

DECISION TREE

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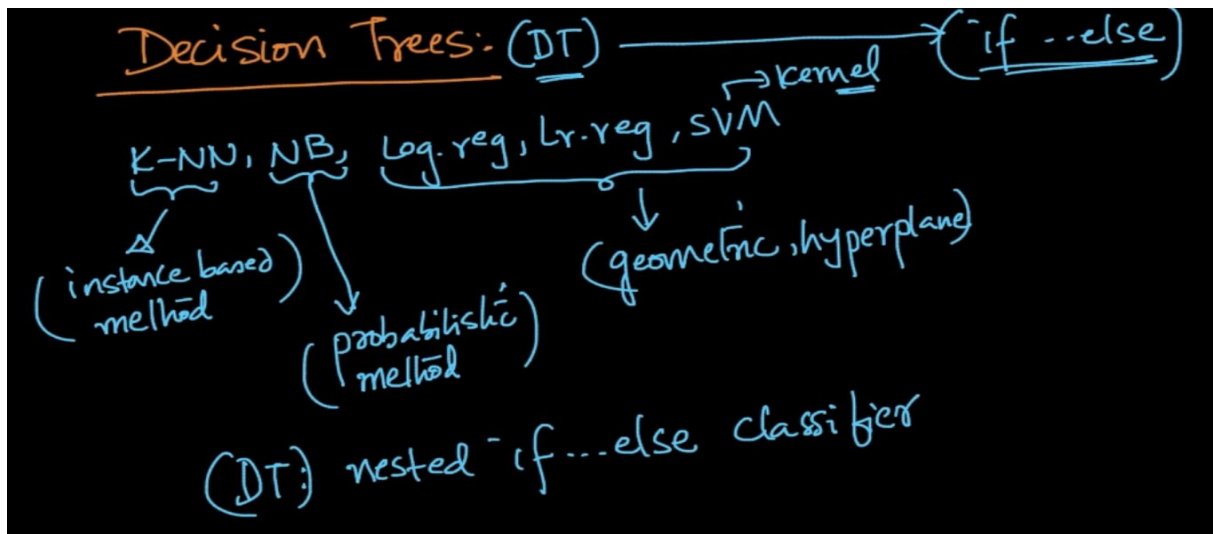
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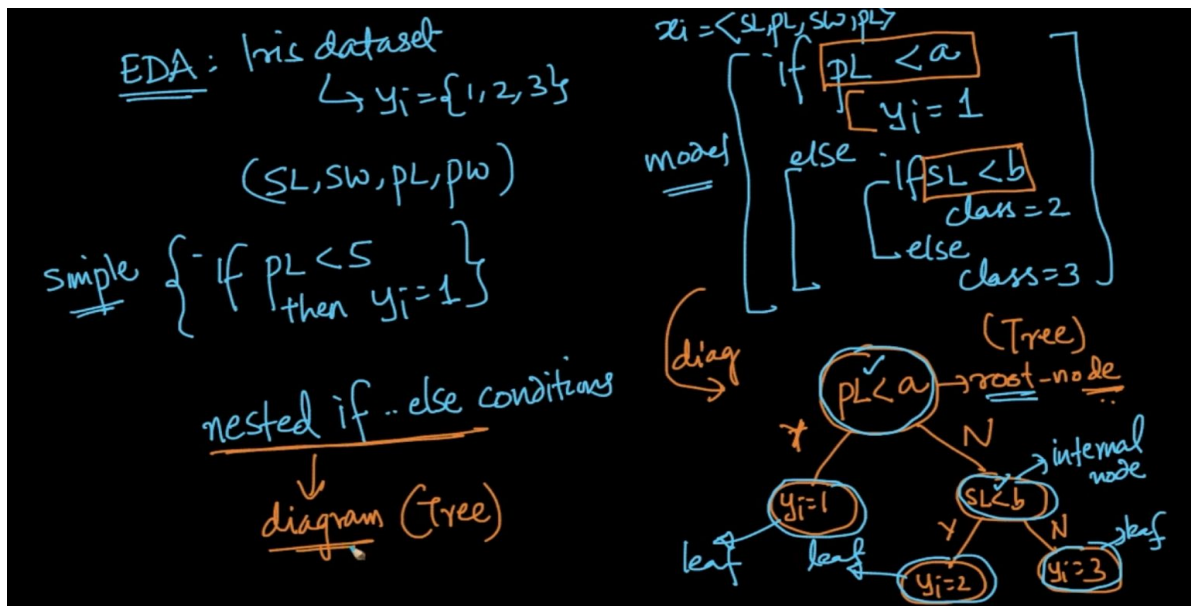
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GEOMETRIC INTUITION

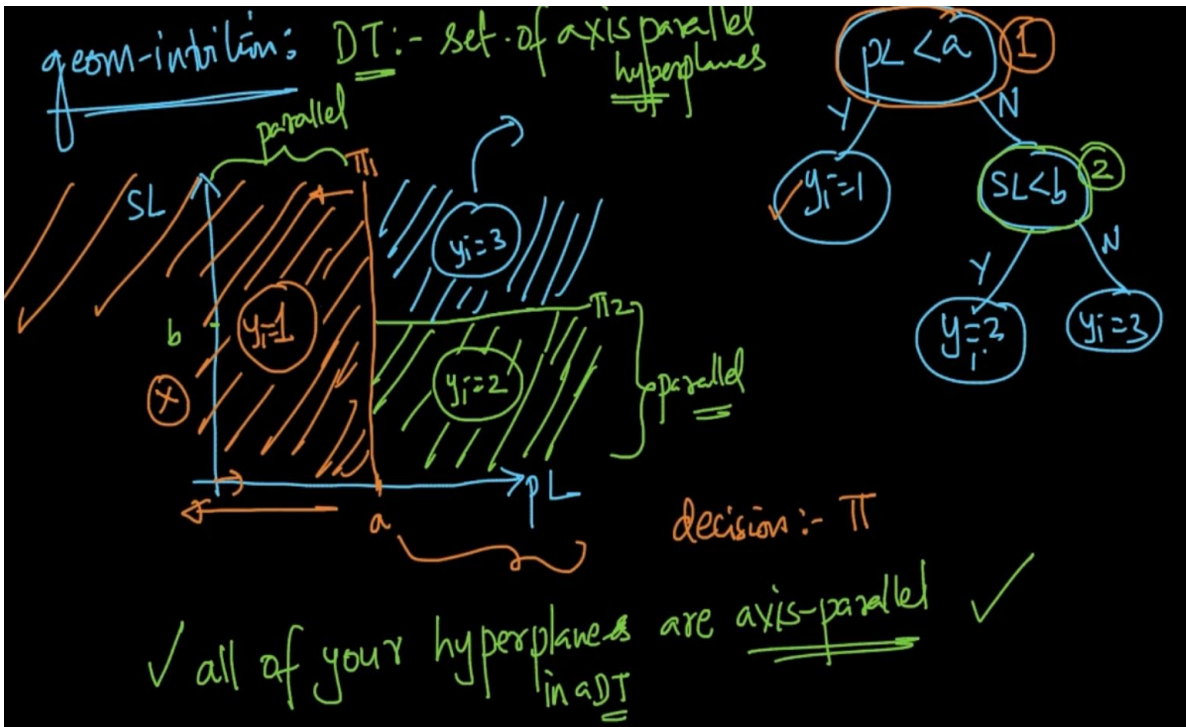


We'd discussed about which **type of methods** the classifiers have .

Decision Tree, it's a nested if Else classifier simply

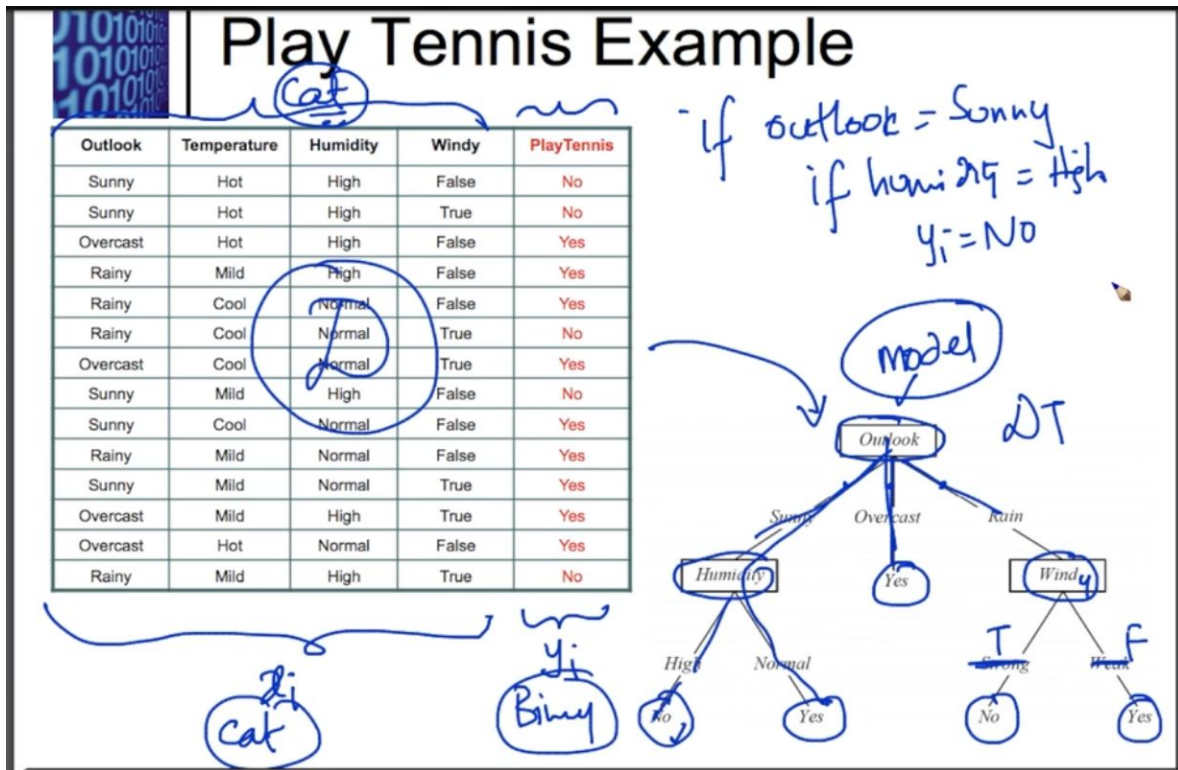


We've a simple nested if-else model for Iris dataset. We are taking the first condition as a root node and from that start building our Decision Tree which is basically diagrammatic representation of Nested if-else model. In DT all the non leaf nodes take a decision and leaf nodes tells us about the class label



We've 2 features in our DT, PL and SL. So we plot a PL-SL graph and in that with every decision we take we draw a hyper-plane (Eg: $PL < a$ then draw a hyperplane π_1 on 'a'. We are satisfying the condition that all $PL < a \Rightarrow y_i = 1$). Same for other decisions. For every decision we've a hyperplane and all the hyperplanes are axis-parallel i.e hyperplanes will always be parallel to axis.

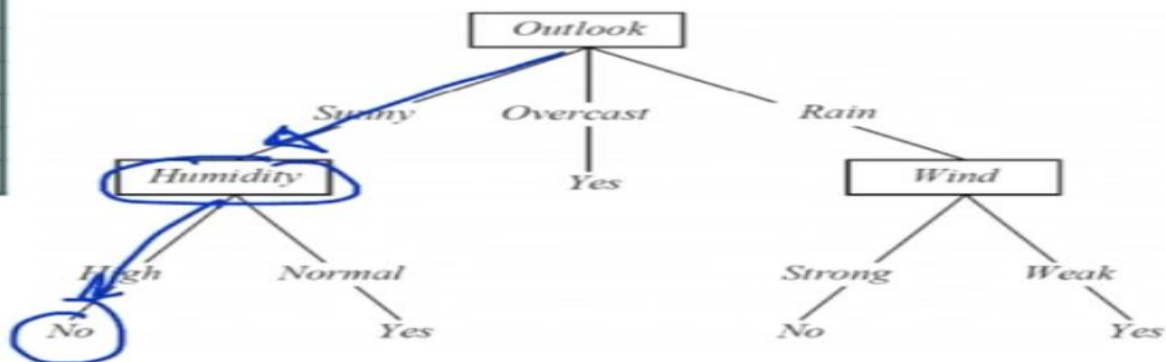
SAMPLE DECISION TREE



It's a dataset given with categorical features and y is binary. We make our model(Decision Tree) using dataset. It works like a nested if-else as seen above.

