Classification Trees

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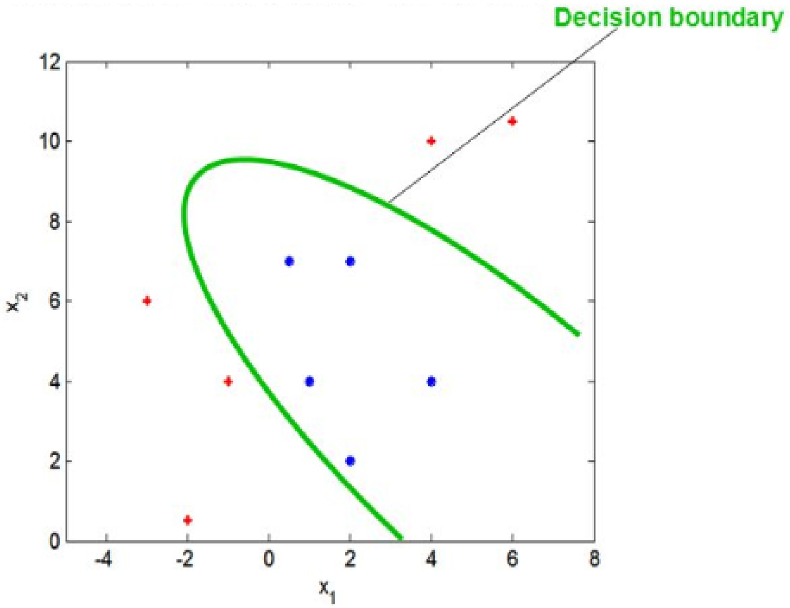
Reading Materials

