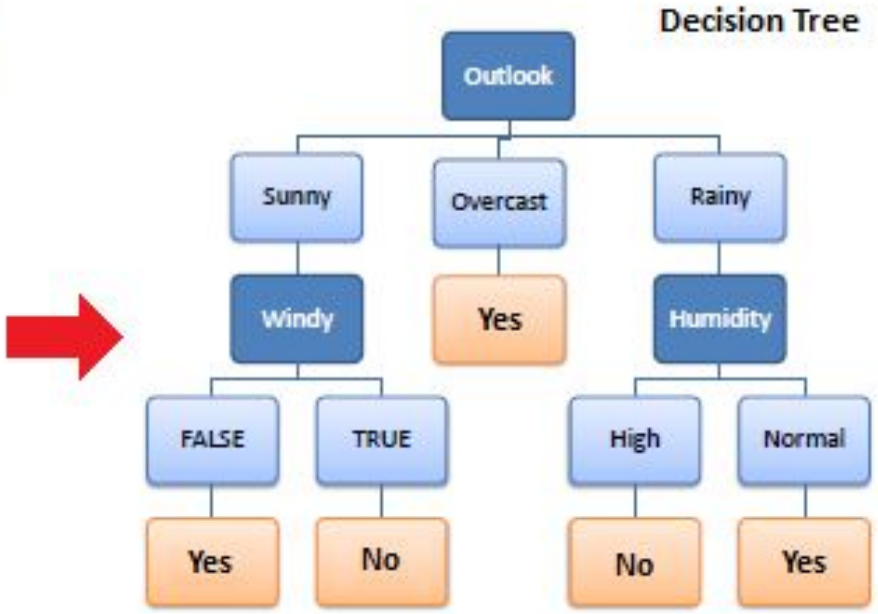
Explainable Rules



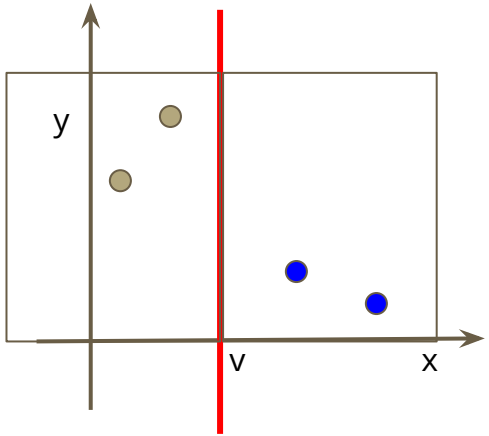
https://heartbeat.fritz.ai/understanding-the-mathematics-behind-decision-trees-22d86d55906

Decision Tree Example

Predictors				Target
Outlook	Temp.	Humidity	Windy	Play Golf
Rainy	Hot	High	False	No
Rainy	Hot	High	True	No
Overcast	Hot	High	False	Yes
Sunny	Mild	High	False	Yes
Sunny	Cool	Normal	False	Yes
Sunny	Cool	Normal	True	No
Overcast	Cool	Normal	True	Yes
Rainy	Mild	High	False	No
Rainy	Cool	Normal	False	Yes
Sunny	Mild	Normal	False	Yes
Rainy	Mild	Normal	True	Yes
Overcast	Mild	High	True	Yes
Overcast	Hot	Normal	False	Yes
Sunny	Mild	High	True	No



Handling Numeric Attributes



- Suppose y is the prediction variable
- x is the feature
- The decision boundary is at value v
- If x > v then use samples on the right
- If x < v use samples on the left
- For classification, voting
- For regression use uniform or weighted average

Decision Tree

- There are many trees possible
  - Always prefer the shortest one
- **What is a good decision tree?**
- For numeric attributes, it is important to decide the value to split
  - binary vs multiway splits
- For categorical variables its the set of the different values
- How to select between multiple attributes?
- How many attributes should be selected?
  - Single or multiple?

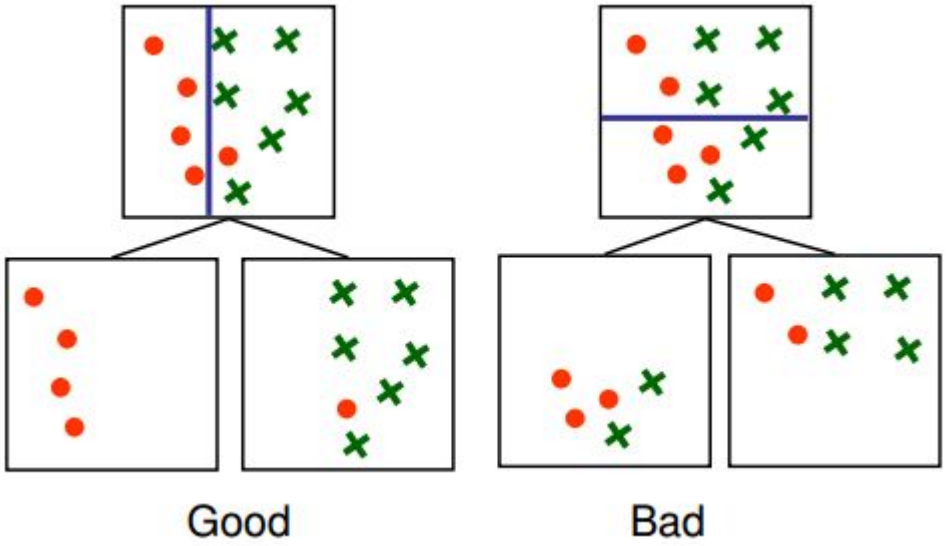
Decision Tree for Regression and Classification

- Classification and Regression Trees
  - Breiman et al 1984
  - Only Binary Splits
  - Uses Gini “measure of impurity”
- Iterative Dichotomiser 3
  - Ross Quinlan, 1986
  - Uses Information Gain, Greedy Algorithm
- C 4.5 by
  - Ross Quinlan, 1993
  - Improved version over ID3
    - Pruning, attributes with different costs, missing values, continuous attributes,

