Decision Tree

Gini Index

Gini Index is a metric to measure how often a randomly chosen element would be incorrectly identified. It means an attribute with lower gini index should be preferred.

Overfitting

Overfitting is a practical problem while building a decision tree model. The model is having an issue of overfitting is considered when the algorithm continues to go deeper and deeper in the to reduce the training set error but results with an increased test set error i.e, Accuracy of prediction for our model goes down. It generally happens when it builds many branches due to outliers and irregularities in data.

Two approaches which we can use to avoid overfitting are:

- Pre-Pruning
- Post-Pruning

Pre-Pruning

In pre-pruning, it stops the tree construction bit early. It is preferred not to split a node if its goodness measure is below a threshold value. But it's difficult to choose an appropriate stopping point.

Post-Pruning

In post-pruning first, it goes deeper and deeper in the tree to build a complete tree. If the tree shows the overfitting problem then pruning is done as a post-pruning step. We use a cross-validation data to check the effect of our pruning. Using cross-validation data, it tests whether expanding a node will make an improvement or not.

If it shows an improvement, then we can continue by expanding that node. But if it shows a reduction in accuracy then it should not be expanded i.e, the node should be converted to a leaf node.

Decision Tree Algorithm Advantages and Disadvantages

Advantages:

1. Decision Trees are easy to explain. It results in a set of rules.
2. It follows the same approach as humans generally follow while making decisions.
3. Interpretation of a complex Decision Tree model can be simplified by its visualizations. Even a naive person can understand logic.
4. The Number of hyper-parameters to be tuned is almost null.

5. It is very interpretable, especially if we need to communicate our findings to a non-technical audience
6. It deals well with noisy or incomplete data
7. It can be used for both regression and classification problems
8.

Disadvantages:

1. There is a high probability of overfitting in Decision Tree.
2. Generally, it gives low prediction accuracy for a dataset as compared to other machine learning algorithms.
3. Information gain in a decision tree with categorical variables gives a biased response for attributes with greater no. of categories.
4. Calculations can become complex when there are many class labels.
5. It can be unstable, meaning that a small change in your data can translate into a big change in your model
6. It tends to overfit, which means low bias but high variance: i.e., might not perform as well on unseen data even if the score on the train data is great

$$\text{Gini} = 1 - \sum_{i=1}^{classes} p(i \mid t)^2$$

Definition of Gini

To calculate Gini, we consider the probability of finding each class after a node, we sum the square of those values and we subtract this amount from 1. For this reason, when a subset is pure (i.e. there is only one class in it), Gini will be 0, because the probability of finding that class is 1 indeed! And in that case, we say we have reached a *leaf*, because there is no need to split anymore as we achieved our goal. But if we look at the picture above, after the root node in

node, we can define the **Information Gain:**

$$\Delta = G(\text{parent}) - \sum_{\text{children}} \frac{N_j}{N} G(\text{child}_j)$$

this is defined as the difference between the Gini of the parent, and the weighted average of the children's Gini. If we refer to the

1. Information Gain

when we use a node in a decision tree to partition the training instances into smaller subsets the entropy changes. Information gain is a measure of this change in entropy. The information gain formula used by ID3 algorithm treats all of the variables the same regardless of their distribution and their importance.

Entropy

Entropy is the measure of uncertainty of a random variable, it characterizes the impurity of an arbitrary collection of examples. The higher the entropy more the information content.

2. Gini Index

- Gini Index is a metric to measure how often a randomly chosen element would be incorrectly identified.
- It means an attribute with lower Gini index should be preferred.
- In Gini Index, we have to choose some random values to categorize each attribute

