Classification Trees

Classification Trees

author: Son Nguyen

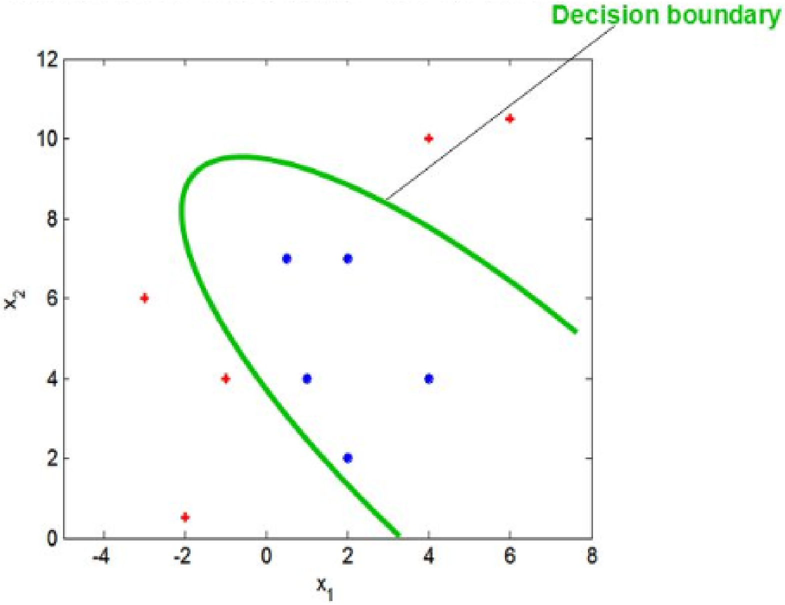
Reading Materials

- Max Kuhn. Chapter 14. Section 14.1

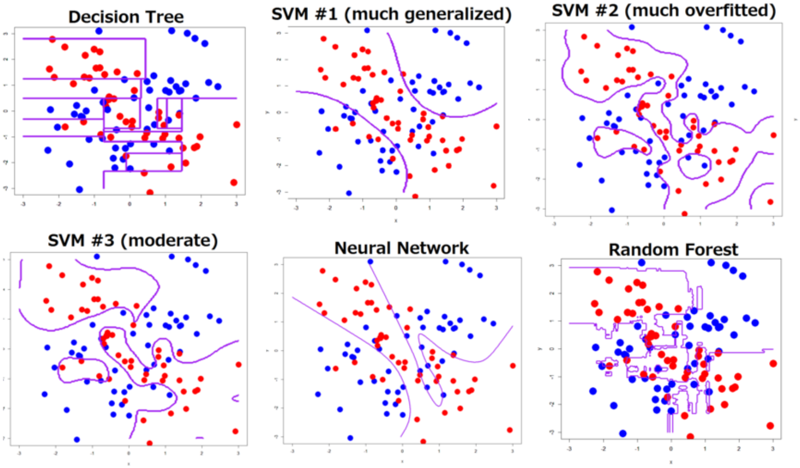
Decision Boundary in Classification

Classification is a process of finding the **decision boundary** that best separates two classes

Decision Boundary in Classification



Decision Boundary in Classification



- SVM = Support Vector Machine

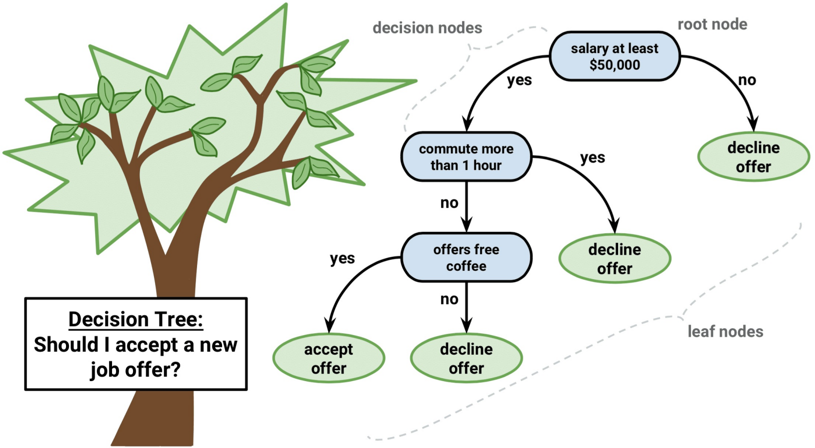
Decision Tree

- Decision Tree for classification is **Classification Tree**
- Decision Tree for Regression is **Regression Tree**

