Final Project

QH20 Water Potability Analysis



Group No. 01

B. Thanushan - S14025

W. S. S. Fernando - \$13990

W. M. C. B. Weerakoon - S14028

1) Abstract

The main objective of this analysis is to build a model to predict the potability of water of a resource using water quality metrics. We are also interested in finding out which factors affect the most for the potability of the water. The dataset consists of data of 3276 different water bodies collected on 10 water quality metrics including the response variable. The descriptive analysis showed that pH value, amount of sulfate, amount of chloramines, and the number of trihalomethanes affect the potability of the water than other factors. Also, some relationships between the water quality metrics have been revealed. Advanced analysis was done by fitting classification techniques such as Logistic Regression, Decision Tree Classifier, Random Forest, and XG-Boost in two different ways. The first way was carried out by changing certain numerical variables to categories and the other way was carried out by taking the numerical values directly. The models with directly used numerical values performed better. The feature selection was applied to find the most important variables for each model. The models were evaluated using the AUC score and accuracy score. The XG-Boost technique outperformed other techniques with a 69.92% accuracy score. A web application was developed for the QH2O water purifier services with the functionality to predict whether the water body is safe for consumption given the values for the given factors. This application can help the water beverages companies who are the clients for QH2O to check whether the water body can be used or not.

2) Table of Contents

1)	Abstract
2)	Table of Contents
3)	List of Figures
4)	List of Tables
5)	Introduction
6)	Description of the Problem.
7)	Description of The Dataset
8)	Descriptive Analysis
I	Analysis of pH5
I	Analysis of Hardness5
I	Analysis of Sulfate6
I	Analysis of Chloramines
I	Analysis of Trihalomethanes
I	Analysis of Turbidity
(Correlation Plot
9)	Advanced Analysis
10)	Discussion and Conclusions
11)	References 10
12`	Appendix and Code

3) List of Figures 4) List of Tables

5) Introduction

Water is a basic human need. Also, water is a vital requirement in the agricultural sector, electricity generation, and many industrial sectors. Although 71% of the earth is covered with water, only around 0.8% of the earth's water is potable. Hence, clean, safe water is a scarce resource that people need to preserve.

The main causes of water pollution are not natural causes but human activities. Around 80% of the worlds' wastewater is dumped back into the water streams. Also, people dump garbage and oil into water streams too. Unsafe water kills more people each year than war and all other forms of violence combined. Since this has become a serious issue in the world, various organizations urge factories to treat their wastewater before releasing them to the environment.

6) Description of the Problem

With all the polluted water resources in the world, a system to identify clean, potable water has become a necessity. We are going to build a model to predict whether the water from different water streams is safe to consume or not. Also, we are interested in finding out which substances in the water that have a major impact on water pollution. Finally, creating a website that will predict whether the water from the stream is potable or not through the built model.

7) Description of The Dataset

Dataset is obtained from the Kaggle website. It consists of data of 3276 different water bodies collected on 10 water quality metrics. Potability is the response variable.

Variable	Type	Description
pH value	Continuous	pH value of the water body.
Hardness	Continuous	The capacity of water to precipitate soap in mg/L
Solids	Continuous	Total dissolved solids in ppm
Chloramines	Continuous	Amount of Chloramines in ppm
Sulfate	Continuous	Amount of Sulfates dissolved in mg/L
Conductivity	Continuous	Electrical conductivity of water in μS/cm
Organic_carbon	Continuous	Amount of organic carbon in ppm
Trihalomethanes	Continuous	Amount of Trihalomethanes in μg/L
Turbidity	Continuous	A measure of the light-emitting property of water in NTU (Nephelometric Turbidity Units)
Potability (Response)	Categorical	Indicates if water is safe for human consumption

Table 7-1: Description of the Dataset

8) Descriptive Analysis

Analysis of pH

According to (World Health Organization, 2007), the pH of most drinking water lies within the range of 6.5–8.5. According to the figure, it is clear that the highest percentage of pH values of potable water falls within this range. Also, it is evident that the pH value is not the only factor for the water to be potable since the water of other pH levels is

fluctuate massively. This happens since a high percentage of data

has pH levels 6.00 - 8.00. The data from this category

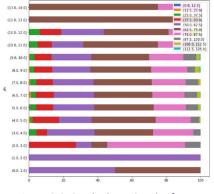


Figure 8-2: Stacked Bar Graph of pH vs. Trihalomethanes

overshadows the fluctuations.

also potable in some percentages.

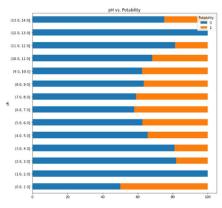


Figure 8-1: Stacked Bar Graph of pH vs. Potability

Even a small change of pH exerts a marked effect on trihalomethanes formation. Therefore, even minute pH fluctuations may result in wide variations of trihalomethanes (Amarasooriya et al, 2018). But in our dataset, even though the

pH levels change, trihalomethane levels do not

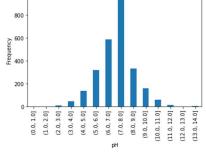


Figure 8-3: Bar Chart of pH

Analysis of Hardness

The simple definition of water hardness is the amount of dissolved calcium and magnesium in the

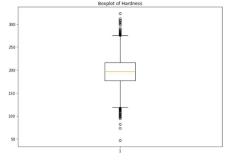


Figure 8-5: Boxplot of Hardness

water (Hardness of Water, 2021). Water supplies with a hardness greater than 200 mg/L are considered poor but have been tolerated by consumers;

those in excess of 500 mg/L are

unacceptable for most domestic purposes (Health Canada, 1995).

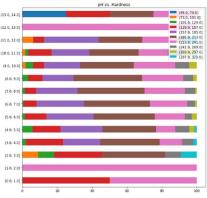


Figure 8-4: Stacked Bar Graph of pH vs. Hardness

According to the figure, the median hardness of the water is just below 200mg/l. It is stated in

300 Hardness Sulfate

200 0 500 1000 1500 2000 2500 3000

(Think Fish, 2013) that dissolved minerals tend to counter the effects of acids in the water, preventing the pH from dropping. Therefore, in most cases, hard water usually has a high (alkaline) pH, whilst soft water has a low (acidic) pH. But this does not reflect in the dataset. This can be due to the sulfate concentration being higher than the level of hardness in water since

Figure 8-6: Scatterplots of Hardness and Sulfate

according to (Sulfate and water quality, n.d.), sulfates are most often related to their ability to form strong acids which change the pH.