Top 10 algorithms in data mining http://www.cs.umd.edu/~samir/498/10Algorithms-08.pdf

Good Split vs Bad Split

- What make a split good?
- The case for classification
  - Entropy
  - Information Gain
  - Gain Ratio
  - Gini Index
- The case for regression
  - Squared Error



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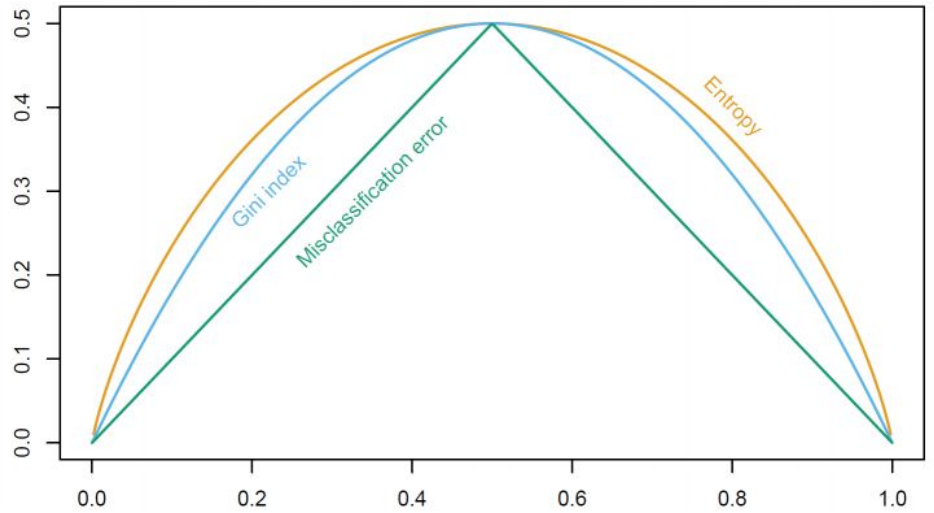
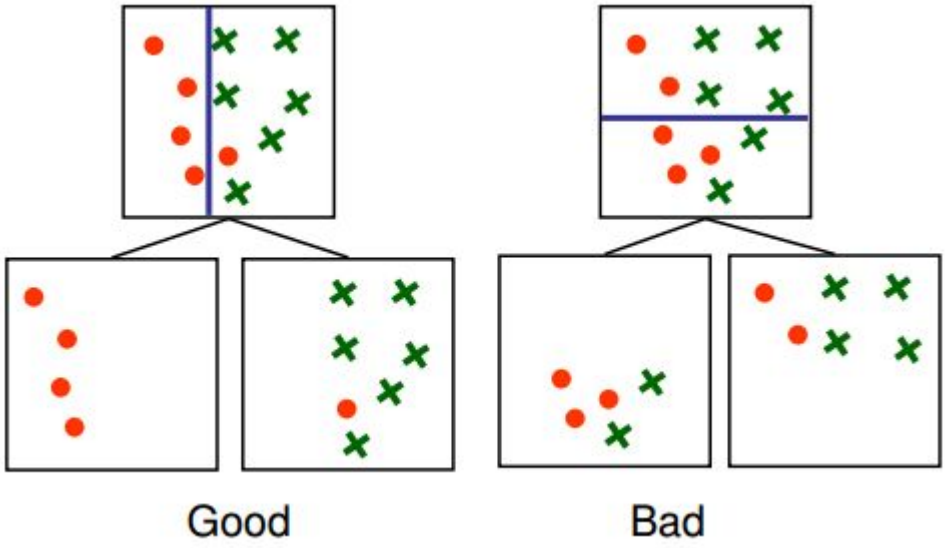


Entropy

$$H(q) = -\sum_{i=1}^{k} p_i log_2(p_i)$$

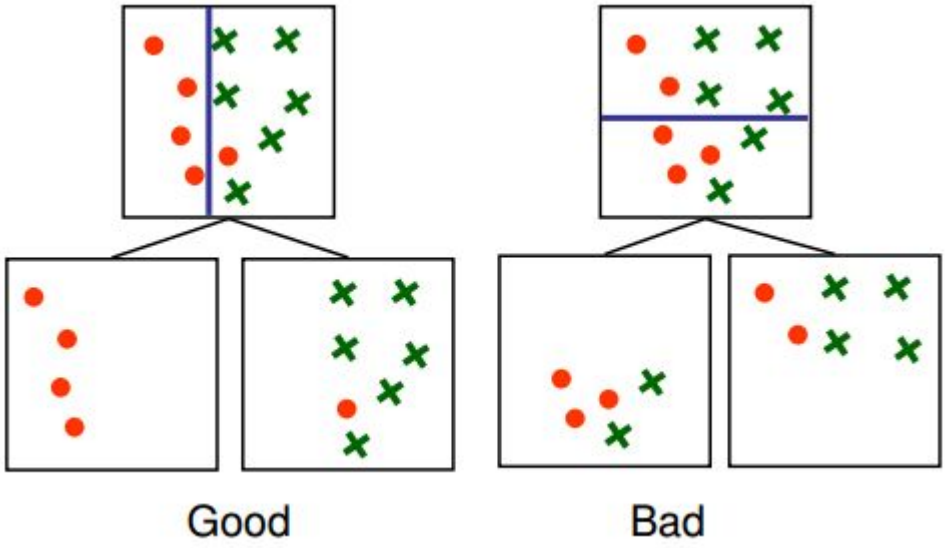
- Measure of disorder in a set
- Find out entropy of each of the rectangles



Information Gain

$$H(q) = -\sum_{i=1}^{k} p_i log_2(p_i)$$

- How much information is gained by a split
- Originally a node have a measure of entropy H(q)
- After the split, the entropy is divided into sets. The gain is the difference.