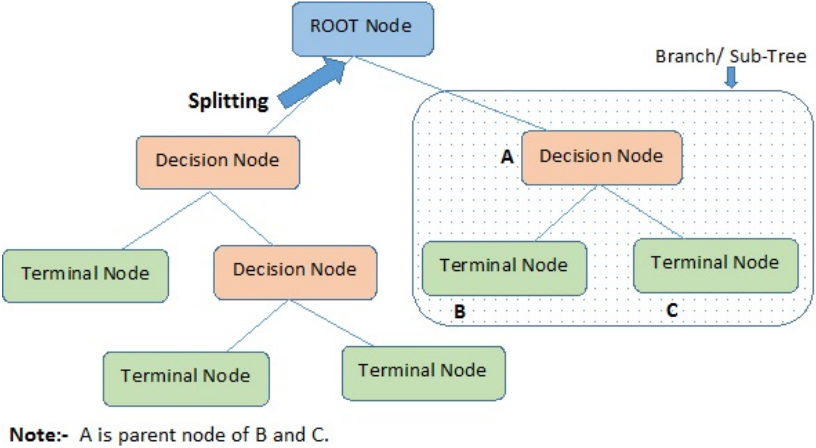
Example of Classification Tree

Link

Example of Classification Tree



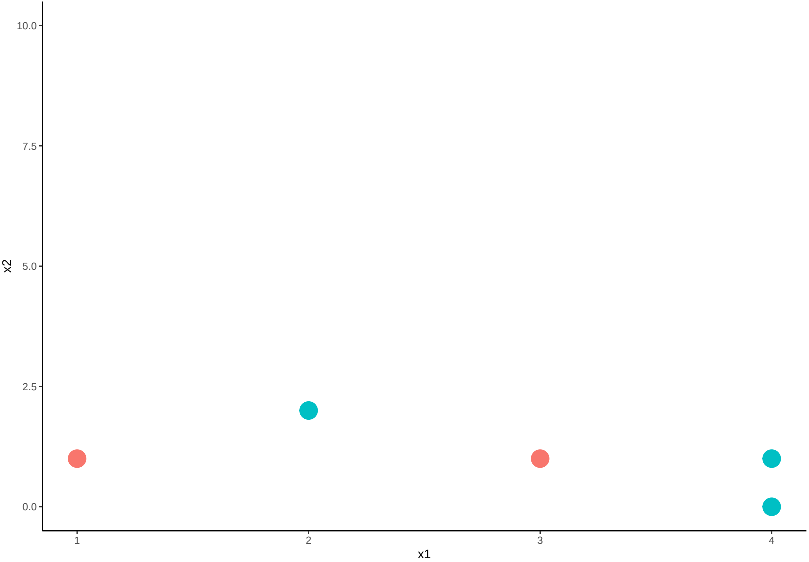
Example of Classification Tree



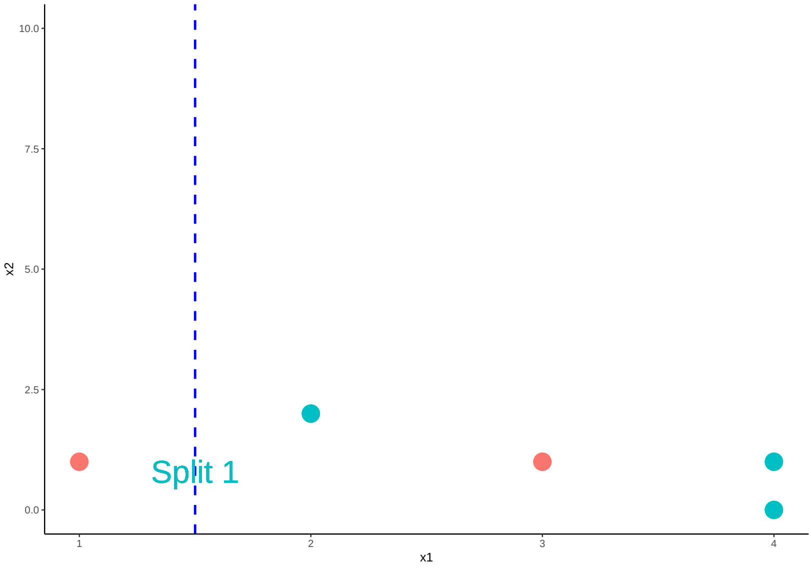
Classification Tree

- In two dimension, classification Tree's decision boundary is a collection of horiontal and vertical line

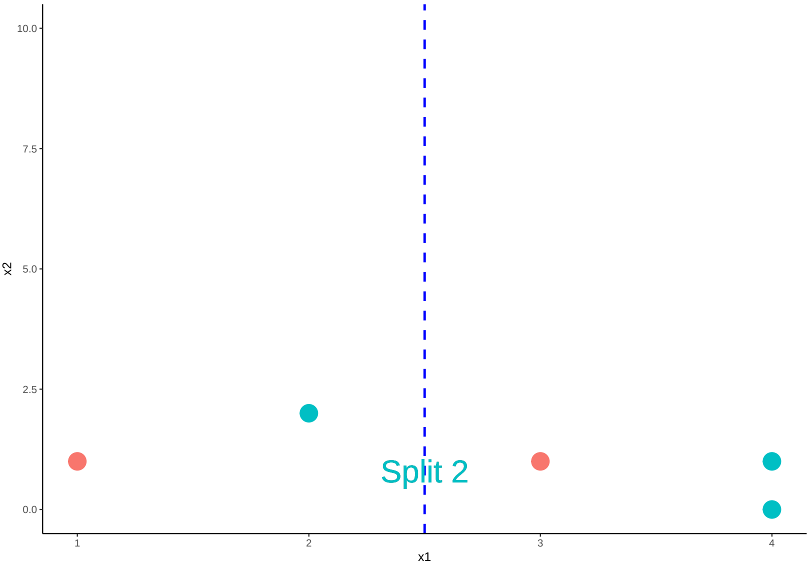
Find a vertical line that best seperate **red** and **green**.