- Max Kuhn. Chapter 14. Section 14.1

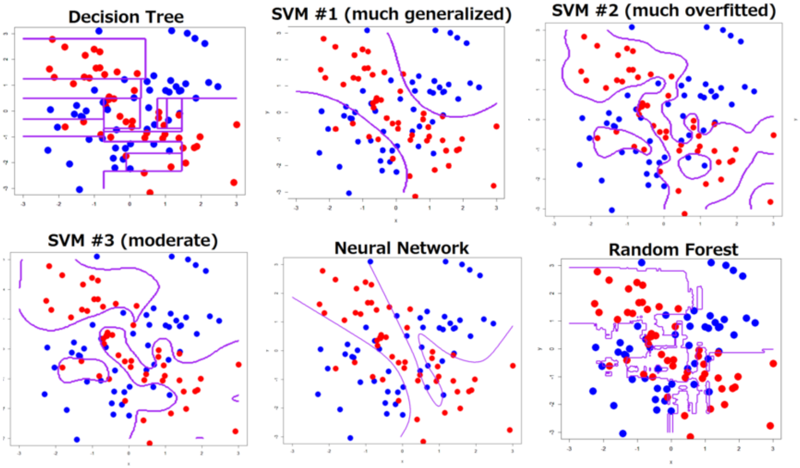
Decision Boundary in Classification

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

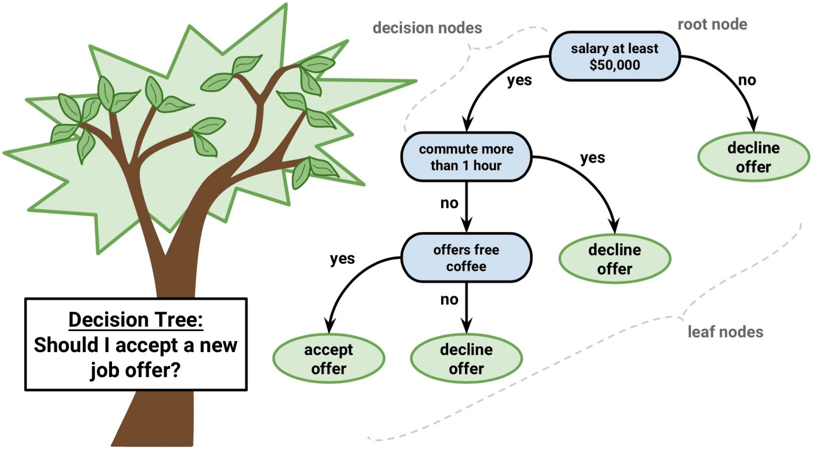
Decision Tree

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

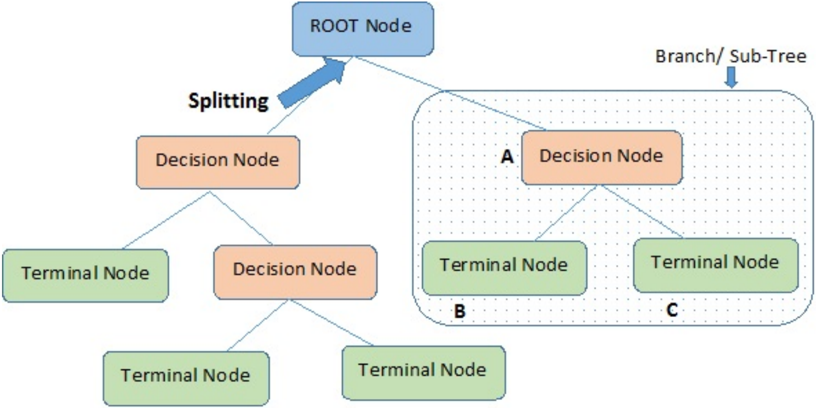
Example of Classification Tree

Link

Example of Classification Tree



Example of Classification Tree

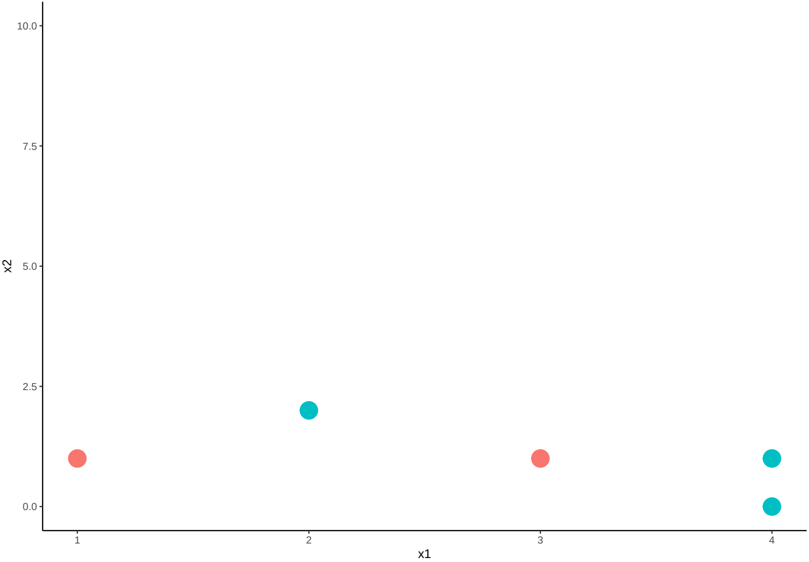


Note:- A is parent node of B and C.