$$Gain(q, V) = H(q) - \sum_{i-1}^{|V|} \frac{N_i}{N_q} H(i)$$

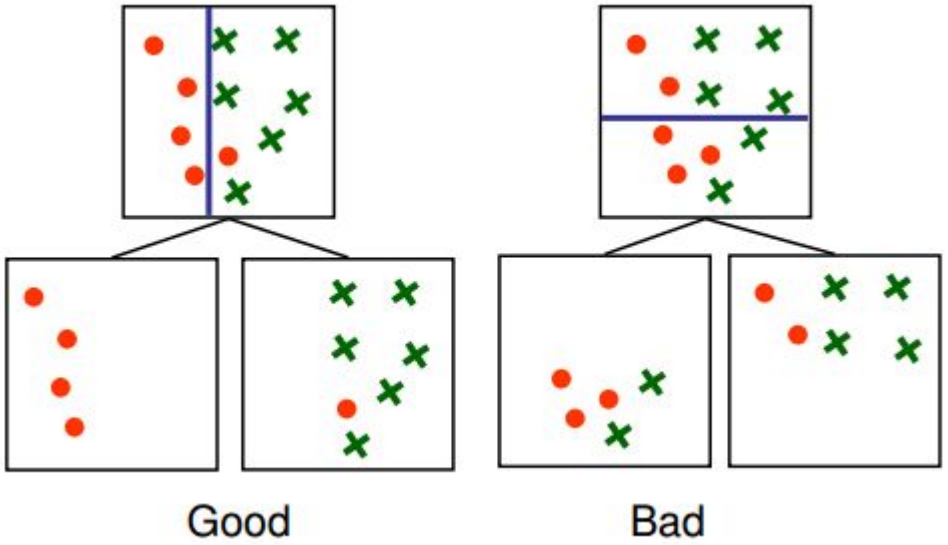
Gain Ratio

$$H(q) = -\sum_{i=1}^{k} p_i log_2(p_i)$$

- IG biases the decision tree against considering attributes with a large number of distinct values
  - E.g. credit card number
- Normalization of Information Gain
- Split Information

$$Split(q, V) = -\sum_{i-1}^{|V|} \frac{N_i}{N_q} log_2(\frac{N_i}{N_q})$$

- Gain Ratio = Information Gain / Split Information

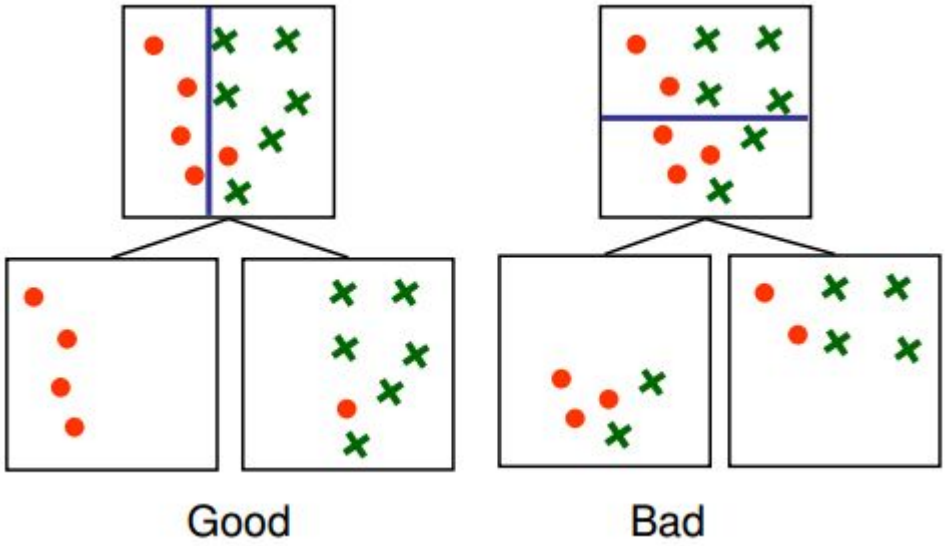


$$Gain(q, V) = H(q) - \sum_{i-1}^{|V|} \frac{N_i}{N_q} H(i)$$

Gini Index

$$Gini(q) = \sum_{i=1}^{k} p_i(1 - p_i)$$

- Gini impurity is a measure of how often a randomly chosen element from the set would be incorrectly labeled if it was randomly labeled according to the distribution of labels in the subset
- Used by CART
- Gain is defined similarly



$$Gain(q, V) = Gini(q) - \sum_{i-1}^{|V|} \frac{N_i}{N_q} Gini(i)$$

An Example

We will work on same dataset in ID3. There are 14 instances of golf playing decisions based on outlook, temperature, humidity and wind factors.

- We will use gini index

Day	Outlook	Temp.	Humidity	Wind	Decision
1	Sunny	Hot	High	Weak	No
2	Sunny	Hot	High	Strong	No
3	Overcast	Hot	High	Weak	Yes
4	Rain	Mild	High	Weak	Yes
5	Rain	Cool	Normal	Weak	Yes
6	Rain	Cool	Normal	Strong	No
7	Overcast	Cool	Normal	Strong	Yes
8	Sunny	Mild	High	Weak	No
9	Sunny	Cool	Normal	Weak	Yes
10	Rain	Mild	Normal	Weak	Yes
11	Sunny	Mild	Normal	Strong	Yes
12	Overcast	Mild	High	Strong	Yes
13	Overcast	Hot	Normal	Weak	Yes
14	Rain	Mild	High	Strong	No

https://sefiks.com/2018/08/27/a-step-by-step-cart-decision-tree-example/

Outlook

Outlook is a nominal feature. It can be sunny, overcast or rain. I will summarize the final decisions for outlook feature.

Outlook	Yes	No	Number of instances
Sunny	2	3	5
Overcast	4	0	4
Rain	3	2	5

$Gini(Outlook=Sunny) = 1 - (2/5)^2 - (3/5)^2 = 1 - 0.16 - 0.36 = 0.48$

$Gini(Outlook=Overcast) = 1 - (4/4)^2 - (0/4)^2 = 0$

$Gini(Outlook=Rain) = 1 - (3/5)^2 - (2/5)^2 = 1 - 0.36 - 0.16 = 0.48$

Then, we will calculate weighted sum of gini indexes for outlook feature.

