water-quality

May 24, 2021

0.1 # Water Quality Prediction

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0.3 Introduction

Water quality refers to the chemical, physical, and biological characteristics of water based on the standards of its usage. The most common standards used to monitor and assess water quality convey the health of ecosystems, safety of human contact, and condition of drinking water. Water quality has a significant impact on water supply and oftentimes determines supply options.

The parameters for water quality are determined by the intended use. Work in the area of water quality tends to be focused on water that is treated for potability, industrial/domestic use, or restoration. Contaminants that may be in untreated water include microorganisms such as viruses, protozoa and bacteria; inorganic contaminants such as salts and metals; organic chemical contaminants from industrial processes and petroleum use; pesticides and herbicides; and radioactive contaminants.

The United States Environmental Protection Agency (EPA) limits the amounts of certain contaminants in tap water provided by US public water systems. The Safe Drinking Water Act authorizes EPA to issue two types of standards:

- Primary standards regulate substances that potentially affect human health.

- Secondary standards prescribe aesthetic qualities, those that affect taste, odor, or appearance.

In this notebook, we try to assess water potability (fit to drink) based on 9 features: 1. **pH**: In chemistry, pH is a scale used to specify the acidity or basicity of an aqueous solution. Acidic solutions (solutions with higher concentrations of H+ ions) are measured to have lower pH values than basic or alkaline solutions. The pH scale is logarithmic and inversely indicates the concentration of hydrogen ions in the solution. At 25 °C, solutions with a pH less than 7 are acidic, and solutions with a pH greater than 7 are basic. Solutions with a pH of 7 at this temperature are neutral. > The pH of most drinking-water lies within the range 6.5 – 8.5.

2. **Hardness**: Water hardness is generally the amount of dissolved calcium and magnesium in water. But in layman's terms, you may notice water hardness when your hands still feel slimy after washing with soap and water, or when your drinking glasses at home become less than crystal clear. Hard water is high in dissolved minerals, largely calcium and magnesium. > Generally, water with the hardness of < 75 mg/L is considered soft and > 150 mg/L is considered hard.

3. **Total Dissolved Solids (TDS)**: Is a measure of the combined total of organic and inorganic substances contained in a liquid. This includes anything present in water other than the pure H2O molecules. These solids are primarily minerals, salts and organic matter that can be a general indicator of water quality. > The TDS of fresh water is < 1000 mg/L. Drinking water generally has a TDS below 500 ppm. Higher TDS Fresh Water is drinkable but taste may be objectionable.

4. **Chloramines**: Chloramines (also known as secondary disinfection) are disinfectants used to treat drinking water and they are most commonly formed when ammonia is added to chlorine to treat drinking water. They provide longer-lasting disinfection as the water moves through pipes to consumers. > According to CDC, Chloramine levels up to 4 mg/L are considered safe in drinking water.

5. **Sulfate**: Sulfate is a chemical commonly found in air, soil and water. Since it is soluble (easily dissolved) in water, sulfate is found at high concentrations in many aquifers. Sulfate is considered a secondary contaminant and nuisance chemical in high enough concentrations. High sulfate levels may also corrode plumbing, particularly copper piping. > A water quality survey carried out on British tap water supplies indicated a mean sulfate concentration of 59.5 mg/L, with a maximum of 236 mg/L. Sulfate levels above 250 mg/L may make the water taste bitter or like medicine.

6. **Conductivity**: Electrical Conductivity of water is its ability to conduct an electric current. Salts or other chemicals that dissolve in water can break down into positively and negatively charged ions. In many cases, conductivity is linked directly to the total dissolved solids (TDS). > Typical drinking water is in the range of 200 – 800 S/cm but in general it is better to not exceed 400 S/cm.

7. **Total Organic Carbon (TOC)**: TOC is a measure of the total amount of carbon in organic compounds in pure water. The produced TOC number indicates Organic materials (natural), Disinfectants and Disinfection byproducts. > Typical TOC values in drinking water should not exceed 2 ppm.

8. **Trihalomethanes (THMs)**: Trihalomethanes are a group of chemicals that can form when organic matter in water is treated with halogen disinfectants such as chlorine. The most common of these chemicals is trichloromethane (also called chloroform), but others, such as

dibromochloromethane, bromodichloromethane, or bromoform can also be found. The sum of these four chemicals is referred to as total trihalomethanes (TTHMs). > The Florida Department of Environmental Protection's drinking water standard for TTHMs is 80 micrograms per liter (80 µg/L).

9. **Turbidity**: Turbidity is the measure of relative clarity of a liquid. It is an optical characteristic of water and is a measurement of the amount of light that is scattered by material in the water when a light is shined through the water sample. The higher the intensity of scattered light, the higher the turbidity. Turbidity is measured in a unit called Nephelometric Turbidity Units (NTUs). > For systems that use conventional or direct filtration, at no time can turbidity (cloudiness of water) go higher than 1 NTUs and for others at no time should exceed 5 NTUs.

Now based on these 9 features we will find whether the water is safe to drink or no (water **Potability** = 0 or 1).

Note: The dataset of this notebook was obtained from https://www.kaggle.com/adityakadiwal/water-potability.

0.4 Python Code

0.4.1 1. Load packages

[1]:
```
import numpy as np
import pandas as pd
import matplotlib.pyplot as plt
import seaborn as sns

from sklearn.preprocessing import StandardScaler, LabelEncoder, OneHotEncoder
from sklearn.compose import ColumnTransformer, make_column_selector,␣
↪make_column_transformer
from sklearn.pipeline import Pipeline
from sklearn.impute import SimpleImputer

from sklearn.model_selection import train_test_split, cross_val_score
from sklearn.ensemble import RandomForestClassifier
from sklearn.neural_network import MLPClassifier

from tensorflow import keras
from tensorflow.keras import layers, callbacks

from sklearn.metrics import confusion_matrix, classification_report,␣
↪mean_absolute_error, accuracy_score
```

0.4.2 2. Load data

[2]:
```
df = pd.read_csv('water_potability.csv')
df.head()
```

[2]:
```
          ph    Hardness        Solids  Chloramines     Sulfate  Conductivity  \
0        NaN  204.890455  20791.318981     7.300212  368.516441    564.308654
1   3.716080  129.422921  18630.057858     6.635246         NaN    592.885359
2   8.099124  224.236259  19909.541732     9.275884         NaN    418.606213
3   8.316766  214.373394  22018.417441     8.059332  356.886136    363.266516
4   9.092223  181.101509  17978.986339     6.546600  310.135738    398.410813

   Organic_carbon  Trihalomethanes  Turbidity  Potability
0       10.379783        86.990970   2.963135           0
1       15.180013        56.329076   4.500656           0
2       16.868637        66.420093   3.055934           0
3       18.436524       100.341674   4.628771           0
4       11.558279        31.997993   4.075075           0
```

[3]:
```
df.info()
```

```
<class 'pandas.core.frame.DataFrame'>
RangeIndex: 3276 entries, 0 to 3275
Data columns (total 10 columns):
 #   Column           Non-Null Count  Dtype
---  ------           --------------  -----
 0   ph               2785 non-null   float64
 1   Hardness         3276 non-null   float64
 2   Solids           3276 non-null   float64
 3   Chloramines      3276 non-null   float64
 4   Sulfate          2495 non-null   float64
 5   Conductivity     3276 non-null   float64
 6   Organic_carbon   3276 non-null   float64
 7   Trihalomethanes  3114 non-null   float64
 8   Turbidity        3276 non-null   float64
 9   Potability       3276 non-null   int64
dtypes: float64(9), int64(1)
memory usage: 256.1 KB
```

[3]:
```
# num of NaNs in dataset in each column
df.isnull().sum()
```

[3]:
```
ph                 491
Hardness             0
Solids               0
Chloramines          0
Sulfate            781
Conductivity         0
Organic_carbon       0
Trihalomethanes    162
Turbidity            0
Potability           0
```

```
dtype: int64
```

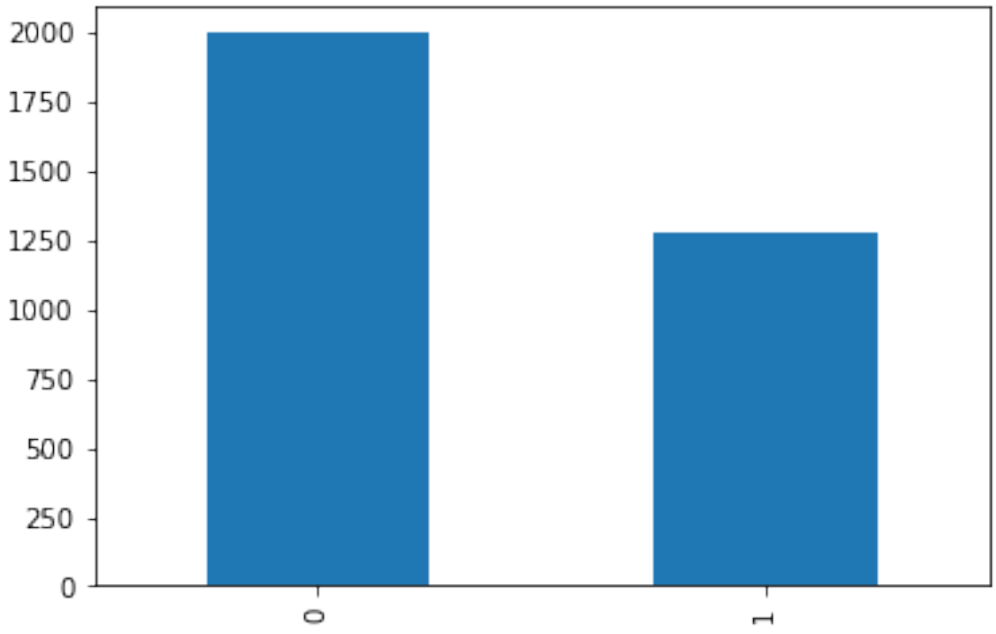
[5]:
```
df['Potability'].unique()
```

[5]:
```
array([0, 1])
```

0.4.3 3. Visualizing Potability (target)

[6]:
```
print(df.Potability.value_counts())
df.Potability.value_counts().plot(kind='bar')
plt.show()
```

```
0    1998
1    1278
Name: Potability, dtype: int64
```



0.4.4 4. Data Statistics

[7]:
```
df.describe()
```

[7]:

	ph	Hardness	Solids	Chloramines	Sulfate	\
count	2785.000000	3276.000000	3276.000000	3276.000000	2495.000000	
mean	7.080795	196.369496	22014.092526	7.122277	333.775777	
std	1.594320	32.879761	8768.570828	1.583085	41.416840	
min	0.000000	47.432000	320.942611	0.352000	129.000000	

25%	6.093092	176.850538	15666.690297	6.127421	307.699498
50%	7.036752	196.967627	20927.833607	7.130299	333.073546
75%	8.062066	216.667456	27332.762127	8.114887	359.950170
max	14.000000	323.124000	61227.196008	13.127000	481.030642

	Conductivity	Organic_carbon	Trihalomethanes	Turbidity	Potability
count	3276.000000	3276.000000	3114.000000	3276.000000	3276.000000
mean	426.205111	14.284970	66.396293	3.966786	0.390110
std	80.824064	3.308162	16.175008	0.780382	0.487849
min	181.483754	2.200000	0.738000	1.450000	0.000000
25%	365.734414	12.065801	55.844536	3.439711	0.000000
50%	421.884968	14.218338	66.622485	3.955028	0.000000
75%	481.792304	16.557652	77.337473	4.500320	1.000000
max	753.342620	28.300000	124.000000	6.739000	1.000000

We can see that 3 columns have missing data: **'ph'**, **'Sulfate'**, and **'Trihalomethanes'**. We need to take care of this first before we move on. The easiest way is to substitute the 'NaN' with the mean value in each column which we will do here.

0.4.5 5. Imputation (handling the missing data points)

[8]:
```
numerical_cols = ['ph', 'Hardness', 'Solids', 'Chloramines', 'Sulfate',␣
↪'Conductivity', 'Organic_carbon',
                  'Trihalomethanes', 'Turbidity']
categorical_cols = ['Potability']

print('numerical_cols:',numerical_cols)
print('numerical_cols:',categorical_cols)
```

```
numerical_cols: ['ph', 'Hardness', 'Solids', 'Chloramines', 'Sulfate',
'Conductivity', 'Organic_carbon', 'Trihalomethanes', 'Turbidity']
numerical_cols: ['Potability']
```

[9]:
```
# Preprocessing for numerical data
numerical_transformer = SimpleImputer(strategy='mean') # the default is mean
preprocessor = ColumnTransformer(transformers=[('num', numerical_transformer,␣
↪numerical_cols)])
```

Here we assume all the columns are significant in predicting the water potability.