$x_q = [\overset{\checkmark}{\text{sunny}}, \underset{\times}{\text{hot}}, \overset{\checkmark}{\text{high}}, \underset{\times}{\text{T}}]$

$y_q = \text{NO}$



How does it work with a new query $x_q = [\text{sunny}, \text{hot}, \text{high}, \text{True}]$ then it'll work through the Decision Tree and follow the path. As it's visible we don't even need two features i.e hot and True

In Decision Tree the main part is to how to construct Decision Tree from Dataset after that

it's very easy to do $x_q \Rightarrow y_q$

BUILDING A DECISION TREE: ENTROPY

$$X.V \quad Y \rightarrow y_1, y_2, y_3, \dots, y_k$$

$$H(Y) = - \sum_{i=1}^k p(y_i) \log_b(p(y_i))$$

$$p(y_i) = P(Y=y_i)$$

$$b = 2 \text{ or } b = e = 2.718$$

$$\log_2 = \lg$$

$$\log_e = \ln$$

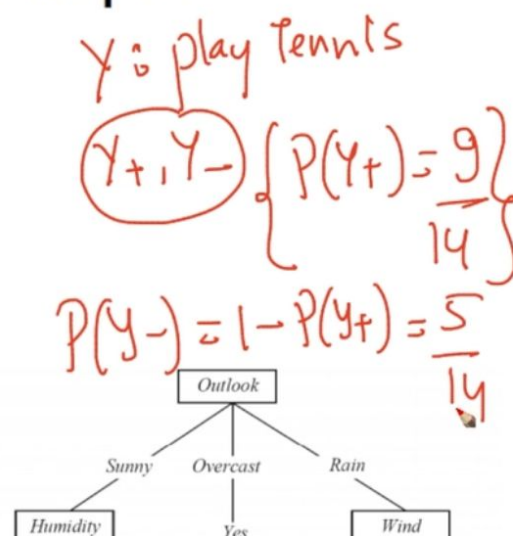
We are given a random variable $Y \rightarrow y_1, y_2, \dots, y_k$ i.e it can have k -values

Entropy : $H(Y) = - \sum_{i=1}^k P(y_i) \log_b(P(y_i))$ where $b = 2$ or e typically. What is $P(y_i)$? It's $P(Y = y_i)$



Play Tennis Example

Outlook	Temperature	Humidity	Windy	PlayTennis
Sunny	Hot	High	False	No
Sunny	Hot	High	True	No
Overcast	Hot	High	False	Yes
Rainy	Mild	High	False	Yes
Rainy	Cool	Normal	False	Yes
Rainy	Cool	Normal	True	No
Overcast	Cool	Normal	True	Yes
Sunny	Mild	High	False	No
Sunny	Cool	Normal	False	Yes
Rainy	Mild	Normal	False	Yes
Sunny	Mild	Normal	True	Yes
Overcast	Mild	High	True	Yes
Overcast	Hot	Normal	False	Yes
Rainy	Mild	High	True	No



There are only 2 classes . So we need only $P(Y_+)$ and $P(Y_-)$ which is calculated

$$H(Y) = - \sum_{i=1}^K p(y_i) \log_2(p(y_i))$$

$$H(Y) = - \left[\frac{9}{14} \log_2\left(\frac{9}{14}\right) + \frac{5}{14} \log_2\left(\frac{5}{14}\right) \right] = 0.94$$

Annotations:

- $\frac{9}{14}$ is labeled $p(y_+)$ and $\frac{5}{14}$ is labeled $p(y_-)$.
- $\frac{9}{14}$ is also labeled $\frac{\# \text{ve p's}}{\text{Total \# p's}}$.
- $\frac{5}{14}$ is labeled $\frac{\% \text{ age of -ve p's in } D}{100}$.
- A box contains the text: $\% \text{ age of +ve p's in } D$.

The Entropy of the above dataset is calculated like this

Properties: $Y \rightarrow y_+, y_-$ (2 class, 2 category)

Case 1:

$$\begin{cases} y_+ \rightarrow 99\% \\ y_- \rightarrow 1\% \end{cases} \quad H(Y) = -0.99 \log_2 0.99 - 0.01 \log_2 0.01 = 0.0801$$

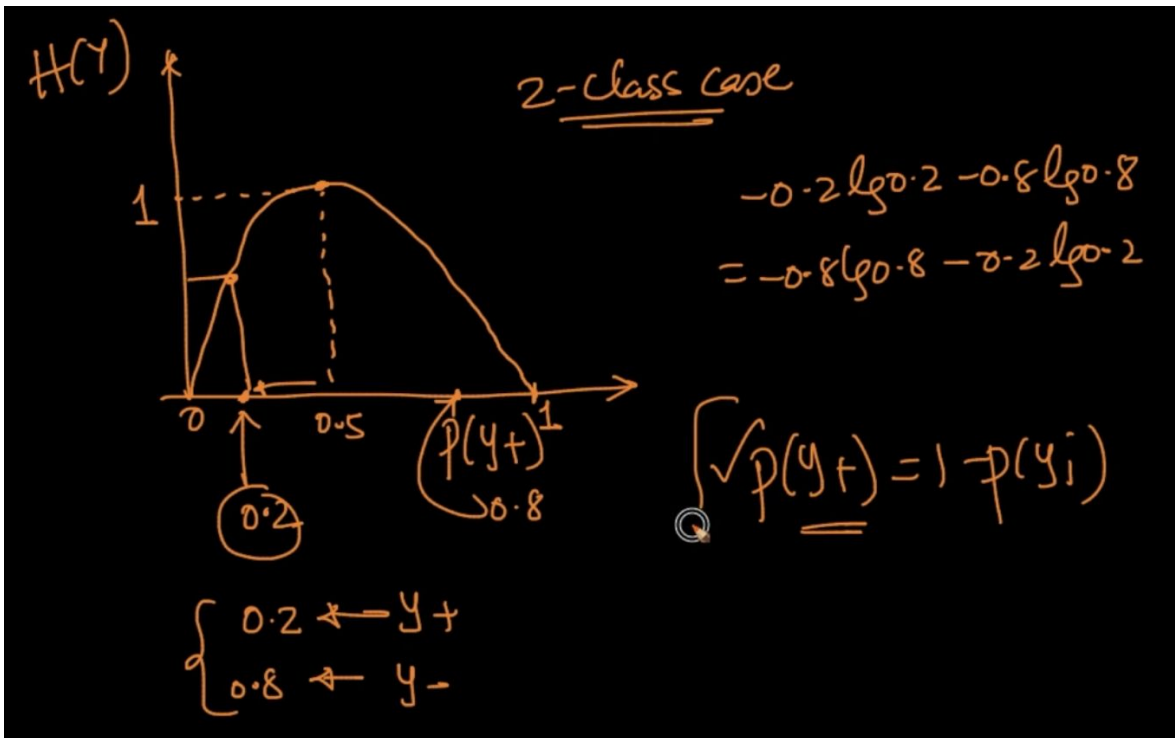
Case 2:

$$\begin{cases} y_+ \rightarrow 50\% \\ y_- \rightarrow 50\% \end{cases} \quad H(Y) = -0.5 \log_2 0.5 - 0.5 \log_2 0.5 = 1$$

Case 3:

$$\begin{cases} y_+ \rightarrow 0\% \\ y_- \rightarrow 100\% \end{cases} \quad H(Y) = 0$$

As we can see if both the classes are equiprobable (case 2) its entropy is max. When 1 class is fully dominating the other class (Case 3) its 0. In case 1 $H(Y)$ decreased



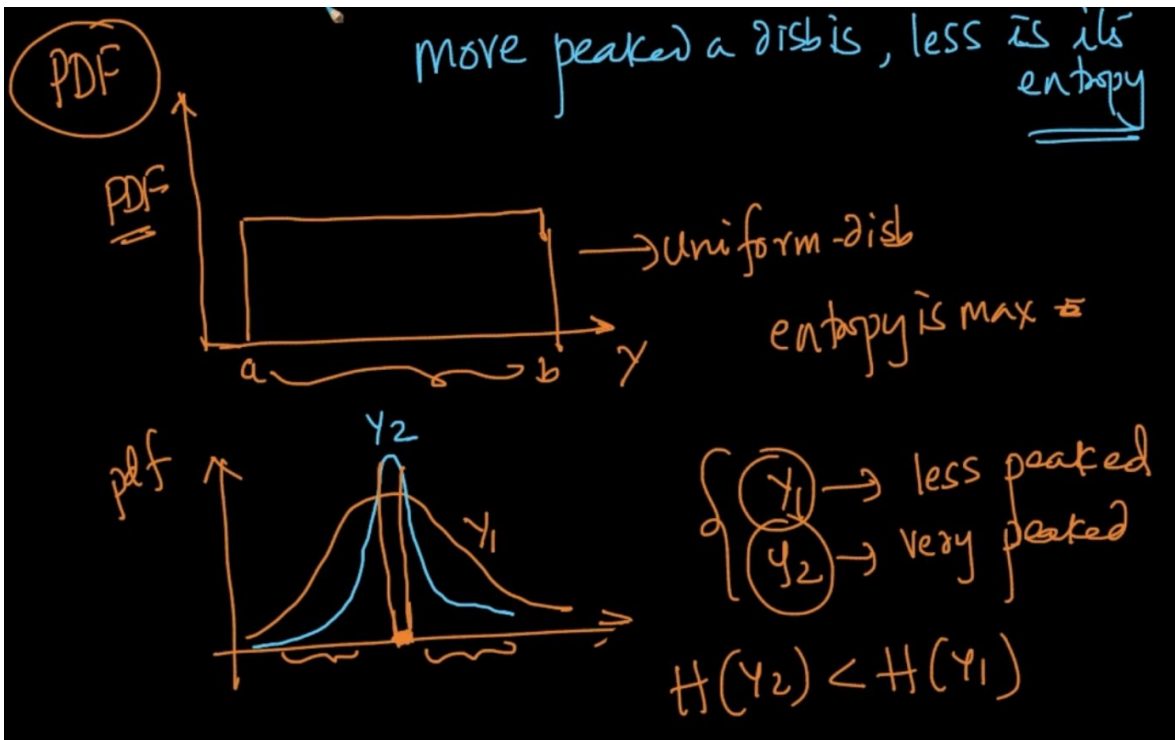
$P(Y_+) = 1 - P(Y_-)$. When we plot the graph of $P(Y_+)$ v/s $H(Y)$. When $P(Y_+) = 0.5$ or equiprobable $H(Y) = 1$ (It's maximum for a 2 class problem). When $P(Y_+) = 0.2$; $P(Y_-) = 0.8$ or we can say one class is dominating, Entropy decreases

$Y \rightarrow y_1, y_2, \dots, y_k$
 equi-probable \rightarrow entropy is maximum

$y_1 \rightarrow$ most probable
 $y_2, y_3, \dots \rightarrow 0$

\rightarrow entropy is minimum

When a random variable Y is given and all its class labels are equiprobable then entropy is maximum. When $y_1 \rightarrow$ most probable and all the other y 's $\rightarrow 0$ Entropy is minimum