Analysis of Sulfate

According to (Oram, n.d.), The SMCL (Secondary Maximum Contaminant Level) for sulfate in drinking water is 250 mg/l. It can be seen that there is a high percentage of potability

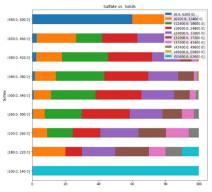


Figure 8-8: Stacked Bar Graph of Sulfate vs. Solids

around 250 mg/l sulfate
levels in the dataset too.

There is a low water
potability percentage in
sulfate levels between 300
mg/l and 460mg/l. This can

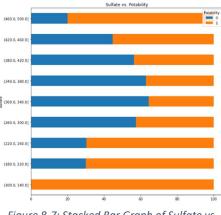
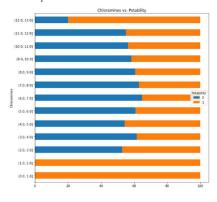


Figure 8-7: Stacked Bar Graph of Sulfate vs.

be due to the high percentage of solids in those levels as according to (Oram, n.d.), elevated total dissolved solids can

result in your water having a bitter or salty taste which affects the potability of water.

Analysis of Chloramines



Chloramine levels up to 4 mg/l or 4 ppm are considered safe in drinking water according to (CDC, 2020). In the dataset, levels up to 3mg/l have a high percentage of potability. But in level 3mg/l to 4mg/l has a low percentage of potability. This is due to the presence of high levels of solid concentration in that level of chloramines since as earlier explained elevated total dissolved Figure 8-9 Stacked Bar Graph of Chloramines vs. Potability solids can result in your water having

a bitter or salty taste which affects the potability of water. Furthermore, (Friedler et al., 2021) stated that the regression coefficient of solids is negative when the level of solids is regressed against the level of chlorine. This implies that the solids in water affect negatively in the process of chlorine disinfection. This can be reflected in the figure since when the level of chloramine concentration is increasing, the level of solid concentration is decreasing.

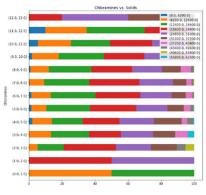
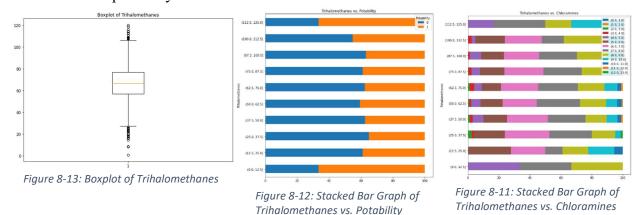


Figure 8-10: Stacked Bar Graph of Chloramines vs. Solids

Analysis of Trihalomethanes

Trihalomethanes are the result of a reaction between the chlorine used for disinfecting tap water and natural organic matter in the water (Hood, 2005). This can be seen from the figure as the level of trihalomethanes increases, the level of chloramines also increases. According to (EPA, 2016), the maximum allowable trihalomethanes level is 100 ppb. Since the level of trihalomethanes of almost all the data is below 100ppb but not all the data is potable, we can declare that other factors affect the water potability than trihalomethanes.



Analysis of Turbidity

Turbidity describes the cloudiness of water caused by suspended particles (WHO, 2017). Also, the WHO establishes that the turbidity of drinking water shouldn't be more than 5 NTU, and should ideally be below 1 NTU. According to the figure, the turbidity of the majority of the data is below 5NTU.

The stacked bar chart of turbidity vs. pH values show that when turbidity is increasing, the level of pH decreases. But, according to

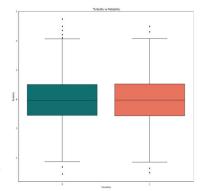


Figure 8-14: Boxplots of Turbidity vs. Potability

(Mohammed, 2015), there is no significant direct influence of pH on turbidity. But when the turbidity is increasing, the conductivity also increases. Hence, there are free ions in the water at high turbidity levels. According to (Hancock, n.d.), the coagulation process to eliminate turbidity requires positive ions. Therefore, there is a possibility of the coagulation process happening at high turbidity levels. It is stated in (Whitman.edu) that the coagulation process releases hydrogen ions into the water. Hence, the pH values of water will be decreased. Therefore, when turbidity is increasing, the pH values will decrease.

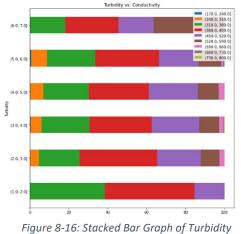


Figure 8-16: Stacked Bar Graph of Turbidity vs. Conductivity

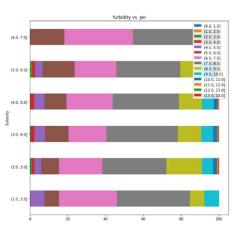


Figure 8-15: Stacked Bar Graph of Turbidity vs. pH

Correlation Plot

There are no significant correlations between variables.

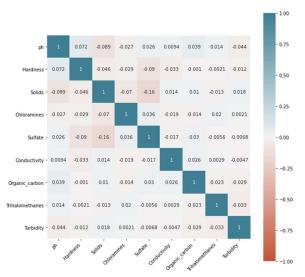


Figure 8-18: Correlation Plot of Predictor Variables

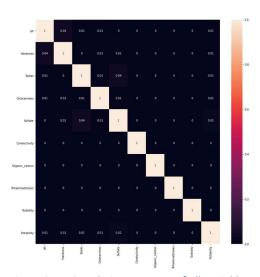


Figure 8-17: Correlation Heatmap of All Variables

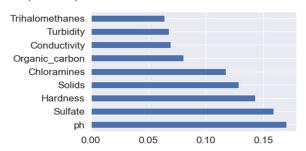
9) Advanced Analysis

It has been concluded to use classification techniques such as Logistic Regression, Decision Tree Classifier, Random Forest, and XG Boosting from the results of the explorative data analysis. The AUC value and the Model Accuracy Score of models are used in evaluating the models. The advanced analysis was performed in two ways. The first way was done by changing some of the numerical variables to categorical variables in a proper way from the findings of a research paper. For example, hardness was classified into soft, slightly hard, moderately hard, hard, and very hard if values lie in between 0-17.1, 17.1-60, 60-120, 120-180, and 180-above respectively. The second way was done by using the numerical variable directly in model fitting. From the results, it was found that using the numerical values directly gave a better result than the first way.