$$GiniIndex = 1 - \sum_j p_j^2$$

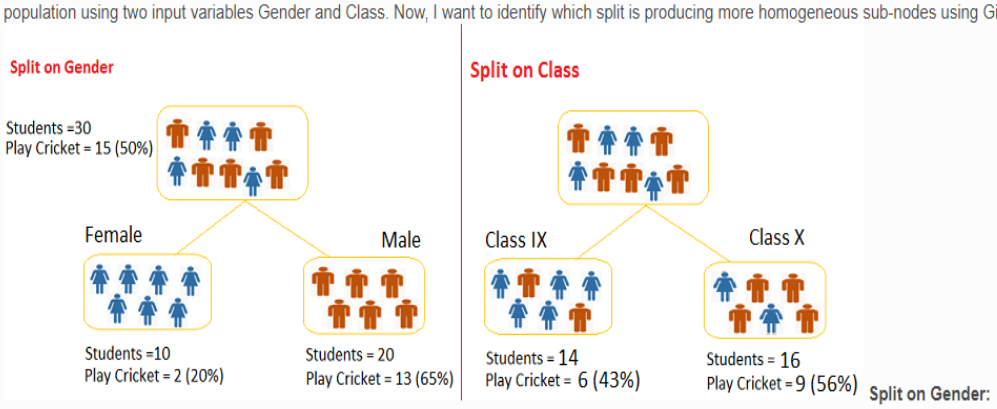
Gini index says,

- If we select two items from a population at random then they must be of same class and probability for this is 1 if population is pure.
- It works with categorical target variable “Success” or “Failure”.
- It performs only Binary splits
- Higher the value of Gini higher the homogeneity.
- CART (Classification and Regression Tree) uses Gini method to create binary splits.

Steps to Calculate Gini for a split

- Calculate Gini for sub-nodes, using formula sum of square of probability for success and failure (p^2+q^2).
- Calculate Gini for split using weighted Gini score of each node of that split

Example: – Referring to example used above, where we want to segregate the students based on target variable (playing cricket or not). In the snapshot below, we split the population using two input variables Gender and Class. Now, I want to identify which split is producing more homogeneous sub-nodes using Gini index.



Split on Gender:

- Calculate, Gini for sub-node Female = (0.2)*(0.2)+(0.8)*(0.8)=0.68
- Gini for sub-node Male = (0.65)*(0.65)+(0.35)*(0.35)=0.55
- Calculate weighted Gini for Split Gender = (10/30)*0.68+(20/30)*0.55 = **0.59**

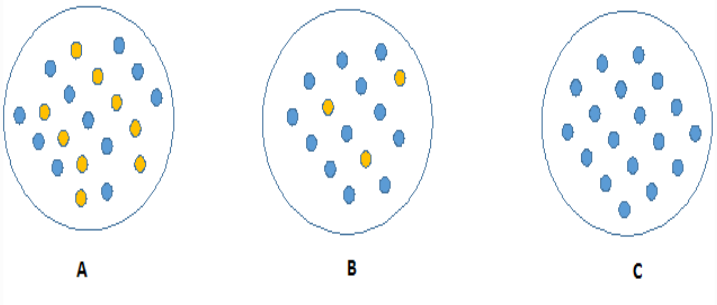
Similar for Split on Class:

- Gini for sub-node Class IX = (0.43)*(0.43)+(0.57)*(0.57)=0.51
- Gini for sub-node Class X = (0.56)*(0.56)+(0.44)*(0.44)=0.51
- Calculate weighted Gini for Split Class = (14/30)*0.51+(16/30)*0.51 = **0.51**

Above, you can see that Gini score for *Split on Gender* is higher than *Split on Class*, hence, the node split will take place on Gender.

Information Gain:

Look at the image below and think which node can be described easily. I am sure, your answer is C because it requires less information as all values are similar. On the other hand, B requires more information to describe it and A requires the maximum information. In other words, we can say that C is a Pure node, B is less Impure and A is more impure.



Now, we can build a conclusion that less impure node requires less information to describe it. And, more impure node requires more information. Information theory is a measure to define this degree of disorganization in a system known as Entropy. If the sample is completely homogeneous, then the entropy is zero and if the sample is an equally divided (50% – 50%), it has entropy of one.

Entropy can be calculated using formula:- $\text{Entropy} = -p \log_2 p - q \log_2 q$

Here p and q is probability of success and failure respectively in that node. Entropy is also used with categorical target variable. It chooses the split which has lowest entropy compared to parent node and other splits. The lesser the entropy, the better it is.

Steps to calculate entropy for a split:

- Calculate entropy of parent node
- Calculate entropy of each individual node of split and calculate weighted average of all sub-nodes available in split.

Example: Let's use this method to identify best split for student example.