[10]:
```
feature_columns_1 = ['ph', 'Hardness', 'Solids', 'Chloramines', 'Sulfate',␣
↪'Conductivity',
                     'Organic_carbon', 'Trihalomethanes', 'Turbidity']
X = df[feature_columns_1]
y = df['Potability']
X_train, X_test, y_train, y_test = train_test_split(X, y, random_state=1)
```

0.4.6 6. Define Model 1: Random Forest Classifier

[11]:
```
model_rfc = RandomForestClassifier(random_state=1)
```

[12]:
```
my_pipeline = Pipeline(steps=[('preprocessor', preprocessor),
                              ('model', model_rfc)])
my_pipeline.fit(X_train, y_train)
preds_test = my_pipeline.predict(X_test)
print('MAE:', mean_absolute_error(y_test, preds_test))
```

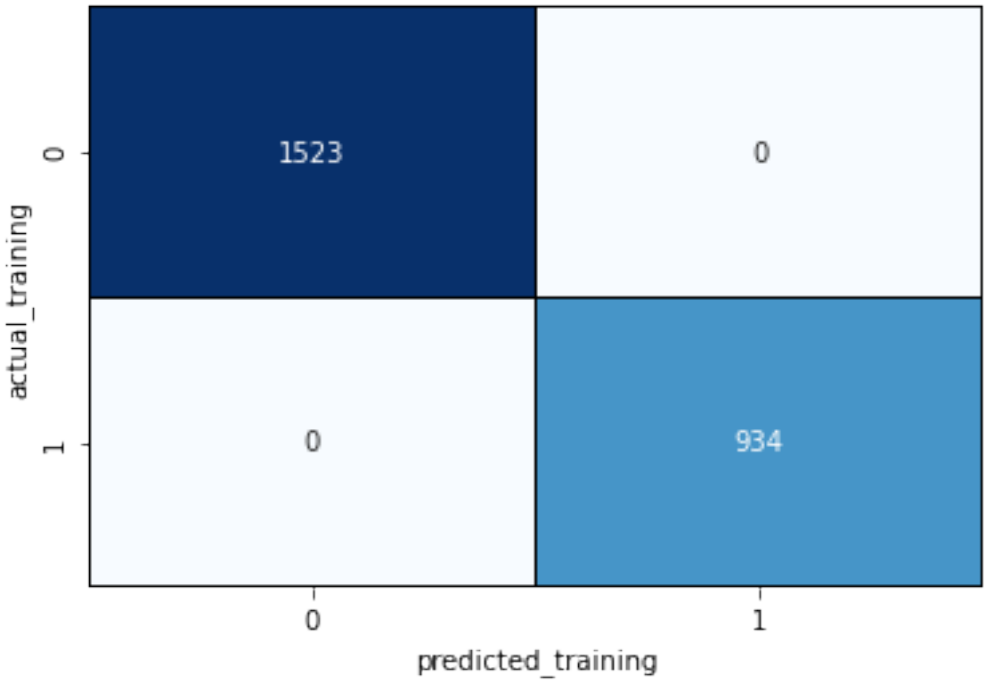
```
MAE: 0.3540903540903541
```

[13]:
```
# cross validate
# Multiply by -1 since sklearn calculates *negative* MAE

# cv = Determines the cross-validation splitting strategy, the default 5-fold␣
 ↪cross validation
scores = -1 * cross_val_score(my_pipeline, X, y,
                              cv=5,
                              scoring='neg_mean_absolute_error')

print(scores)
print(scores.mean())
```

```
[0.39634146 0.35419847 0.35114504 0.39541985 0.33129771]
0.3656805064233848
```

0.4.7 7. Analyze the Results: Random Forest Classifier

[37]:
```
# Train dataset
preds_train = my_pipeline.predict(X_train)
conf_train = confusion_matrix(y_train, preds_train)
ax = plt.axes()
sns.heatmap(conf_train, cmap='Blues', annot=True,
            cbar=False, fmt='d',
            linecolor='black',
            linewidths=0.1)
ax.set(xlabel='predicted_training', ylabel = 'actual_training')
plt.show()
```



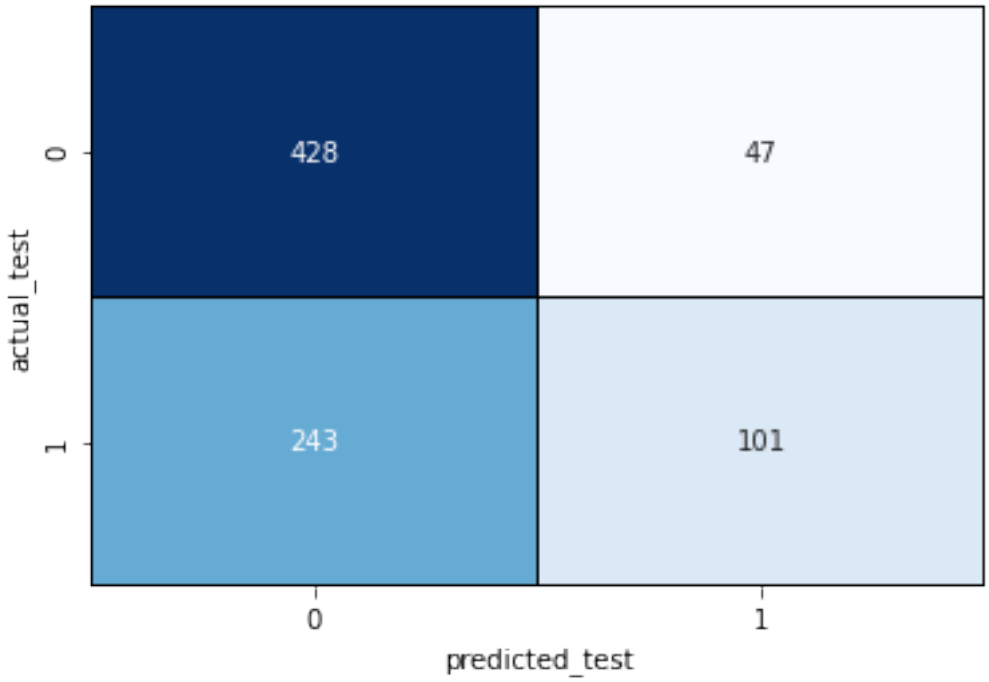
[33]:
```
print(classification_report(y_train, preds_train))
print('accuracy =',accuracy_score(y_train, preds_train))
```

```
              precision    recall  f1-score   support

           0       1.00      1.00      1.00      1523
           1       1.00      1.00      1.00       934

    accuracy                           1.00      2457
   macro avg       1.00      1.00      1.00      2457
weighted avg       1.00      1.00      1.00      2457

accuracy = 1.0
```

It seems that there is an overfitting to the train data.

[36]:
```
# Test dataset
conf_test = confusion_matrix(y_test, preds_test)
ax = plt.axes()
sns.heatmap(conf_test, cmap='Blues', annot=True,
            cbar=False, fmt='d',
            linecolor='black',
            linewidths=0.1)
ax.set(xlabel='predicted_test', ylabel = 'actual_test')
plt.show()
```

```
print(conf_test)
```




```
[[428  47]
 [243 101]]
```

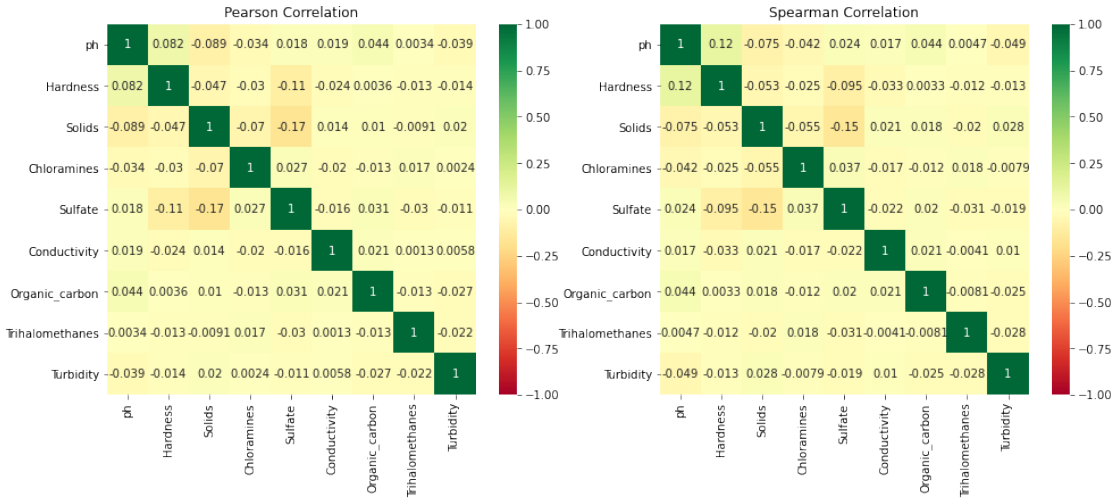
[34]:
```
print(classification_report(y_test, preds_test))
print('accuracy =',accuracy_score(y_test, preds_test))
```

```
              precision    recall  f1-score   support

           0       0.64      0.90      0.75       475
           1       0.68      0.29      0.41       344

    accuracy                           0.65       819
   macro avg       0.66      0.60      0.58       819
weighted avg       0.66      0.65      0.61       819

accuracy = 0.645909645909646
```

0.4.8 8. Improving the model by looking at the correlation diagrams

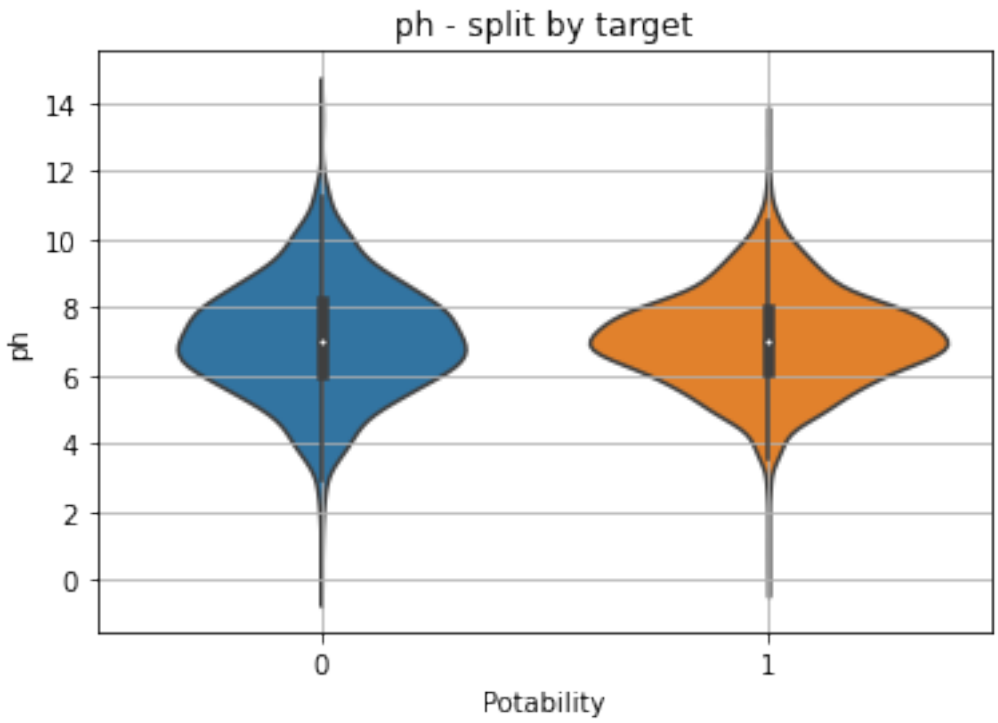
[38]:
```
corr_pearson = df[feature_columns_1].corr(method='pearson')
corr_spearman = df[feature_columns_1].corr(method='spearman')

plt.figure(figsize=(16,6))
```