There were 491, 781, and 162 missing values in PH, Sulfate, and Trihalomethanes respectively. These values were less than 30% from the dataset and the variables were normally distributed. Hence, the missing values were imputed with the mean. The logistic regression is sensitive to outliers. Therefore, the outliers were handled by the capping method since the number of observations was small. The tree-based methods were not sensitive to outliers. Hence, the data was used without capping the outliers when fitting tree-based methods. The feature selection was done using recursive feature elimination.

The variables PH, hardness, chloramines, organic carbon, and turbidity were selected as the important variables in logistic regression. The parameters C and solver were chosen as 1 and 'lbfgs' by parameter tuning. The variables sulfate, solids, hardness, PH, and chloramines were selected as the important variables in the Decision Tree Method. The max depth, max features, min samples leaf, and min sample split were chosen as 9, auto, 5, and 0.01 respectively from parameter tuning. The variables PH, sulfate, hardness, solids, and chloramines were selected as

the important variables in Random Forest Model. The criterion, max features, max depth, and the number of estimators were chosen as 'Gini', 9, auto, and 300 from parameter tuning. The variables PH, sulfate, hardness, solids, and



chloramines were selected as the important *Figure 9-1: Feature Importance Plot of the XGBoost Model* variables in Random Forest Model. The gamma, learning rate, max depth, number of estimators,

and sub-sample were chosen as 0.1, 0.01, 8, 300, and 0.6 respectively from parameter tuning. The table shows the AUC scores and accuracy scores of the models. The figure shows the important variable plot of the XGBoost Model.

Models	AUC score	Accuracy Score
Logistic Regression	0.5	0.5991
Decision Tree	0.5720	0.6372
Random Forest	0.6069	0.6723
XG boost	0.6473	0.6992

Table 0-1: AUC Scores and the Accuracy Scores of the Models

10) Discussion and Conclusions

The main objective of the study is to predict whether the water body is safe for human consumption. The second objective is to find the factors that affect water purity. The objectives were achieved by the descriptive and advanced analysis.

The PH value, Sulfate, Hardness, Solids, and chloramines are the factors that mostly impact whether the water body can be used for the consumption or not since these variables were chosen as the important variables in most of the techniques. The XG boost model was selected as the best model to predict whether the water body is safe for human consumption. A website was created with the prediction feature using the best model.

In the advanced analysis, several ways have been tried to improve the model but no improvements were found in the accuracy and AUC scores. Therefore, it is suggested to take more observations to improve the model.

11) References

World Health Organisation. (2007). pH in drinking-water. *Guidelines for Drinking Water Quality*, 2(2), 1–7.

http://www.who.int/water_sanitation_health/dwq/chemicals/ph_revised_2007_clean_version.pdf

Usgs.gov. 2021. *Hardness of Water*. [online] Available at: https://www.usgs.gov/special-topic/water-science-school/science/hardness-water?qt-science_center_objects=0#qt-science_center_objects>.

Health Canada. (1995). Sources and Levels of Hardness. *World Health*, 1979(February 1979), 40–43.

Think Fish. 2013. [online] Available at: https://www.thinkfish.co.uk/article/testing-for-ph-and-hardness-in-an-aquarium>.

State.ky.us. n.d. *Sulfate and water quality*. [online] Available at: http://www.state.ky.us/nrepc/water/ramp/rmso4.htm>.

Oram, B., n.d. *Sulfate, Hydrogen Sulfide, Sulfate Reducing Bacteria - How to Identify and Manage*. [online] Water Research Center. Available at: https://www.water-research.net/index.php/sulfates.

Cdc.gov. 2020. Water Disinfection with Chlorine and Chloramine | Public Water Systems | Drinking Water | Healthy Water | CDC. [online] Available at: https://www.cdc.gov/healthywater/drinking/public/water disinfection.html.

Friedler, E., Chavez, D. F., Alfiya, Y., Gilboa, Y., & Gross, A. (2021). Impact of suspended solids and organic matter on chlorine and UV disinfection efficiency of greywater. *Water (Switzerland)*, 13(2). https://doi.org/10.3390/w13020214

Hood, E., 2005. Tap Water and Trihalomethanes: Flow of Concerns Continues. *Environmental Health Perspectives*, 113(7).

Archive.epa.gov. 2016. *EPA* | *Envirofacts* | *ICR* | *Regulations*. [online] Available at: https://archive.epa.gov/enviro/html/icr/web/html/regulations.html>.

Amarasooriya, A., Weragoda, S., Makehelwala, M. and Weerasooriya, R., 2018. Occurrence of trihalomethane in relation to treatment technologies and water quality under tropical conditions. *H2Open Journal*, 1(1), pp.69-83.

WHO. (2017). WATER QUALITY AND HEALTH - REVIEW OF TURBIDITY: Information for regulators and water suppliers. *Who/Fwc/Wsh/17.01*, 10. https://www.who.int/water_sanitation_health/publications/turbidity-information-200217.pdf

Mohammed, S., 2015. Effect of pH on the Turbidity Removal of Wastewater. *OALib*, 02(12), pp.1-9.

Hancock, N., n.d. Conventional Water Treatment: Coagulation and Filtration — Safe Drinking Water Foundation. [online] Safe Drinking Water Foundation. Available at: https://www.safewater.org/fact-sheets-1/2017/1/23/conventional-water-treatment>.

Whitman.edu. n.d. [online] Available at: https://www.whitman.edu/chemistry/edusolns software/AlkalinityBackground.pdf>.