$Gini(Outlook) = (5/14) \times 0.48 + (4/14) \times 0 + (5/14) \times 0.48 = 0.171 + 0 + 0.171 = 0.342$

https://sefiks.com/2018/08/27/a-step-by-step-cart-decision-tree-example/

Temperature

Temperature is a nominal feature and it could have 3 different values: Cool, Hot and Mild. Let's summarize decisions for temperature feature.

Temperature	Yes	No	Number of instances
Hot	2	2	4
Cool	3	1	4
Mild	4	2	6

$Gini(Temp=Hot) = 1 - (2/4)^2 - (2/4)^2 = 0.5$

$Gini(Temp=Cool) = 1 - (3/4)^2 - (1/4)^2 = 1 - 0.5625 - 0.0625 = 0.375$

$Gini(Temp=Mild) = 1 - (4/6)^2 - (2/6)^2 = 1 - 0.444 - 0.111 = 0.445$

We'll calculate weighted sum of gini index for temperature feature

$Gini(Temp) = (4/14) \times 0.5 + (4/14) \times 0.375 + (6/14) \times 0.445 = 0.142 + 0.107 + 0.190 = 0.439$

https://sefiks.com/2018/08/27/a-step-by-step-cart-decision-tree-example/

Humidity

Humidity is a binary class feature. It can be high or normal.

Humidity	Yes	No	Number of instances
High	3	4	7
Normal	6	1	7

$Gini(Humidity=High) = 1 - (3/7)^2 - (4/7)^2 = 1 - 0.183 - 0.326 = 0.489$

$Gini(Humidity=Normal) = 1 - (6/7)^2 - (1/7)^2 = 1 - 0.734 - 0.02 = 0.244$

Weighted sum for humidity feature will be calculated next

$Gini(Humidity) = (7/14) \times 0.489 + (7/14) \times 0.244 = 0.367$

https://sefiks.com/2018/08/27/a-step-by-step-cart-decision-tree-example/

Wind

Wind is a binary class similar to humidity. It can be weak and strong.

Wind	Yes	No	Number of instances
Weak	6	2	8
Strong	3	3	6

$$Gini(Wind=Weak) = 1 - (6/8)^2 - (2/8)^2 = 1 - 0.5625 - 0.062 = 0.375$$

$$Gini(Wind=Strong) = 1 - (3/6)^2 - (3/6)^2 = 1 - 0.25 - 0.25 = 0.5$$

$$Gini(Wind) = (8/14) \times 0.375 + (6/14) \times 0.5 = 0.428$$

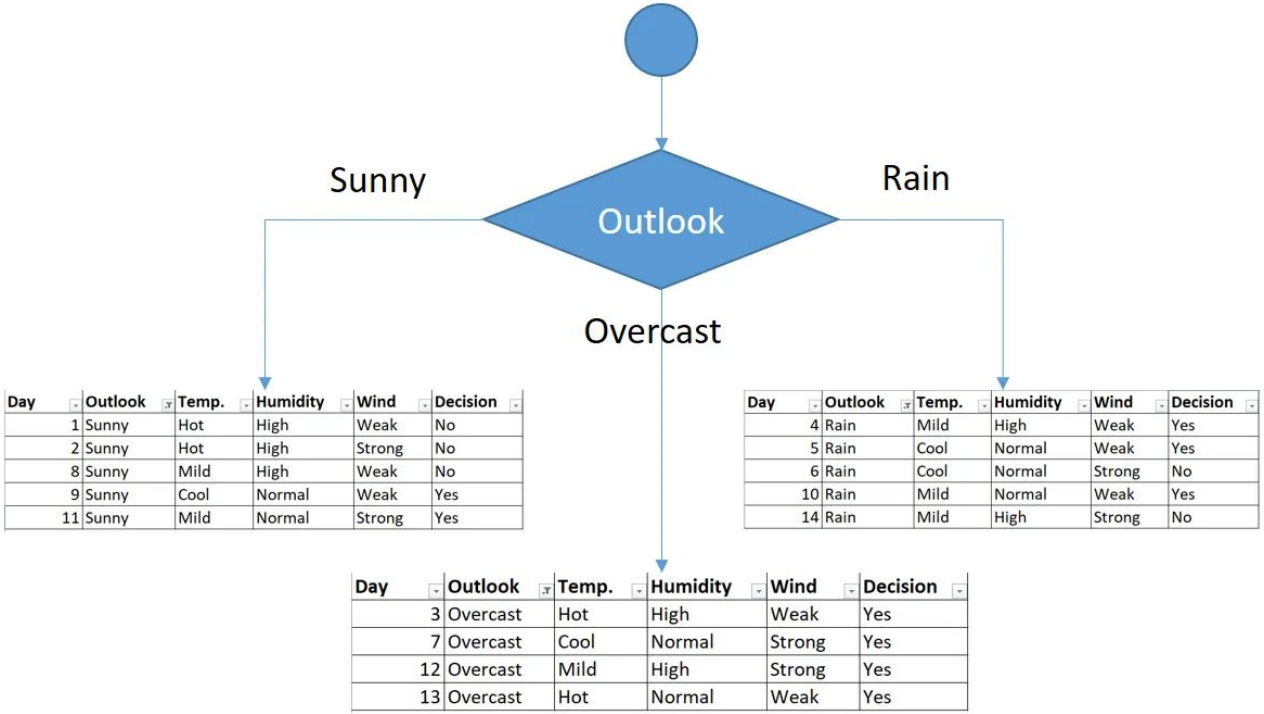
https://sefiks.com/2018/08/27/a-step-by-step-cart-decision-tree-example/