- Entropy for parent node = -(15/30) log2 (15/30) – (15/30) log2 (15/30) = **1**. Here 1 shows that it is a impure node.
- Entropy for Female node = -(2/10) log2 (2/10) – (8/10) log2 (8/10) = 0.72 and for male node, -(13/20) log2 (13/20) – (7/20) log2 (7/20) = **0.93**
- Entropy for split Gender = Weighted entropy of sub-nodes = (10/30)*0.72 + (20/30)*0.93 = **0.86**
- Entropy for Class IX node, -(6/14) log2 (6/14) – (8/14) log2 (8/14) = 0.99 and for Class X node, -(9/16) log2 (9/16) – (7/16) log2 (7/16) = 0.99.
- Entropy for split Class = (14/30)*0.99 + (16/30)*0.99 = **0.99**

Above, you can see that entropy for *Split on Gender* is the lowest among all, so the tree will split on *Gender*. We can derive information gain from entropy as **1- Entropy.**

Decision Tree - Classification

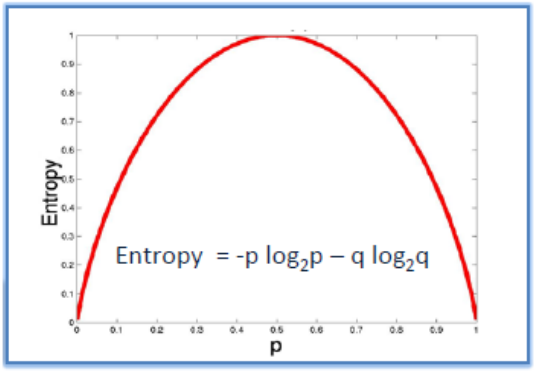
Decision tree builds classification or regression models in the form of a tree structure. It breaks down a dataset into smaller and smaller subsets while at the same time an associated decision tree is incrementally developed. The final result is a tree with **decision nodes** and **leaf nodes**. A decision node (e.g., Outlook) has two or more branches (e.g., Sunny, Overcast and Rainy). Leaf node (e.g., Play) represents a classification or decision. The topmost decision node in a tree which corresponds to the best predictor called **root node**. Decision trees can handle both categorical and numerical data.

Algorithm

The core algorithm for building decision trees called **ID3** by J. R. Quinlan which employs a top-down, greedy search through the space of possible branches with no backtracking. ID3 uses *Entropy* and *Information Gain* to construct a decision tree. In ZeroR model there is no predictor, in OneR model we try to find the single best predictor, naive Bayesian includes all predictors using Bayes' rule and the independence assumptions between predictors but decision tree includes all predictors with the dependence assumptions between predictors.

Entropy

A decision tree is built top-down from a root node and involves partitioning the data into subsets that contain instances with similar values (homogenous). ID3 algorithm uses entropy to calculate the homogeneity of a sample. If the sample is completely homogeneous the entropy is zero and if the sample is an equally divided it has entropy of one.



Entropy = $-0.5 \log_2 0.5 - 0.5 \log_2 0.5 = 1$

To build a decision tree, we need to calculate two types of entropy using frequency tables as follows:

a) Entropy using the frequency table of one attribute:

$$E(S) = \sum_{i=1}^{c} - p_i \log_2 p_i$$

Play Golf	
Yes	No
9	5

Entropy(PlayGolf) = Entropy (5,9)
= Entropy (0.36, 0.64)
= - (0.36 $\log_2$ 0.36) - (0.64 $\log_2$ 0.64)
= 0.94

b) Entropy using the frequency table of two attributes:

$$E(T, X) = \sum_{c \in X} P(c) E(c)$$

		Play Golf		
		Yes	No	
Outlook	Sunny	3	2	5
	Overcast	4	0	4
	Rainy	2	3	5
				14

E(PlayGolf, Outlook) = **P**(Sunny)***E**(3,2) + **P**(Overcast)***E**(4,0) + **P**(Rainy)***E**(2,3)
= (5/14)*0.971 + (4/14)*0.0 + (5/14)*0.971
= 0.693

Information Gain

The information gain is based on the decrease in entropy after a dataset is split on an attribute. Constructing a decision tree is all about finding attribute that returns the highest information gain (i.e., the most homogeneous branches).

Step 1: Calculate entropy of the target.

Entropy(PlayGolf) = Entropy (5,9)
= Entropy (0.36, 0.64)
= - (0.36 $\log_2$ 0.36) - (0.64 $\log_2$ 0.64)
= 0.94

Step 2: The dataset is then split on the different attributes. The entropy for each branch is calculated. Then it is added proportionally, to get total entropy for the split. The resulting entropy is subtracted from the entropy before the split. The result is the Information Gain, or decrease in entropy.