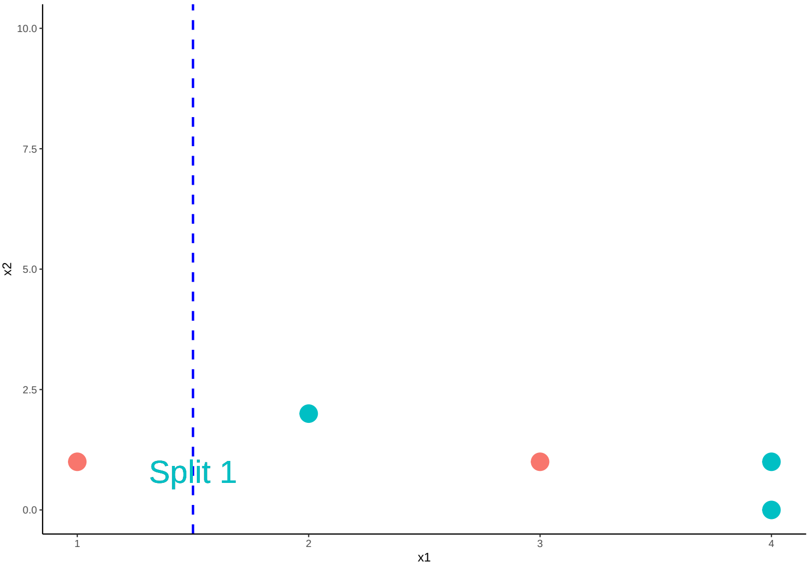
Classification Tree

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

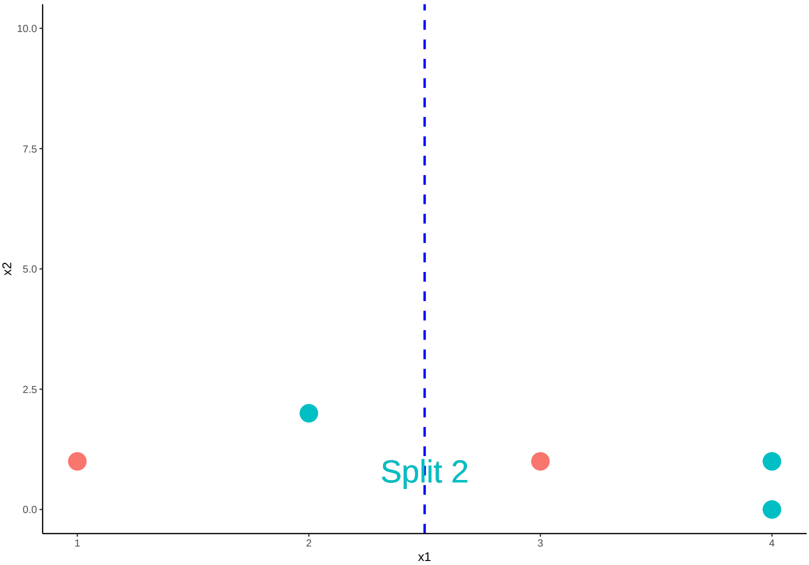
Find a vertical line that best seperate **red** and **green**.



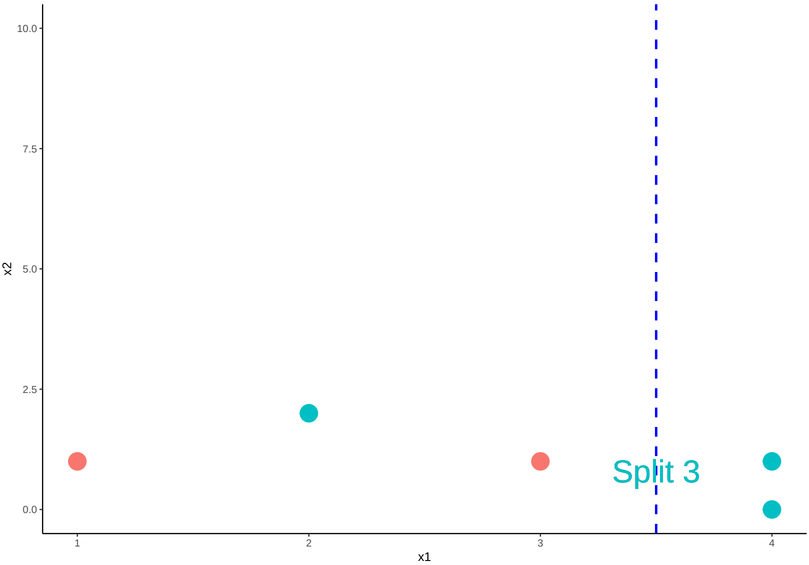
One way to seperate the reds and greens



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.