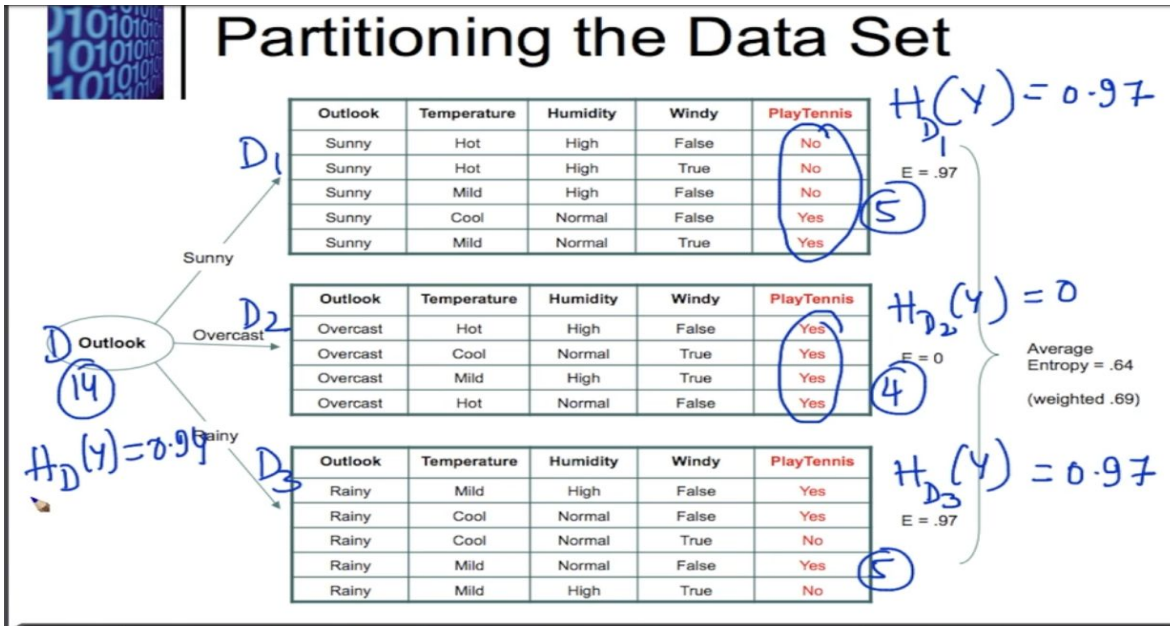


In the first figure all the values are uniformly distributed so entropy is maximum

In the second one, y_2 is very peaked i.e it can only take small set of values and Probability of taking other values is less whereas y_1 is less peaked meaning it can take more values which means y_1 tending towards equiprobability. So, we can clearly say $H(y_2) < H(y_1)$

More peaked a distribution is less is its entropy

BUILDING A DECISION TREE : INFORMATION GAIN



We divide the Dataset based on Root Node "Outlook" which is a categorical feature having 3 discrete values = [Sunny, Overcast, Rainy]. Now we calculate the Entropies of the divided datasets.

Information Gain Calculation:

$$IG(Y, outlook) = \left(\frac{5}{7} \times 0.97 \right) - (0.94) = 1.6$$

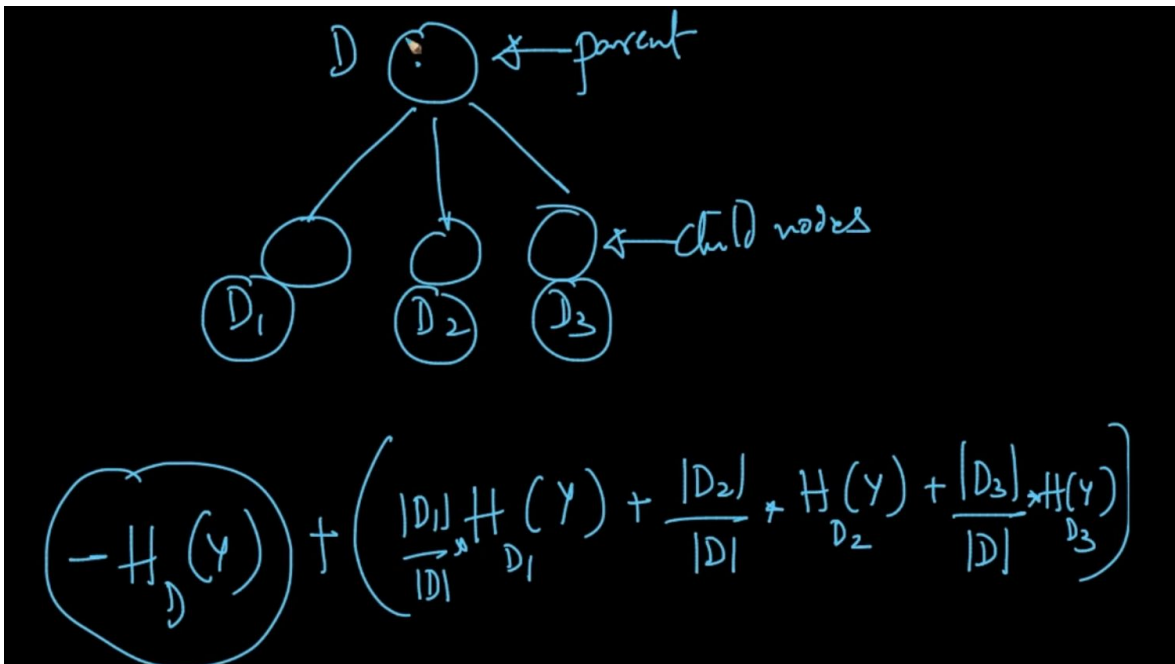
Weighted entropy after D1, D2, D3:

$$\left(\frac{5}{14} \times 0.97 \right) + \left(\frac{4}{14} \times 0 \right) + \left(\frac{5}{14} \times 0.97 \right)$$

Final Calculation:

$$\frac{5}{7} \times 0.97 = 0.69$$

Information Gain by 'Outlook' : $IG(Y, \text{Outlook})$ is calculated as above . First we summate all the Entropies for the divided dataset and Entropy for the dataset is used for IG



This is how Information Gain is calculated where D_1, D_2, D_3 are no. of points in the divided datasets respectively and D is total no. of features/rows

The diagram shows a variable 'Y' being split into categories 'Y1, Y2, ..., Yk'. Above each category is a circled label 'D1, D2, ..., Dk'. An arrow points from 'Y' to the categories, with the word 'var' written above it. Below this, the general formula for Information Gain is written:

$$IG(Y, \text{var}) = \sum_{i=1}^k \frac{|D_i|}{|D|} * H_{D_i}(Y) - H_D(Y)$$

$$IG(Y, \text{var}) = \sum_{i=1}^k \frac{|D_i|}{|D|} * H_{D_i}(Y) - H_D(Y)$$

GINI IMPURITY

Gini Impurity \sim similar to Entropy

$$I_G(Y) = 1 - \sum_{i=1}^K (p(y_i))^2 \quad Y \rightarrow \begin{matrix} y_+ \\ y_- \end{matrix}$$

$$Y \rightarrow y_1, y_2, y_3, \dots, y_K$$

Case 2: $p(y_+) = 1$
 $p(y_-) = 0$

$$I_G(Y) = 1 - (1 + 0) = 0$$

$H(Y) \uparrow$

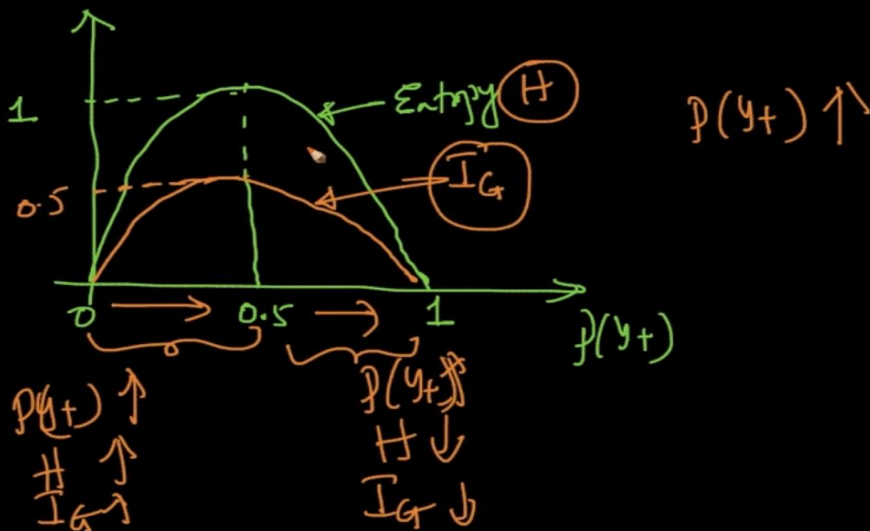
Case 1: $p(y_+) = 0.5$
 $p(y_-) = 0.5$

$$I_G(Y) = 1 - (0.25 + 0.25) = 0.5$$

$$H(Y) = 1$$

$$I_G(Y) = 1 - \sum_{i=1}^K (P(y_i))^2. \text{ We've discussed different cases there}$$

2-category case: y_+, y_- $p(y_+) = 1 - p(y_-)$



As seen, Entropy and Gini Impurity are very similar except the max value of $I_G = 0.5$

The image shows a handwritten comparison of Gini Impurity and Entropy on a blackboard. On the left, the Gini Impurity formula $I_G(Y)$ is circled in blue. Next to it, a bracketed note says "more computationally efficient" with an arrow pointing to the formula. The formula is $1 - (p_{y+})^2 - (p_{y-})^2$, with the squares circled in blue. An arrow points down from this formula to a circled blue label "no-log". Below this, "SKlearn: - DT" is written with "DT" circled in blue. On the right, the Entropy formula $H(Y)$ is circled in blue and crossed out with a blue 'X'. Below it, the formula is written as $-\sum p(y) \log_2(p(y))$, with the \log_2 terms circled in blue. An arrow points up from a circled blue label "log" to the \log_2 terms.

$$I_G(Y) = 1 - (p_{y+})^2 - (p_{y-})^2$$

more computationally efficient

no-log

SKlearn: - DT

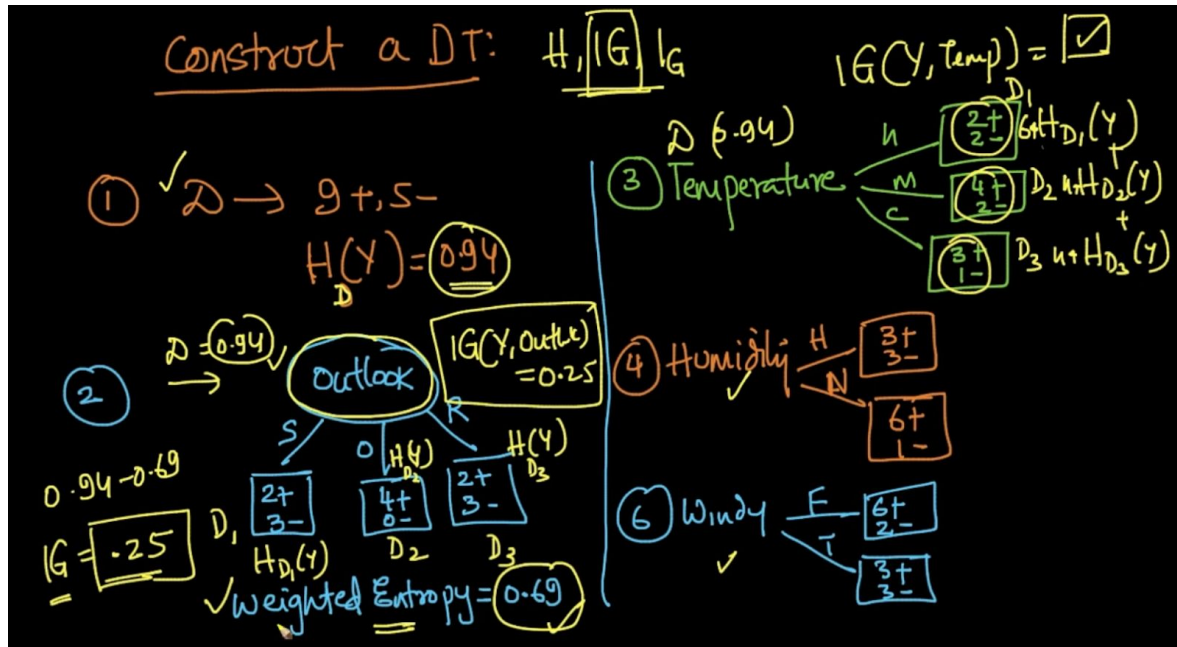
$$H(Y) = -\sum p(y) \log_2(p(y))$$

log

So if they are very similar then why do people prefer Gini's impurity ?