		Play Golf	
		Yes	No
Outlook	Sunny	3	2
	Overcast	4	0
	Rainy	2	3
Gain = 0.247			

		Play Golf	
		Yes	No
Temp.	Hot	2	2
	Mild	4	2
	Cool	3	1
Gain = 0.029			

		Play Golf	
		Yes	No
Humidity	High	3	4
	Normal	6	1
Gain = 0.152			

		Play Golf	
		Yes	No
Windy	False	6	2
	True	3	3
Gain = 0.048			

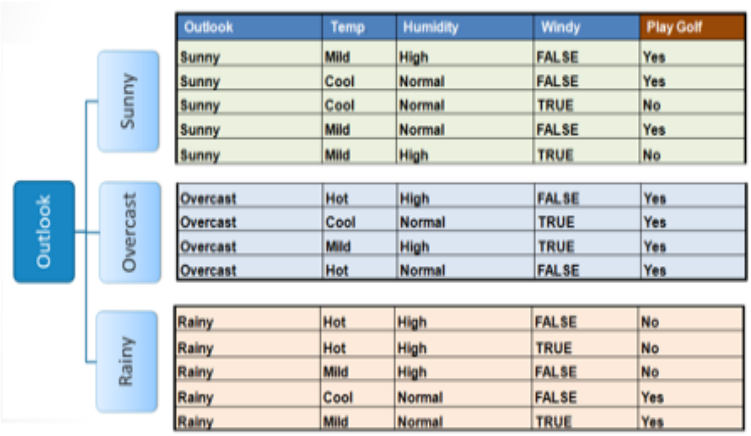
$$Gain(T,X) = Entropy(T) - Entropy(T,X)$$

G(PlayGolf, Outlook) = **E**(PlayGolf) – **E**(PlayGolf, Outlook)

= 0.940 – 0.693 = 0.247

Step 3: Choose attribute with the largest information gain as the decision node, divide the dataset by its branches and repeat the same process on every branch.

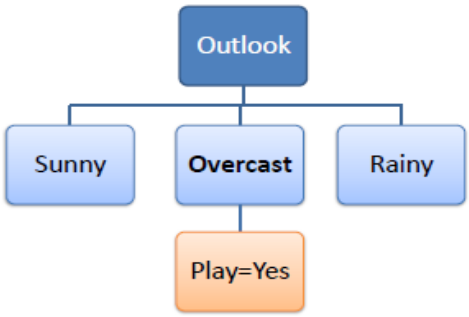
★		Play Golf	
		Yes	No
Outlook	Sunny	3	2
	Overcast	4	0
	Rainy	2	3
Gain = 0.247			



Outlook	Temp	Humidity	Windy	Play Golf
Sunny	Mild	High	FALSE	Yes
Sunny	Cool	Normal	FALSE	Yes
Sunny	Cool	Normal	TRUE	No
Sunny	Mild	Normal	FALSE	Yes
Sunny	Mild	High	TRUE	No
Overcast	Hot	High	FALSE	Yes
Overcast	Cool	Normal	TRUE	Yes
Overcast	Mild	High	TRUE	Yes
Overcast	Hot	Normal	FALSE	Yes
Rainy	Hot	High	FALSE	No
Rainy	Hot	High	TRUE	No
Rainy	Mild	High	FALSE	No
Rainy	Cool	Normal	FALSE	Yes
Rainy	Mild	Normal	TRUE	Yes

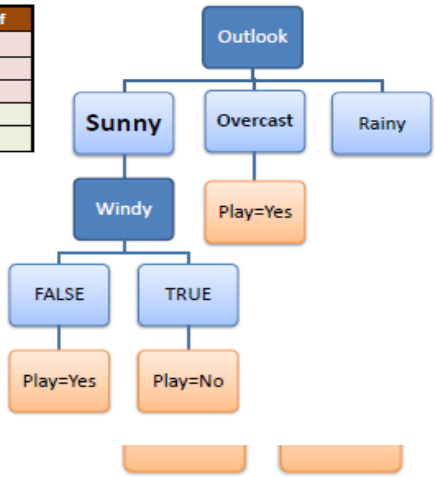
Step 4a: A branch with entropy of 0 is a leaf node.