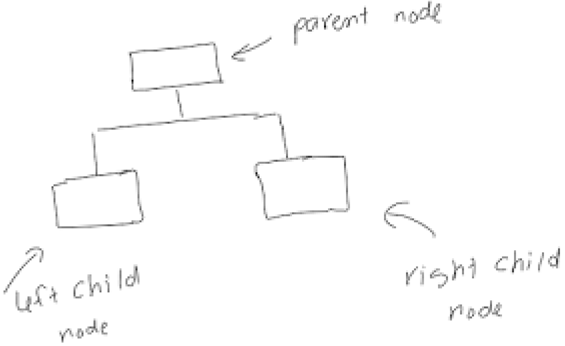
Impurity Measure

- 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.

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

By Gini Index: $I = 1 - p_0^2 - p_1^2$

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

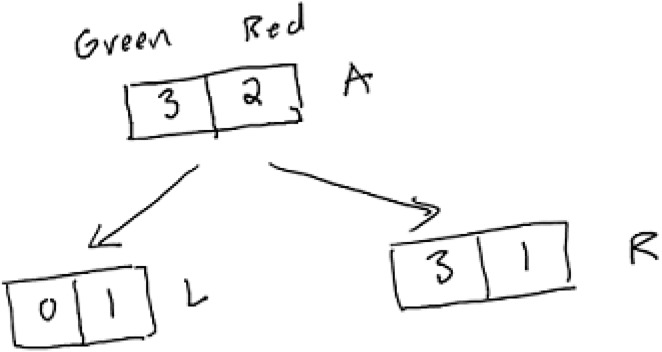
Calculation

- 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

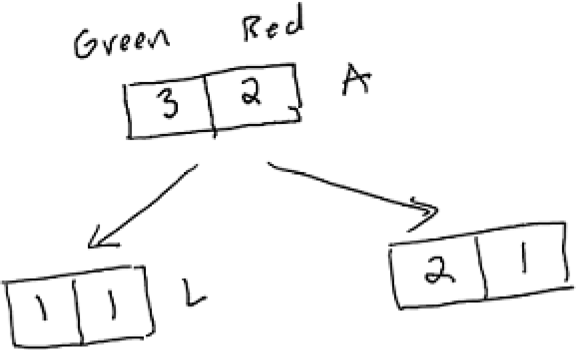
- Node *child left,* L: $p_0 = \frac{0}{1} = 0, p_1 = \frac{1}{1} = 1$. Thus, $I_L = \min(0, 1) = 0$
- Node *child right,* R: $p_0 = \frac{3}{4}, p_1 = \frac{1}{4}$. Thus, $I_R = \min(\frac{3}{4}, \frac{1}{4}) = \frac{1}{4}$
- Children Impurity of Split 1:

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

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

Split 2: Impurity by Classification Error

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



Split 2: Impurity by Classification Error

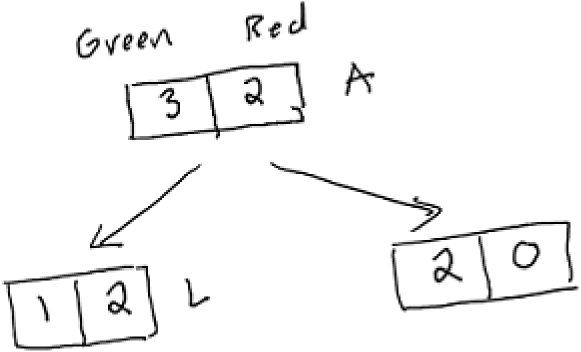
- Node *child left,* L: $p_0 = \frac{1}{2}, p_1 = \frac{1}{2}$. Thus, $I_L = \frac{1}{2}$
- Node *child right,* R: $p_0 = \frac{2}{3}, p_1 = \frac{1}{3}$. Thus, $I_R = \min(\frac{2}{3}, \frac{1}{3}) = \frac{1}{3}$
- Children Impurity of Split 2:

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

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

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:

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

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

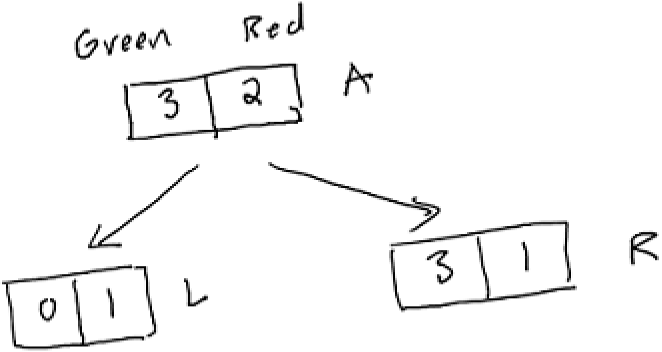
Comparing Impurity by Classification Error