It's because as seen in the formula we take out squares in I_G but in $H(Y)$ we use log and computing squares is computationally more efficient than computing logs. That's why Gini is preferred

CONSTRUCT A DECISION TREE: BUILDING A DECISION TREE



We calculate the Entropy of all the dataset. After that we have to decide the feature for Root Nodes. So for choosing that we choose one, we decide the feature use that as a Root Node and partition the data based on that and calculate the Entropies and their combined Weighted Entropies using the individual Entropies. We do it for all and calculate $IG(Y, \text{Feature})$. It is shown below

$$IG(Y, f) = H_D(Y) - \sum_{i=1}^k \frac{|D_i|}{|D|} H_D(Y)$$

$D \rightarrow$

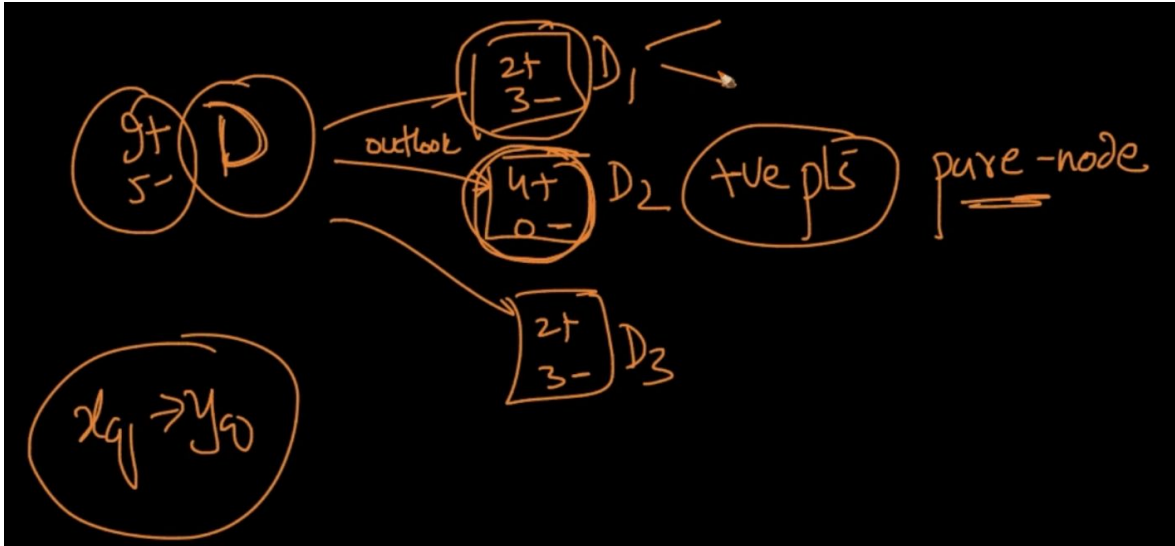
$IG(Y, outlook) = 0.25$

$IG(Y, Temp) = -$

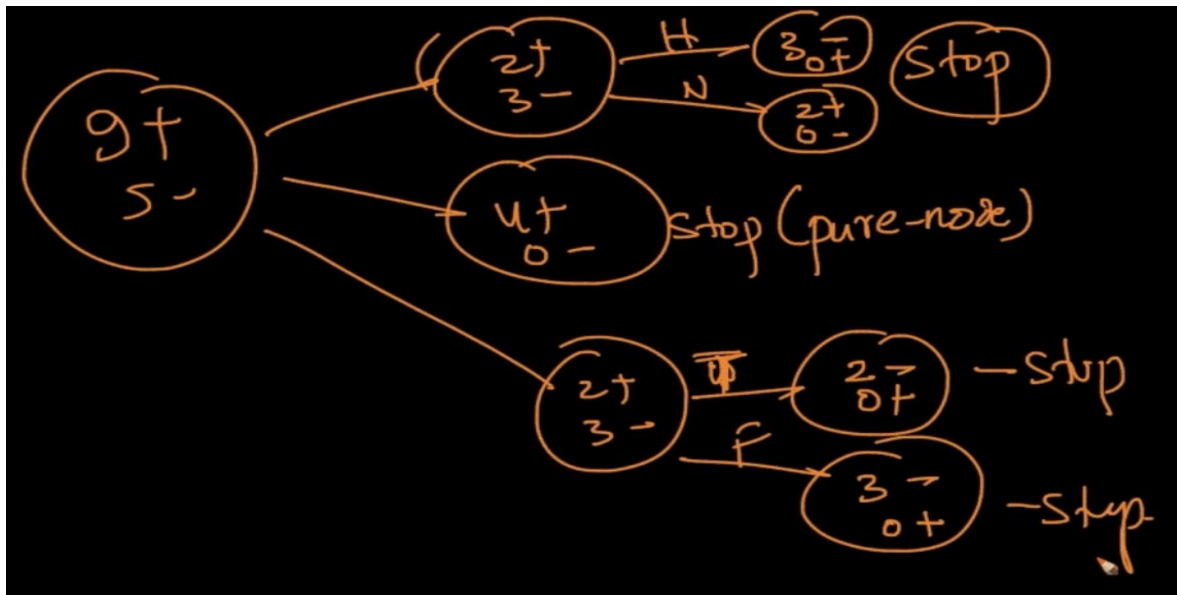
$IG(Y, Humidity) = -$

$IG(Y, Windy) = -$

\rightarrow Choosing the root node



We decide Feature "Outlook" as it has the maximum IG. In the divided Dataset, D_2 is a pure node since it has only +ve points and for the other Datasets we partition further by using the remaining features and calculating their Information Gain and selecting the Maximum Information Gain



D_1 has 2+ and 3- and if we break it up by 'Humidity' we can see the dataset is further divided and we get pure nodes. Same procedure for D_3 . We divide it on the basis of 'Windy'. So our DT is completed using IG as criteria

depth of the tree \uparrow ; overfitting \uparrow
 (few pts)
 depth is small \Rightarrow underfit
 DT: - hyperparam: - depth \rightarrow CV

So our depth of the Tree is a hyper-parameter and we can know the right depth by Cross Validation

BUILDING A DECISION TREE : SPLITTING NUMERICAL FEATURES

Splitting numerical features
 Construct a DT: - Splitting a node \rightarrow IG
 IG: $\begin{cases} \text{entropy} \\ \text{Gini impurity} \end{cases} \rightarrow \text{computationally efficient}$

The most important step in constructing a DT is Splitting a node and we did that by using IG - We used Entropy for it but we can use Gini Impurity as well since it's computationally efficient. But we've a problem here since we only dealt with Categorical Features and Discrete Random Variables and constructing a DT is easy because we splitted with the categories but what if we'd Numerical data

f_1		y
2.2	1	2
2.6	1	3
3.5	0	
3.8	0	
4.6	1	
5.3	0	

n pts

f_1 : numerical
 ↳ integer
 ↳ real value

① Sort the numerical feature in asc-order

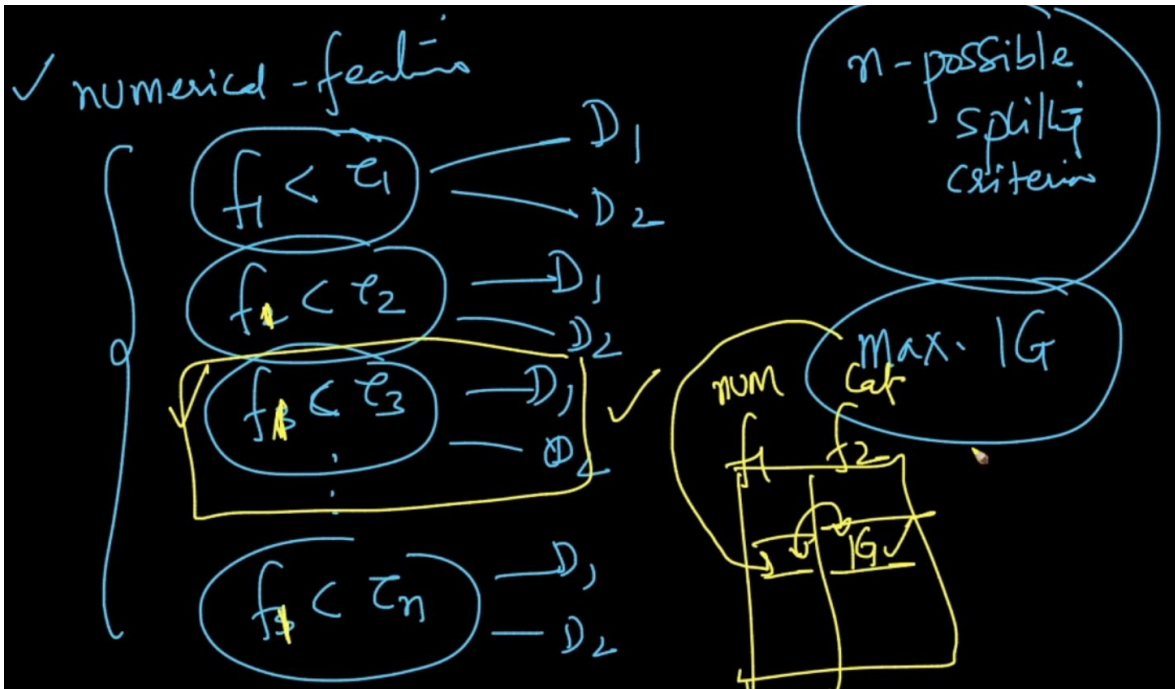
②

$f_1 < 2.2$
 $f_1 < 2.6$
 $f_1 < 3.5$
 $f_1 < 3.8$

$f_1 < 4.6$
 $f_1 < 5.3$

n possible variations

If we've numerical features like above then first we sort in ascending order and create Datasets using conditions like above. For Ex: If $f_1 < 3.5$ then we've 2 pts below it and 4 points above it. We can have a partitioned dataset . We can do it for every value. If we've 'n' points in a dataset then we've 'n' possibilities

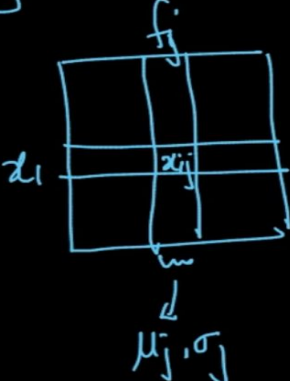


Sp for n points we can create partitioned datasets by applying Thresholds and we select the one which has maximum Information Gain. If we've 2 features f_1 and f_2 we compare the IG and select feature but since there are ' n ' possibilities it can get time consuming

FEATURE STANDARDIZATION

Feature Standardization:

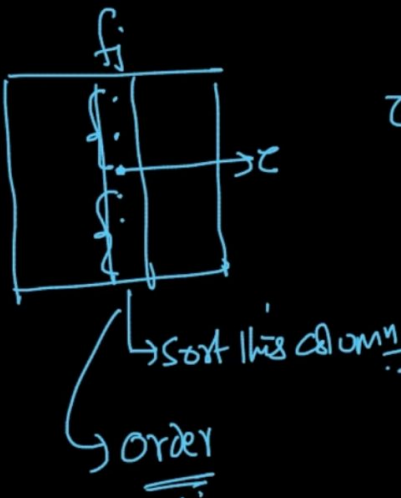
Logistic regression } → feature std'n
SVM }


$$x'_{ij} = \frac{x_{ij} - \mu_j}{\sigma_j}$$

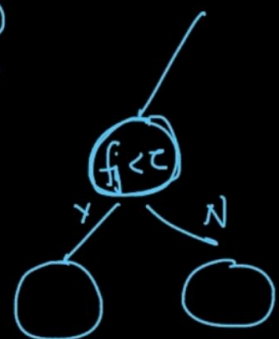
In the Logistic Regression, SVM we did feature Standardization like above