Temp	Humidity	Windy	Play Golf
Hot	High	FALSE	Yes
Cool	Normal	TRUE	Yes
Mild	High	TRUE	Yes
Hot	Normal	FALSE	Yes

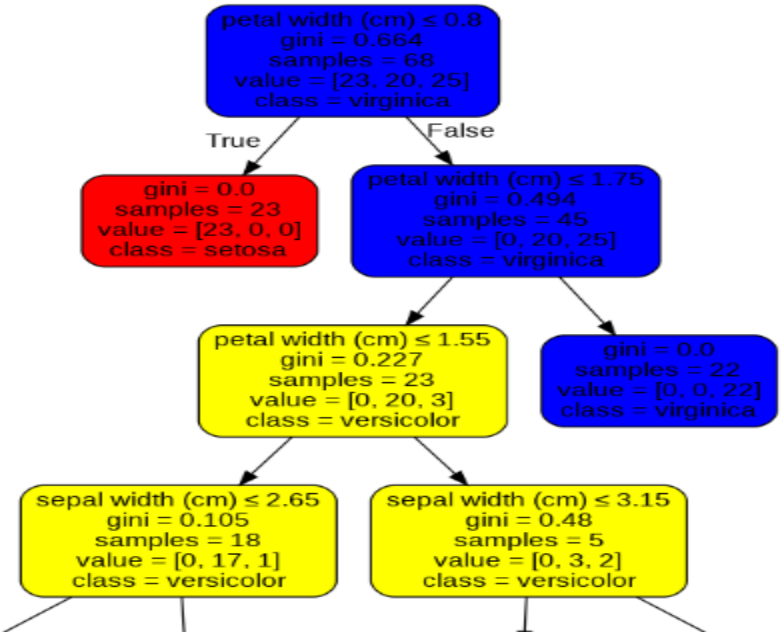


Step 4b: A branch with entropy more than 0 needs further splitting.

Temp	Humidity	Windy	Play Golf
Mild	High	FALSE	Yes
Cool	Normal	FALSE	Yes
Mild	Normal	FALSE	Yes
Cool	Normal	TRUE	No
Mild	High	TRUE	No



Step 5: The ID3 algorithm is run recursively on the non-leaf branches, until all data is classified.



This plot on the left is the same as the previous one but with the **first decision boundary** of the tree : `petal width = 0.8 cm`.

How was this decision boundary decided ?

> A decision boundary is decided by testing all the possible decision boundaries splitting the dataset and choosing the one that minimizes the Gini impurity of the two splits.

*What is **Gini impurity** ?*

Gini impurity is a metric that measures the probability from a randomly chosen element (here an iris) to be incorrectly classified, i.e. the probability of choosing an element times the probability of being misclassified. If we sum over all J possible classes we have the Gini impurity :

$$\sum_{i=1}^{J} p_i \sum_{k!=i} p_k = \sum_{i=1}^{J} p_i(1-p_i) = \sum_{i=1}^{J}(p_i - p_i^2) = \sum_{i=1}^{J} p_i - \sum_{i=1}^{J} p_i^2 = 1 - \sum_{i=1}^{J} p_i^2$$

But the algorithm has no intuition. So how does it find the best split ?

- **It will try all the possible boundaries along all the features**, i.e. all the axes *petal width* and *sepal width*.
- For each split the algorithm will compute the Gini impurity of the two groups created.
- Finally it will choose the decision boundary that gives the lowest Gini impurity for the two groups (either summing the Gini impurity for each group or doing a mean).

Let's get back to the first node and the first split

In the case of the root node, the algorithm has found that among all the possible splits the split with `petal width = 0.8 cm` gives the lowest Gini impurity.
The Gini impurity for the left leaf is :

$$1 - p_{se}^2 - p_{ve}^2 - p_{vi}^2 = 1 - p_{se}^2 = 1 - (\frac{23}{23})^2 = 0$$

We verify this result with the tree graph. This result is not surprising because in the left leaf which matches the left part of the graph we only have *setosa* iris, so the group is very homogeneous and Gini impurity is a measure of homogeneity.

- **Decision tree algorithms use information gain to split a node. Gini index or entropy is the criterion for calculating information gain.**

Both gini and entropy are measures of impurity of a node. A node having multiple classes is impure whereas a node having only one class is pure. Entropy in statistics is analogous to entropy in thermodynamics where it signifies disorder. If there are multiple classes in a node, there is disorder in that node.