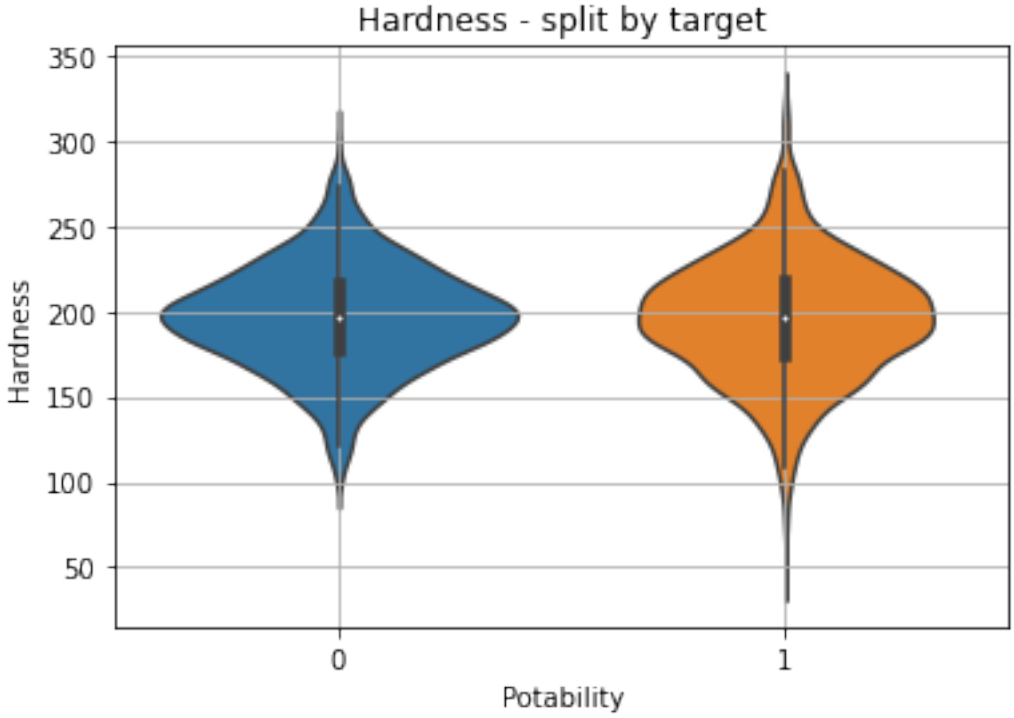
```
ax1 = plt.subplot(1,2,1)
sns.heatmap(corr_pearson, annot=True, cmap='RdYlGn', vmin=-1, vmax=+1)
plt.title('Pearson Correlation')

ax2 = plt.subplot(1,2,2, sharex=ax1)
sns.heatmap(corr_spearman, annot=True, cmap='RdYlGn', vmin=-1, vmax=+1)
plt.title('Spearman Correlation')
plt.show()
```

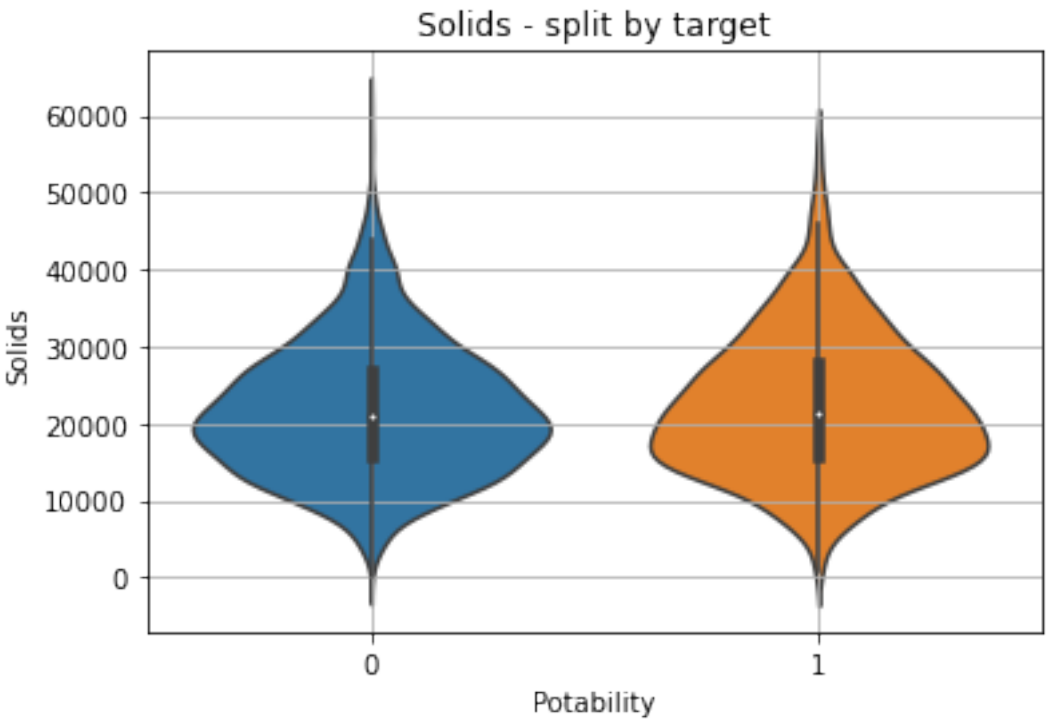


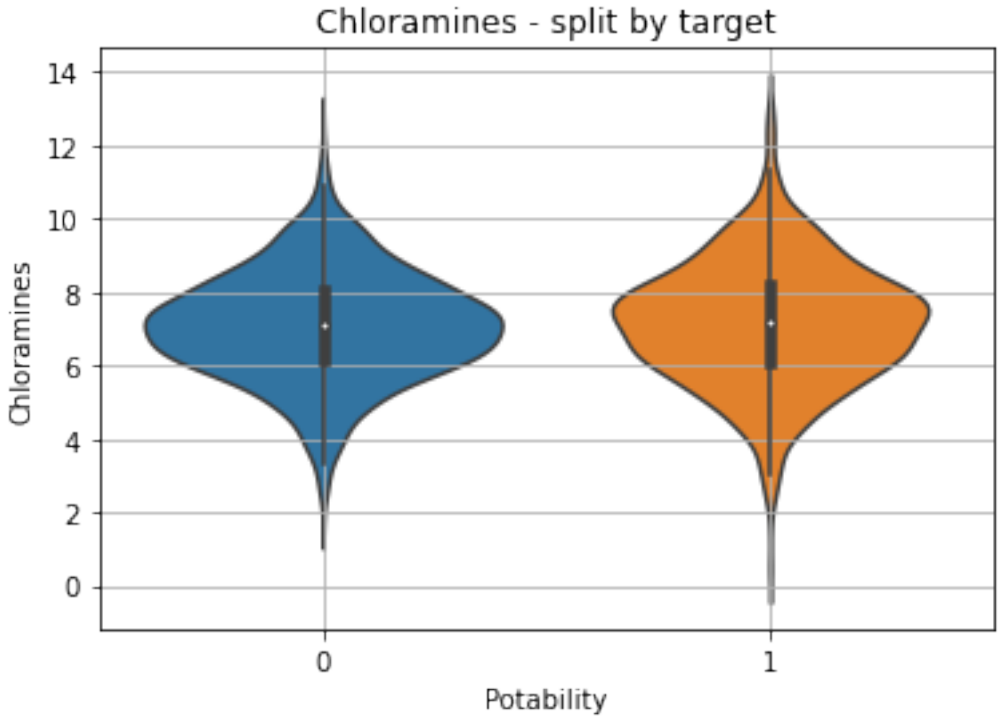
Surprisingly, it is clear that there is little to no correlation between the features. Now let's plot our target against each feature separately.

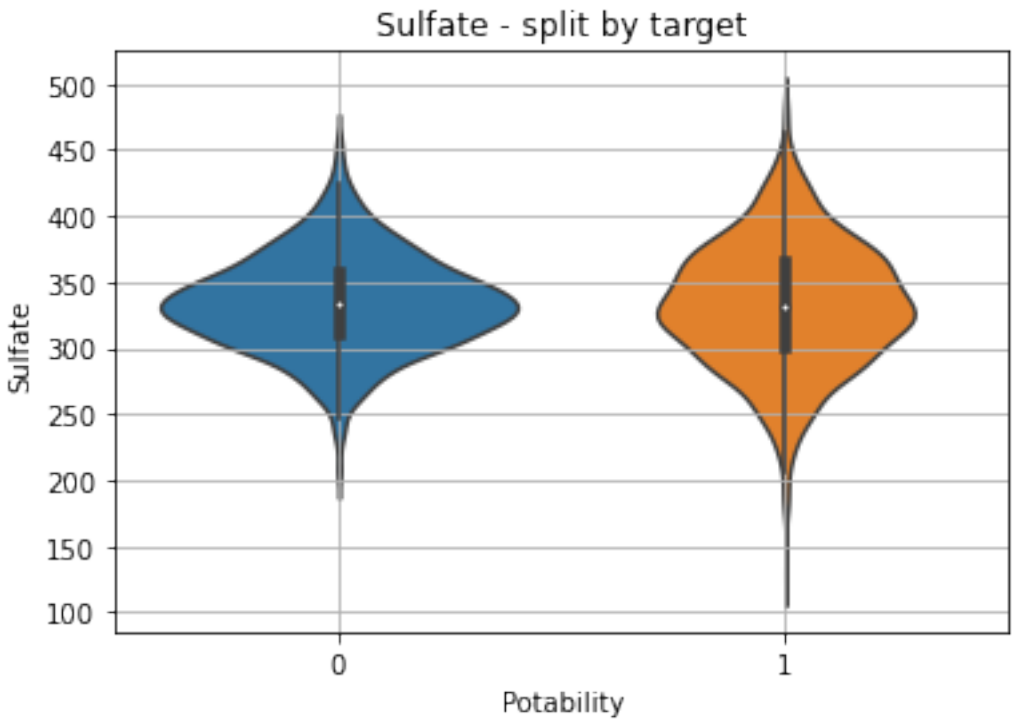
[39]:
```
# Target vs Features
for f in feature_columns_1:
    plt.figure(figsize=(6,4))
    sns.violinplot(y=f, x='Potability', data=df)
    my_title = f + ' - split by target'
    plt.title(my_title)
    plt.grid()
```