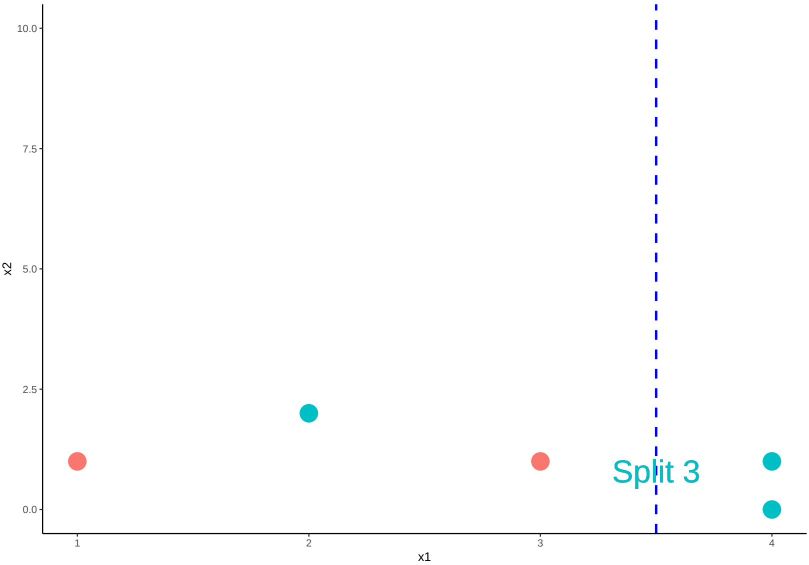
One way to seperate the reds and greens



One way to seperate the reds and greens



One way to seperate the reds and greens



Question

- **Question**: Which is the best split?

Partial Answer

- It looks like Split 1 and 3 are better than Split 2 since it misclassifies less

Partial Answer

- Which is the better split between Split 1 and Split 3?

Partial Answer

- We need to find a way to measure *how good a split is*

Impurity Measure

- The impurity of a node (**a node = a subset of the data or the original data**) measure how uncertain the node is.

Impurity Measure

- For example, node A with 50% reds and 50% greens would be more uncertained than node B with 90% reds and 10% greens. Thus, node A has greater impurity than node B.

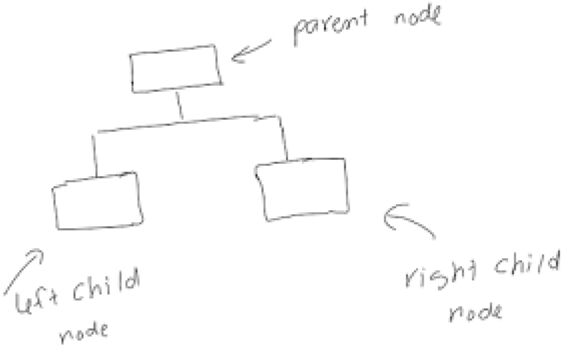
Impurity Measure

- More uncertained = Greater impurity

Children Impurity

- A split resulting smaller children impurity is a **better split**

Children Impurity ($I_{children}$)



$$I_{children} = \frac{N_{left}}{N} I_{left} + \frac{N_{right}}{N} I_{right}$$

- N_{left} and N_{right} are the number of points in the left child node and right child node, respectively.
- $N_{left} + N_{right} = N$

Impurity Measure

- Impurity can be measured by: classification error, Gini Index, and Entropy.

Impurity Measure

- Let p_0 and p_1 be the proportion of class 0 and class 1 in a node.

$$\text{By Classification Error: } I = min\{p_0, p_1\}$$

$$\text{By Gini Index: } I = 1 - p_0^2 - p_1^2$$

$$\text{By Entropy: } I = -p_0 \log_2(p_0) - p_1 \log_2(p_1)$$

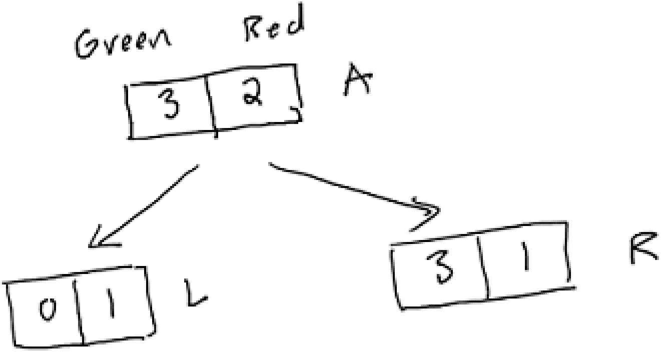
Calculation

- Let's calculate the Children Impurity ($I_{children}$) of the three splits to decide which split is the best

Split 1: Impurity by Classification Error

- Let **green** and **red** be class 0 and class 1, respectively.

For Split 1: $N = 5, N_{left} = 1, N_{right} = 4$



Split 1: Impurity by Classification Error

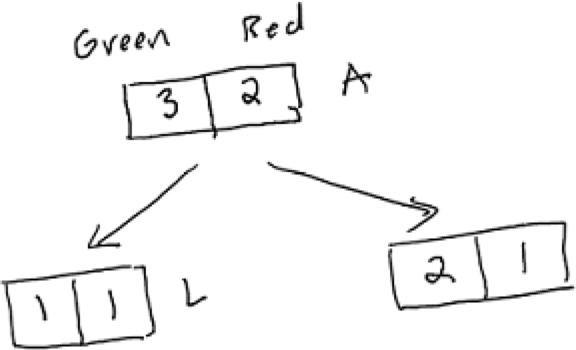
- Node *child left*, L: $p_0 = \frac{0}{1} = 0, p_1 = \frac{1}{1} = 1$. Thus, $I_L = \min(0, 1) = 0$
- Node *child right*, R: $p_0 = \frac{3}{4}, p_1 = \frac{1}{4}$. Thus, $I_R = \min(\frac{3}{4}, \frac{1}{4}) = \frac{1}{4}$
- Children Impurity of Split 1:

$$I_{children} = \frac{N_{left}}{N} I_L + \frac{N_{right}}{N} I_R$$

$$= \frac{1}{5} \cdot 0 + \frac{4}{5} \cdot \frac{1}{4} = 0.2$$

Split 2: Impurity by Classification Error

For Split 2: $N = 5, N_{left} = 2, N_{right} = 3$



Split 2: Impurity by Classification Error

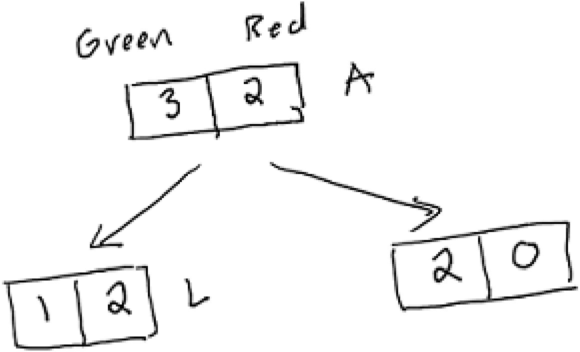
- Node *child left*, L: $p_0 = \frac{1}{2}, p_1 = \frac{1}{2}$. Thus, $I_L = \frac{1}{2}$
- Node *child right*, R: $p_0 = \frac{2}{3}, p_1 = \frac{1}{3}$. Thus, $I_R = \min(\frac{2}{3}, \frac{1}{3}) = \frac{1}{3}$
- Children Impurity of Split 2:

$$I_{children} = \frac{N_{left}}{N} I_L + \frac{N_{right}}{N} I_R$$

$$= \frac{2}{5} \cdot \frac{1}{2} + \frac{3}{5} \cdot \frac{1}{3} = 0.4$$

Split 3: Impurity by Classification Error

For Split 3: $N = 5, N_{left} = 3, N_{right} = 2$



Split 3: Impurity by Classification Error

- Node *child left*, L: $p_0 = \frac{1}{3}, p_1 = \frac{2}{3}$. Thus, $I_A = \min(\frac{1}{3}, \frac{2}{3}) = \frac{1}{3}$
- Node *child right*, R: $p_0 = \frac{2}{2}, p_1 = \frac{0}{2}$. Thus, $I_R = \min(1, 0) = 0$
- Children Impurity of Split 3:

$$I_{children} = \frac{N_{left}}{N} I_L + \frac{N_{right}}{N} I_R$$

$$= \frac{3}{5} \cdot \frac{1}{3} + \frac{2}{5} \cdot 0 = 0.2$$

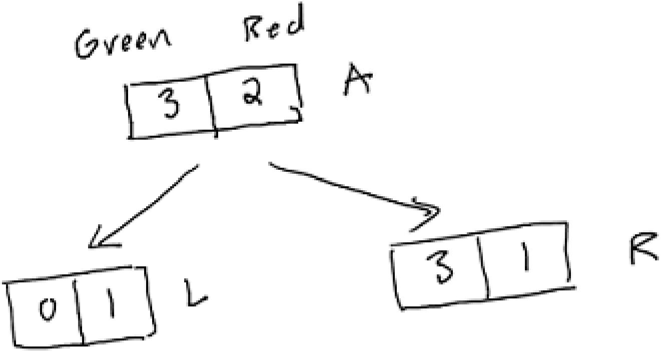
Comparing Impurity by Classification Error

	$I_{children}$
Split 1	0.2
Split 2	0.4
Split 3	0.2

- By classification error, Split 1 and Split 3 are tie as the best because they have the same Children Impurity ($I_{children}$).

Split 1: Impurity by Gini Index

For Split 1: $N = 5, N_{left} = 1, N_{right} = 4$



Split 1: Impurity by Gini Index

- Node *child left*, L: $p_0 = \frac{0}{1} = 0, p_1 = \frac{1}{1} = 1$. Thus,

$$I_L = 1 - 0^2 - 1^2 = 0$$

- Node *child right*, R: $p_0 = \frac{3}{4}, p_1 = \frac{1}{4}$. Thus,

$$I_R = 1 - (\frac{3}{4})^2 - (\frac{1}{4})^2 = 0.375$$

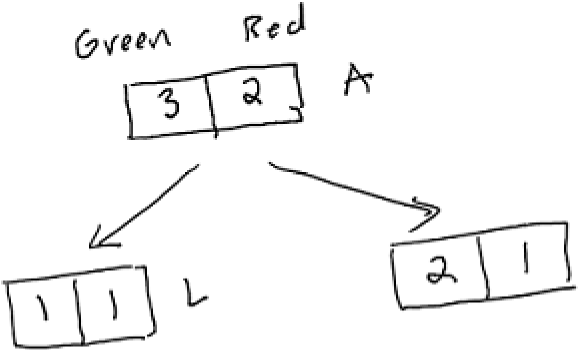
- Children Impurity of Split 1:

$$I_{children} = \frac{N_{left}}{N} I_L + \frac{N_{right}}{N} I_R$$

$$= \frac{1}{5} \cdot 0 + \frac{4}{5} \cdot 0.375 = 0.3$$

Split 2: Impurity by Gini Index

For Split 2: $N = 5, N_{left} = 2, N_{right} = 3$



Split 2: Impurity by Gini Index

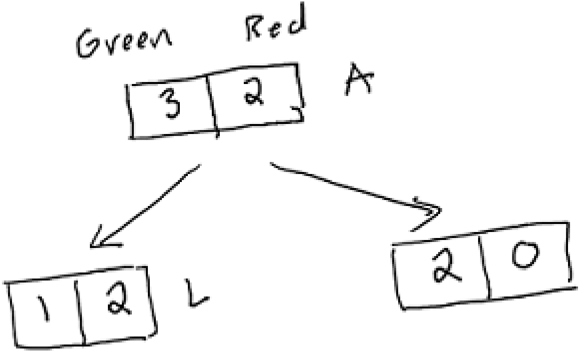
- Node *child left*, L: $p_0 = \frac{1}{2}, p_1 = \frac{1}{2}$. Thus, $I_L = 1 - (\frac{1}{2})^2 - (\frac{1}{2})^2 = 0.5$
- Node *child right*, R: $p_0 = \frac{2}{3}, p_1 = \frac{1}{3}$. Thus, $I_R = 1 - (\frac{2}{3})^2 - (\frac{1}{3})^2 = 0.44$
- Children Impurity of Split 2:

$$I_{children} = \frac{N_{left}}{N} I_L + \frac{N_{right}}{N} I_R$$

$$= \frac{2}{5} \cdot \frac{1}{2} + \frac{3}{5} \cdot 0.44 = 0.464$$

Split 3: Impurity by Gini Index

For Split 3: $N = 5, N_{left} = 3, N_{right} = 2$



Split 3: Impurity by Gini Index

- Node *child left*, L: $p_0 = \frac{1}{3}, p_1 = \frac{2}{3}$. Thus, $I_A = 1 - (\frac{1}{3})^2 - (\frac{2}{3})^2 = 0.44$
- Node *child right*, R: $p_0 = \frac{2}{2}, p_1 = \frac{0}{2}$. Thus, $I_R = 1 - 0^2 - 1^2 = 0$
- Children Impurity of Split 3:

$$I_{children} = \frac{N_{left}}{N} I_L + \frac{N_{right}}{N} I_R$$

$$= \frac{3}{5} \cdot 0.44 + \frac{2}{5} \cdot 0 = 0.184$$

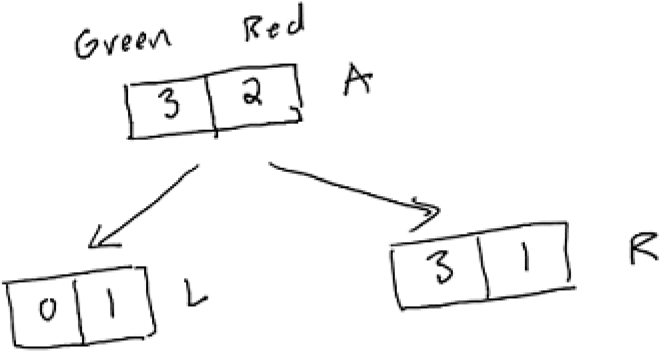
Comparing Impurity by Gini Index

	$I_{children}$
Split 1	0.3
Split 2	0.464
Split 3	0.184

- By Gini Index, Split 3 is the best because it has the smallest Children Impurity ($I_{children}$).

Split 1: Impurity by Entropy

For Split 1: $N = 5, N_{left} = 1, N_{right} = 4$



Split 1: Impurity by Entropy

- Node *child left*, L: $p_0 = \frac{0}{1} = 0, p_1 = \frac{1}{1} = 1$. Thus, $I_L = 0$
- Node *child right*, R: $p_0 = \frac{3}{4}, p_1 = \frac{1}{4}$. Thus,

$$I_R = -log_2(\frac{3}{4}) - log_2(\frac{1}{4}) = 0.811$$

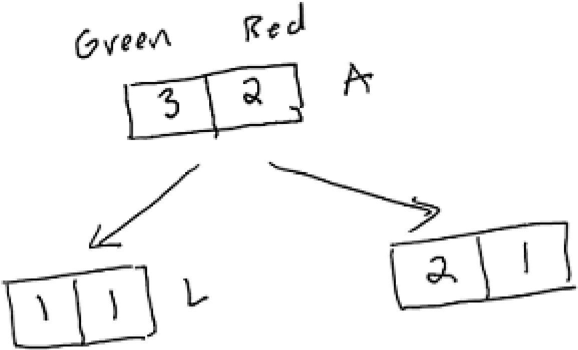
- Children Impurity of Split 1:

$$I_{children} = \frac{N_{left}}{N} I_L + \frac{N_{right}}{N} I_R$$

$$= \frac{1}{5} \cdot 0 + \frac{4}{5} \cdot 0.811 = 0.649$$

Split 2: Impurity by Entropy

For Split 2: $N = 5, N_{left} = 2, N_{right} = 3$



Split 2: Impurity by Entropy

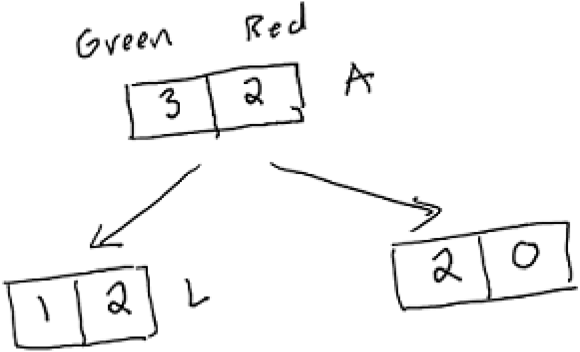
- Node *child left,* L: $p_0 = \frac{1}{2}, p_1 = \frac{1}{2}$. Thus, $I_L = -log_1(\frac{1}{2}) - log_2(\frac{1}{2}) = 1$
- Node *child right,* R: $p_0 = \frac{2}{3}, p_1 = \frac{1}{3}$. Thus, $I_R = -log_2(\frac{2}{3}) - log_2(\frac{1}{3}) = 0.918$
- Children Impurity of Split 2:

$$I_{children} = \frac{N_{left}}{N} I_L + \frac{N_{right}}{N} I_R$$

$$= \frac{2}{5} \cdot 1 + \frac{3}{5} \cdot 0.918 = 0.951$$

Split 3: Impurity by Entropy

For Split 3: $N = 5, N_{left} = 3, N_{right} = 2$



Split 3: Impurity by Entropy

- Node *child left*, L: $p_0 = \frac{1}{3}, p_1 = \frac{2}{3}$. Thus, $I_A = -log_2(\frac{1}{3}) - log_2(\frac{2}{3}) = 0.918$
- Node *child right*, R: $p_0 = \frac{2}{2}, p_1 = \frac{0}{2}$. Thus, $I_R = 0$
- Children Impurity of Split 3:

$$I_{children} = \frac{N_{left}}{N} I_L + \frac{N_{right}}{N} I_R$$

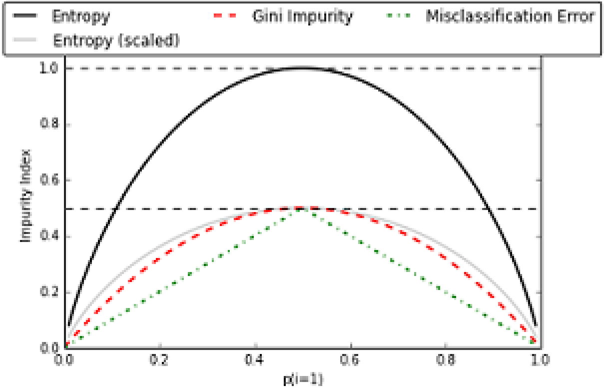
$$= \frac{3}{5} \cdot 0.918 + \frac{2}{5} \cdot 0 = 0.551$$

Comparing Impurity by Entropy

	$I_{children}$
Split 1	0.649
Split 2	0.951
Split 3	0.551

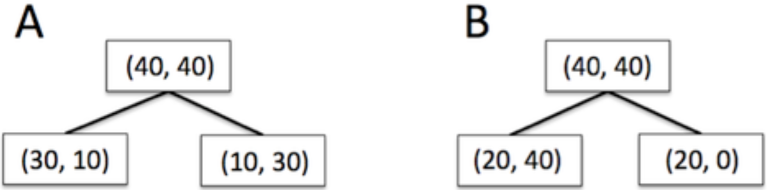
- By Gini Index, Split 3 is the best because it has the smallest Children Impurity ($I_{children}$).

Comparing Impurity Measures



- Relation between impurity and the class probabilities. All impurity measures are maximized at $p_1 = 1/2$ and minimized at $p_1 = 0$ and $p_1 = 1$.

Another Example



- Which split is better?

Decide the best split using Chi-Square test of Independence

- Besides Children Impurity, one can use the Chi-square, χ^2, test of independence to decide the best split.

Review of Chi-Square test of Independence

- Let X and Y be two categorical variables.
- We want to test if X and Y are independent/associated
  - H_0: X and Y are independent
  - H_α : X and Y are dependent
- Test statistic:

$$\sum \frac{(e_i - o_i)^2}{e_i} \sim \chi^2 \text{ distribution with degree of freedom} (n-1)(m-1)$$

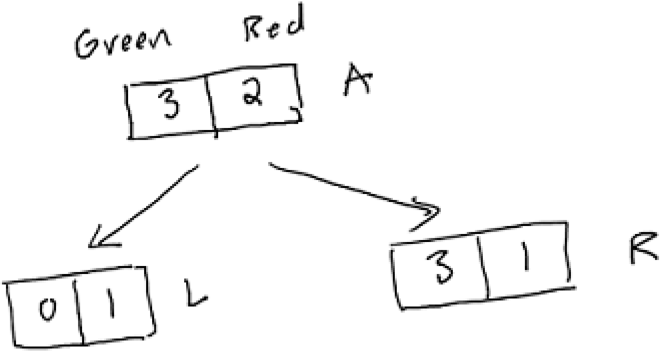
Review of Chi-Square test of Independence

- In our context, the greater the χ^2 value, the smaller the $p - value$
- The smaller the $p - value$, the more dependent the two variables are. Thus the better the split is.
- Therefore, we look for the split with the **greatest χ^2 value.**

Applying to Our Example

- We will calculate the χ^2 values of the three splits.
- The best split is the split with the greatest χ^2 value.

Split 1



	Greens	Reds	Total
Left Branch	0	1	1
Right Branch	3	1	4
Total	3	2	

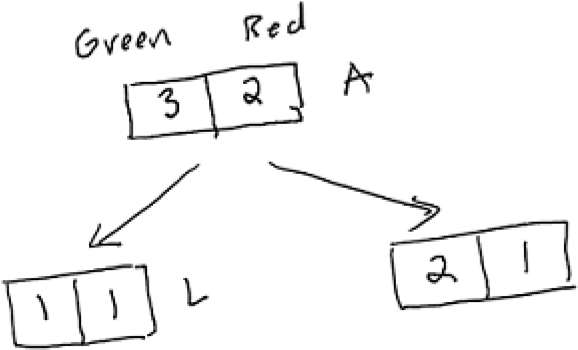
Split 1

$$\chi^2 = \frac{(e_1 - o_1)^2}{e_1} + \frac{(e_2 - o_2)^2}{e_2} + \frac{(e_3 - o_3)^2}{e_3} + \frac{(e_4 - o_4)^2}{e_4}$$