12) Appendix and Code

```
plt.title("Histogram of Hardness")
# In[37]:
fig = plt.figure(figsize = (10, 7))
plt.title("Boxplot of Hardness")
plt.boxplot(train["Hardness"])
                                                                                                                                                                                                                                                                                                                                                                                                              sns.boxplot(x="Potability", y =
train[col], data=train, palette= my_pal)
plt.title(f' {col} vs Potability')
plt.figure(figsize=(15,15))
# In[2]:
import numpy as np
import pandas as pd
import matplotlib.pyplot as plt
import scipy.stats as stats
from sklearn.model_selection import
train_test_split
# In[10]:
data=pd.read_csv/mp./ca.
                                                                                                                                                                                                                                                                                                                                                                                                             pl.figure(figsize=(15,15))
# In[120]:
bucket_ph = np.linspace(0, 14, 15)
bucket_ph
# In[121]:
train["ph"] = pd.cut(train["ph"],
bucket_ph)
train.head()
# In[100]:
                                                                                                                                                                                                              In[38]:
                                                                                                                                                                                                       # In[38]:
plt.hist(train["Solids"], color="tomato")
plt.title("Histogram of Solids")
                                                                                                                                                                                                      pit.title("Histogram or Solids")
# In[39]:
fig = plt.figure(figsize = (10, 7))
plt.title("Boxplot of Solids")
plt.boxplot(train["Solids"])
# In[40]:
# In[109]:
data=pd.read_csv("D:/Studies/ST 4052 -
Statistical Learning II/Final
Project/water_potability.CSV")
# Tr(110)
                                                                                                                                                                                                                                                                                                                                                                                                              # In[100]:
train["ph"].value_counts().sort_index().plo
                                                                                                                                                                                                      plt.boxplot(train["Solids"])
# In[40]:
plt.hist(train["Chloramines"],
color="tomato")
plt.title("Histogram of Chloramines")
# In[41]:
fig = plt.figure(figsize = (10, 7))
plt.title("Boxplot of Chloramines")
plt.boxplot(train["Chloramines"])
# In[41]:
                                                                                                                                                                                                                                                                                                                                                                                                             train["ph"].value_count
t.bar()
plt.xlabel("pH")
plt.ylabel("Frequency")
plt.title("pH")
# In[116]:
# In[110]:
data.head()
# In[5]:
data.isna().any()
 data.isna().sum()
                                                                                                                                                                                                                                                                                                                                                                                                             ph_Pot = pd.crosstab(index=train["ph"],
columns=train["Potability"])
 data.isna().sum()/len(data)
                                                                                                                                                                                                                                                                                                                                                                                                             ph_Pot
# In[117]:
ph_Pot = ph_Pot.div(ph_Pot.sum(axis = 1),
axis = 0)*100
                                                                                                                                                                                                      in(42):
in(42):
plt.hist(train["Sulfate"], color="tomato")
plt.title("Histogram of Sulfate")
if In(43):
if p = plt.figure(figsize = (10, 7))
plt.title("Boxplot of Sulfate")
plt.boxplot(train["Sulfate"])
if In(44):
plt.hist(train["Conductivity"],
color="comato")
plt.title("Histogram of Conductivity")
if In(45):
if
                                                                                                                                                                                                             In[42]:
# In[8]:
data_1=data.dropna(how="any")
data_1.head()
                                                                                                                                                                                                                                                                                                                                                                                                              ph_Pot
# In[138]:
 stats.probplot(data 1["ph"], dist="norm",
                                                                                                                                                                                                                                                                                                                                                                                                             # In[138]:
ph_Pot.plot(kind = "barh", stacked = True,
figsize=(10, 10))
plt.title ("pH vs. Potability")
# In[123]:
ph_Pot1 = pd.crosstab(index=train["ph"),
columns=train["Potability"]).transpose()
plot=plt)
plt.show()
pit.snow()
# In[9]:
stats.probplot(data_1["Sulfate"],
dist="norm", plot=plt)
plt.show()
                                                                                                                                                                                                      plt.title("Histogram of Conductivity")
# In[45]:
fig = plt.figure(figsize = (10, 7))
plt.bixplot ("Boxplot of Conductivity")
plt.boxplot (train["Conductivity"])
# In[103]:
plt.hist(train["Organic_carbon"],
color="tomato")
plt.title("Histogram of Organic Carbon")
# In[105]:
                                                                                                                                                                                                                                                                                                                                                                                                            stats.probplot(data_1["Trihalomethanes"],
dist="norm", plot=plt)
dist="norm", plot=pit)
plt.show()
# In[111]:
# split into train test sets
craim, test =
train_test_split(data,test_size=0.2,random_
state= 20)
                                                                                                                                                                                                      plt.title("Histogram of Organic Carbon")
# In[105]:
fig = plt.figure(figsize = (10, 7))
plt.title("Boxplot of Organic Carbon")
plt.boxplot(train["Organic_carbon"])
# In[48]:
plt.hist(train["Trihalomethanes"],
color="tomato")
plt.title("Histogram of Trihalomethanes")
# In[51]:
state= 20)
# In[114]:
train.shape
# In[115]:
test.shape
# In[94]:
                                                                                                                                                                                                                                                                                                                                                                                                             plt.title("pH vs. Potability")
plt.legend(loc='upper right')
# In[122]:
bucket Har = np.linspace(45, 325, 11)
bucket Har
# In[123]:
                                                                                                                                                                                                                                                                                                                                                                                                            # In[123]:
    train["Hardness"] =
    pd.cut(train["Hardness"], bucket_Har)
    train.head()
# In[29]:
    train["Hardness"].value_counts().sort_index
().plot.bar()
    plt.xlabel("Hardness")
    plt.ylabel("Frequency")
    plt.title("Hardness")
# In[33]:
    Har_Pot =
    pd.crosstab(index=train["Hardness"],
    columns=train["Potability"])
    Har_Pot
 train.isna().anv()
 # In[16]:
                                                                                                                                                                                                        # In[51]:
fig = plt.figure(figsize =(10, 7))
plt.title("Boxplot of Trihalomethan
   test.isna().anv()
                                                                                                                                                                                                      pl.title("Boxplot of Trihalomethanes")
plt.boxplot(train["Trihalomethanes"])
# In[52]:
 train.isna().sum()
                                                                                                                                                                                                       # In[52]:
plt.hist(train["Turbidity"],
 test.isna().sum()
 # In[19]:
                                                                                                                                                                                                        color="tomato")
                                                                                                                                                                                                      color="tomato")
plt.title("Histogram of Turbidity")
# In[53]:
fig = plt.figure(figsize = (10, 7))
plt.title("Boxplot of Turbidity")
plt.boxplot(train["Turbidity"])
# In[62]:
  train.isna().sum()/len(train)
tlain.isia().sum()/len(tlain)
# In[20]:
test.isna().sum()/len(test)
# In[116]:
train["ph"].fillna(train["ph"].mean(),inpla
                                                                                                                                                                                                                                                                                                                                                                                                             Har_Pot # In[34]:

# In[34]:

Har_Pot = Har_Pot.div(Har_Pot.sum(axis = 1), axis = 0)*100

Har_Pot # In[35]:

Har_Pot.plot(kind = "barh", stacked = True, firsize=(10.10)
 ce=True)
                                                                                                                                                                                                      train.head()
 train.nead()
f In[17]:
train["Sulfate"].fillna(train["Sulfate"].me
an(),inplace=True)
train.head()
 # In[118]:
train["Trihalomethanes"].fillna(train["Trih
                                                                                                                                                                                                                                                                                                                                                                                                             Har_Pot.piot(kind = "Dain", stacked = Trifigsize=(10, 10))
plt.title("Hardness vs. Potability")
# In[124]:
Har Potl =
pd.crosstab(index=train["Hardness"],
columns=train["Potability"]).transpose()
Har Porl
                                                                                                                                                                                                       # plotting legend
 alomethanes"].mean(),inplace=True)
                                                                                                                                                                                                      plt.legend()
# plot title
plt.title('Potability')
 train.head()
train.nead()
# In[119:
train.isna().any()
# In[102]:
plt.hist(train["ph"], color="tomato")
                                                                                                                                                                                                        # showing the plot
  plt.title("Histogram of pH")
                                                                                                                                                                                                                                                                                                                                                                                                             fig = plt.figure(figsize = (10, 7))
plt.title("Boxplot of ru")
                                                                                                                                                                                                             In[466]:
                                                                                                                                                                                                         import seaborn as sns
                                                                                                                                                                                                      import seaborn as sns
# In[83]:
my_pal = {1: "tomato", 0: "teal"}
for i,col in enumerate(train):
                                                                                                                                                                                                                                                                                                                                                                                                             Har_Pot1
# In[38]:
Har_Pot1.plot(kind = "bar", stacked = True,
figsize=(10, 10))
# In[36]:
plt.hist(train["Hardness"], color="tomato")
```