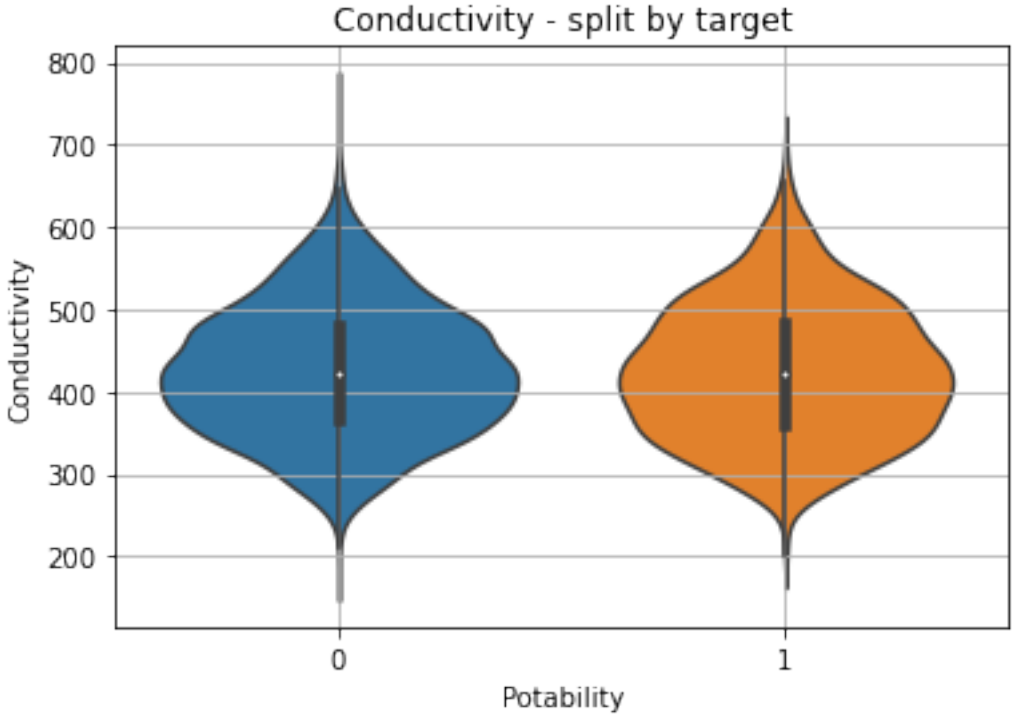

ph - split by target
ph
14
12
10
8
6
4
2
0
0
1
Potability

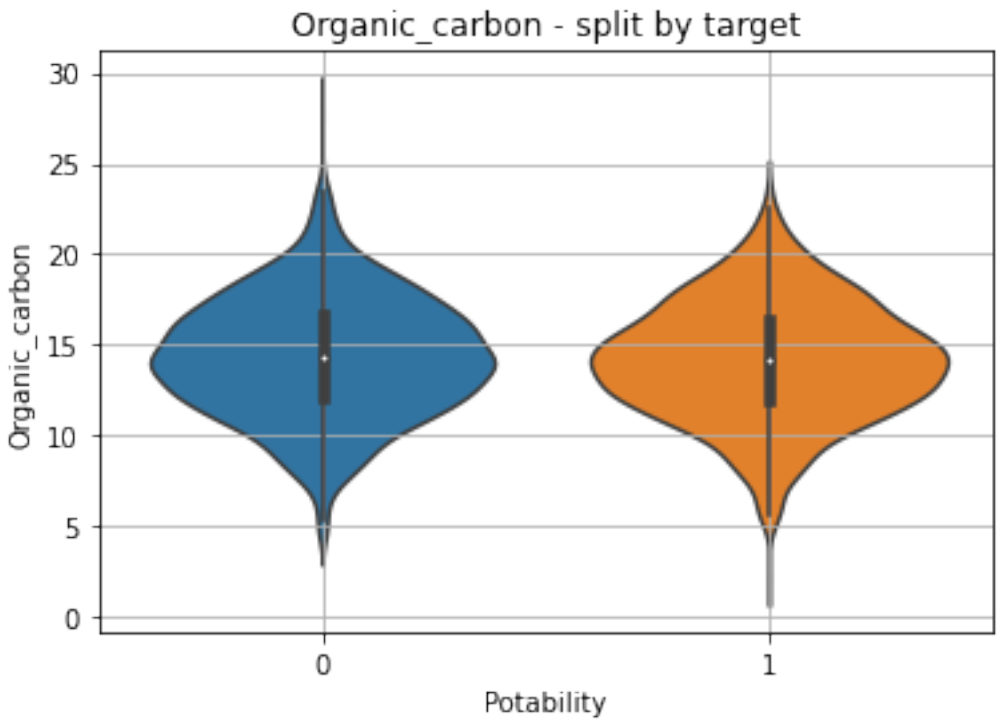

Hardness - split by target
Hardness
350
300
250
200
150
100
50
0
1
Potability

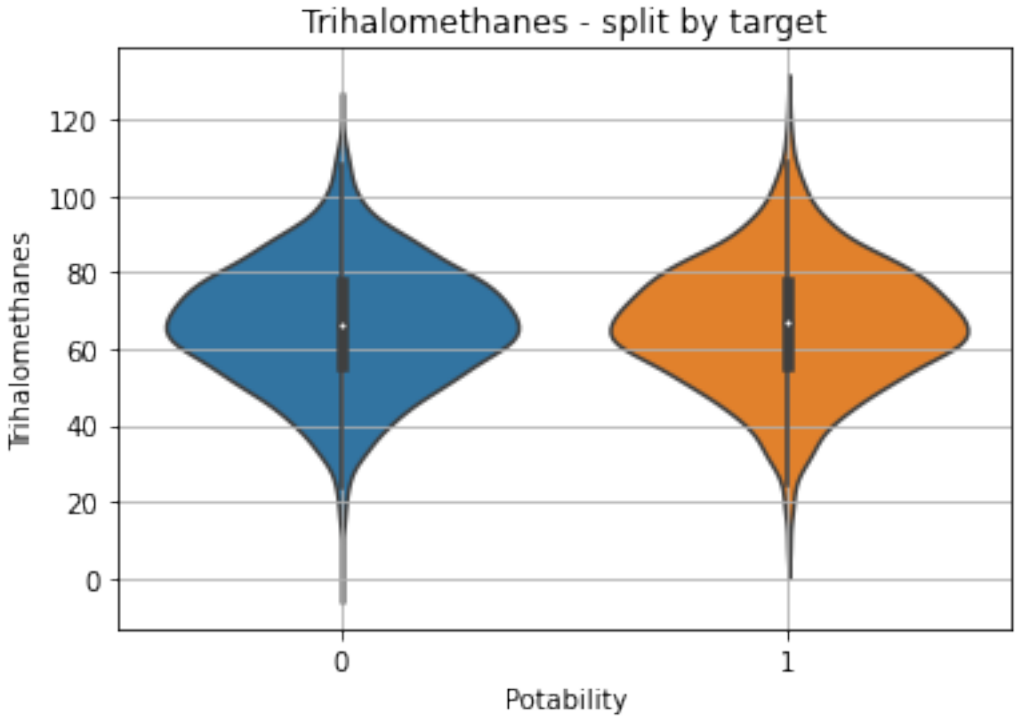

Solids - split by target
60000
50000
40000
30000
20000
10000
0
Solids
0
1
Potability

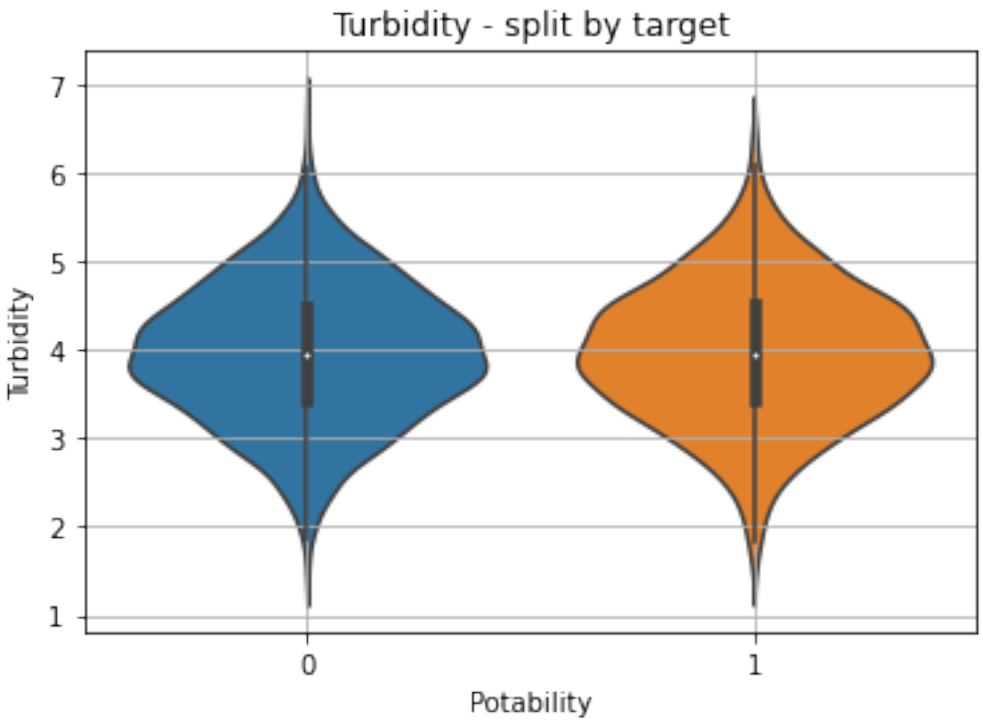

Chloramines - split by target
14
12
10
8
6
4
2
0
Chloramines
0
1
Potability


Sulfate - split by target
Sulfate
500
450
400
350
300
250
200
150
100
0
1
Potability


Conductivity - split by target
Conductivity
800
700
600
500
400
300
200
0
1
Potability


Organic_carbon - split by target
Organic_carbon
30
25
20
15
10
5
0
0
1
Potability


Trihalomethanes - split by target
Trihalomethanes
120
100
80
60
40
20
0
0
1
Potability



It seems that the diagram of Potability is significantly not affected by some of the features suggesting that some of these features might not be important in predicting Potability of water.

0.4.9 9. Modification

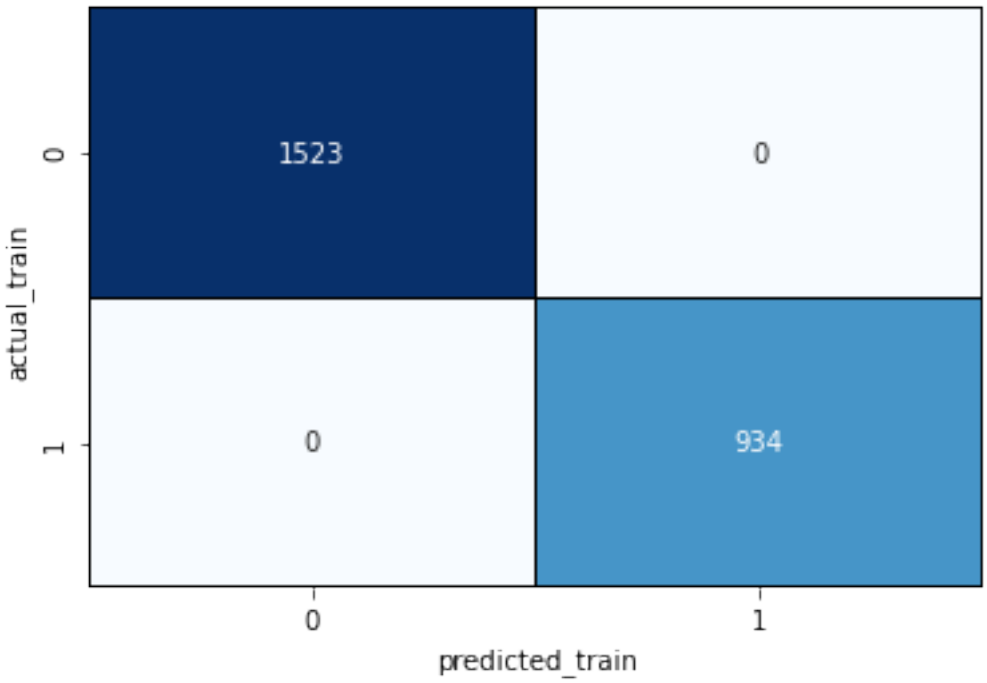
0.4.10 9.1. Changing features, keeping the same model

[40]:
```
feature_columns_2 = ['ph', 'Hardness', 'Solids', 'Chloramines', 'Sulfate']
X = df[feature_columns_2]
y = df['Potability']
X_train, X_test, y_train, y_test = train_test_split(X, y, random_state=1)

# Preprocessing for numerical data
numerical_transformer = SimpleImputer(strategy='mean') # the default is mean
preprocessor = ColumnTransformer(transformers=[('num', numerical_transformer,␣
 ↪feature_columns_2)])

model_rfc = RandomForestClassifier(random_state=1)
my_pipeline = Pipeline(steps=[('preprocessor', preprocessor),
                              ('model', model_rfc)])
my_pipeline.fit(X_train, y_train)
preds_test = my_pipeline.predict(X_test)
print('MAE:', mean_absolute_error(y_test, preds_test))
```

```
# cross validate
# Multiply by -1 since sklearn calculates *negative* MAE

# cv = Determines the cross-validation splitting strategy, the default 5-fold␣
 ↪cross validation
scores = -1 * cross_val_score(my_pipeline, X, y,
                              cv=5,
                              scoring='neg_mean_absolute_error')

print(scores)
print(scores.mean())
```

```
MAE: 0.3308913308913309
[0.41768293 0.3480916  0.36183206 0.41526718 0.35114504]
0.3788037609383727
```

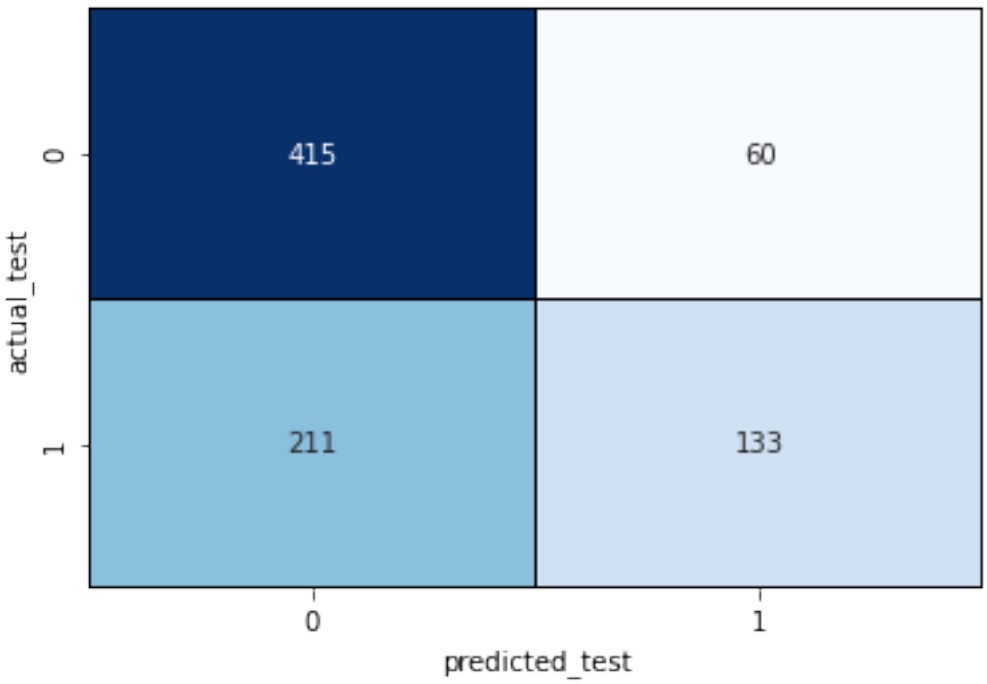
[46]:
```
# Train
preds_train = my_pipeline.predict(X_train)
conf_train = confusion_matrix(y_train, preds_train)
ax = plt.axes()
sns.heatmap(conf_train, cmap='Blues', annot=True,
            cbar=False, fmt='d',
            linecolor='black',
            linewidths=0.1)
ax.set(xlabel='predicted_train', ylabel = 'actual_train')
plt.show()
```



[42]:
```
print(classification_report(y_train, preds_train))
print('accuracy =',accuracy_score(y_train, preds_train))
```

```
              precision    recall  f1-score   support

           0       1.00      1.00      1.00      1523
           1       1.00      1.00      1.00       934

    accuracy                           1.00      2457
   macro avg       1.00      1.00      1.00      2457
weighted avg       1.00      1.00      1.00      2457

accuracy = 1.0
```

[45]:
```
# Test
conf_test = confusion_matrix(y_test, preds_test)
ax = plt.axes()
sns.heatmap(conf_test, cmap='Blues', annot=True,
            cbar=False, fmt='d',
            linecolor='black',
            linewidths=0.1)
ax.set(xlabel='predicted_test', ylabel = 'actual_test')
plt.show()
```



[44]:
```
print(classification_report(y_test, preds_test))
print('accuracy =',accuracy_score(y_test, preds_test))
```

```
              precision    recall  f1-score   support

           0       0.66      0.87      0.75       475
           1       0.69      0.39      0.50       344

    accuracy                           0.67       819
   macro avg       0.68      0.63      0.62       819
weighted avg       0.67      0.67      0.65       819

accuracy = 0.6691086691086691
```

As can be seen, there is a small improvement in predicting 'Potability=1' by just removing some of the irrelavant columns: the overall accuracy has improved from **0.65** to **0.67**.