	$I_{children}$
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,

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

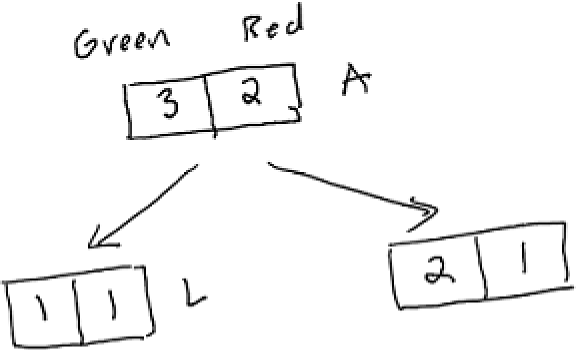
- Children Impurity of Split 1:

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

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

Split 2: Impurity by Gini Index

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



Split 2: Impurity by Gini Index

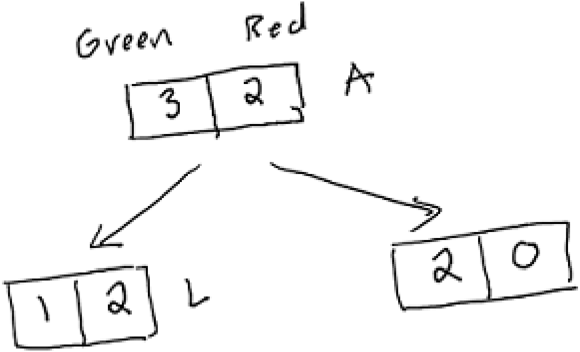
- Node *child left,* L: $p_0 = \frac{1}{2}, p_1 = \frac{1}{2}$. Thus, $I_L = 1 - (\frac{1}{2})^2 - (\frac{1}{2})^2 = 0.5$
- Node *child right,* R: $p_0 = \frac{2}{3}, p_1 = \frac{1}{3}$. Thus, $I_R = 1 - (\frac{2}{3})^2 - (\frac{1}{3})^2 = 0.44$
- Children Impurity of Split 2:

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

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

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:

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

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

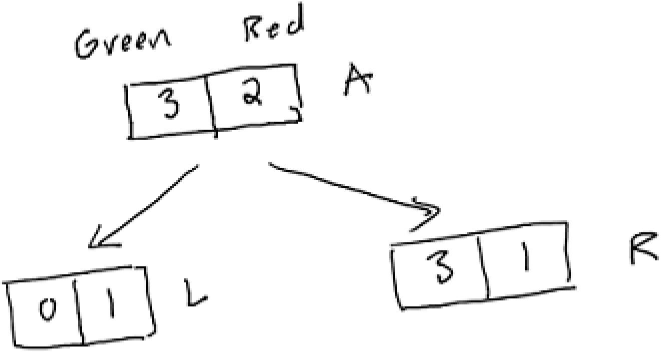
Comparing Impurity by Gini Index

	$I_{children}$
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,

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

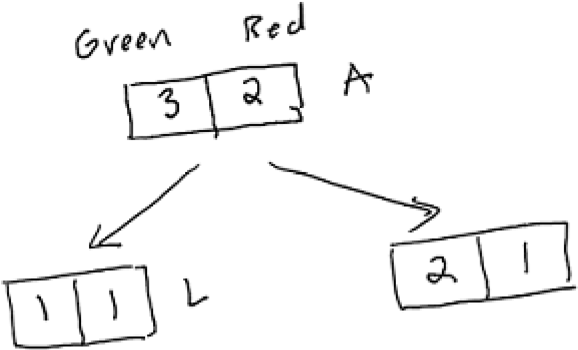
- Children Impurity of Split 1:

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

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

Split 2: Impurity by Entropy

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



Split 2: Impurity by Entropy

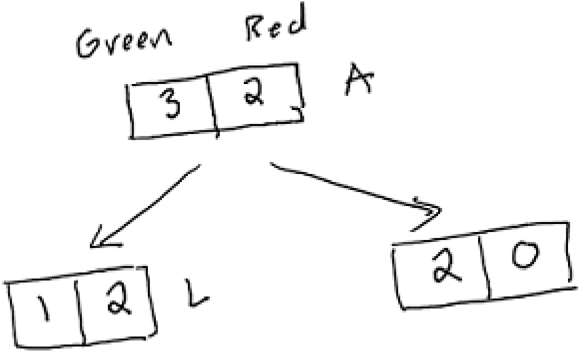
- Node *child left*, L: $p_0 = \frac{1}{2}, p_1 = \frac{1}{2}$. Thus, $I_L = -log_1(\frac{1}{2}) - log_2(\frac{1}{2}) = 1$
- Node *child right*, R: $p_0 = \frac{2}{3}, p_1 = \frac{1}{3}$. Thus, $I_R = -log_2(\frac{2}{3}) - log_2(\frac{1}{3}) = 0.918$
- Children Impurity of Split 2:

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

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

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:

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

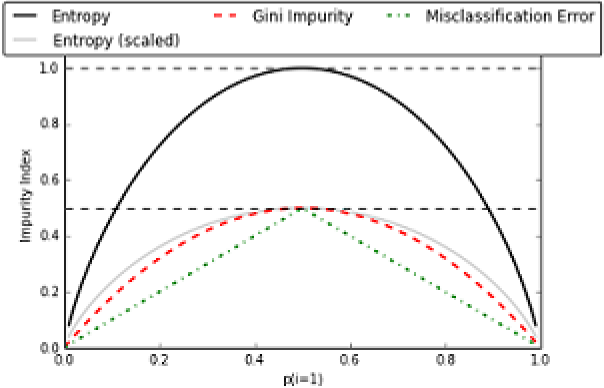
$$= \frac{3}{5} \cdot 0.918 + \frac{2}{5} \cdot 0 = 0.551$$

Comparing Impurity by Entropy

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

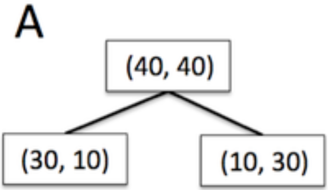
- By Gini Index, Split 3 is the best because it has the smallest Children Impurity ($I_{children}$).

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:

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

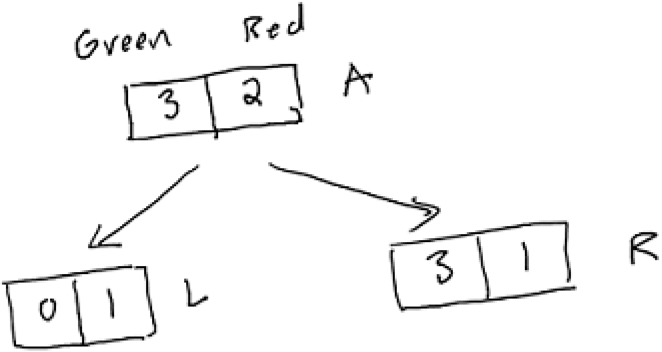
Review of Chi-Square test of Independence