Information gain is the entropy of parent node minus sum of weighted entropies of child nodes. Weight of a child node is number of samples in the node/total samples of all child nodes.

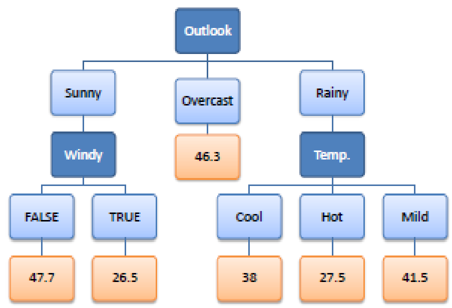
When to use Information Gain and When to use Gini Index

Choice of impurity measure has little effect on the performance of decision tree induction algorithms. This is because many impurity measures are quite consistent with each other. There are merely any difference between these two criteria. Gini plays the same role as entropy in information gain, rather than information gain itself, which makes the problem much simpler.

Decision Tree - Regression

Decision tree builds regression or classification models in the form of a tree structure. It breaks down a dataset into smaller and smaller subsets while at the same time an associated decision tree is incrementally developed. The final result is a tree with **decision nodes** and **leaf nodes**. A decision node (e.g., Outlook) has two or more branches (e.g., Sunny, Overcast and Rainy), each representing values for the attribute tested. Leaf node (e.g., Hours Played) represents a decision on the numerical target. The topmost decision node in a tree which corresponds to the best predictor called **root node**. Decision trees can handle both categorical and numerical data.

Predictors				Target
Outlook	Temp	Humidity	Windy	Hours Played
Rainy	Hot	High	False	25
Rainy	Hot	High	True	30
Overcast	Hot	High	False	46
Sunny	Mild	High	False	45
Sunny	Cool	Normal	False	52
Sunny	Cool	Normal	True	23
Overcast	Cool	Normal	True	43
Rainy	Mild	High	False	35
Rainy	Cool	Normal	False	38
Sunny	Mild	Normal	False	46
Rainy	Mild	Normal	True	48
Overcast	Mild	High	True	52
Overcast	Hot	Normal	False	44
Sunny	Mild	High	True	30



Decision Tree Algorithm

The core algorithm for building decision trees called **ID3** by J. R. Quinlan which employs a top-down, greedy search through the space of possible branches with no backtracking. The ID3 algorithm can be used to construct a decision tree for regression by replacing Information Gain with *Standard Deviation Reduction*.

Standard Deviation

A decision tree is built top-down from a root node and involves partitioning the data into subsets that contain instances with similar values (homogenous). We use standard deviation to calculate the homogeneity of a numerical sample. If the numerical sample is completely homogeneous its standard deviation is zero.

a) Standard deviation for **one** attribute:

Hours Played
25
30
46
45
52
23
43
35
38
46
48
52
44
30

$$Count = n = 14$$

$$Average = \bar{x} = \frac{\sum x}{n} = 39.8$$

$$Standard\ Deviation = S = \sqrt{\frac{\sum(x-\bar{x})^2}{n}} = 9.32$$

$$Coeffeicient\ of\ Variation = CV = \frac{S}{\bar{x}} * 100\% = 23\%$$

- Standard Deviation (**S**) is for tree building (branching).
- Coefficient of Deviation (**CV**) is used to decide when to stop branching. We can use Count (**n**) as well.
- Average (**Avg**) is the value in the leaf nodes.

b) Standard deviation for **two** attributes (target and predictor):

$$S(T,X) = \sum_{c \in X} P(c)S(c)$$

		Hours Played (StDev)	Count
Outlook	Overcast	3.49	4
	Rainy	7.78	5
	Sunny	10.87	5
			14

S(Hours, Outlook) = **P**(Sunny)***S**(Sunny) + **P**(Overcast)***S**(Overcast) + **P**(Rainy)***S**(Rainy)

= (4/14)*3.49 + (5/14)*7.78 + (5/14)*10.87

= 7.66

Standard Deviation Reduction

The standard deviation reduction is based on the decrease in standard deviation after a dataset is split on an attribute. Constructing a decision tree is all about finding attribute that returns the highest standard deviation reduction (i.e., the most homogeneous branches).

Step 1: The standard deviation of the target is calculated.

Standard deviation (Hours Played) = 9.32

Step 2: The dataset is then split on the different attributes. The standard deviation for each branch is calculated. The resulting standard deviation is subtracted from the standard deviation before the split. The result is the standard deviation reduction.