0.4.11 9.2. Playing around with the Random Forest Classifier parameters

9.2.1. max_leaf_nodes

[57]:
```
# 1. max_leaf_nodes
mae_accuracy = []
for i in range(2,101):
    model_rfc = RandomForestClassifier(max_leaf_nodes=i, random_state=1)
    my_pipeline = Pipeline(steps=[('preprocessor', preprocessor),
                                  ('model', model_rfc)])
    my_pipeline.fit(X_train, y_train)
    preds_train = my_pipeline.predict(X_train)
    #print('MAE Train:', mean_absolute_error(y_train, preds_train))
    preds_test = my_pipeline.predict(X_test)
    #print('MAE Test:', mean_absolute_error(y_test, preds_test))

    # we add num of leaf, mae_test, mae_train, and accuracy to our list
    mae_accuracy.append([i,mean_absolute_error(y_test,␣
 ↪preds_test),mean_absolute_error(y_train, preds_train),
                         accuracy_score(y_test, preds_test)])

# sort by MAE Test
mae_accuracy.sort(key = lambda x: x[1])
# Top 3 MAE
print('Top 3 models sorted by least MAE:',mae_accuracy[0:3])
max_leaf_mae = mae_accuracy[0][0]
print('optimal max leaf :',max_leaf_mae)
print('\n')
# sort by Accuracy Test
mae_accuracy.sort(key = lambda x: x[3], reverse=True)
```

```
# Top 3 MAE
print('Top 3 models sorted by best accuracy:',mae_accuracy[0:3])
max_leaf_accuracy = mae_accuracy[0][0]
print('optimal max leaf :',max_leaf_accuracy)
```

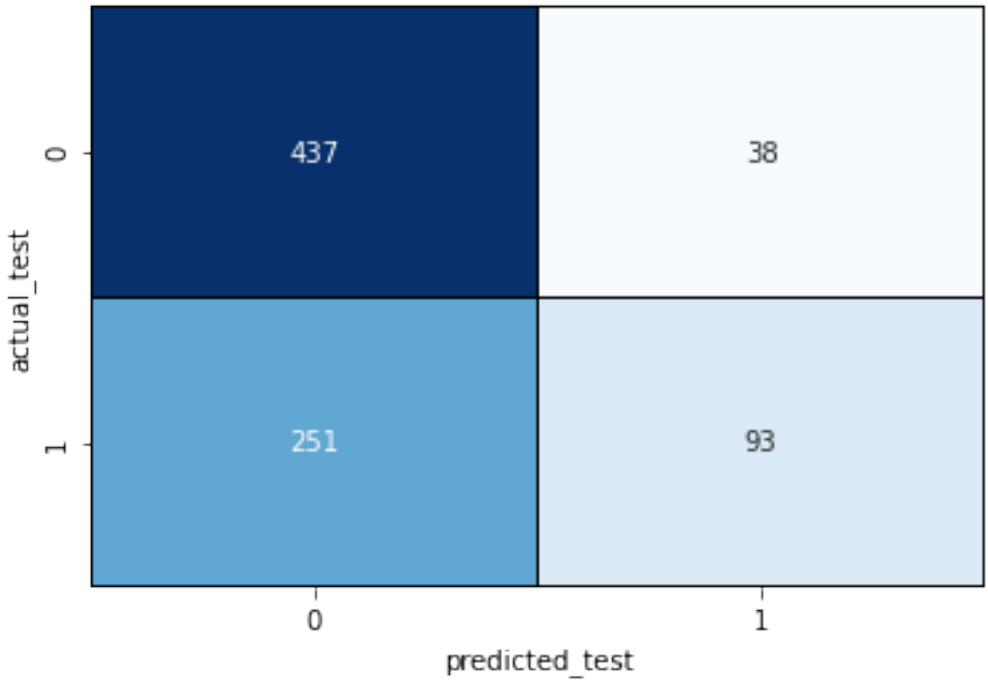
```
Top 3 models sorted by least MAE: [[89, 0.3528693528693529, 0.18274318274318274,
0.6471306471306472], [88, 0.3540903540903541, 0.18315018315018314,
0.645909645909646], [90, 0.3540903540903541, 0.1807081807081807,
0.645909645909646]]
optimal max leaf : 89
```

```
Top 3 models sorted by best accuracy: [[89, 0.3528693528693529,
0.18274318274318274, 0.6471306471306472], [88, 0.3540903540903541,
0.18315018315018314, 0.645909645909646], [90, 0.3540903540903541,
0.1807081807081807, 0.645909645909646]]
optimal max leaf : 89
```

It is clear that both MAE (lowest MAE) and accuracy (highest accuracy) give the same number of max_leaf_nodes. So **max_leaf_nodes = 89** gives us the lowest MAE and highest accuracy.

Now let's set the number of **max_leaf_nodes = 89** and remodel our system.

[53]:
```
model_rfc = RandomForestClassifier(max_leaf_nodes=89, random_state=1)
my_pipeline = Pipeline(steps=[('preprocessor', preprocessor),
                              ('model', model_rfc)])
my_pipeline.fit(X_train, y_train)
preds_test = my_pipeline.predict(X_test)

# Test
conf_test = confusion_matrix(y_test, preds_test)
ax = plt.axes()
sns.heatmap(conf_test, cmap='Blues', annot=True,
            cbar=False, fmt='d',
            linecolor='black',
            linewidths=0.1)
ax.set(xlabel='predicted_test', ylabel = 'actual_test')
plt.show()

print(classification_report(y_test, preds_test))
print('accuracy =',accuracy_score(y_test, preds_test))
```



	precision	recall	f1-score	support
0	0.64	0.92	0.75	475
1	0.71	0.27	0.39	344
accuracy			0.65	819
macro avg	0.67	0.60	0.57	819
weighted avg	0.67	0.65	0.60	819

accuracy = 0.6471306471306472

9.2.2. n_estimators

[55]:
```
# 2. n_estimators
mae_accuracy = []
for i in range(1,101):
    model_rfc = RandomForestClassifier(max_leaf_nodes=89, n_estimators=i,␣
 ↪random_state=1)
    my_pipeline = Pipeline(steps=[('preprocessor', preprocessor),
                                  ('model', model_rfc)])
    my_pipeline.fit(X_train, y_train)
    preds_train = my_pipeline.predict(X_train)
    #print('MAE Train:', mean_absolute_error(y_train, preds_train))
    preds_test = my_pipeline.predict(X_test)
    #print('MAE Test:', mean_absolute_error(y_test, preds_test))
```

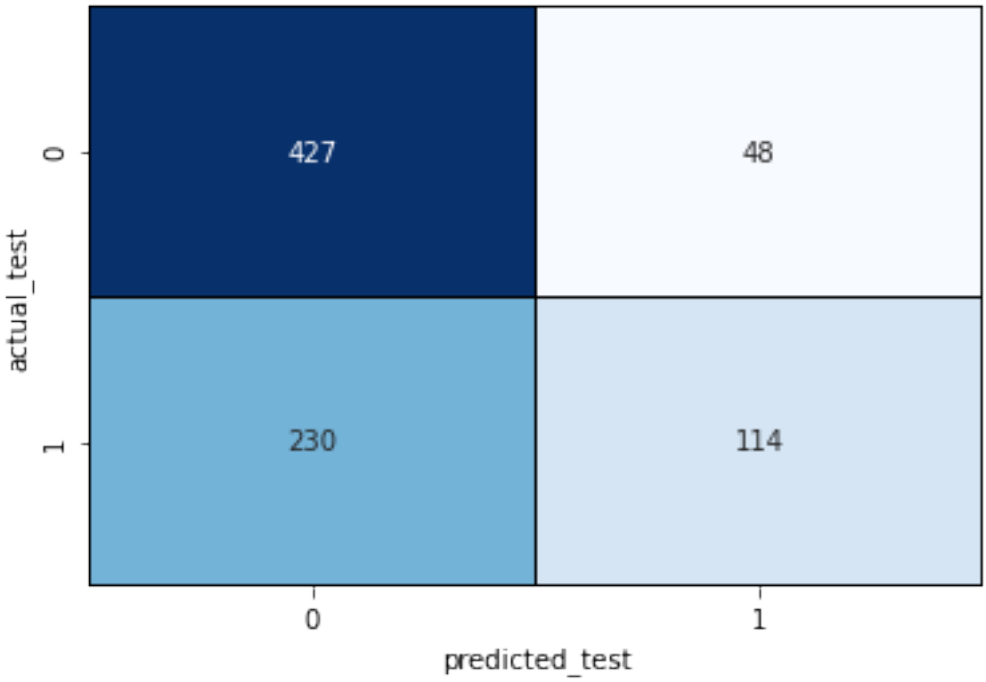
```
    mae_accuracy.append([i,mean_absolute_error(y_test,␣
 ↪preds_test),mean_absolute_error(y_train, preds_train),
                         accuracy_score(y_test, preds_test)])

# sort by MAE Test
mae_accuracy.sort(key = lambda x: x[1])
# Top 3 MAE
print('Top 3 models sorted by least MAE:',mae_accuracy[0:3])
n_estimators = mae_accuracy[0][0]
print('optimal n_estimators :',n_estimators)
print('\n')
# sort by Accuracy Test
mae_accuracy.sort(key = lambda x: x[3], reverse=True)
# Top 3 MAE
print('Top 3 models sorted by best accuracy:',mae_accuracy[0:3])
n_estimators = mae_accuracy[0][0]
print('optimal n_estimators :',n_estimators)
```

```
Top 3 models sorted by least MAE: [[15, 0.33943833943833945, 0.1908831908831909,
0.6605616605616605], [34, 0.34065934065934067, 0.18233618233618235,
0.6593406593406593], [29, 0.3418803418803419, 0.1794871794871795,
0.6581196581196581]]
optimal n_estimators : 15


Top 3 models sorted by best accuracy: [[15, 0.33943833943833945,
0.1908831908831909, 0.6605616605616605], [34, 0.34065934065934067,
0.18233618233618235, 0.6593406593406593], [29, 0.3418803418803419,
0.1794871794871795, 0.6581196581196581]]
optimal n_estimators : 15
```

Now let's set the **n_estimators = 15** and remodel our system.