- $i = 1$ (Cell 1): $e_1 = \frac{1 \cdot 3}{5}$, $o_1 = 0$
- $i = 2$ (Cell 2): $e_2 = \frac{1 \cdot 2}{5}$, $o_2 = 1$
- $i = 3$ (Cell 3): $e_3 = \frac{3 \cdot 4}{5}$, $o_3 = 3$
- $i = 4$ (Cell 4): $e_4 = \frac{2 \cdot 4}{5}$, $o_4 = 1$
- Plug in, we have:

$$\chi^2 = 1.875$$

Split 2



	Greens	Reds	Total
Left Branch	1 (Cell 1)	1 (Cell 2)	2
Right Branch	2 (Cell 3)	1 (Cell 4)	3
Total	3	2	

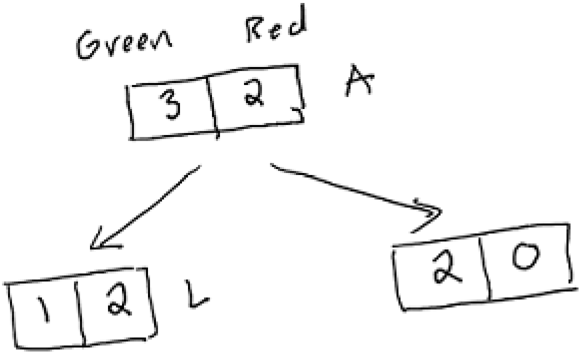
Split 2

$$\chi^2 = \frac{(e_1 - o_1)^2}{e_1} + \frac{(e_2 - o_2)^2}{e_2} + \frac{(e_3 - o_3)^2}{e_3} + \frac{(e_4 - o_4)^2}{e_4}$$

- $i = 1$ (Cell 1): $e_1 = \frac{2 \cdot 3}{5}$, $o_1 = 1$
- $i = 2$ (Cell 2): $e_2 = \frac{2 \cdot 2}{5}$, $o_2 = 1$
- $i = 3$ (Cell 3): $e_3 = \frac{3 \cdot 3}{5}$, $o_3 = 2$
- $i = 4$ (Cell 4): $e_4 = \frac{3 \cdot 2}{5}$, $o_4 = 1$
- Plug in, we have:

$$\chi^2 = 0.139$$

Split 3



	Greens	Reds	Total
Left Branch	1 (Cell 1)	2 (Cell 2)	3
Right Branch	2 (Cell 3)	0 (Cell 4)	2
Total	3	2	

Split 3

$$\chi^2 = \frac{(e_1 - o_1)^2}{e_1} + \frac{(e_2 - o_2)^2}{e_2} + \frac{(e_3 - o_3)^2}{e_3} + \frac{(e_4 - o_4)^2}{e_4}$$

- (Cell 1): $e_1 = \frac{2 \cdot 3}{5}$, $o_1 = 1$
- (Cell 2): $e_2 = \frac{2 \cdot 2}{5}$, $o_2 = 2$
- (Cell 3): $e_3 = \frac{3 \cdot 3}{5}$, $o_3 = 2$
- (Cell 4): $e_4 = \frac{3 \cdot 2}{5}$, $o_4 = 0$
- Plug in, we have:

$$\chi^2 = 2.222$$

Comparing the three splits

	χ^2
Split 1	1.875
Split 2	0.139
Split 3	2.222

- Split 3 is the best because it has the greatest χ^2!

Logworth

- The quality of the split can be measured by **Logworth**
- Formula:

$$logworth = -log(p_{value})$$

- The greater the logworth, the better the split

Logworth

	χ^2	p-value	logworth
Split 1	1.875	0.114	0.943
Split 2	0.139	0.998	0.0008
Split 3	2.222	0.088	1.055

- Greatest χ^2 = Lowest $p - value$ = Greatest logworth = Best Split
- Split 3 is the best split!

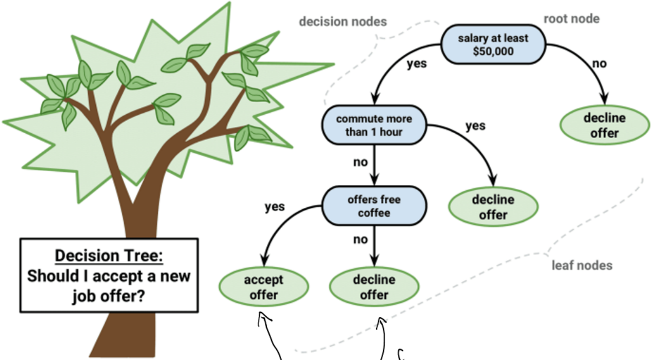
What happens after the first split?

- After the first split, the data are divided into to subsets.
- The splitting process is repeated for each subset.
- The process ends when a stopping criteria is satisfied

Stopping Criteria

- Minimum Leaf Size: The minimum of observations in the leaves
- Maximum Number of Leaves
- Maximum Depth
- Others

Stopping Criteria



Depth = 3

Leaf

Leaf

Decision Tree Algorithm - How to grow a tree

- Step 1: Calculate the Children Impurity or $p - value$ of all possible splits at all variables
- Step 2: Select the split that give the minimum Children Impurity or lowest $p - value$ to split the data into two subdata D_1 and D_2
- Repeat *Step 1* and *Step 2* to both D_1 and D_2.
- Until a stopping criteria is satisfied

Complexity of Decision Tree

- A complexity of a tree can be measured by the number of leaves the tree has
- The more leaves a tree has, the more complex the tree is.
- A complex tree may be **overfitted**, i.e. having low training error but high testing error.