Decision Trees: - not a distance based method

{ do not need }
to perform
feat. std'n

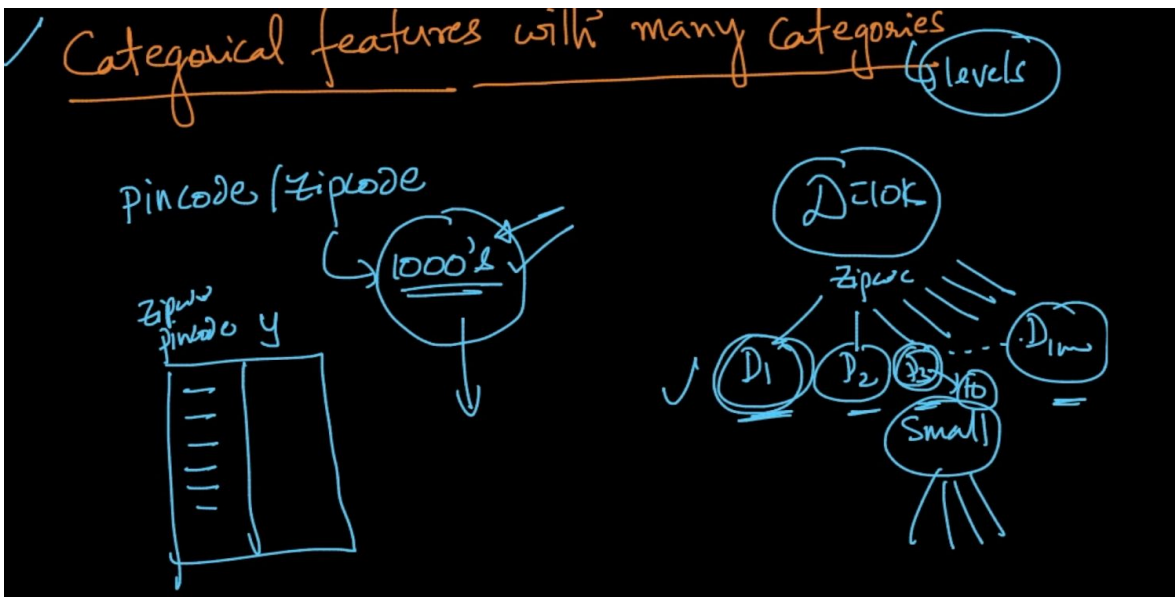


Threshold

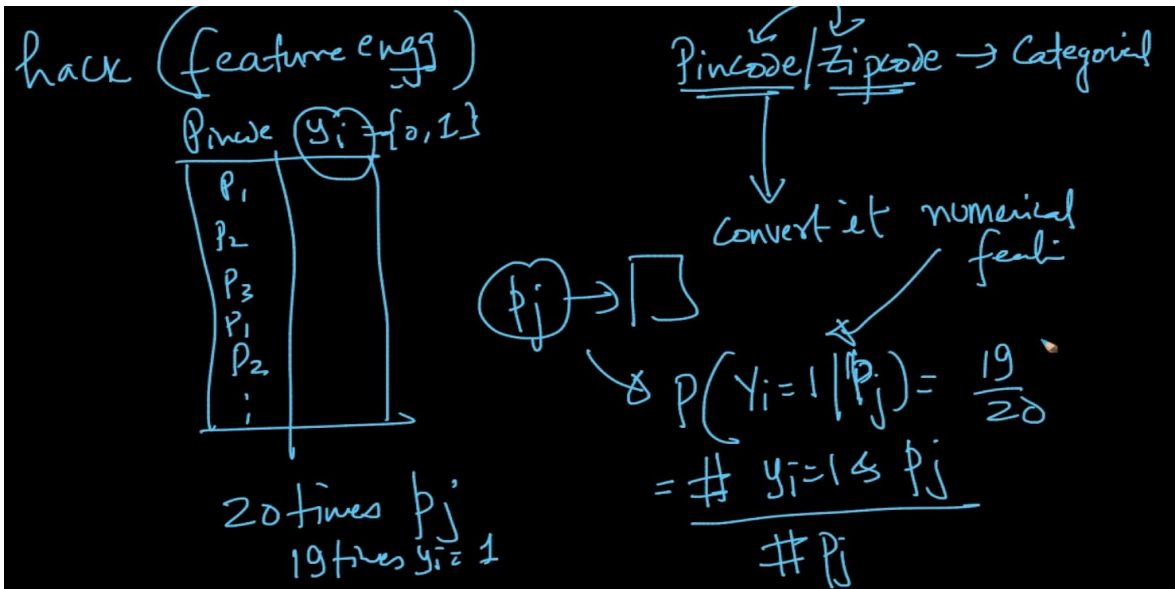


In Decision Trees we don't need to do Feature Standardization since it's not a distance based method like other ML algorithms we only care about whether something is greater than something or not. This is one of the great aspect of DT

CATEGORICAL FEATURES WITH MANY CATEGORIES



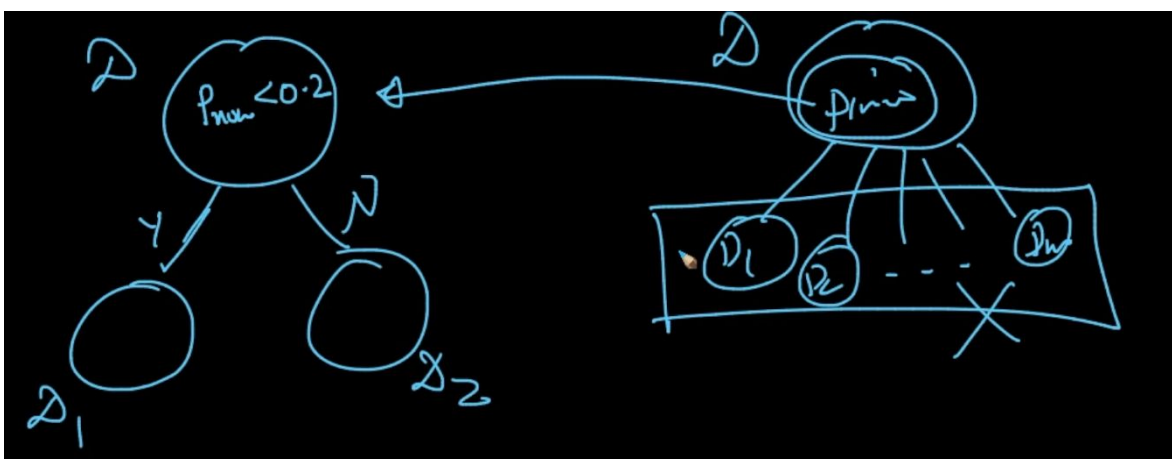
A Pincode is a Categorical feature since it can't be compared and it can be in 1000's in number so we will create 1000's of partitioned datasets which can be trivial



We can convert our Categorical Feature to a Numerical Feature . We convert it like above where $P(y_i = 1 | P_j)$ i.e Probability of $y_i = 1$ given Pincode P_j = No of points where $y_i = 1$ and P_j / No. of points where Pincode is P_j

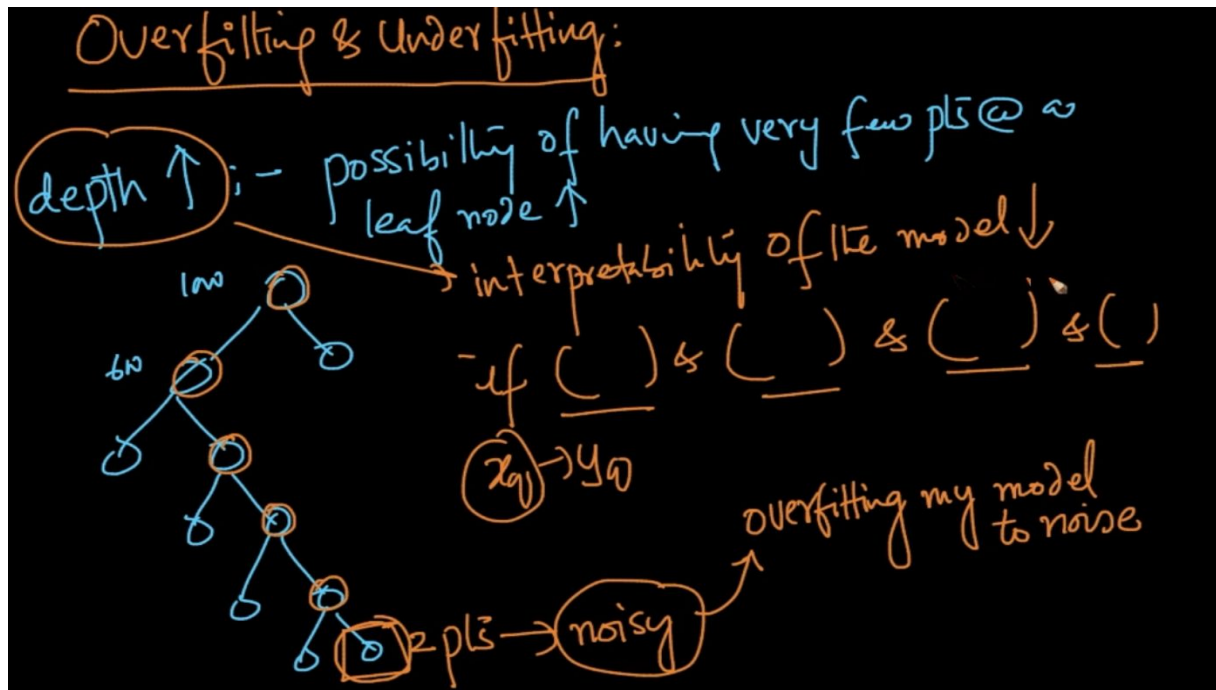
$p_j \rightarrow \text{numerical feature} = P(y_i=1 | p_j)$
 $\mathcal{D} \rightarrow \text{remove pincode feature}$
 \downarrow
 numerical features
 $p_i \& p_j$

So we are removing PinCode feature by converting it into Numerical Feature.

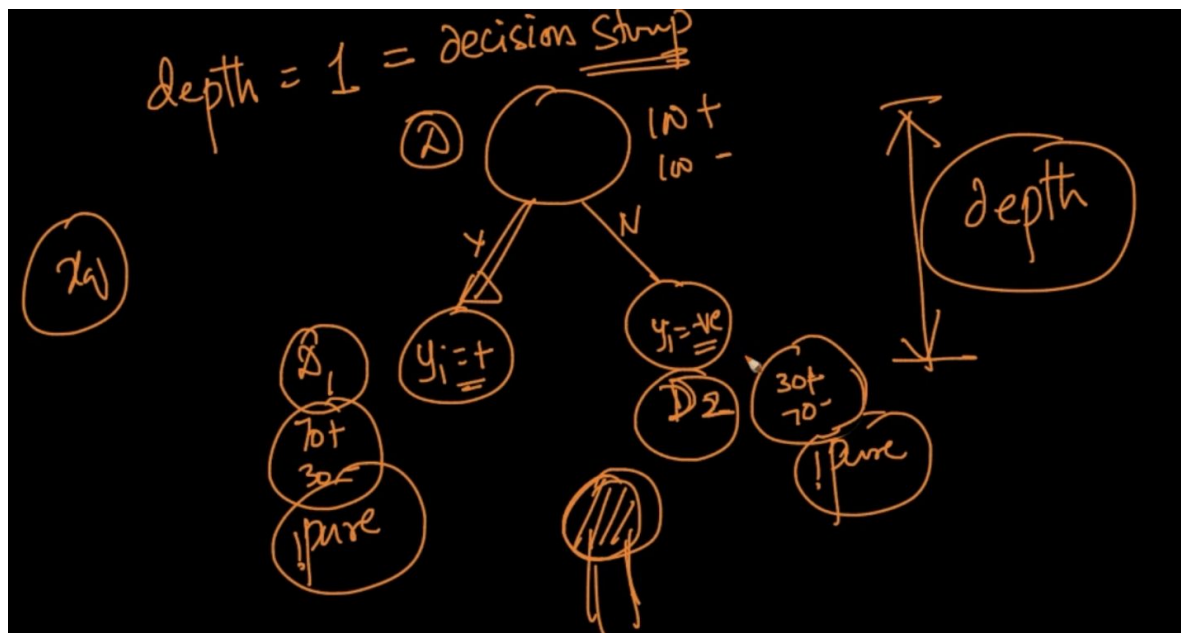


After converting The pincodes to Probability like above $P_{numerical} < 0.2$ we create the ideal partitions and getting rid of the problem of Data Sparsity