		Hours Played (StDev)
Outlook	Overcast	3.49
	Rainy	7.78
	Sunny	10.87
SDR=1.66		

		Hours Played (StDev)
Temp.	Cool	10.51
	Hot	8.95
	Mild	7.65
SDR=0.17		

		Hours Played (StDev)
Humidity	High	9.36
	Normal	8.37
SDR=0.28		

		Hours Played (StDev)
Windy	False	7.87
	True	10.59
SDR=0.29		

$$SDR(T,X) = S(T) - S(T,X)$$

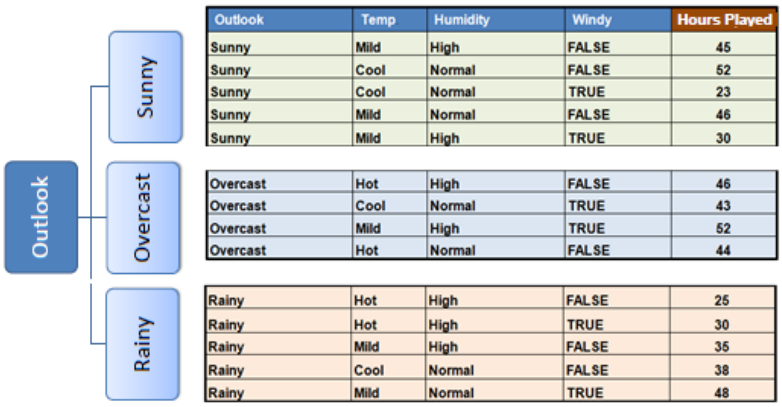
SDR(Hours , Outlook) = **S**(Hours) – **S**(Hours, Outlook)

= 9.32 – 7.66 = 1.66

Step 3: The attribute with the largest standard deviation reduction is chosen for the decision node.

		Hours Played (StDev)
Outlook	Overcast	3.49
	Rainy	7.78
	Sunny	10.87
SDR=1.66		

Step 4a: The dataset is divided based on the values of the selected attribute. This process is run recursively on the non-leaf branches, until all data is processed.



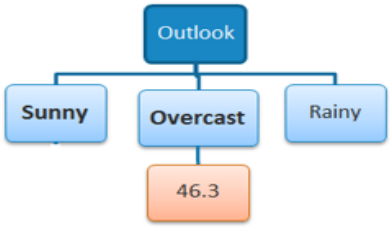
Outlook	Temp	Humidity	Windy	Hours Played
Sunny	Mild	High	FALSE	45
Sunny	Cool	Normal	FALSE	52
Sunny	Cool	Normal	TRUE	23
Sunny	Mild	Normal	FALSE	46
Sunny	Mild	High	TRUE	30
Overcast	Hot	High	FALSE	46
Overcast	Cool	Normal	TRUE	43
Overcast	Mild	High	TRUE	52
Overcast	Hot	Normal	FALSE	44
Rainy	Hot	High	FALSE	25
Rainy	Hot	High	TRUE	30
Rainy	Mild	High	FALSE	35
Rainy	Cool	Normal	FALSE	38
Rainy	Mild	Normal	TRUE	48

In practice, we need some termination criteria. For example, when coefficient of deviation (**CV**) for a branch becomes smaller than a certain threshold (e.g., 10%) and/or when too few instances (**n**) remain in the branch (e.g., 3).

Step 4b: "Overcast" subset does not need any further splitting because its CV (8%) is less than the threshold (10%). The related leaf node gets the average of the "Overcast" subset.

Outlook - Overcast

		Hours Played (StDev)	Hours Played (AVG)	Hours Played (CV)	Count
Outlook	Overcast	3.49	46.3	8%	4
	Rainy	7.78	35.2	22%	5
	Sunny	10.87	39.2	28%	5



Step 4c: However, the "Sunny" branch has an CV (28%) more than the threshold (10%) which needs further splitting. We select "Windy" as the best best node after "Outlook" because it has the largest SDR.