[56]:
```
model_rfc = RandomForestClassifier(max_leaf_nodes=89, n_estimators=15,␣
 ↪random_state=1)
my_pipeline = Pipeline(steps=[('preprocessor', preprocessor),
                              ('model', model_rfc)])
my_pipeline.fit(X_train, y_train)
preds_test = my_pipeline.predict(X_test)

# Test
conf_test = confusion_matrix(y_test, preds_test)
ax = plt.axes()
sns.heatmap(conf_test, cmap='Blues', annot=True,
            cbar=False, fmt='d',
            linecolor='black',
            linewidths=0.1)
ax.set(xlabel='predicted_test', ylabel = 'actual_test')
```

```
plt.show()

print(classification_report(y_test, preds_test))
print('accuracy =',accuracy_score(y_test, preds_test))
```




```
              precision    recall  f1-score   support

           0       0.65      0.90      0.75       475
           1       0.70      0.33      0.45       344

    accuracy                           0.66       819
   macro avg       0.68      0.62      0.60       819
weighted avg       0.67      0.66      0.63       819

accuracy = 0.6605616605616605
```

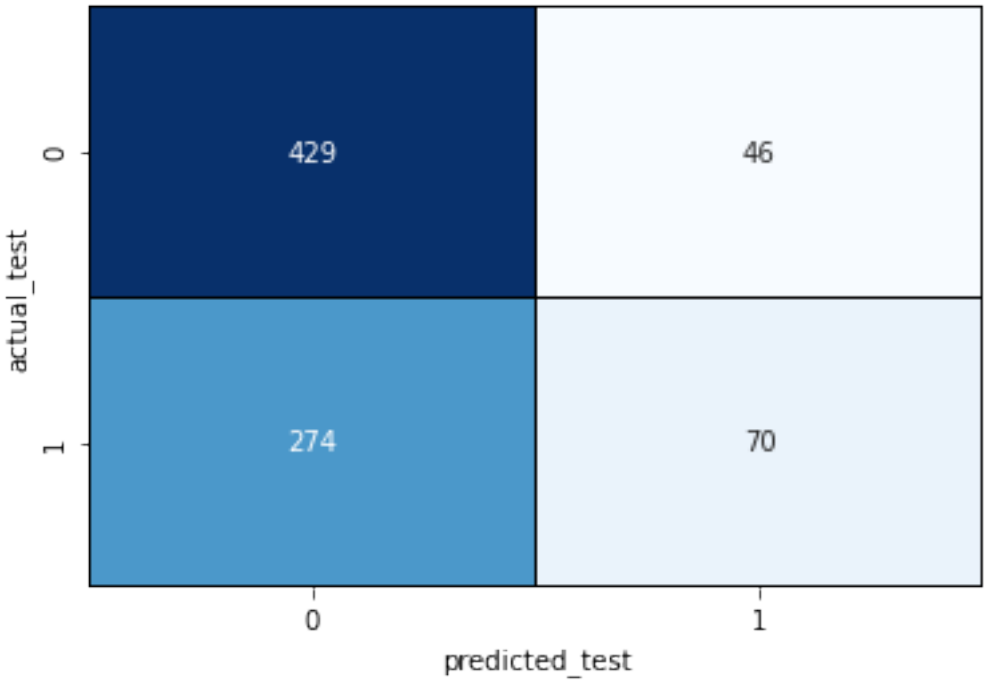
It is clear that **max_leaf_nodes** and **n_estimators** have small influence on the final accuracy. It seems that we need to change our model.

0.4.12 10. Define Model 2: Multi-layer Perceptron Classifier

Note: Here, similar to what we did to our previous model, we play around with the parameters and find the optimal ones. We found that **hidden_layer_sizes = 263** gives us the highest accuracy. (we searched up to 500) However, this number is still less than the accuracy which we obtained from the Random Forest Classifier model. Also, early stopping did not really affect the final accuracy.

[97]:
```
# As a reminder
feature_columns_1 = ['ph', 'Hardness', 'Solids', 'Chloramines', 'Sulfate',␣
 ↪'Conductivity',
                     'Organic_carbon', 'Trihalomethanes', 'Turbidity']
X = df[feature_columns_1]
y = df['Potability']
X_train, X_test, y_train, y_test = train_test_split(X, y, random_state=1)

numerical_transformer = SimpleImputer(strategy='mean') # the default is mean
preprocessor = ColumnTransformer(transformers=[('num', numerical_transformer,␣
 ↪feature_columns_1)])

# Model
#acc = []
#for i in range(1,301):
model_mlp = MLPClassifier(hidden_layer_sizes=263, activation='relu',␣
 ↪solver='adam',
                          batch_size='auto', max_iter=500,
                          random_state=1, tol=0.0001)
my_pipeline = Pipeline(steps=[('preprocessor', preprocessor),
                              ('model', model_mlp)])
my_pipeline.fit(X_train, y_train)
preds_test = my_pipeline.predict(X_test)
acc.append([i, accuracy_score(y_test, preds_test)])
print('MAE:', mean_absolute_error(y_test, preds_test))

#acc.sort(key = lambda x: x[1], reverse=True)
#print('Top 3 :', acc[0:3])
#hid_lay_optimal = acc[0][0]

# Test
conf_test = confusion_matrix(y_test, preds_test)
ax = plt.axes()
sns.heatmap(conf_test, cmap='Blues', annot=True,
            cbar=False, fmt='d',
            linecolor='black',
            linewidths=0.1)
ax.set(xlabel='predicted_test', ylabel = 'actual_test')
plt.show()

print(classification_report(y_test, preds_test))
print('accuracy =',accuracy_score(y_test, preds_test))
```

```
MAE: 0.3907203907203907
```



	precision	recall	f1-score	support
0	0.61	0.90	0.73	475
1	0.60	0.20	0.30	344
accuracy			0.61	819
macro avg	0.61	0.55	0.52	819
weighted avg	0.61	0.61	0.55	819

accuracy = 0.6092796092796092

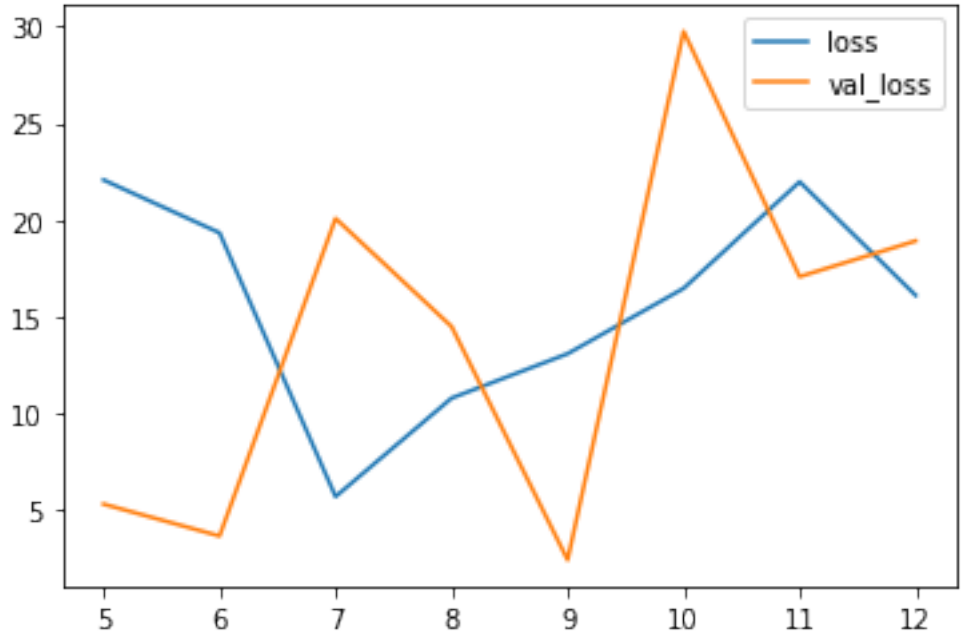
0.4.13 11. Define Model 3: Deep Neural Network

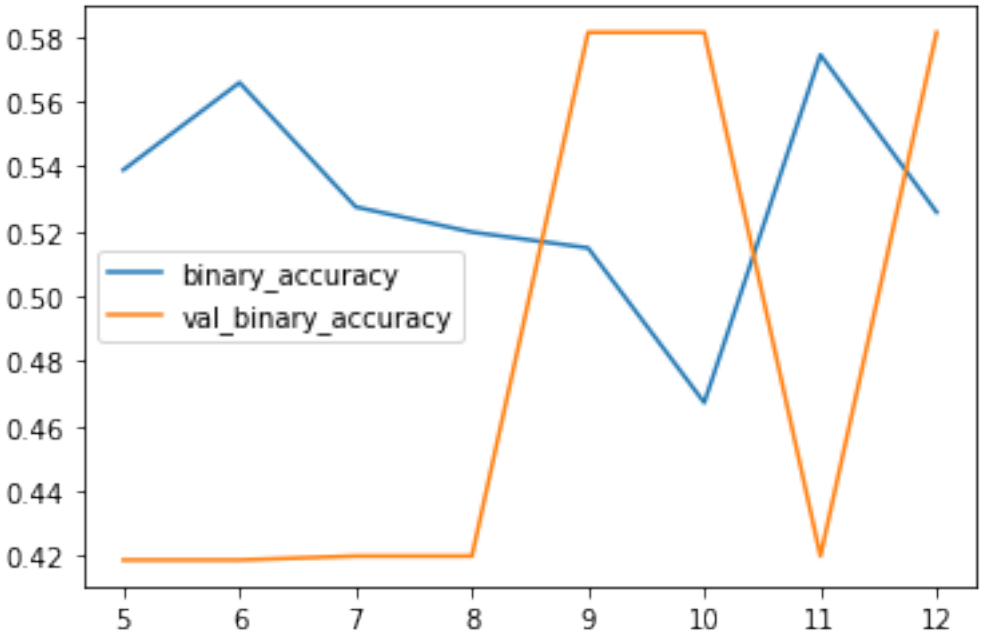
[125]:
```
feature_columns_1 = ['ph', 'Hardness', 'Solids', 'Chloramines', 'Sulfate',␣
 ↪'Conductivity',
                     'Organic_carbon', 'Trihalomethanes', 'Turbidity']
X = df[feature_columns_1]
y = df['Potability']
X_train, X_test, y_train, y_test = train_test_split(X, y, random_state=1)

numerical_transformer = SimpleImputer(strategy='mean') # the default is mean
preprocessor = ColumnTransformer(transformers=[('num', numerical_transformer,␣
 ↪feature_columns_1)])

# preprocessing
```

```
#preprocessor = make_column_transformer((StandardScaler(), # numerical data
#                                        make_column_selector(dtype_include=np.
 ↪number)),
#                                       (OneHotEncoder(sparse=False), #␣
 ↪categorical data
#                                       ␣
 ↪make_column_selector(dtype_include=object)))

model_dnn = keras.Sequential([layers.Dense(64, activation='relu',␣
 ↪input_shape=[9]),
                              layers.Dense(64, activation='relu'),
                              layers.Dense(64, activation='relu'),
                              layers.Dense(64, activation='relu'),
                              layers.Dense(64, activation='relu'),
                              layers.Dense(1, activation='sigmoid')])

model_dnn.compile(optimizer='adam',
                  loss='binary_crossentropy',
                  metrics=['binary_accuracy'])

early_stopping = keras.callbacks.EarlyStopping(patience=10,
                                               min_delta=0.001,
                                               restore_best_weights=True)

X_train = preprocessor.fit_transform(X_train)
X_test = preprocessor.transform(X_test)


history = model_dnn.fit(X_train, y_train,
                        validation_data=(X_test, y_test),
                        batch_size=512,
                        epochs=1000,
                        callbacks=[early_stopping],
                        verbose=0) # hide the output because we have so many␣
 ↪epochs

history_df = pd.DataFrame(history.history)
# Start the plot at epoch 5
history_df.loc[5:, ['loss', 'val_loss']].plot()
history_df.loc[5:, ['binary_accuracy', 'val_binary_accuracy']].plot()

print(("Best Validation Loss: {:0.4f}" +\
      "\nBest Validation Accuracy: {:0.4f}")\
      .format(history_df['val_loss'].min(),
              history_df['val_binary_accuracy'].max()))
```

```
Best Validation Loss: 1.3753
```

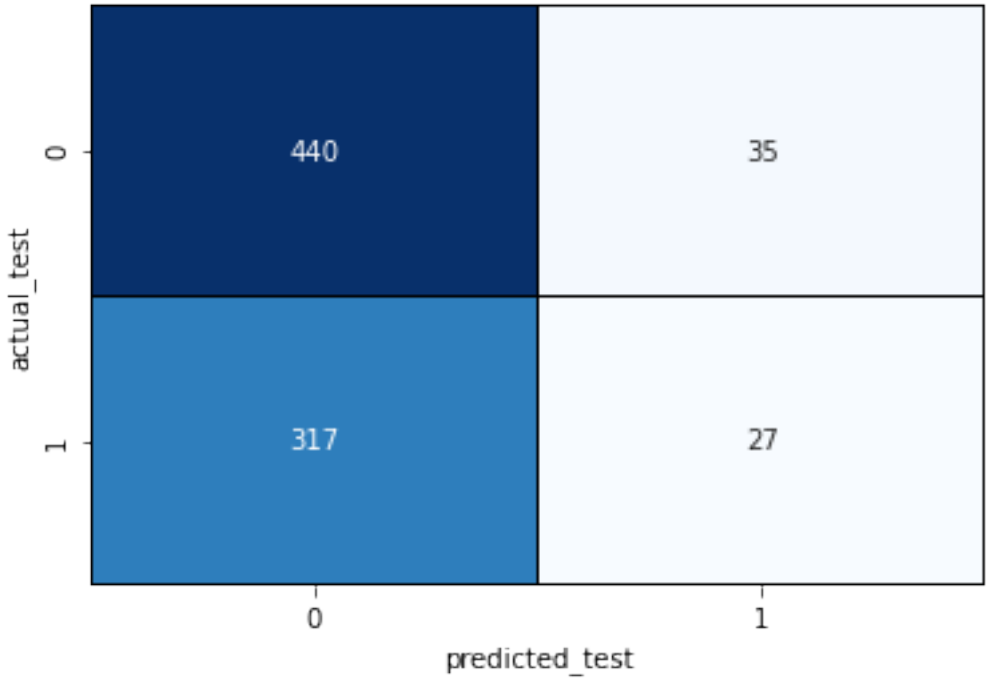
```
Best Validation Accuracy: 0.5812
```