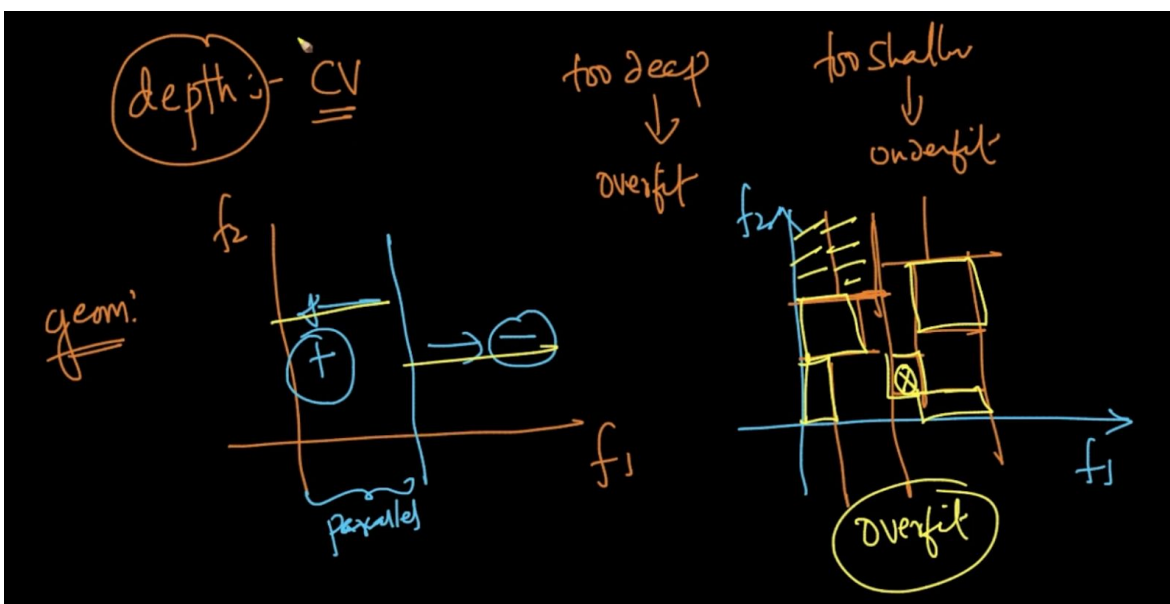
OVERFITTING AND UNDERFITTING



If the depth of the tree is very high then the possibility of few points at leaf node \uparrow which means we might overfit our model and interpretability of model \downarrow since many if conditions.

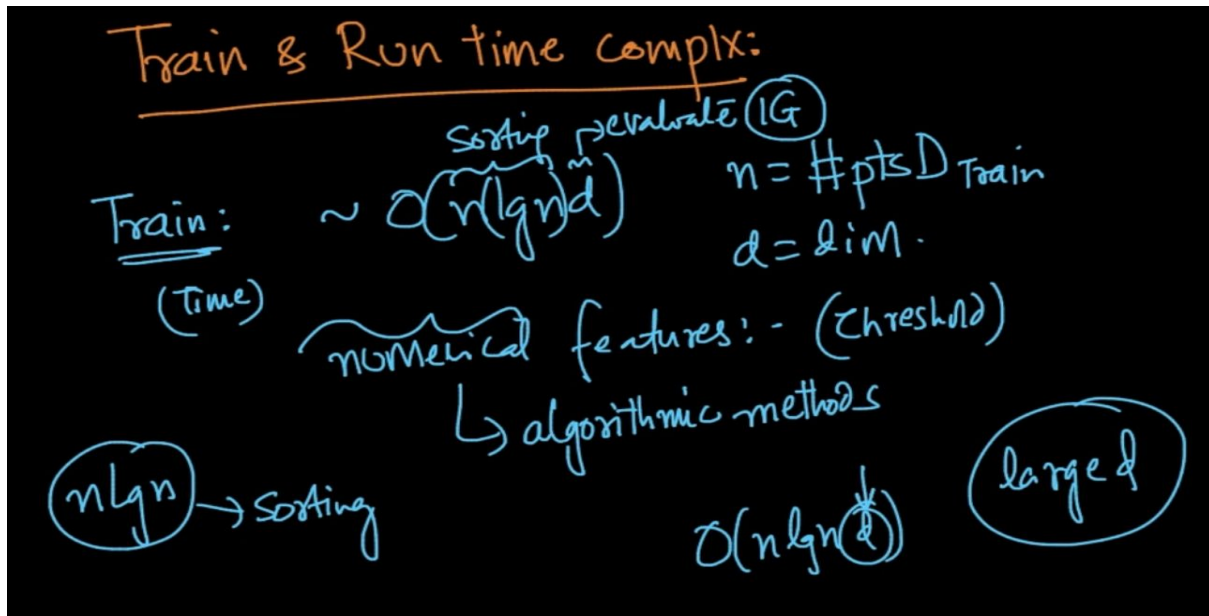


In a low depth tree suppose if we've 70+ve , 30 -ve points in D_1 and 70 -ve , 30 +ve points in D_2 we declare D_1 as +ve and D_2 as -ve although both are impure nodes



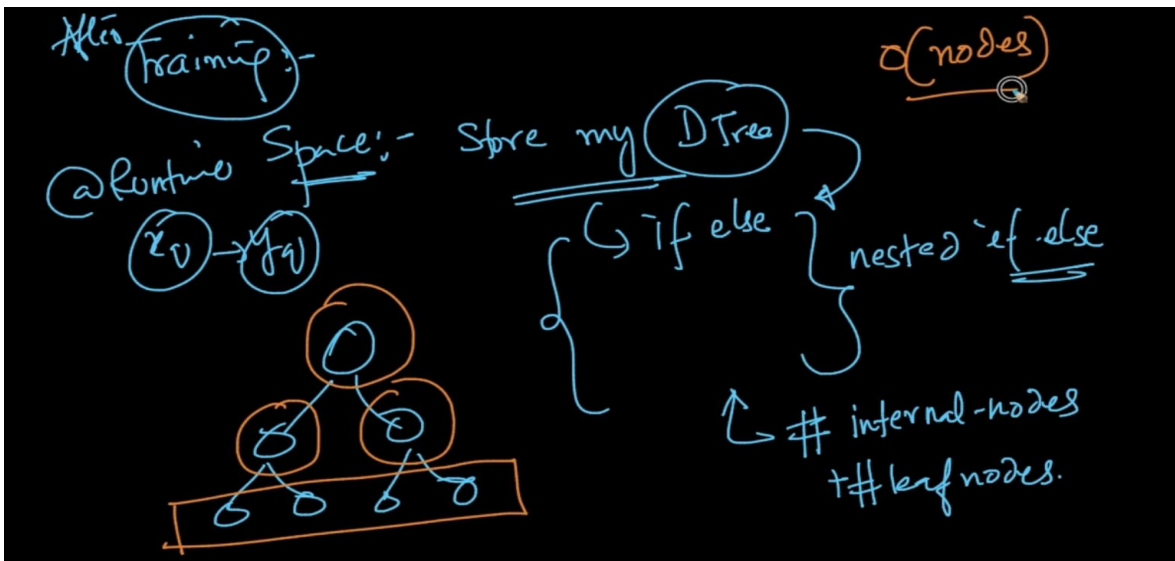
In the left figure , it is underfitting since only one axis parallel is dividing the dataset and in right there are many axis parallels so there can be an area where there's only 1 point and we might predict a query's class label using 1 point which is overfitting . So in order to decide the right depth we do Cross Validation

TRAIN AND RUN TIME COMPLEXITY

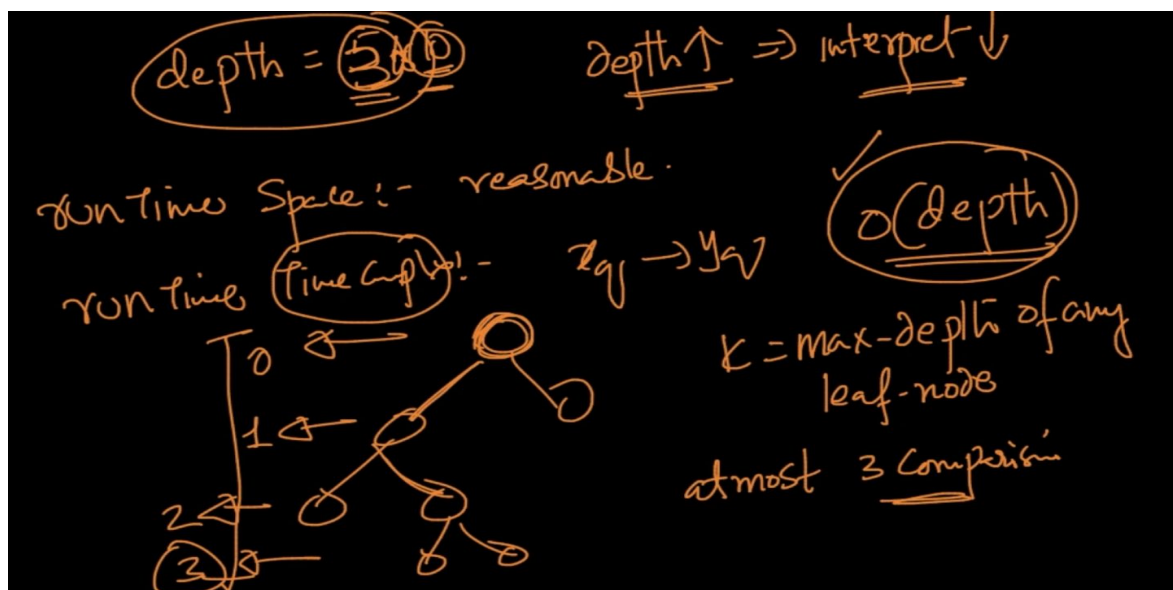


Train : $O(n * (\log n) * d)$ where n = No. of points in Training Dataset and d = dimensions

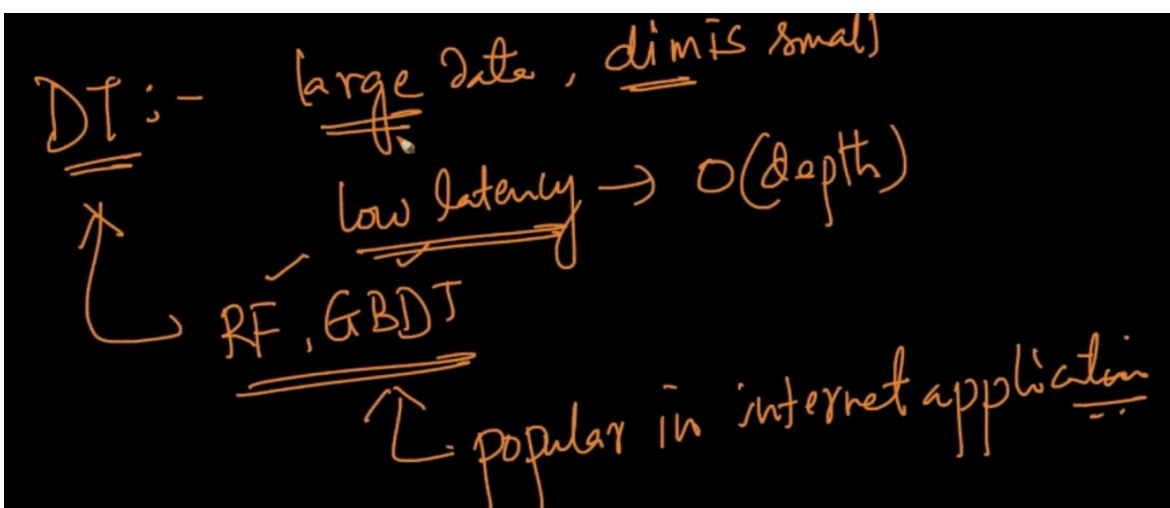
We've come up with algorithmic methods for Numerical Features. So, $(n * \log(n))$ should be for sorting since sorting has Time Complexity : $O(n * \log(n))$ and d is a multiplier since at every stage we've to compare the features so if our ' d ' is very large then Decision Tree isn't a great option



After Training : The Run Time Space Complexity :- Just to store a Decision Tree and it's not hard since a **Decision Tree** is basically a **nested if - else** and **storing** it is **No. of Internal Nodes + No. of leaf Nodes** which takes **very less** space = $O(\text{nodes})$ which is not too hard if you've **reasonable depth** of Decision Tree