<pre>plt.title("Hardness vs. Potability") plt.legend(loc='upper right')</pre>	<pre>Har_Chll.plot(kind = "bar", stacked = True, figsize=(10, 10))</pre>	Har_Org1 # In[187]:
# In[125]:	plt.title("Chloramines vs. Potability")	<pre>Har_Tril = Har_Tril.div(Har_Tril.sum(axis =</pre>
bucket_Sol = np.linspace(0, 62000, 11)	plt.legend(loc='upper right')	1), axis = 0)*100
<pre>bucket_Sol # In[126]:</pre>	<pre># In[159]: for i,col in enumerate(train):</pre>	Har_Tri1 # In[188]:
train["Solids"] = pd.cut(train["Solids"],	Tot 1,001 in chamerate (crain).	Har Turl = Har Turl.div(Har Turl.sum(axis =
bucket_Sol)	train[col].value_counts().sort_index().plot	1), axis = 0) *100
train.head() # In[127]:	<pre>.bar() plt.xlabel(f"{col}")</pre>	Har_Turl # In[189]:
bucket Chl = np.linspace(0, 14, 15)	plt.ylabel("Frequency")	Har Sull.plot(kind = "bar", stacked = True,
bucket_Ch1	plt.title(f"{col}")	figsize=(10, 10))
# In[128]:	plt.figure(figsize=(10,10))	plt.title("Sulfer vs. Potability")
<pre>train["Chloramines"] = pd.cut(train["Chloramines"], bucket_Chl)</pre>	# In[163]: Har Sul =	<pre>plt.legend(loc='upper right') # In[190]:</pre>
train.head()	pd.crosstab(index=train["Sulfate"],	Har Con1.plot(kind = "bar", stacked = True,
# In[129]:	columns=train["Potability"])	figsize=(10, 10))
<pre>bucket_Sul = np.linspace(100, 500, 11) bucket_Sul</pre>	Har_Sul # In[164]:	<pre>plt.title("Conductivity vs. Potability") plt.legend(loc='upper right')</pre>
# In[130]:	Har Con =	# In[191]:
<pre>train["Sulfate"] = pd.cut(train["Sulfate"],</pre>	pd.crosstab(index=train["Conductivity"],	<pre>Har_Org1.plot(kind = "bar", stacked = True,</pre>
<pre>bucket_Sul) train.head()</pre>	columns=train["Potability"]) Har Con	<pre>figsize=(10, 10)) plt.title("Organic Carbon vs. Potability")</pre>
# In[131]:	# In[165]:	plt.legend(loc='upper right')
bucket_Con = np.linspace(100, 800, 11)	Har_Org =	# In[192]:
bucket_Con	pd.crosstab(index=train["Organic_carbon"],	Har_Tril.plot(kind = "bar", stacked = True,
<pre># In[132]: train["Conductivity"] =</pre>	columns=train["Potability"]) Har Org	<pre>figsize=(10, 10)) plt.title("Trihalomethane vs. Potability")</pre>
pd.cut(train["Conductivity"], bucket_Con)	# In[166]:	plt.legend(loc='upper right')
train.head()	Har_Tri =	# In[193]:
# In[133]: bucket Org = np.linspace(0, 30, 11)	<pre>pd.crosstab(index=train["Trihalomethanes"], columns=train["Potability"])</pre>	<pre>Har_Turl.plot(kind = "bar", stacked = True, figsize=(10, 10))</pre>
bucket Org	Har Tri	plt.title("Turbidity vs. Potability")
# In[134]:	# In[167]:	plt.legend(loc='upper right')
train["Organic_carbon"] =	Har_Tur =	# In[458]:
pd.cut(train["Organic_carbon"], bucket_Org) train.head()	<pre>pd.crosstab(index=train["Turbidity"], columns=train["Potability"])</pre>	<pre>ph_Sul = pd.crosstab(index=train["Turbidity"],</pre>
# In[135]:	Har_Tur	columns=train["Conductivity"])
bucket_Tri = np.linspace(0, 125, 11)	# In[168]:	ph_Sul
<pre>bucket_Tri # In[136]:</pre>	<pre>Har_Sul = Har_Sul.div(Har_Sul.sum(axis = 1), axis = 0)*100</pre>	<pre># In[459]: ph Sul = ph Sul.div(ph Sul.sum(axis = 1),</pre>
train["Trihalomethanes"] =	Har Sul	axis = 0)*100
pd.cut(train["Trihalomethanes"],	# In[169]:	ph_Sul
bucket_Tri) train.head()	<pre>Har_Con = Har_Con.div(Har_Con.sum(axis = 1), axis = 0)*100</pre>	<pre># In[462]: ph Sul.plot(kind = "barh", stacked = True,</pre>
# In[137]:	Har Con	figsize=(10, 10))
bucket_Tur = np.linspace(1, 7, 7)	# In[170]:	plt.title("Turbidity vs. Conductivity")
bucket_Tur	Har_Org = Har_Org.div(Har_Org.sum(axis =	plt.legend(loc='upper right')
<pre># In[138]: train["Turbidity"] =</pre>	1), axis = 0)*100 Har Org	<pre># In[488]: def cramers_v(x, y):</pre>
pd.cut(train["Turbidity"], bucket Tur)	# In[171]:	x = np.array(x)
train.head()	Har_Tri = Har_Tri.div(Har_Tri.sum(axis =	y = np.array(y)
# In[139]:	1), axis = 0)*100 Har Tri	<pre>confusion_matrix = pd.crosstab(x, y) chi2 =</pre>
<pre>train["Solids"].value_counts().sort_index() .plot.bar()</pre>	# In[172]:	stats.chi2 contingency(confusion matrix)[0]
plt.xlabel("Solids")	Har Tur = Har Tur.div(Har Tur.sum(axis =	<pre>n = confusion_matrix.sum().sum()</pre>
plt.ylabel("Frequency")	1), axis = 0)*100	phi2 = chi2/n
plt.title("Solids") # In[140]:	Har_Tur # In[268]:	$r,k = confusion_matrix.shape$ phi2corr = max(0, phi2-((k-1)*(r-