The first split

Feature	Gini index
Outlook	0.342
Temperature	0.439
Humidity	0.367
Wind	0.428

https://sefiks.com/2018/08/27/a-step-by-step-cart-decision-tree-example/

The first split: Outlook



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2	Sunny	Hot	High	Strong	No
8	Sunny	Mild	High	Weak	No
9	Sunny	Cool	Normal	Weak	Yes
11	Sunny	Mild	Normal	Strong	Yes

Day	Outlook	Temp.	Humidity	Wind	Decision
4	Rain	Mild	High	Weak	Yes
5	Rain	Cool	Normal	Weak	Yes
6	Rain	Cool	Normal	Strong	No
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Day	Outlook	Temp.	Humidity	Wind	Decision
3	Overcast	Hot	High	Weak	Yes
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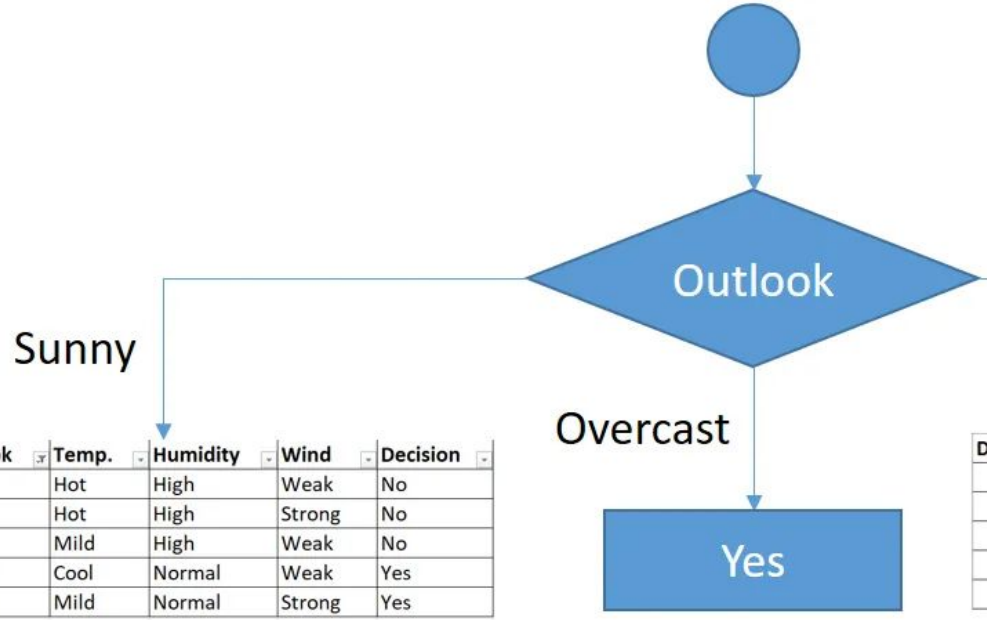
The first split:Outlook



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Recursive Partitioning

A sub dataset

Day	Outlook	Temp.	Humidity	Wind	Decision
1	Sunny	Hot	High	Weak	No
2	Sunny	Hot	High	Strong	No
8	Sunny	Mild	High	Weak	No
9	Sunny	Cool	Normal	Weak	Yes
11	Sunny	Mild	Normal	Strong	Yes

https://sefiks.com/2018/08/27/a-step-by-step-cart-decision-tree-example/

Outlook sunny & Temperature

Temperature	Yes	No	Number of instances
Hot	0	2	2
Cool	1	0	1
Mild	1	1	2

Gini(Outlook=Sunny and Temp.=Hot) = $1 - (0/2)^2 - (2/2)^2 = 0$

Gini(Outlook=Sunny and Temp.=Cool) = $1 - (1/1)^2 - (0/1)^2 = 0$

Gini(Outlook=Sunny and Temp.=Mild) = $1 - (1/2)^2 - (1/2)^2 = 1 - 0.25 - 0.25 = 0.5$

Gini(Outlook=Sunny and Temp.) = $(2/5)x0 + (1/5)x0 + (2/5)x0.5 = 0.2$

https://sefiks.com/2018/08/27/a-step-by-step-cart-decision-tree-example/

Outlook sunny & Humidity

Humidity	Yes	No	Number of instances
High	0	3	3
Normal	2	0	2

$$\text{Gini(Outlook=Sunny and Humidity=High)} = 1 - (0/3)^2 - (3/3)^2 = 0$$

$$\text{Gini(Outlook=Sunny and Humidity=Normal)} = 1 - (2/2)^2 - (0/2)^2 = 0$$

$$\text{Gini(Outlook=Sunny and Humidity)} = (3/5)\text{x}0 + (2/5)\text{x}0 = 0$$