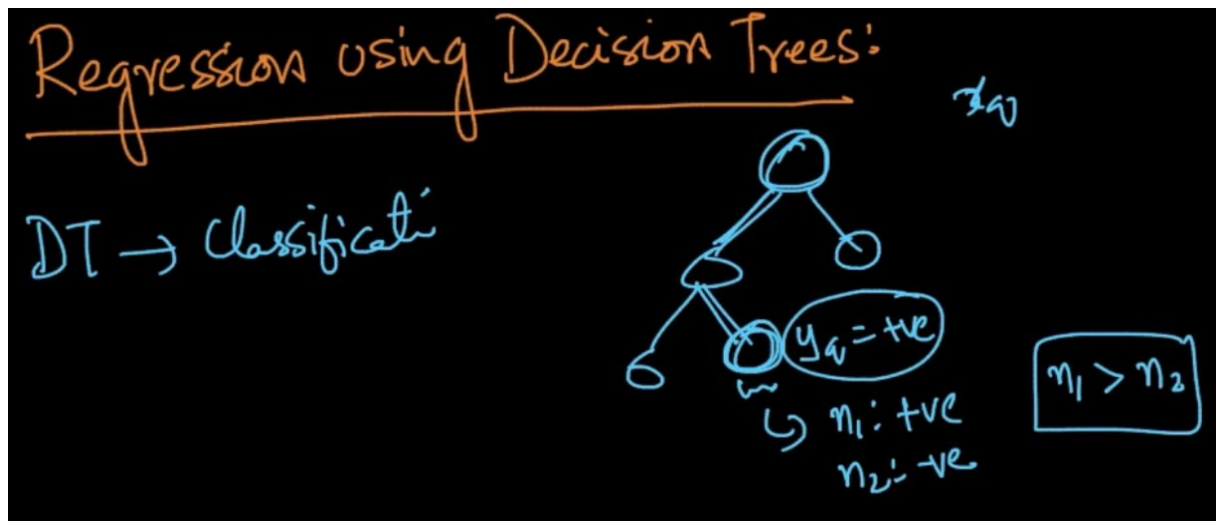


Our decision Tree has only depth = 5 or 10 because as depth \uparrow = interpretability \downarrow
 Runtime Time Complexity : It is just '**k**' where k = maximum depth of any leaf node
 Ex:- In the above Tree ' k ' = 3 because it has depth = 3 . So it's $O(\text{depth})$

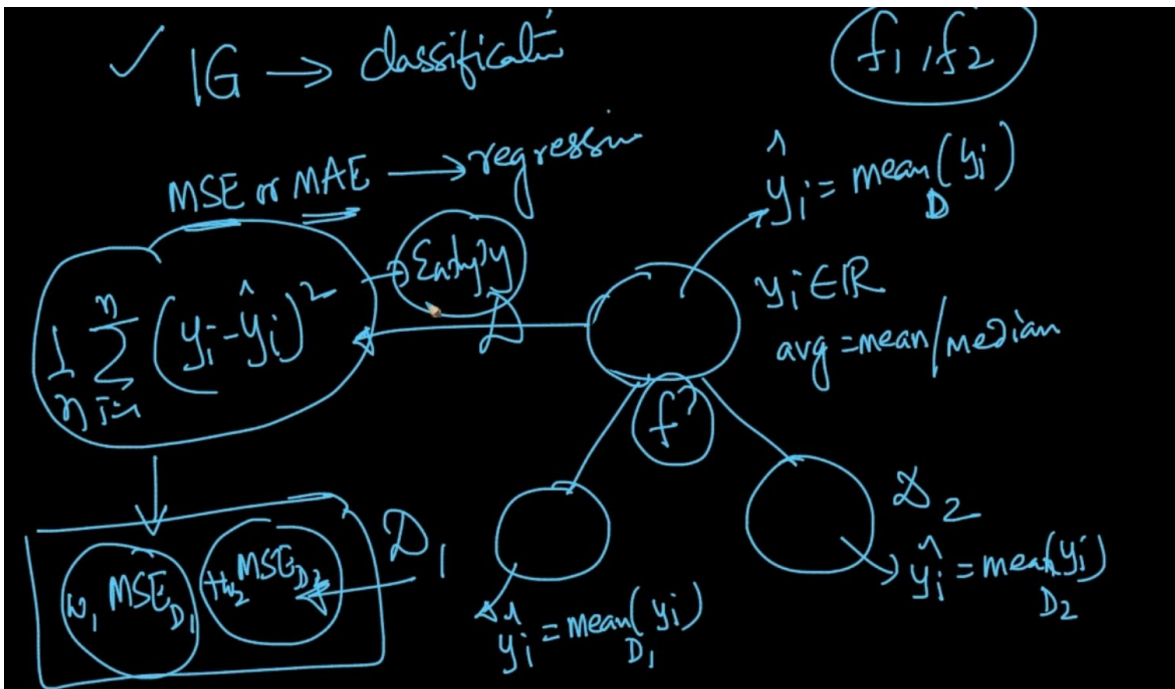


Decision Tree is good when we've the above features. Random Forest(RF), Gradient Boosting Decision Tree (GBDT) are different Decision Trees which are very popular

REGRESSION USING DECISION TREES

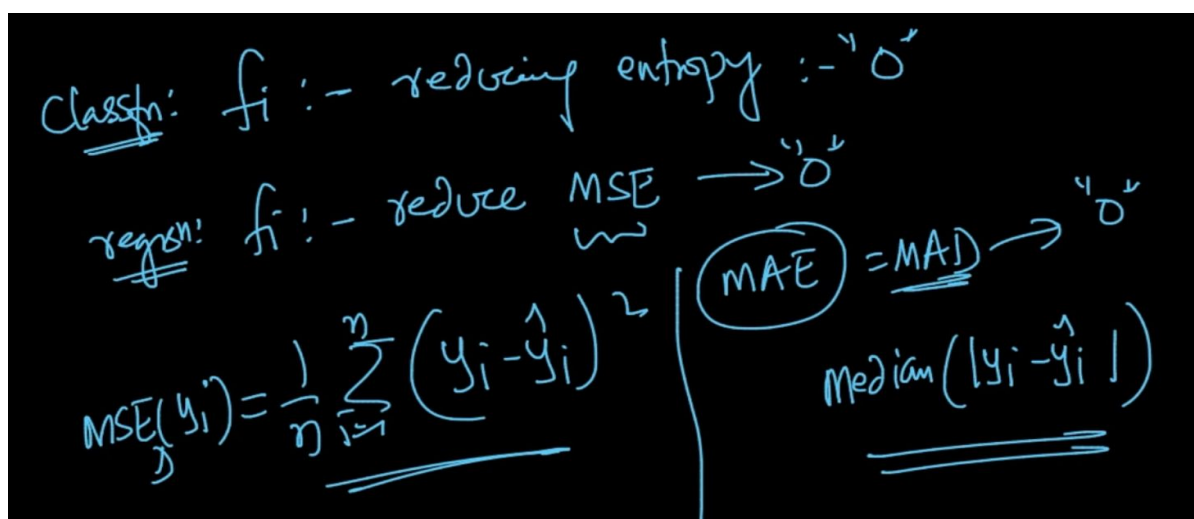


In Classification, in the leaf node $n_1: +ve$ and $n_2: -ve$ and $n_1 > n_2$ so if a new query x_q arrives at that leaf node it's $y_q = +ve$ since $n_1 > n_2$

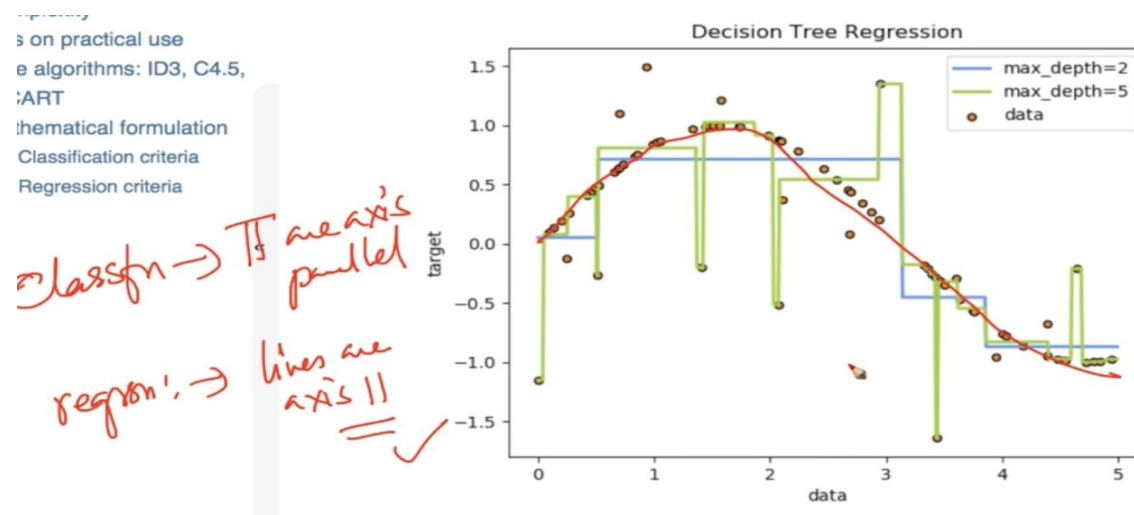


In Classification we used IG for feature selection. In Regression, we use Mean Squared Error or Mean Absolute Error. For the root node we take $\hat{y}_i = \text{mean}_D(y_i)$ i.e avg/median. Then we divide the dataset with some feature and for D_1 $\hat{y}_i = \text{mean}_{D_1}(y_i)$ for all 'y' in D_1

Same for D_2 . How do we decide which feature to use for breaking ? Just like IG we use Mean Squared Error (MSE) : $\frac{1}{n} \sum_{i=1}^n (y_i - \hat{y}_i)^2$ which is like Entropy and then we calculate $w_1 MSE_{D_1} + w_2 MSE_{D_2}$. Suppose we've features f_1, f_2 we split by both and whichever reduces $w_1 MSE_{D_1} + w_2 MSE_{D_2}$ we select that feature



In classification we wanted to reduce Entropy :- "0" and in Regression we wanted to reduce MSE/MAE - 0

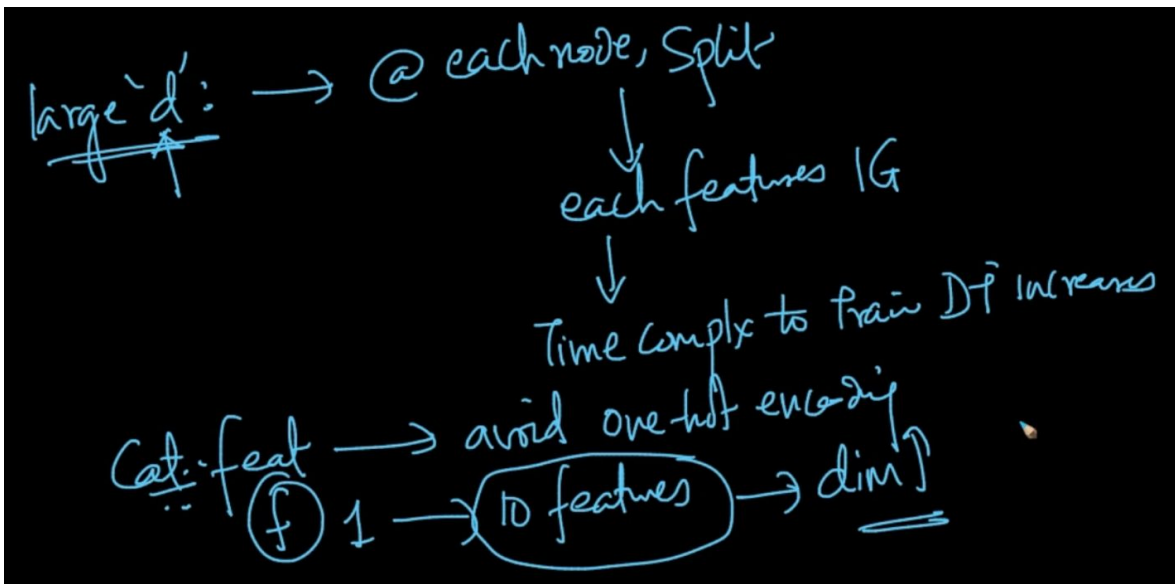


The red smooth curve is the ideal function but in Decision Trees when depth = 2 we get blue which is underfitting and depth = 5 (green) which is overfitting. In Classification and Regression with Decision Trees lines are axis-parallel