- 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	

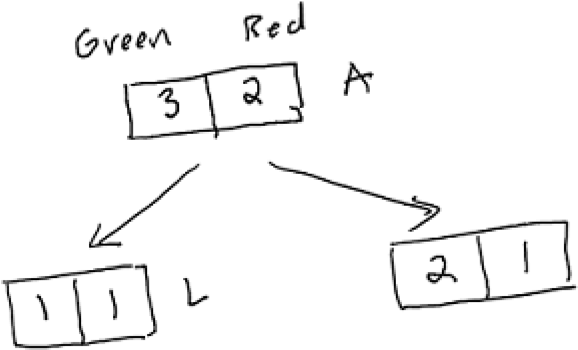
Split 1

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

- $i = 1$ (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



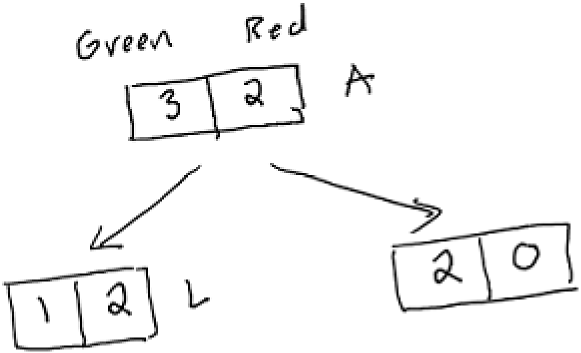
	Greens	Reds	Total
Left Branch	1 (Cell 1)	1 (Cell 2)	2
Right Branch	2 (Cell 3)	1 (Cell 4)	3
Total	3	2	

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!

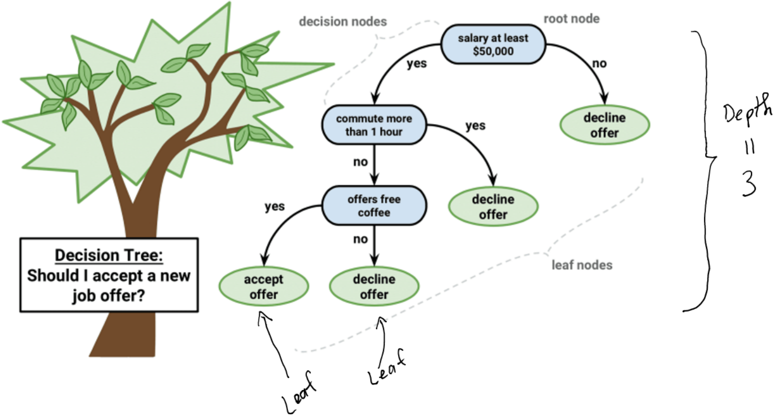
What happens after the first split?

- 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



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.