https://sefiks.com/2018/08/27/a-step-by-step-cart-decision-tree-example/

Outlook sunny & Wind

Wind	Yes	No	Number of instances
Weak	1	2	3
Strong	1	1	2

Gini(Outlook=Sunny and Wind=Weak) = $1 - (1/3)^2 - (2/3)^2 = 0.266$

Gini(Outlook=Sunny and Wind=Strong) = $1- (1/2)^2 - (1/2)^2 = 0.2$

Gini(Outlook=Sunny and Wind) = $(3/5)\text{x}0.266 + (2/5)\text{x}0.2 = 0.466$

https://sefiks.com/2018/08/27/a-step-by-step-cart-decision-tree-example/

The second split

Feature	Gini index
Temperature	0.2
Humidity	0
Wind	0.466

Sunny

High

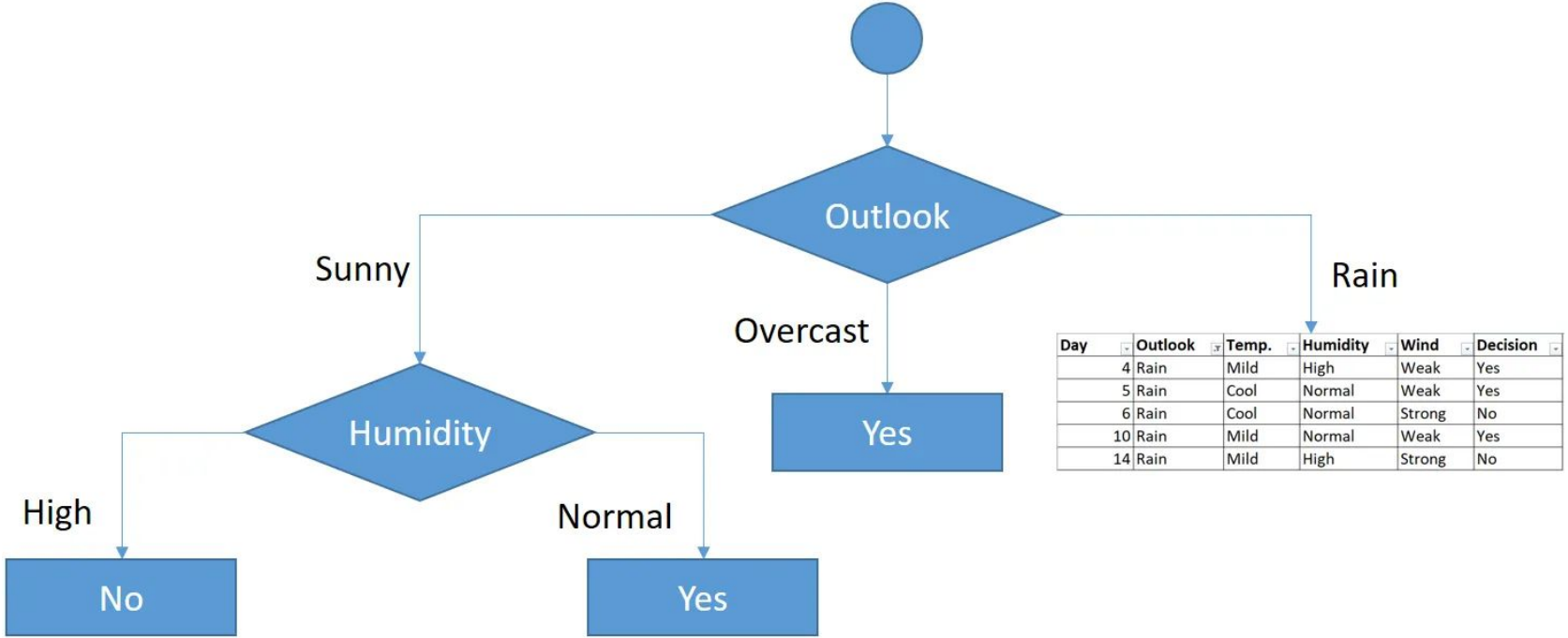
Day	Outlook	Temp.	Humidity	Wind	Decision
1	Sunny	Hot	High	Weak	No
2	Sunny	Hot	High	Strong	No
8	Sunny	Mild	High	Weak	No

Normal

Day	Outlook	Temp.	Humidity	Wind	Decision
9	Sunny	Cool	Normal	Weak	Yes
11	Sunny	Mild	Normal	Strong	Yes

https://sefiks.com/2018/08/27/a-step-by-step-cart-decision-tree-example/

The second split



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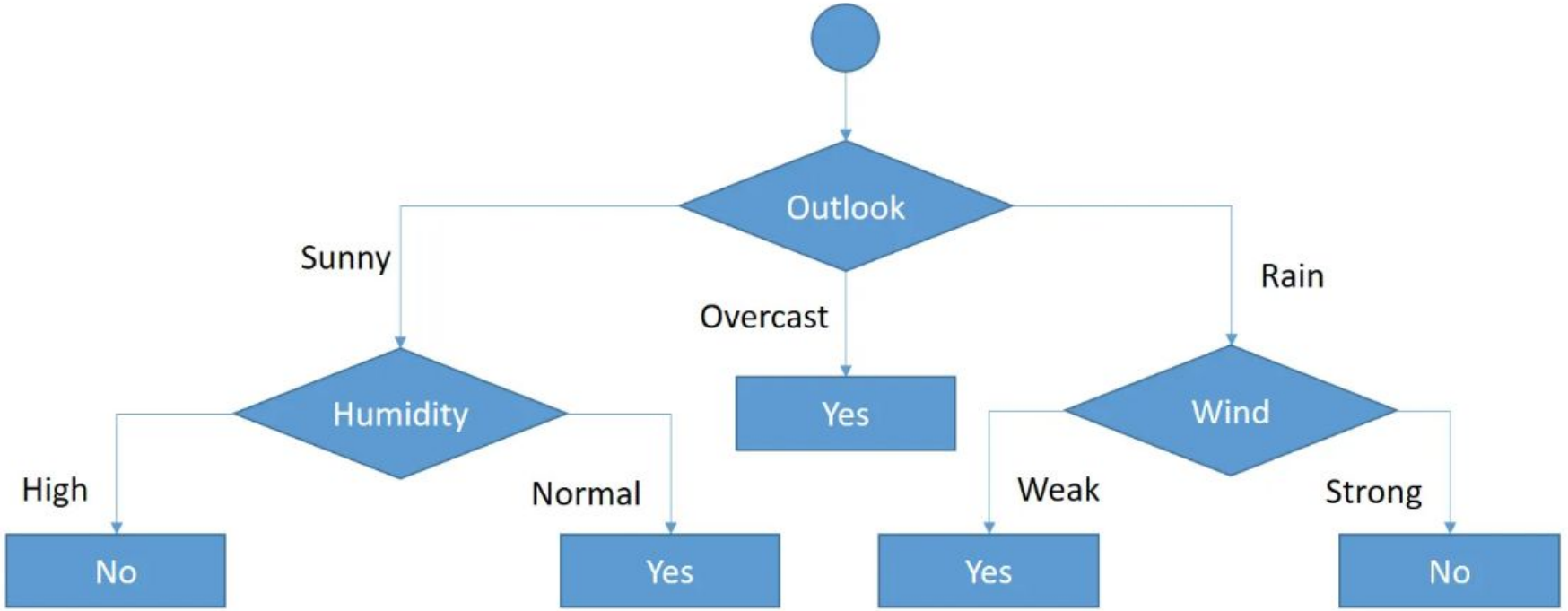
The final tree