CASES



If we've Imbalanced data we need to balance it because it impacts Entropy Calculation



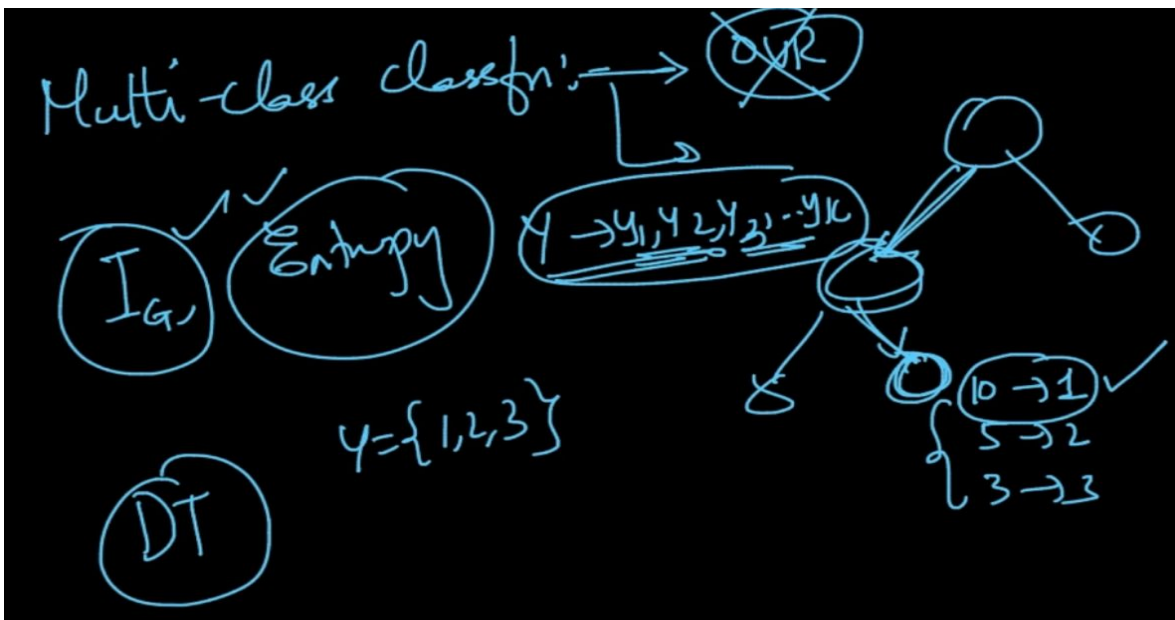
If we've large 'dimensions' we need to split for every feature for IG and if 'd' is large then Time complexity increases dramatically

If we've Categorical Features we need to avoid one-hot encoding because suppose we've a categorical feature f with 10 distinct values with one-hot encoding it'll be converted to 10 features

✓ Categorical feat → numerical feat
 lots of levels
 ✓ $P(y_i=1 | f=C_1)$ ✓
Similarity Matrix :- DT need the features explicitly

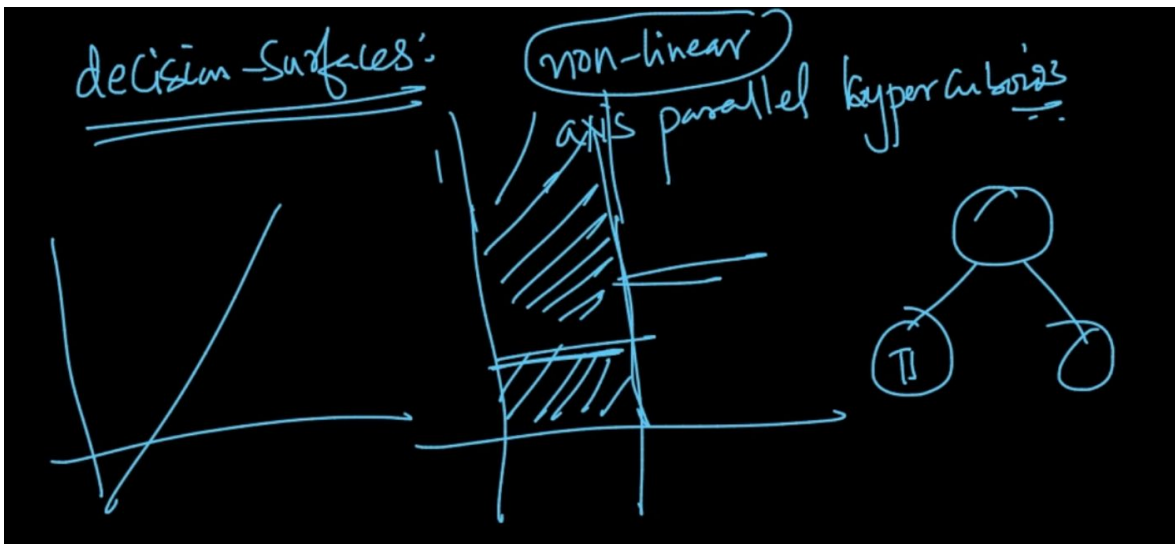
So if we've Categorical features with lot of categories we convert them into a numerical feature $P(y = 1 | f = C_1)$ where C is category

We can't use Similarity Matrix since DT needs the features explicitly for Entropy calculation

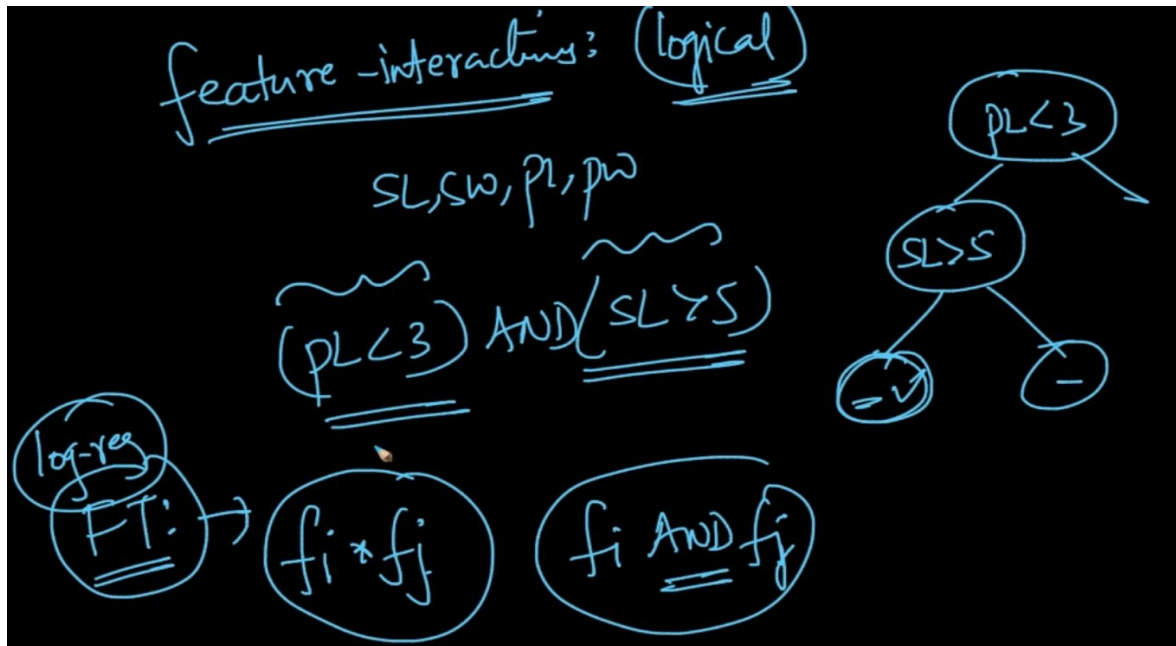


For multiclass classification we don't need to do One v/s Rest because suppose $y = \{1, 2, 3\}$

So if a query arrives at a leaf where 1 -> 10 pts, 2 -> 5 pts and 3 -> 3 pts it's $y = 1$ since it has majority



Decision Surfaces : They are axis parallel hypercuboids. Here there;s no just 1 hyperplane separating but multiple hyperplanes where each decision surface corresponds to Decision nodes

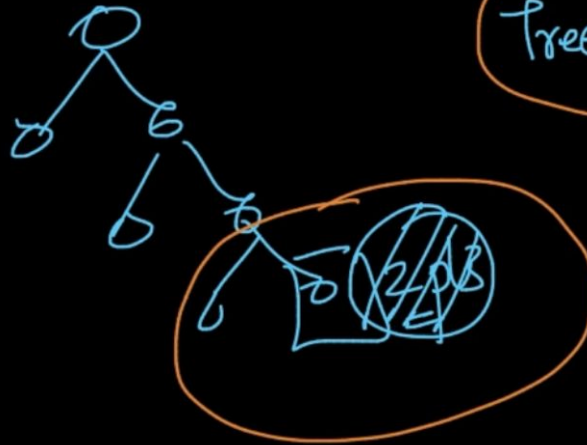


Feature Interactions : If a new query arrives at leaf nodes with $(PL < 3)$ AND $(SL > 5)$ Then features PL, SL are interacting with each other

Outliers?

depth ↑ :- outlier will impact

Tree Constable

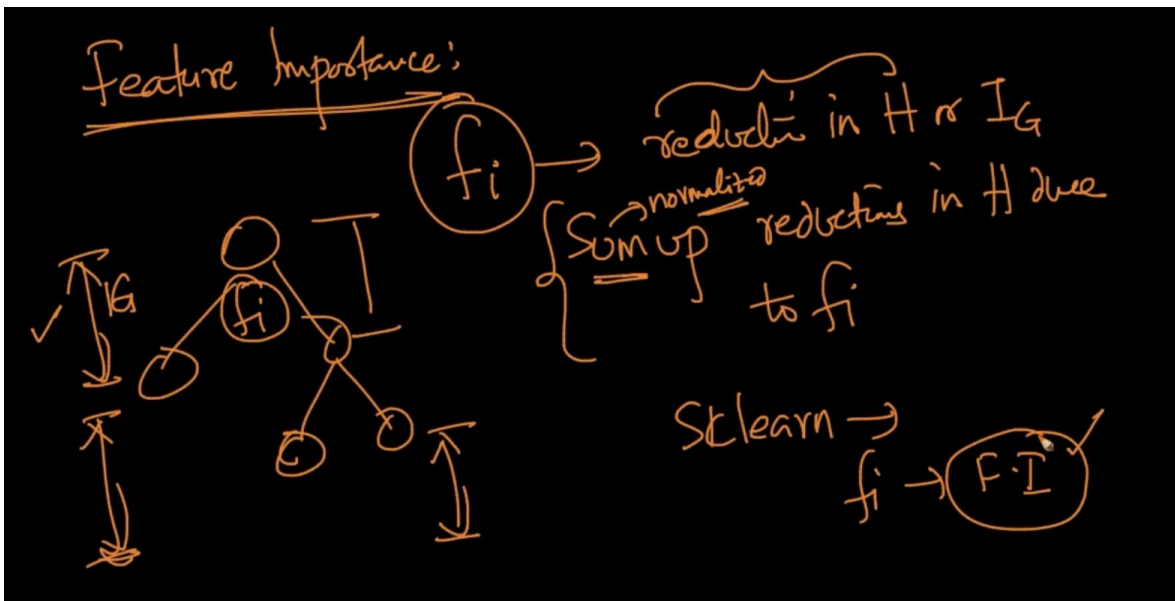


If the depth of the tree increases then Outliers affect Decision Trees

Interpretability:-

[illegible]

Decision Trees are super Interpretable since it's just Nested if-else which are very easy to understand if the depth is not too large



Feature Importance : A feature f_i tells us about reduction in IG or H . We sum up reductions in H due to f_i . SO whichever features gives the maximum reduction is an important feature