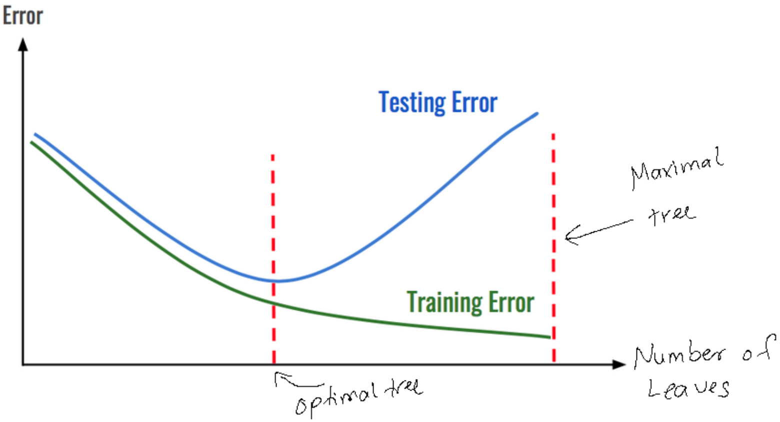
Prunning a tree

- For any given data, one can construct a tree that achives 0 misclassification on training data
- After growing the tree one needs to prune it to avoid overfittted

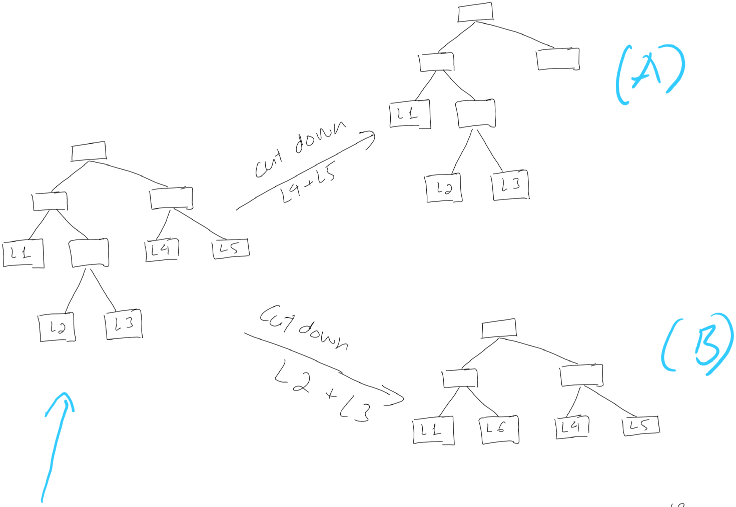
Prunning a tree

- The tree with maximum number of leaves is called the **maximal tree** (still satisfied the stopping rule)
- From the **maximal tree**, leaves are cut down, one by one, to obatined all possible subtrees
- The subtree with lowest error on validation data, is the **optimal tree**

Maximal vs Optimal Tree



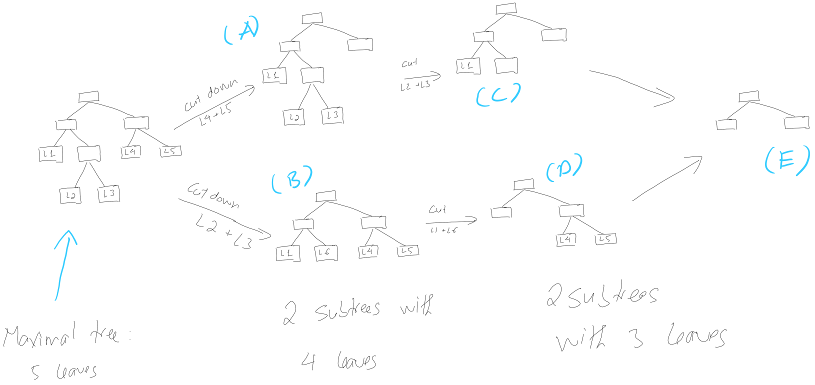
Example of Tree Prunning



Maximal tree:
5 leaves

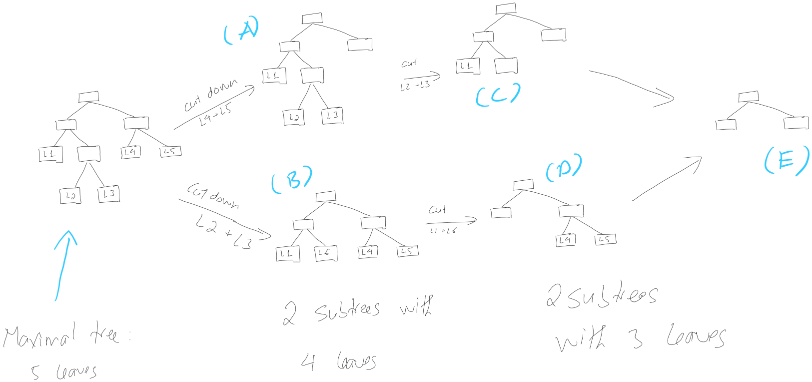
2 subtrees with
4 leaves

Example of Tree Prunning



- All the subtrees A, B, C, D, and E will be validated with the validation data to find the **optimal tree**
- The **optimal tree** could be the **maximal tree**!

Question



- What if both B and C give the lowest error on the validation data? Which tree should be selected as the final model?