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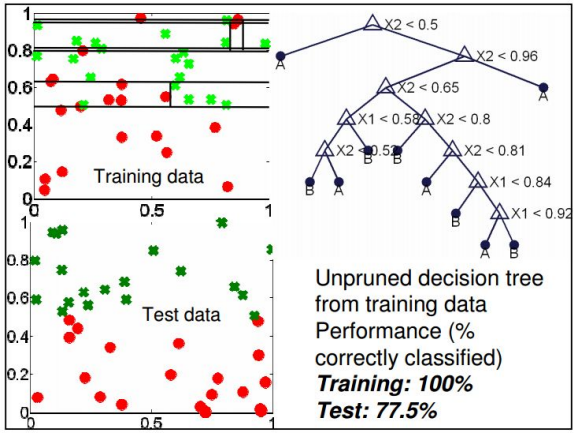
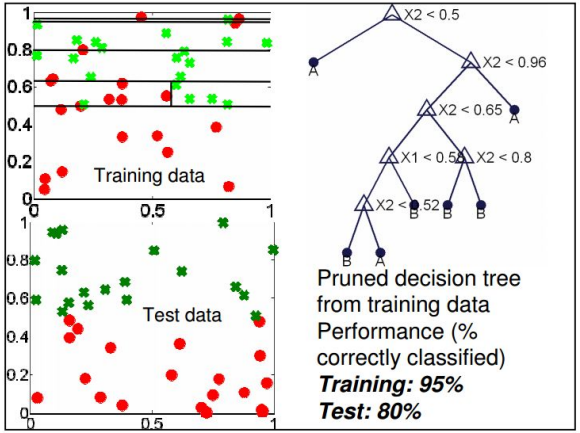
Decision Tree Overfitting

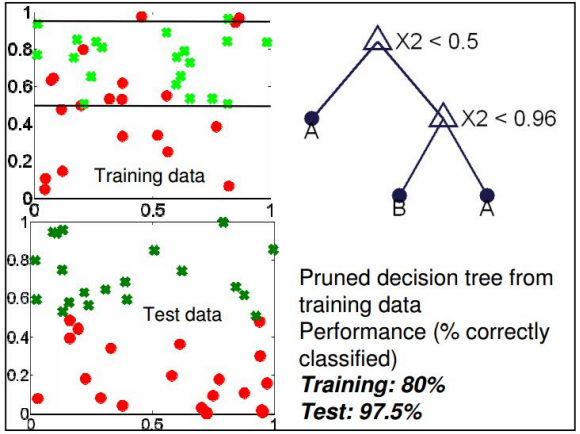
- Pre-Pruning
  - Maximum number of leaf nodes
  - Maximum depth of the tree
  - Minimum number of training instances at a leaf node
- Post-Pruning
  - Another strategy to avoid overfitting in decision trees is to first grow a full tree, and then prune it based on a previously held-out validation dataset.
  - Use statistical Tests

Tree Pruning: Validation Set

- Prune using a hold out validation dataset







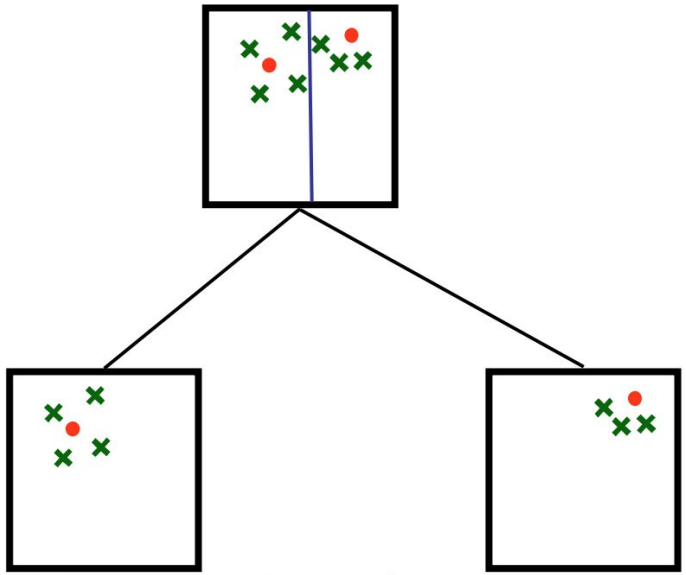
https://www.cs.cmu.edu/afs/cs.cmu.edu/academic/class/15381-s06/www/DTs2.pdf

Detecting Useless Splits

$$\hat{p}_k = p \times \frac{p_k + n_k}{p + n}$$
$$\hat{n}_k = n \times \frac{p_k + n_k}{p + n}$$

- Try Chi Square Test
- Check the statistic to find any significance gain achieved by the split
- Is there any difference with the arbitrary split?

$$\Delta = \sum_{k=1}^{d} \frac{(p_k - \hat{p}_k)^2}{\hat{p}_k} + \frac{(n_k - \hat{n}_k)^2}{\hat{n}_k}$$