Har Sol =	Har Sul.plot(kind = "barh", stacked = True,	1))/(n-1))
pd.crosstab(index=train["Solids"],	figsize=(10, 10))	rcorr = r - ((r-1)**2) / (n-1)
columns=train["Potability"]) Har Sol	<pre>plt.title("Sulfate vs. Potability") # In[174]:</pre>	kcorr = k - ((k-1)**2) / (n-1)
# In[141]:	Har Con.plot(kind = "barh", stacked = True,	return np.sqrt(phi2corr/min((kcorr- 1),(rcorr-1)))
Har Sol = Har Sol.div(Har Sol.sum(axis =	figsize=(10, 10))	columns = train.columns
1), axis = 0)*100	plt.title("Conductivity vs. Potability")	cramersv =
Har_Sol # In[142]:	<pre># In[175]: Har_Org.plot(kind = "barh", stacked = True,</pre>	<pre>pd.DataFrame(index=train.columns,columns=tr ain.columns)</pre>
Har_Sol.plot(kind = "barh", stacked = True,	figsize=(10, 10))	cramersv
figsize=(10, 10))	plt.title("Organic Carbon vs. Potability")	# In[487]:
<pre>plt.title("Solids vs. Potability") # In[143]:</pre>	<pre># In[176]: Har_Tri.plot(kind = "barh", stacked = True,</pre>	<pre>fig = plt.figure(figsize=(15,15)) sns.heatmap(cramersv, annot=True)</pre>
# IN[145]. Har Sol1 =	figsize=(10, 10))	fig.savefig('catcorr.jpg',
pd.crosstab(index=train["Solids"],	plt.title("Trihalomethanes vs. Potability")	bbox_inches='tight', dpi=150)
columns=train["Potability"]).transpose() Har Sol1	<pre># In[177]: Har_Tur.plot(kind = "barh", stacked = True,</pre>	plt.show() # In[476]:
# In[145]:	figsize=(10, 10))	from scipy.stats import chi2_contingency
Har Sol1 = Har Sol1.div(Har Sol1.sum(axis =	plt.title("Turbidity vs. Potability")	def cramers_V(var1,var2) :
1), axis = 0)*100	# In[179]:	crosstab =np.array(pd.crosstab(var1,var2,
Har_Sol1 # In[146]:	<pre>Har_Sul1 = pd.crosstab(index=train["Sulfate"],</pre>	rownames=None, colnames=None)) # Cross table building
Har_Soll.plot(kind = "bar", stacked = True,	columns=train["Potability"]).transpose()	stat = chi2_contingency(crosstab)[0] #
figsize=(10, 10))	Har_Sul1	Keeping of the test statistic of the Chi2
<pre>plt.title("Solids vs. Potability") plt.legend(loc='upper right')</pre>	# In[180]: Har Con1 =	<pre>test obs = np.sum(crosstab) # Number of</pre>
# In[147]:	pd.crosstab(index=train["Conductivity"],	observations
train["Chloramines"].value_counts().sort_in	columns=train["Potability"]).transpose()	mini = min(crosstab.shape)-1 # Take the
dex().plot.bar()	Har_Con1 # In[181]:	minimum value between the columns and the rows of the cross table
plt.xlabel("Chloramines") plt.ylabel("Frequency")	# IN[101]. Har Org1 =	return (stat/(obs*mini))
plt.title("Chloramines")	pd.crosstab(index=train["Organic_carbon"],	# In[477]:
# In[148]:	columns=train["Potability"]).transpose()	rows= []
<pre>Har_Chl = pd.crosstab(index=train["Chloramines"],</pre>	Har_Org1 # In[182]:	for var1 in train: col = []
columns=train["Potability"])	Har Tril =	for var2 in train :
Har_Chl	pd.crosstab(index=train["Trihalomethanes"],	cramers =cramers_V(train[var1],
<pre># In[149]: Har_Chl = Har_Chl.div(Har_Chl.sum(axis =</pre>	<pre>columns=train["Potability"]).transpose() Har Tril</pre>	<pre>train[var2]) # Cramer's V test col.append(round(cramers,2)) # Keeping</pre>
1), axis = 0)*100	# In[183]:	of the rounded value of the Cramer's V
Har_Chl	Har_Tur1 =	rows.append(col)
# In[150]:	pd.crosstab(index=train["Turbidity"],	gramora regulta =
<pre>Har_Chl.plot(kind = "barh", stacked = True, figsize=(10, 10))</pre>	<pre>columns=train["Potability"]).transpose() Har Turl</pre>	<pre>cramers_results = np.array(rows) df = pd.DataFrame(cramers results, columns</pre>
plt.title("Chloramines vs. Potability")	# In[184]:	= train.columns, index =train.columns)
# In[151]:	Har_Sull = Har_Sull.div(Har_Sull.sum(axis =	df
<pre>Har_Chl1 = pd.crosstab(index=train["Chloramines"],</pre>	1), axis = 0)*100 Har Sull	<pre># In[480]: fig = plt.figure(figsize=(15,15))</pre>
columns=train["Potability"]).transpose()	# In[185]:	sns.heatmap(df, annot=True)
Har_Chl1	<pre>Har_Con1 = Har_Con1.div(Har_Con1.sum(axis =</pre>	fig.savefig('catcorr.jpg',
<pre># In[152]: Har Chl1 = Har Chl1.div(Har Chl1.sum(axis =</pre>	1), axis = 0)*100 Har Con1	<pre>bbox_inches='tight', dpi=150) plt.show()</pre>
1), $axis = 0)*100$	# In[186]:	# In[481]:
Har_Chl1	Har Org1 = Har Org1.div(Har Org1.sum(axis =	import scipy.stats as ss
# In[153]:	1), axis = 0)*100	