Outlook - Sunny

Temp	Humidity	Windy	Hours Played
Mild	High	FALSE	45
Cool	Normal	FALSE	52
Cool	Normal	TRUE	23
Mild	Normal	FALSE	46
Mild	High	TRUE	30
			S = 10.87
			AVG = 39.2
			CV = 28%

		Hours Played (StDev)	Count
Temp	Cool	14.50	2
	Mild	7.32	3

SDR = 10.87-((2/5)*14.5 + (3/5)*7.32) = **0.678**

		Hours Played (StDev)	Count
Humidity	High	7.50	2
	Normal	12.50	3

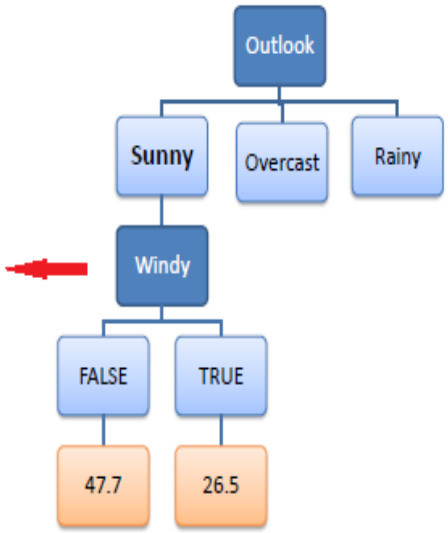
SDR = 10.87-((2/5)*7.5 + (3/5)*12.5) = **0.370**

		Hours Played (StDev)	Count
Windy	False	3.09	3
	True	3.50	2

SDR = 10.87-((3/5)*3.09 + (2/5)*3.5) = **7.62**

Because the number of data points for both branches (FALSE and TRUE) is equal or less than 3 we stop further branching and assign the average of each branch to the related leaf node.

Temp	Humidity	Windy	Hours Played
Mild	High	FALSE	45
Cool	Normal	FALSE	52
Mild	Normal	FALSE	46
Cool	Normal	TRUE	23
Mild	High	TRUE	30



Step 4d: Moreover, the "rainy" branch has an CV (22%) which is more than the threshold (10%). This branch needs further splitting. We select "Windy" as the best best node because it has the largest SDR.

Outlook - Rainy

Temp	Humidity	Windy	Hours Played
Hot	High	FALSE	**25**
Hot	High	TRUE	**30**
Mild	High	FALSE	**35**
Cool	Normal	FALSE	**38**
Mild	Normal	TRUE	**48**
			S = 7.78
			AVG = 35.2
			CV = 22%

		Hours Played (StDev)	Count
Temp	Cool	0	1
	Hot	2.5	2
	Mild	6.5	2

SDR = 7.78 - ((1/5)*0+(2/5)*2.5 + (2/5)*6.5) = **4.18**

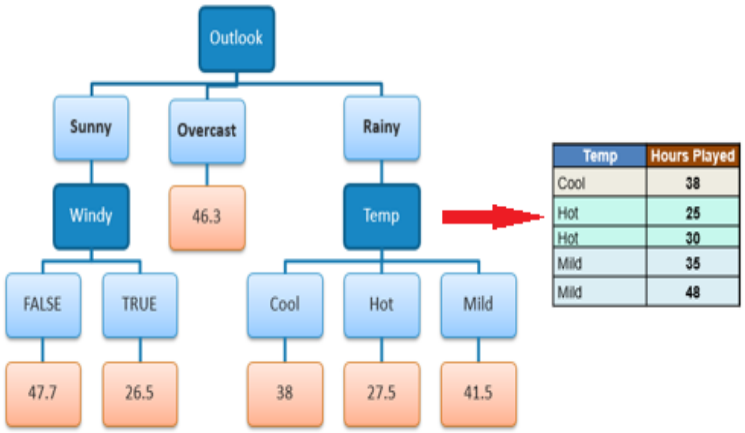
		Hours Played (StDev)	Count
Humidity	High	4.1	3
	Normal	5.0	2

SDR = 7.78 - ((3/5)*4.1 + (2/5)*5.0) = **3.32**

		Hours Played (StDev)	Count
Windy	False	5.6	3
	True	9.0	2

SDR = 7.78 - ((3/5)*5.6 + (2/5)*9.0) = **0.82**

Because the number of data points for all three branches (Cool, Hot and Mild) is equal or less than 3 we stop further branching and assign the average of each branch to the related leaf node.



Temp	Hours Played
Cool	**38**
Hot	**25**
Hot	**30**
Mild	**35**
Mild	**48**

When the number of instances is more than one at a *leaf node* we calculate the *average* as the final value for the target.