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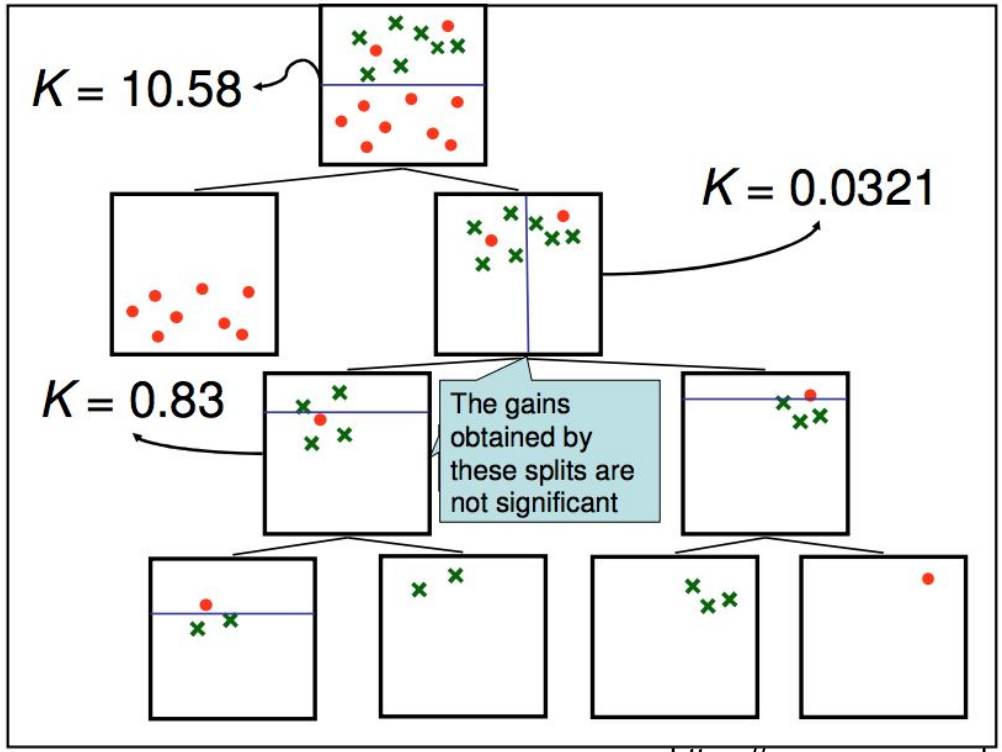

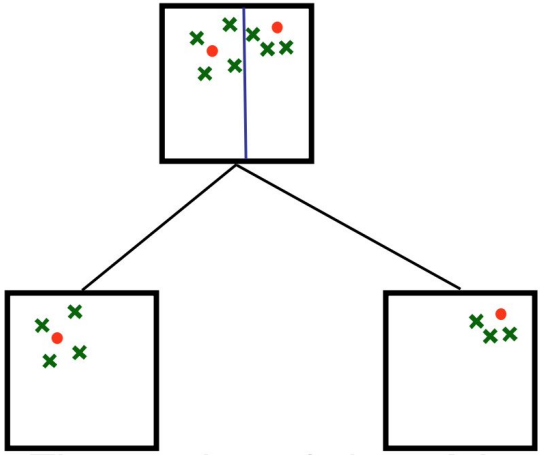

$$\hat{p}_k = p \times \frac{p_k + n_k}{p + n}$$

$$\hat{n}_k = n \times \frac{p_k + n_k}{p + n}$$

$$\Delta = \sum_{k=1}^{d} \frac{(p_k - \hat{p}_k)^2}{\hat{p}_k} + \frac{(n_k - \hat{n}_k)^2}{\hat{n}_k}$$

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Decision Tree

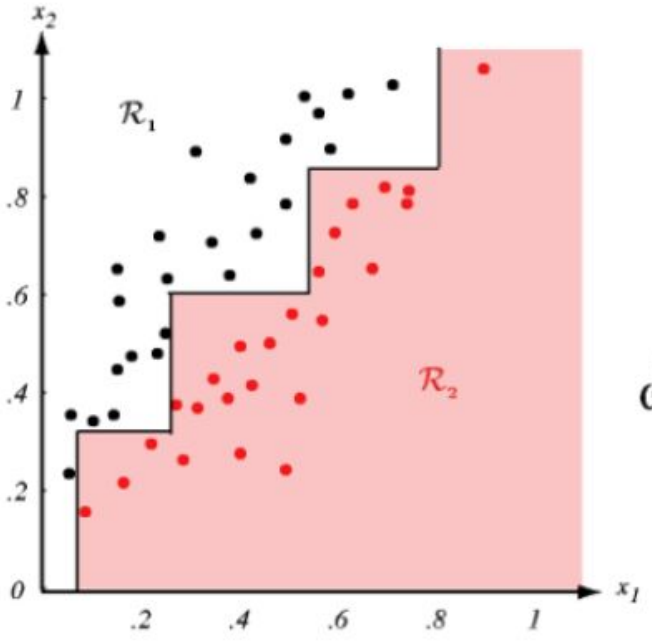
Pros

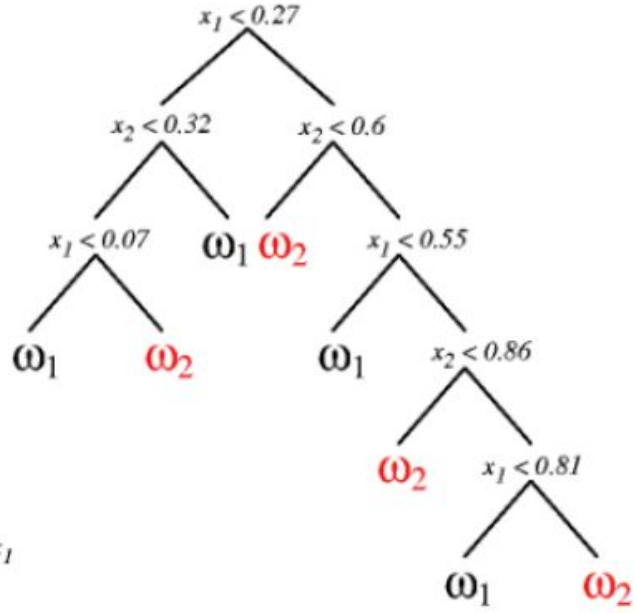
- Interpretable and Simple
- Handles all types of data
- Handles missing values
- Less pre-processing required
- Fast computation
- non-parametric

Cons

- NP-complete
- Not stable
- Often Overfits
- High bias
- Not suitable for structured data

Multi-Variable Split?





Multi-Variable Split?