<pre>def cramers_corrected_stat(confusion_matrix): """ calculate Cramers V statistic for categorial-categorial association.</pre>	<pre>plt.title('Feature Importances') plt.barh(range(len(indices)), importances[indices], color='b', align='center')</pre>	<pre>final_xgb = XGBClassifier(base_score=0.5, booster='gbtree', colsample_bylevel=1, colsample_bynode=1, colsample_bytree=1, gamma=0.1, gpu_id=-1,</pre>
uses correction from Bergsma and Wicher,	<pre>plt.yticks(range(len(indices)), [features[i] for i in indices])</pre>	<pre>importance_type='gain', interaction_constraints='',</pre>
Journal of the Korean Statistical Society 42 (2013): 323-328	<pre>plt.xlabel('Relative Importance') plt.show()</pre>	learning_rate=0.01, max_delta_step=0, max_depth=8,
chi2 =	<pre>important_feat = list(feat_imp_DT.nlargest(5).index)</pre>	<pre>min_child_weight=1, monotone_constraints='()',</pre>
ss.chi2_contingency(confusion_matrix)[0]	X_train_imp = X_train.loc[:,important_feat] X_test_imp = X_test.loc[:,important_feat]	n_estimators=300, n_jobs=4,
n = confusion_matrix.sum() phi2 = chi2/n	grid_search.fit(X_train_imp, Y_train)	nthread=4, num_parallel_tree=1, random_state=20, reg_alpha=0,
$r, k = confusion_matrix.shape$ phi2corr = max(0, phi2 - ((k-1)*(r-	<pre>DT_clf_imp = DecisionTreeClassifier(max_depth = 9,</pre>	<pre>reg_lambda=1, scale_pos_weight=1,</pre>
1))/ $(n-1)$) rcorr = r - $((r-1)**2)/(n-1)$	<pre>max_features = 'auto', min_samples_leaf = 5, min samples split=0.01,random state=20)</pre>	<pre>tree_method='exact', validate_parameters=1,</pre>
<pre>kcorr = k - ((k-1)**2)/(n-1) return np.sqrt(phi2corr / min((kcorr-</pre>	<pre>DT_clf_imp.fit(X_train_imp, Y_train) Y_pred_imp = DT_clf_imp.predict(X_test_imp)</pre>	<pre>final_xgb.fit(X_train_xgb, Y_train) y pred xgb = final xgb.predict(X test xgb)</pre>
1), (rcorr-1))) # In[482]:	<pre>print('Model accuracy score: {0:0.4f}'. format(accuracy score(Y test, Y pred imp)))</pre>	print ('Model accuracy score: {0:0.4f}'. format(accuracy score(Y test, y pred xgb)))
<pre>confusion_matrix = pd.crosstab(train[column1], train[column2])</pre>	false positive rate, true positive rate, thresholds = roc curve(Y test, Y pred imp)	false_positive_rate, true_positive_rate,
import pandas as pd	roc_auc = auc(false_positive_rate,	<pre>thresholds = roc_curve(Y_test, y_pred_xgb) roc_auc = auc(false_positive_rate,</pre>
<pre>import matplotlib.pyplot as plt import numpy as np</pre>	<pre>true_positive_rate) print(confusion_matrix(Y_test, Y_pred_imp))</pre>	true_positive_rate)
import seaborn as sns	<pre>print(classification_report(Y_test,</pre>	<pre>#handling outliers #finding the Q1(25 percentile) and Q3(75</pre>
from sklearn.model_selection import train test split	#random forest	<pre>percentile) q1 = train["ph"].quantile(0.25)</pre>
from sklearn.preprocessing import StandardScaler	<pre>param_grid_RF = { 'n_estimators': [100,200,300,400,500],</pre>	<pre>q2 = train["ph"].quantile(0.75) #finding out the value of Inter Quartile</pre>
from sklearn.linear_model import	'max_features': ['auto', 'sqrt',	Range
LogisticRegression from sklearn.ensemble import	'log2'], 'max_depth' : [6,7,8,9,10],	IQR = q2 - q1 #defining max and min limits
RandomForestClassifier from sklearn.tree import	'criterion' :['gini', 'entropy'] }	$\max_{\text{limit}} = q2 + (1.5 * IQR)$ $\min_{\text{limit}} = q1 - (1.5 * IQR)$
DecisionTreeClassifier	<pre>RFC = RandomForestClassifier(random state=20)</pre>	#capping
%matplotlib inline	<pre>Grid_rf= GridSearchCV(estimator=RFC, param_grid=param_grid_RF, cv= 5,n_jobs=-</pre>	<pre>train_ph= pd.DataFrame(np.where(train["ph"] > max_limit, max_limit,</pre>
<pre>df = pd.read_csv('water_potability.csv') df.shape</pre>	<pre>1,verbose =1,scoring='roc_auc') Grid rf.fit(X train, Y train)</pre>	<pre>(np.where(train["ph"] < min_limit, min limit, train["ph"]))), columns=["ph"])</pre>
df.head() df.isnull().sum()	Grid_rf.best_params_ RF =	train_ph
train.isnull().mean()*100	RandomForestClassifier(n estimators=400, max	#finding the Q1(25 percentile) and Q3(75 percentile)
<pre>train, test = train_test_split(df,test_size=0.2,random_st</pre>	_features='auto',max_depth=10,criterion='en tropy', random_state=20 ,verbose = 1)	<pre>q1 = train['Hardness'].quantile(0.25) q2 = train['Hardness'].quantile(0.75)</pre>
ate= 20)	<pre>feat_imp_RF = pd.Series(RF.feature_importances_,</pre>	#finding out the value of Inter Quartile Range
<pre>train['ph'] = train['ph'].fillna(train['ph'].mean())</pre>	<pre>index=X_train.columns) feat imp RF.nlargest(15).plot(kind='barh')</pre>	IQR = q2 - q1 #defining max and min limits
<pre>test['ph'] = test['ph'].fillna(train['ph'].mean())</pre>	<pre>important_feat = list(feat_imp_RF.nlargest(5).index)</pre>	$\max_{1 \text{ imit}} = q2 + (1.5 * IQR)$ $\min_{1 \text{ imit}} = q1 - (1.5 * IQR)$
<pre>train['Sulfate'] = train['Sulfate'].fillna(train['Sulfate'].me</pre>	X train imp = X train.loc[:,important feat] X test imp = X test.loc[:,important feat]	#capping