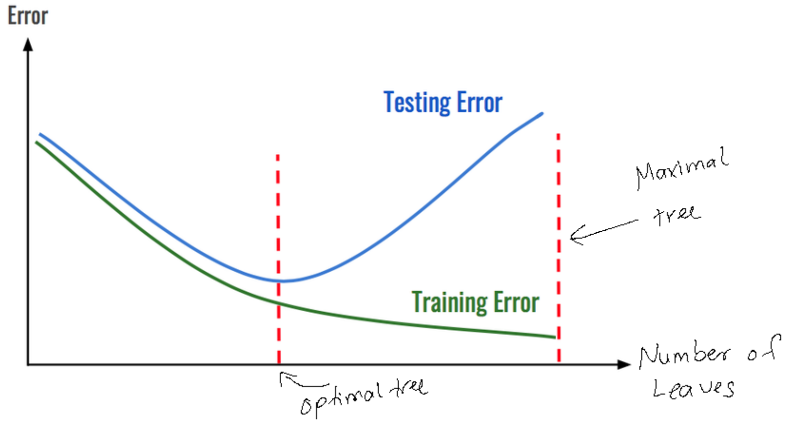
Prunning a tree

- 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

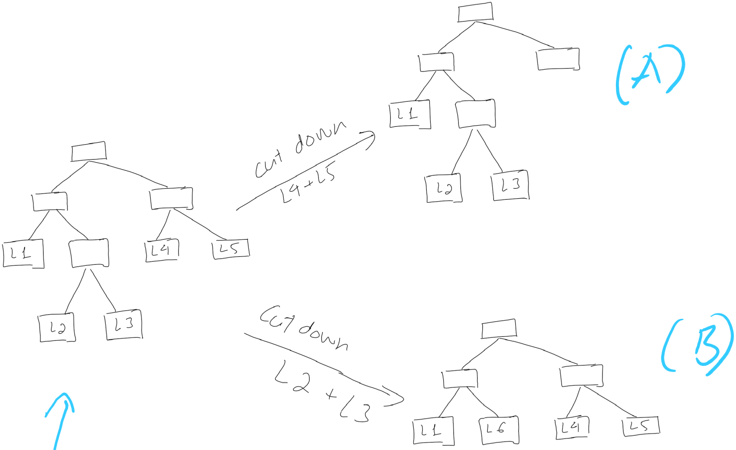
Prunning a tree

- 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



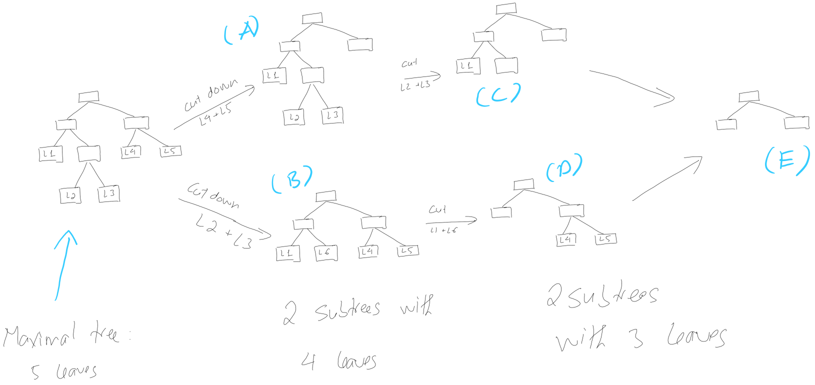
Example of Tree Prunning



Maximal tree: 5 leaves

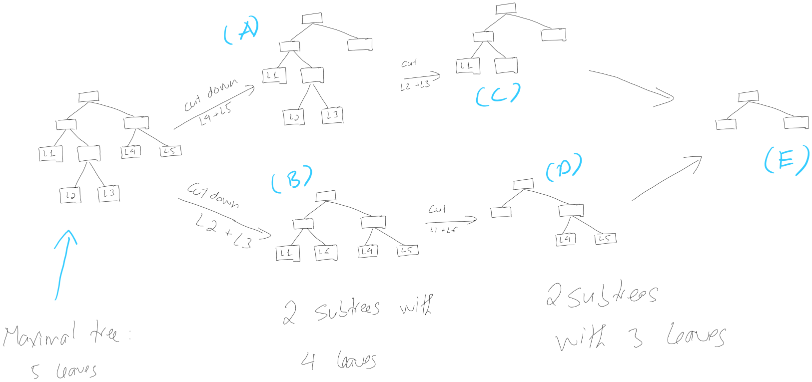
2 subtrees with 4 leaves

Example of Tree Prunning



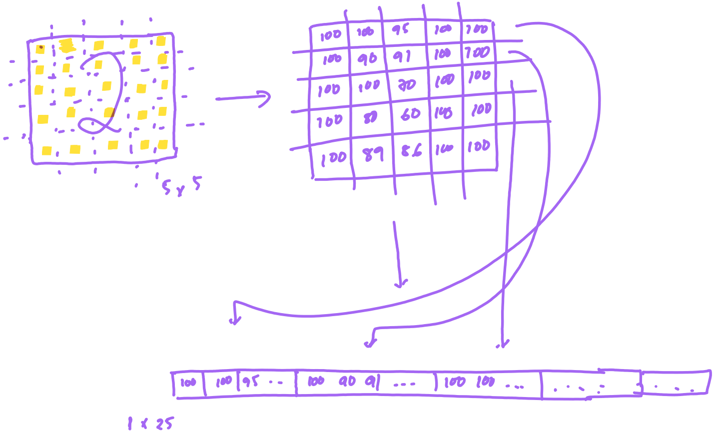
- All the subtrees A, B, C, D, and E will be validated with the validation data to find the **optimal tree**
- The **optimal tree** could be the **maximal tree**!

Question



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

Goal:


5 x 5
100 100 95 100 100
100 90 91 100 100
100 100 70 100 100
100 80 60 100 100
100 89 86 100 100
100 100 95 .. 100 90 91 ... 100 100 ...
1 x 25