[133]:
```
preds_test = model_dnn.predict(X_test)

for i in range(len(preds_test)):
```

```
    if (preds_test[i] < 0.5):
        preds_test[i] = 0
    else:
        preds_test[i] = 1

# Test
conf_test = confusion_matrix(y_test, preds_test)
ax = plt.axes()
sns.heatmap(conf_test, cmap='Blues', annot=True,
            cbar=False, fmt='d',
            linecolor='black',
            linewidths=0.1)
ax.set(xlabel='predicted_test', ylabel = 'actual_test')
plt.show()

print(classification_report(y_test, preds_test))
print('accuracy =',accuracy_score(y_test, preds_test))
```




```
              precision    recall  f1-score   support

           0       0.58      0.93      0.71       475
           1       0.44      0.08      0.13       344

    accuracy                           0.57       819
   macro avg       0.51      0.50      0.42       819
```

```
weighted avg       0.52      0.57      0.47       819

accuracy = 0.5702075702075702
```

0.4.14 12. Data Imputation: another approach

It seems that substituting the missing data with the mean value will make the final prediction biased toward more potability. The reason is that the mean value is usually an acceptable value for the water to be safe to drink. However, if for a missing feature value the corresponding potability is 0 (and since we do not have any missing potability values) by replacing the missing feature with the mean value we are actually making the data prediction worse.

So instead of replacing all NaNs with the mean value we first look at the potability. If the potability is 0 then we replace the missing value with the max value (meaning that the water is not desirable to drink) and if the potability is 1 then we replace the NaN with the mean value.

[4]:
```
missing_cols = ['ph', 'Sulfate', 'Trihalomethanes']

for i in range(len(df)):
    if (pd.isna(df['ph'][i]) and df['Potability'][i] == 0):
        df['ph'][i] = df.describe()['ph']['max']
    elif (pd.isna(df['ph'][i]) and df['Potability'][i] == 1):
        df['ph'][i] = df.describe()['ph']['mean']

    if (pd.isna(df['Sulfate'][i]) and df['Potability'][i] == 0):
        df['Sulfate'][i] = df.describe()['Sulfate']['max']
    elif (pd.isna(df['Sulfate'][i]) and df['Potability'][i] == 1):
        df['Sulfate'][i] = df.describe()['Sulfate']['mean']

    if (pd.isna(df['Trihalomethanes'][i]) and df['Potability'][i] == 0):
        df['Trihalomethanes'][i] = df.describe()['Trihalomethanes']['max']
    elif (pd.isna(df['Trihalomethanes'][i]) and df['Potability'][i] == 1):
        df['Trihalomethanes'][i] = df.describe()['Trihalomethanes']['mean']

df.isnull().sum()
```

```
<ipython-input-4-296d39367db8>:5: SettingWithCopyWarning:
A value is trying to be set on a copy of a slice from a DataFrame

See the caveats in the documentation: https://pandas.pydata.org/pandas-
docs/stable/user_guide/indexing.html#returning-a-view-versus-a-copy
  df['ph'][i] = df.describe()['ph']['max']
<ipython-input-4-296d39367db8>:10: SettingWithCopyWarning:
A value is trying to be set on a copy of a slice from a DataFrame

See the caveats in the documentation: https://pandas.pydata.org/pandas-
docs/stable/user_guide/indexing.html#returning-a-view-versus-a-copy
  df['Sulfate'][i] = df.describe()['Sulfate']['max']
<ipython-input-4-296d39367db8>:15: SettingWithCopyWarning:
```

```
A value is trying to be set on a copy of a slice from a DataFrame

See the caveats in the documentation: https://pandas.pydata.org/pandas-
docs/stable/user_guide/indexing.html#returning-a-view-versus-a-copy
  df['Trihalomethanes'][i] = df.describe()['Trihalomethanes']['max']
<ipython-input-4-296d39367db8>:7: SettingWithCopyWarning:
A value is trying to be set on a copy of a slice from a DataFrame

See the caveats in the documentation: https://pandas.pydata.org/pandas-
docs/stable/user_guide/indexing.html#returning-a-view-versus-a-copy
  df['ph'][i] = df.describe()['ph']['mean']
<ipython-input-4-296d39367db8>:12: SettingWithCopyWarning:
A value is trying to be set on a copy of a slice from a DataFrame

See the caveats in the documentation: https://pandas.pydata.org/pandas-
docs/stable/user_guide/indexing.html#returning-a-view-versus-a-copy
  df['Sulfate'][i] = df.describe()['Sulfate']['mean']
<ipython-input-4-296d39367db8>:17: SettingWithCopyWarning:
A value is trying to be set on a copy of a slice from a DataFrame

See the caveats in the documentation: https://pandas.pydata.org/pandas-
docs/stable/user_guide/indexing.html#returning-a-view-versus-a-copy
  df['Trihalomethanes'][i] = df.describe()['Trihalomethanes']['mean']
```

[4]:
```
ph                0
Hardness          0
Solids            0
Chloramines       0
Sulfate           0
Conductivity      0
Organic_carbon    0
Trihalomethanes   0
Turbidity         0
Potability        0
dtype: int64
```

[5]:
```
df.describe()
```

[5]:

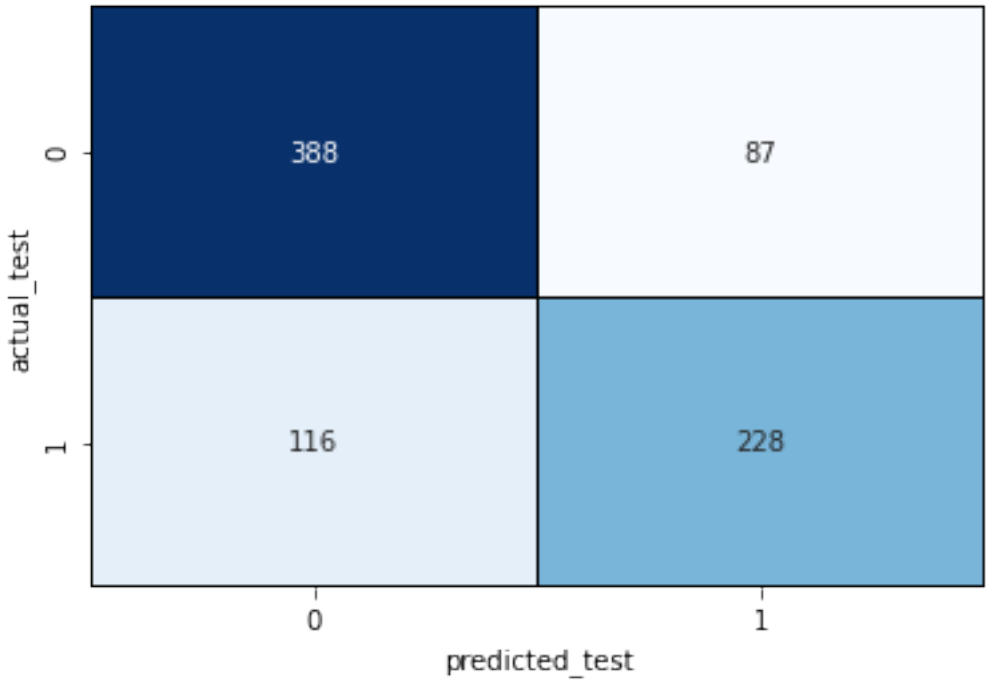
	ph	Hardness	Solids	Chloramines	Sulfate	\
count	3276.000000	3276.000000	3276.000000	3276.000000	3276.000000	
mean	7.765504	196.369496	22014.092526	7.122277	356.936395	
std	2.508442	32.879761	8768.570828	1.583085	63.415209	
min	0.000000	47.432000	320.942611	0.352000	129.000000	
25%	6.277673	176.850538	15666.690297	6.127421	317.094638	
50%	7.341889	196.967627	20927.833607	7.130299	343.302742	
75%	8.439712	216.667456	27332.762127	8.114887	378.230674	
max	14.000000	323.124000	61227.196008	13.127000	481.030642	

	Conductivity	Organic_carbon	Trihalomethanes	Turbidity	Potability
count	3276.000000	3276.000000	3276.000000	3276.000000	3276.000000
mean	426.205111	14.284970	68.294745	3.966786	0.390110
std	80.824064	3.308162	18.802058	0.780382	0.487849
min	181.483754	2.200000	0.738000	1.450000	0.000000
25%	365.734414	12.065801	56.647656	3.439711	0.000000
50%	421.884968	14.218338	67.304132	3.955028	0.000000
75%	481.792304	16.557652	78.230106	4.500320	1.000000
max	753.342620	28.300000	124.000000	6.739000	1.000000

12.1. Random Forest Classifier

[6]:
```
feature_columns_1 = ['ph', 'Hardness', 'Solids', 'Chloramines', 'Sulfate',␣
 ↪'Conductivity',
                     'Organic_carbon', 'Trihalomethanes', 'Turbidity']
X = df[feature_columns_1]
y = df['Potability']
X_train, X_test, y_train, y_test = train_test_split(X, y, random_state=1)

model_rfc = RandomForestClassifier(random_state=1)

# Preprocessing for numerical data: here it does not matter as we do not have␣
 ↪any NaN
numerical_transformer = SimpleImputer(strategy='mean') # the default is mean
preprocessor = ColumnTransformer(transformers=[('num', numerical_transformer,␣
 ↪feature_columns_1)])

my_pipeline = Pipeline(steps=[('preprocessor', preprocessor),
                              ('model', model_rfc)])
my_pipeline.fit(X_train, y_train)
preds_test = my_pipeline.predict(X_test)
print('MAE:', mean_absolute_error(y_test, preds_test))

# Test
conf_test = confusion_matrix(y_test, preds_test)
ax = plt.axes()
sns.heatmap(conf_test, cmap='Blues', annot=True,
            cbar=False, fmt='d',
            linecolor='black',
            linewidths=0.1)
ax.set(xlabel='predicted_test', ylabel = 'actual_test')
plt.show()

print(classification_report(y_test, preds_test))
print('accuracy =',accuracy_score(y_test, preds_test))
```

```
MAE: 0.24786324786324787
```



	precision	recall	f1-score	support
0	0.77	0.82	0.79	475
1	0.72	0.66	0.69	344
accuracy			0.75	819
macro avg	0.75	0.74	0.74	819
weighted avg	0.75	0.75	0.75	819

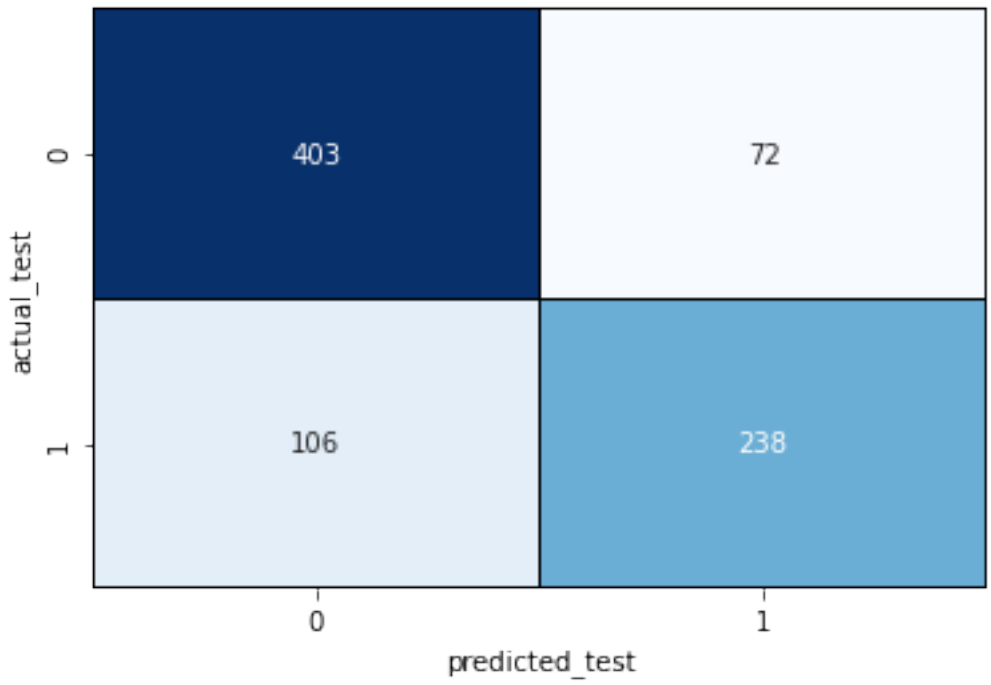
```
accuracy = 0.7521367521367521
```

Now we can see a significant improvement here! Now let's use another set of features, which was shown previously that might be better descriptors, and see if we can do better!