an())	<pre>Grid_rf= GridSearchCV(estimator=RFC,</pre>	train_Hardness=
<pre>test['Sulfate'] = test['Sulfate'].fillna(train['Sulfate'].mea</pre>	<pre>param_grid=param_grid_RF, cv= 5,n_jobs=- 1,verbose =1,scoring='roc_auc')</pre>	<pre>pd.DataFrame(np.where(train['Hardness'] > max_limit, max_limit,</pre>
n()) train['Trihalomethanes'] =	$\begin{array}{ll} \operatorname{Grid}_{-}\operatorname{rf.fit}(X_\operatorname{train}_\operatorname{imp},\ \overline{Y}_\operatorname{train}) \\ \operatorname{Grid}_{-}\operatorname{rf.best}_\operatorname{params}_ \end{array}$	<pre>(np.where(train['Hardness'] < min_limit, min_limit, train['Hardness']))),</pre>
<pre>train['Trihalomethanes'].fillna(train['Trih alomethanes'].mean())</pre>	<pre>RF = RandomForestClassifier(n estimators=300,max</pre>	columns=["Hardness"]) train Hardness
<pre>test['Trihalomethanes'] = test['Trihalomethanes'].fillna(train['Triha</pre>	_features='auto',max_depth=9,criterion='gin i', random state=20 ,verbose = 1)	<pre>frames = [train ph,train Hardness,train Solids,train</pre>
<pre>lomethanes'].mean()) X train = train.iloc[:,:-1]</pre>	<pre>RF.fit(X_train imp, Y_train) Y_pred_imp = RF.predict(X_test_imp)</pre>	_Chloramines,train_Sulfate,train_Conductivity,train_Organic_carbon,
<pre>X_train = train.iloc[:,-1:] X_test = test.iloc[:,:-1]</pre>	print('Model accuracy score: {0:0.4f}'.	train Trihalomethanes, train Turbidity, train
Y_test = test.iloc[:,-1:]	<pre>format(accuracy_score(Y_test, Y_pred_imp))) false_positive_rate, true_positive_rate,</pre>	_Potability]
from sklearn.tree import	<pre>thresholds = roc_curve(Y_test, Y_pred_imp) roc_auc = auc(false_positive_rate,</pre>	<pre>new_train = pd.concat(frames, axis=1, join='inner')</pre>
DecisionTreeClassifier from sklearn import metrics	<pre>true_positive_rate) print(confusion matrix(Y test, Y pred imp))</pre>	#logistic regression
from sklearn.metrics import roc_curve, auc from sklearn.metrics import accuracy_score	<pre>print(classification_report(Y_test, Y_pred_imp))</pre>	<pre>LR = LogisticRegression(random_state=20) LR.fit(X_train, Y_train)</pre>
from sklearn.model_selection import GridSearchCV	#xgboost	#feature selection sing rfe from sklearn feature selection import RFE
from sklearn.metrics import roc_curve, auc from sklearn.metrics import	import xgboost as xgb from xgboost import XGBClassifier	rfe = RFE(LR, 5) fit = rfe.fit(X_train, Y_train)
confusion_matrix	<pre>xgb_model = XGBClassifier(</pre>	print("Num Features: %d" % fit.n_features_)
from sklearn.metrics import classification_report	random_state=20,learning_rate=0.01,eval_met ric='auc')	<pre>print("Selected Features: %s" % fit.support_)</pre>
params = {	<pre># fit the model with the training data xgb_model.fit(X_train,Y_train)</pre>	<pre>print("Feature Ranking: %s" % fit.ranking_) columns = list(X_train.columns)</pre>
'max_depth': [2, 3, 4, 5,6,7,8,9,10], 'min_samples_leaf': [5, 8, 12, 15, 20],	<pre>feat_imp_xgb = pd.Series(xgb_model.feature_importances_,</pre>	<pre>imp_feat =[] for i in range(len(columns)):</pre>
'max_features' : ['auto', 'sqrt', 'log2'],	<pre>index=X_train.columns) feat_imp_xgb.nlargest(15).plot(kind='barh')</pre>	<pre>if (fit.support_[i] == True): imp feat.append(columns[i])</pre>
'min_samples_split' : [0.01,0.05,0.1]	<pre>imp_feat_xgb = list(feat_imp_xgb.nlargest(5).index)</pre>	<pre>imp_feat X_train_imp = X_train.loc[:,imp_feat]</pre>
clf TUNED =	<pre>X train_xgb = X train.loc[:,imp_feat_xgb] X test xgb = X test.loc[:,imp_feat xgb]</pre>	X test_imp = X test.loc[:,imp_feat] LR = LogisticRegression(random state=20)
DecisionTreeClassifier(random_state=20)	params_xgb = {	params = {
<pre>grid_search = GridSearchCV(estimator=clf_TUNED,</pre>	'max_depth': [4,5,6,7,8], 'n_estimators': [100,200,300,400,500],	'solver': ['lbfgs', 'liblinear', 'sag', 'saga'],
param_grid=params,cv=5,	'learning_rate': [0.1, 0.01, 0.05], 'subsample':[i/10.0 for i in	'C' : [1.0,0.5, 0.1,0.05, 0.01]
n_jobs=-1, verbose=1, scoring =	range(6,8)], 'gamma':[i/10.0 for i in range(0,3)],	<pre>grid_search = GridSearchCV(estimator=LR,</pre>
"accuracy") grid search.fit(X train, Y train)	} estimator = XGBClassifier(param_grid=params, cv=5, n jobs=-1,
grid_search.best_params_	random_state=20, nthread=4	<pre>verbose=1, scoring = "accuracy") grid_search.fit(X_train_imp, Y_train)</pre>
DT_clf = DecisionTreeClassifier(max_depth =)	LR_tuned =
7, max_features = 'auto', min_samples_leaf = 5,	<pre>grid_search_xgb = GridSearchCV(estimator=estimator,</pre>	LogisticRegression(C=1,solver='lbfgs',random_state=20)
min_samples_split=0.01,random_state=20) DT_clf.fit(X_train, Y_train)	param_grid=params_xgb,	<pre>LR_tuned.fit(X_train_imp, Y_train) Y_pred_imp = LR_tuned.predict(X_test_imp)</pre>
<pre>Y_pred = DT_clf.predict(X_test)</pre>	cv=5, n_jobs=-1, verbose=1)	
<pre>features = X_train.columns importances = DT_clf.feature_importances_ indices = np.argsort(importances)</pre>	<pre>grid_search_xgb.fit(X_train_xgb, Y_train) grid_search_xgb.best_params_</pre>	