[7]:
```
feature_columns_2 = ['ph', 'Hardness', 'Solids', 'Chloramines', 'Sulfate']
X = df[feature_columns_2]
y = df['Potability']
X_train, X_test, y_train, y_test = train_test_split(X, y, random_state=1)

model_rfc = RandomForestClassifier(random_state=1)

# Preprocessing for numerical data: here it does not matter as we do not have␣
 ↪any NaN
numerical_transformer = SimpleImputer(strategy='mean') # the default is mean
```

```
preprocessor = ColumnTransformer(transformers=[('num', numerical_transformer,␣
 ↪feature_columns_2)])

my_pipeline = Pipeline(steps=[('preprocessor', preprocessor),
                              ('model', model_rfc)])
my_pipeline.fit(X_train, y_train)
preds_test = my_pipeline.predict(X_test)
print('MAE:', mean_absolute_error(y_test, preds_test))

# Test
conf_test = confusion_matrix(y_test, preds_test)
ax = plt.axes()
sns.heatmap(conf_test, cmap='Blues', annot=True,
            cbar=False, fmt='d',
            linecolor='black',
            linewidths=0.1)
ax.set(xlabel='predicted_test', ylabel = 'actual_test')
plt.show()

print(classification_report(y_test, preds_test))
print('accuracy =',accuracy_score(y_test, preds_test))
```

```
MAE: 0.21733821733821734
```




```
              precision    recall  f1-score   support
```

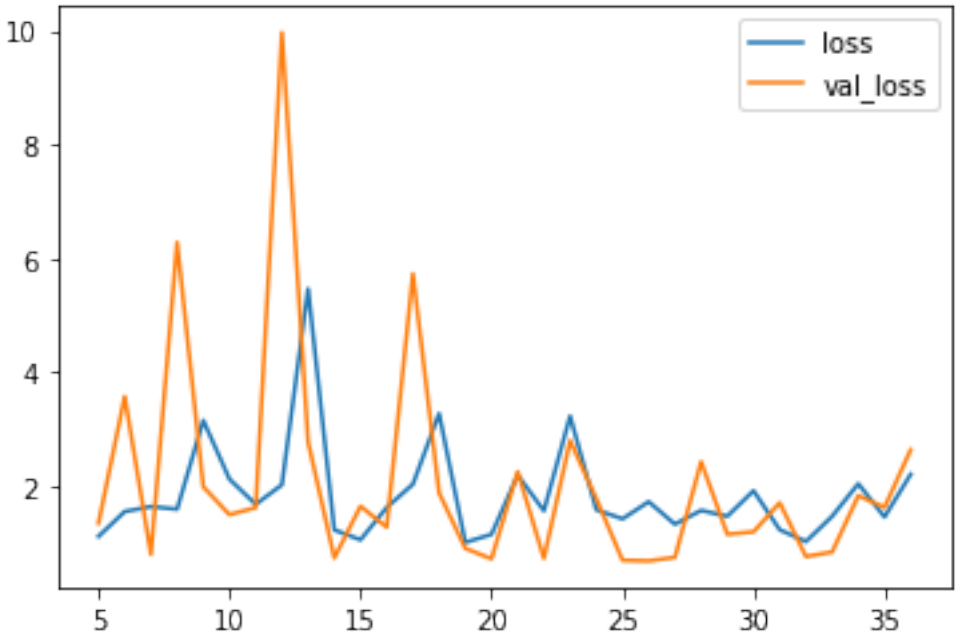
```
              0       0.79      0.85      0.82       475
              1       0.77      0.69      0.73       344

       accuracy                           0.78       819
      macro avg       0.78      0.77      0.77       819
   weighted avg       0.78      0.78      0.78       819

accuracy = 0.7826617826617827
```

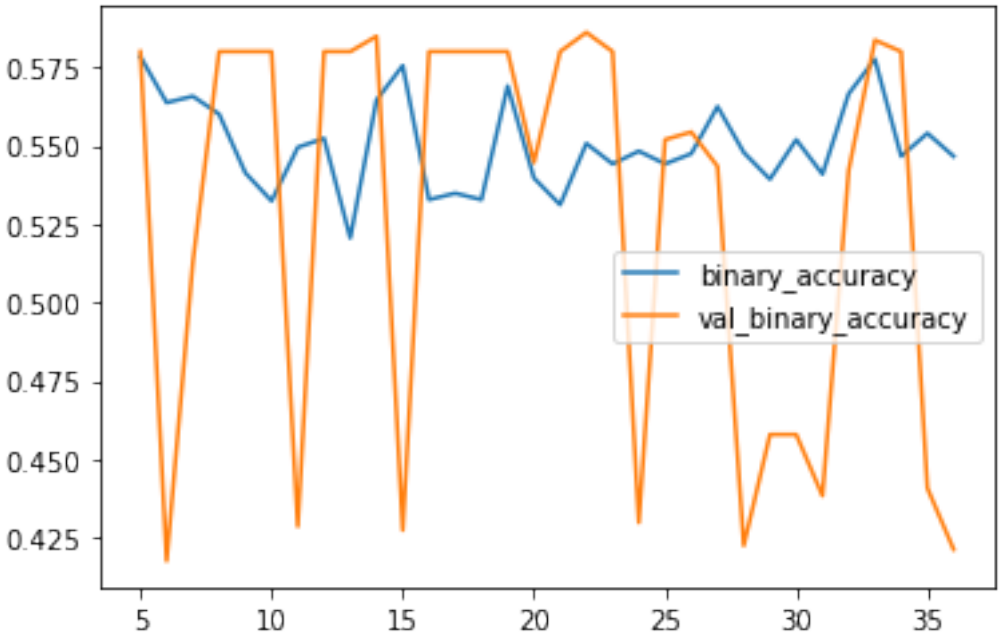
Yes! As you can see the final accuracy is **0.78**. So far, we have been able to increase the accuracy from **0.58** all the way to **0.78**.

[37]:
```
feature_columns_1 = ['ph', 'Hardness', 'Solids', 'Chloramines', 'Sulfate',␣
 ↪'Conductivity',
                     'Organic_carbon', 'Trihalomethanes', 'Turbidity']
X = df[feature_columns_1]
y = df['Potability']
X_train, X_test, y_train, y_test = train_test_split(X, y, random_state=1)

print(df.isnull().sum())

numerical_transformer = SimpleImputer(strategy='mean') # the default is mean
preprocessor = ColumnTransformer(transformers=[('num', numerical_transformer,␣
 ↪feature_columns_1)])

# preprocessing
#preprocessor = make_column_transformer((StandardScaler(), # numerical data
#                                        make_column_selector(dtype_include=np.
 ↪number)),
#                                       (OneHotEncoder(sparse=False), #␣
 ↪categorical data
#                                       ␣
 ↪make_column_selector(dtype_include=object)))

model_dnn = keras.Sequential([layers.Dense(8, activation='relu',␣
 ↪input_shape=[9]),
                          layers.Dense(8, activation='relu'),
                          layers.Dense(8, activation='relu'),
                          layers.Dense(1, activation='sigmoid')])

model_dnn.compile(optimizer='adam',
                  loss='binary_crossentropy',
                  metrics=['binary_accuracy'])

early_stopping = keras.callbacks.EarlyStopping(patience=10,
                                               min_delta=0.001,
```

```
                                                restore_best_weights=True)

X_train = preprocessor.fit_transform(X_train)
X_test = preprocessor.transform(X_test)


history = model_dnn.fit(X_train, y_train,
                        validation_data=(X_test, y_test),
                        batch_size=32,
                        epochs=1000,
                        callbacks=[early_stopping],
                        verbose=0) # hide the output because we have so many␣
 ↪epochs

history_df = pd.DataFrame(history.history)
# Start the plot at epoch 5
history_df.loc[5:, ['loss', 'val_loss']].plot()
history_df.loc[5:, ['binary_accuracy', 'val_binary_accuracy']].plot()

print(("Best Validation Loss: {:0.4f}" +\
      "\nBest Validation Accuracy: {:0.4f}")\
      .format(history_df['val_loss'].min(),
              history_df['val_binary_accuracy'].max()))
```

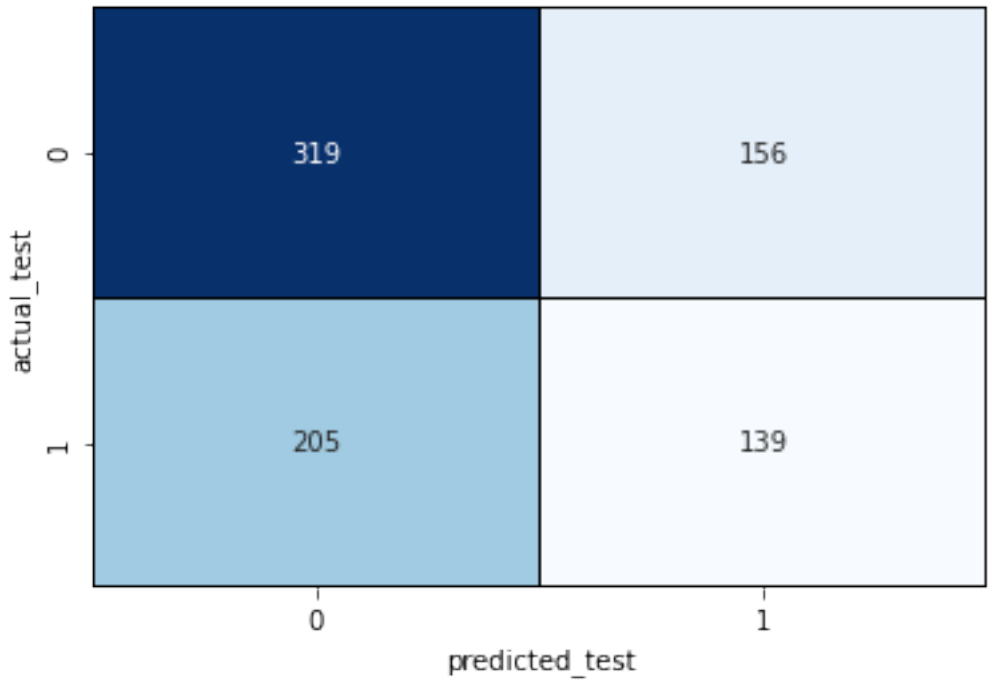
```
ph                 0
Hardness           0
Solids             0
Chloramines        0
Sulfate            0
Conductivity       0
Organic_carbon     0
Trihalomethanes    0
Turbidity          0
Potability         0
dtype: int64
Best Validation Loss: 0.6941
Best Validation Accuracy: 0.6068
```





[32]:
```
preds_test = model_dnn.predict(X_test)

for i in range(len(preds_test)):
    if (preds_test[i] < 0.5):
```

```
        preds_test[i] = 0
    else:
        preds_test[i] = 1

# Test
conf_test = confusion_matrix(y_test, preds_test)
ax = plt.axes()
sns.heatmap(conf_test, cmap='Blues', annot=True,
            cbar=False, fmt='d',
            linecolor='black',
            linewidths=0.1)
ax.set(xlabel='predicted_test', ylabel = 'actual_test')
plt.show()

print(classification_report(y_test, preds_test))
print('accuracy =',accuracy_score(y_test, preds_test))
```




```
              precision    recall  f1-score   support

           0       0.61      0.67      0.64       475
           1       0.47      0.40      0.44       344

    accuracy                           0.56       819
   macro avg       0.54      0.54      0.54       819
weighted avg       0.55      0.56      0.55       819
```

```
accuracy = 0.5592185592185592
```

0.4.15 13. Summary

In summary, we used 3 different models and tried different hyperparameters to obtain the best results. Moreover, we used different input features and handled missing data points to enhance the final accuracy of test dataset. By doing all of that, we have been able to increase the accuracy from **0.58** all the way to **0.78**.

[ ]: