Week 4: Interpretable Machine Learning for Data Science

Problem: You have been mandated by a large wine-making company in Valais to discover the key chemical factors that determine the quality of wine and build an interpretable model that will help their cellar masters make decisions daily.

Settings things up (15')

This week will require quite a lot of autonomy on your part, but we will guide you with this high-level notebook. First, take the following steps:

- Install Poetry.
- Then use Poetry to create a virtual environment:

  ```
  poetry install
  ```

- Then restart VS Code and add the kernel that corresponds to the environment created by Poetry.

Then, let's set up black, which is a highly encouraged best-practice for all your Python projects. That way, you never have to worry and debate about code formatting anymore. By using it, you agree to cede control over minutiae of hand-formatting. In return, Black gives you speed, determinism, and freedom from `pycodestyle` nagging about formatting. You will save time and mental energy for more important matters.

```
# install lib to import data
!pip install ucimlrepo
```

```
!poetry install
!poetry run ipython kernel install --user --name=w4-xai-ds
```

```
Installing dependencies from lock file

No dependencies to install or update
Installed kernelspec w4-xai-ds in /home/franciscoribeiro/.local/share/jupyter/
kernels/w4-xai-ds
```

```
import jupyter_black

jupyter_black.load()
```

Here are the libraries you will most likely need and use during this week:

- `numpy` for basic scientific computing and `scipy` for statistical testing.
- `pandas` or `polars` for dataset manipulation. Polars is highly recommended, because it is awesome. Instructions below will refer to the Polars API.
- `seaborn` for statistical data visualization, but `matplotlib` is always needed anyway. Use both!
- `shap` will be used for interpretability.
- `sklearn` and `xgboost` will be used for training models. You may import them later when you need them.

```
# import all libs to use in this notebook
import numpy as np
import scipy
import pandas as pd
import seaborn as sb
import matplotlib.pyplot as plt
import shap
import sklearn
import xgboost as xgb
from ucimlrepo import fetch_ucirepo
```

```
import seaborn as sns
from sklearn.decomposition import PCA
from sklearn.preprocessing import StandardScaler
from sklearn.cluster import KMeans
from sklearn.metrics import mutual_info_score, accuracy_score, f1_score
from sklearn.linear_model import LogisticRegression
from sklearn.model_selection import train_test_split
from sklearn import linear_model
from sklearn.pipeline import make_pipeline
from sklearn.model_selection import GridSearchCV
import shap
from sklearn.metrics import confusion_matrix, classification_report
```

Fetch the data (15')

Here we have a very nice package that can do everything for us (aka `ucimlrepo`). Let's use it!

Take a look at the website for details.

```
# fetch dataset
wine_quality = fetch_ucirepo(id=186)

df = wine_quality.data.original

# data (as pandas dataframes)
X = wine_quality.data.features
y = wine_quality.data.targets


wineColor = df["color"]

# metadata
print(wine_quality.metadata)

# variable information
print(wine_quality.variables)
```

```
                    name     role         type demographic  \
0          fixed_acidity  Feature   Continuous        None
1       volatile_acidity  Feature   Continuous        None
2            citric_acid  Feature   Continuous        None
3         residual_sugar  Feature   Continuous        None
4              chlorides  Feature   Continuous        None
5    free_sulfur_dioxide  Feature   Continuous        None
6   total_sulfur_dioxide  Feature   Continuous        None
7                density  Feature   Continuous        None
8                     pH  Feature   Continuous        None
9              sulphates  Feature   Continuous        None
10               alcohol  Feature   Continuous        None
11               quality   Target      Integer        None
12                 color    Other  Categorical        None

               description units missing_values
0                     None  None             no
1                     None  None             no
2                     None  None             no
3                     None  None             no
4                     None  None             no
5                     None  None             no
```

```
6                     None  None             no
7                     None  None             no
8                     None  None             no
9                     None  None             no
10                    None  None             no
11  score between 0 and 10  None             no
12            red or white  None             no
```

```
# Check original data set
df.head()
```

```
   fixed_acidity  volatile_acidity  citric_acid  residual_sugar  chlorides  \
0            7.4              0.70         0.00             1.9      0.076
1            7.8              0.88         0.00             2.6      0.098
2            7.8              0.76         0.04             2.3      0.092
3           11.2              0.28         0.56             1.9      0.075
4            7.4              0.70         0.00             1.9      0.076

   free_sulfur_dioxide  total_sulfur_dioxide  density    pH  sulphates  \
0                 11.0                  34.0   0.9978  3.51       0.56
1                 25.0                  67.0   0.9968  3.20       0.68
2                 15.0                  54.0   0.9970  3.26       0.65
3                 17.0                  60.0   0.9980  3.16       0.58
4                 11.0                  34.0   0.9978  3.51       0.56

   alcohol  quality color
0      9.4        5   red
1      9.8        5   red
2      9.8        5   red
3      9.8        6   red
4      9.4        5   red
```

Now, let's check that the data have the correct shape to ensure they have been loaded as expected.

Calculate how many samples and features we have in total, how many are red or white wines, how many are good or bad wines, etc.

```
# Count the number of red and white wines
red_wine_count = df[df["color"] == "red"].shape[0]
white_wine_count = df[df["color"] == "white"].shape[0]

print(f"Number of red wines: {red_wine_count}")
print(f"Number of white wines: {white_wine_count}")
```

```
Number of red wines: 1599
Number of white wines: 4898
```

```
# Count the number of good and bad wines
goodWine = df[df["quality"] >= 6].shape[0]
badWines = df[df["quality"] < 6].shape[0]

print(f"Number of good wines: {goodWine}")
print(f"Number of bad wines: {badWines}")
```

```
Number of good wines: 4113
Number of bad wines: 2384
```

```
print(X.shape)
print(y.shape)
```

```
(6497, 11)
(6497, 1)
```

```
X. describe()
```

```
       fixed_acidity  volatile_acidity  citric_acid  residual_sugar  \
count    6497.000000       6497.000000  6497.000000     6497.000000
mean        7.215307          0.339666     0.318633        5.443235
std         1.296434          0.164636     0.145318        4.757804
min         3.800000          0.080000     0.000000        0.600000
25%         6.400000          0.230000     0.250000        1.800000
50%         7.000000          0.290000     0.310000        3.000000
75%         7.700000          0.400000     0.390000        8.100000
max        15.900000          1.580000     1.660000       65.800000

         chlorides  free_sulfur_dioxide  total_sulfur_dioxide      density  \
count  6497.000000          6497.000000           6497.000000  6497.000000
mean      0.056034            30.525319            115.744574     0.994697
std       0.035034            17.749400             56.521855     0.002999
min       0.009000             1.000000              6.000000     0.987110
25%       0.038000            17.000000             77.000000     0.992340
50%       0.047000            29.000000            118.000000     0.994890
75%       0.065000            41.000000            156.000000     0.996990
max       0.611000           289.000000            440.000000     1.038980

                pH    sulphates      alcohol
count  6497.000000  6497.000000  6497.000000
mean      3.218501     0.531268    10.491801
std       0.160787     0.148806     1.192712
min       2.720000     0.220000     8.000000
25%       3.110000     0.430000     9.500000
50%       3.210000     0.510000    10.300000
75%       3.320000     0.600000    11.300000
max       4.010000     2.000000    14.900000
```

```
y.describe()
```

```
           quality
count  6497.000000
mean      5.818378
std       0.873255
min       3.000000
25%       5.000000
50%       6.000000
75%       6.000000
max       9.000000
```

Data Exploration (1h30)

We now will inspect the features one-by-one, and try to understand their dynamics, especially between white and red wines.

- Use `Dataframe.describe` to display statistics on each feature. Do the same for red wines only, and white wines only. Do you notice any clear difference?
- Compute the effect size by computing the strictly standardized mean difference (SSMD) between the red and white wines for each feature.

```
X.describe()
```

```
       fixed_acidity  volatile_acidity  citric_acid  residual_sugar  \
count    6497.000000       6497.000000  6497.000000     6497.000000
mean        7.215307          0.339666     0.318633        5.443235
std         1.296434          0.164636     0.145318        4.757804
```

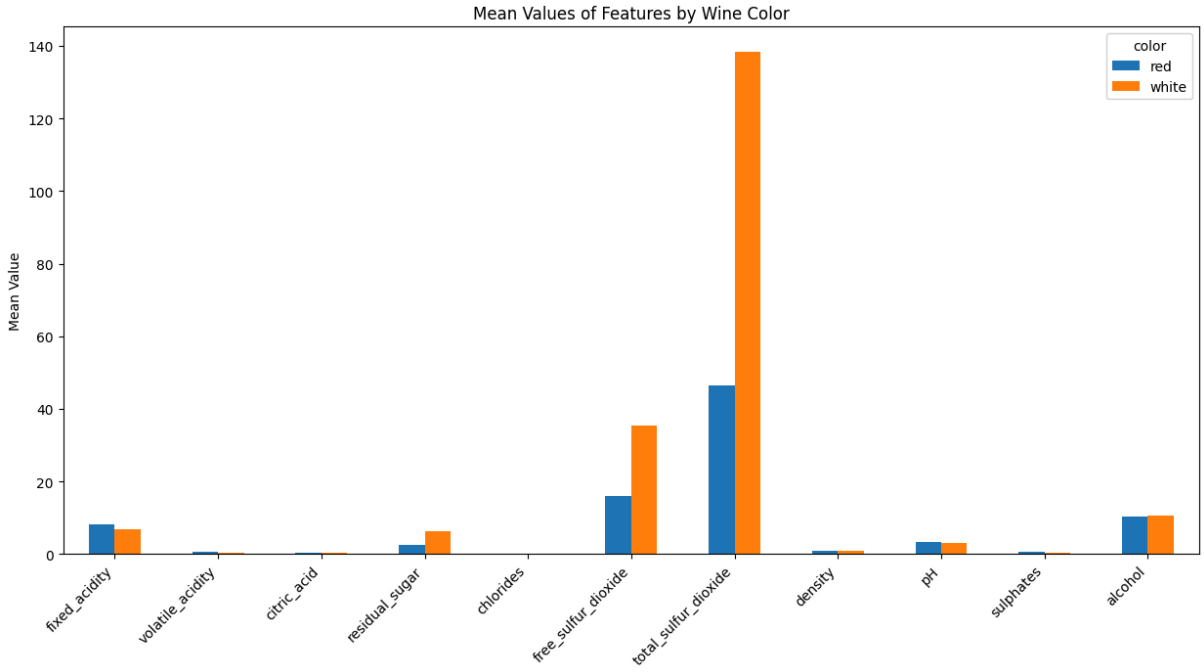
```
min         3.800000          0.080000     0.000000        0.600000
25%         6.400000          0.230000     0.250000        1.800000
50%         7.000000          0.290000     0.310000        3.000000
75%         7.700000          0.400000     0.390000        8.100000
max        15.900000          1.580000     1.660000       65.800000

         chlorides  free_sulfur_dioxide  total_sulfur_dioxide      density  \
count  6497.000000          6497.000000           6497.000000  6497.000000
mean      0.056034            30.525319            115.744574     0.994697
std       0.035034            17.749400             56.521855     0.002999
min       0.009000             1.000000              6.000000     0.987110
25%       0.038000            17.000000             77.000000     0.992340
50%       0.047000            29.000000            118.000000     0.994890
75%       0.065000            41.000000            156.000000     0.996990
max       0.611000           289.000000            440.000000     1.038980

                pH    sulphates      alcohol
count  6497.000000  6497.000000  6497.000000
mean      3.218501     0.531268    10.491801
std       0.160787     0.148806     1.192712
min       2.720000     0.220000     8.000000
25%       3.110000     0.430000     9.500000
50%       3.210000     0.510000    10.300000
75%       3.320000     0.600000    11.300000
max       4.010000     2.000000    14.900000
```

```
# See mean and std for red and white
df[df["color"] == "red"].describe()
df_red = df[df["color"] == "red"]
```

```
df[df["color"] == "white"].describe()
df_white = df[df["color"] == "white"]
```

```
numeric_features = [
    "fixed_acidity",
    "volatile_acidity",
    "citric_acid",
    "residual_sugar",
    "chlorides",
    "free_sulfur_dioxide",
    "total_sulfur_dioxide",
    "density",
    "pH",
    "sulphates",
    "alcohol",
]
```

```
# Calculating the mean values for red and white wines
mean_values = df.groupby("color")[numeric_features].mean().transpose()

# Plotting the barplot comparing mean values between red and white
mean_values.plot(kind="bar", figsize=(15, 7))
plt.title("Mean Values of Features by Wine Color")
plt.ylabel("Mean Value")
plt.xticks(rotation=45, ha="right")
plt.show()
```



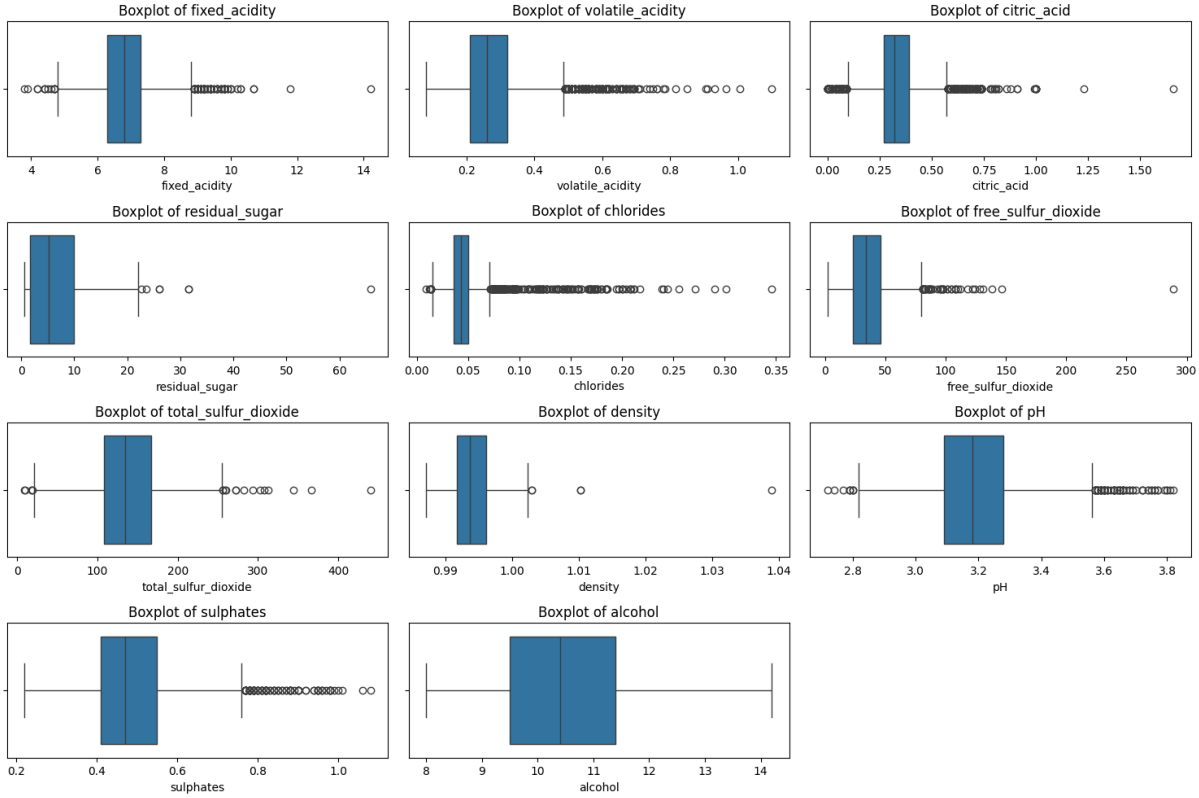
differences between red and white

- we can see big differences between white wine and red whine in the features
- *total_sulfur_dioxide* : We can see that mean of sulfur dioxide is almost 3 times higer in red wine that in white wine
- There is a significant imbalance between 'good' and 'bad' wines, with the majority of wines being classified as 'bad' based on the quality score.

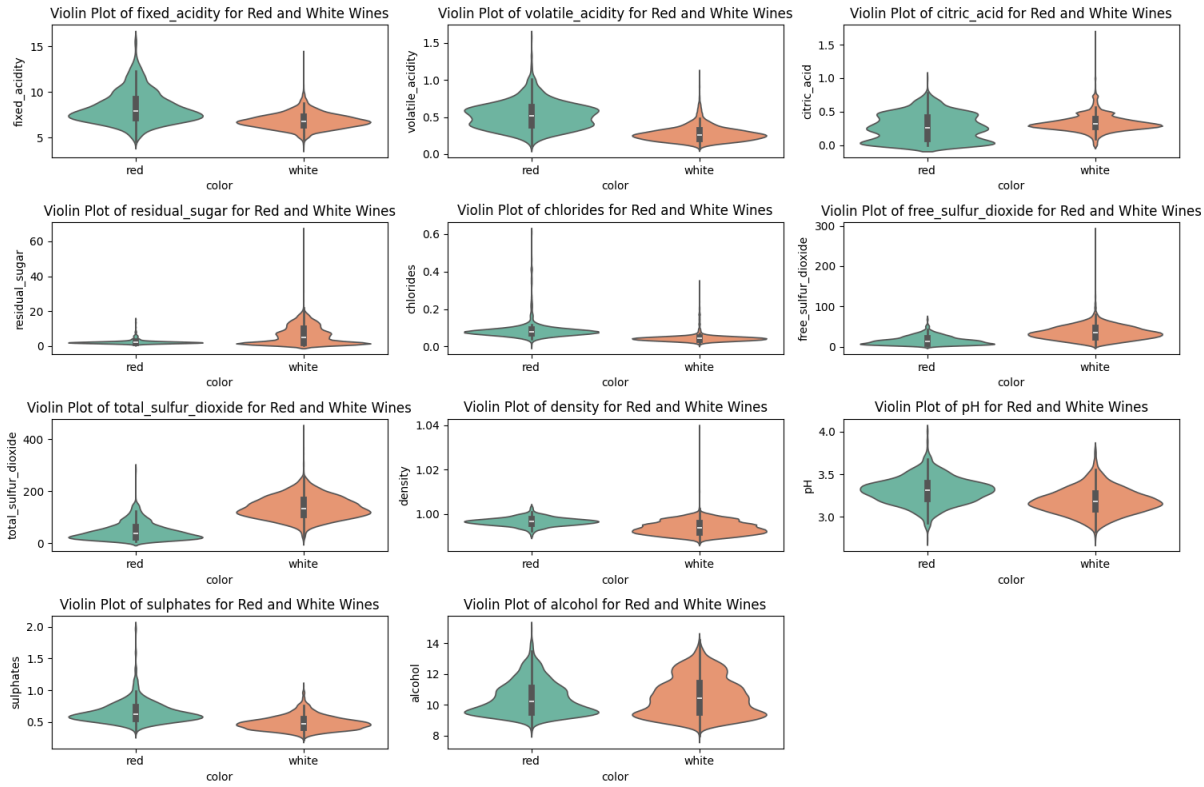
Now let's go a bit deeper into the same analysis, using more visual tools:

- For every feature, plot boxplots, violinplots or histograms for red and white wines. What can you infer? **If you feel a bit more adventurous**, plot the Cumulative Distribution Function (CDF) of the feature for white and red wines, and compute the Kullback-Leibler divergence (or entropy) between them. Explain why this might be useful.
- Plot the correlation matrix of all features as heatmaps, one for red and one for white wines. How do they differ? What can you infer?

```
# plotting through seaborn
plt.figure(figsize=(15, 10))
for i, feature in enumerate(numeric_features, 1):
    plt.subplot(4, 3, i)
    sns.boxplot(x=df_white[feature])
    plt.title(f"Boxplot of {feature}")
plt.tight_layout()
plt.show()
```

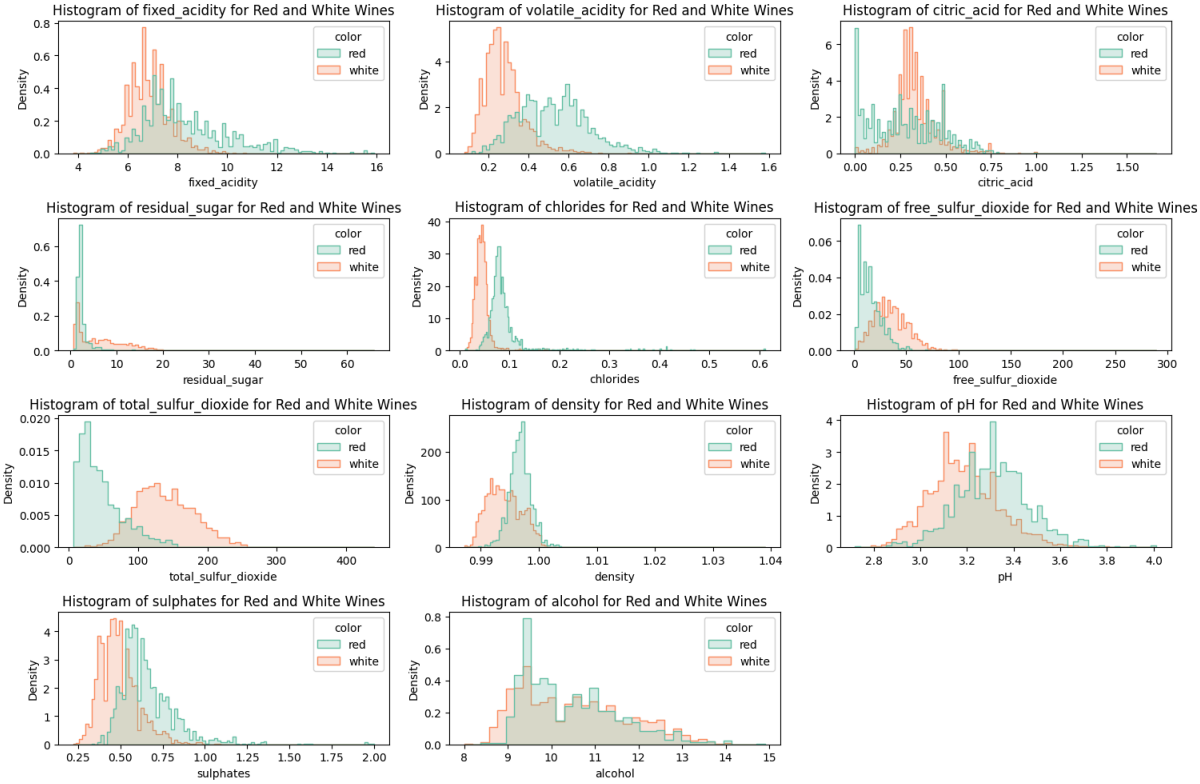



```
# Set up figure for Violin Plots
plt.figure(figsize=(15, 10))
for i, feature in enumerate(numeric_features, 1):
    plt.subplot(4, 3, i)
    sns.violinplot(x="color", y=feature, data=df, palette="Set2")
    plt.title(f"Violin Plot of {feature} for Red and White Wines")
plt.tight_layout()
plt.show()
```

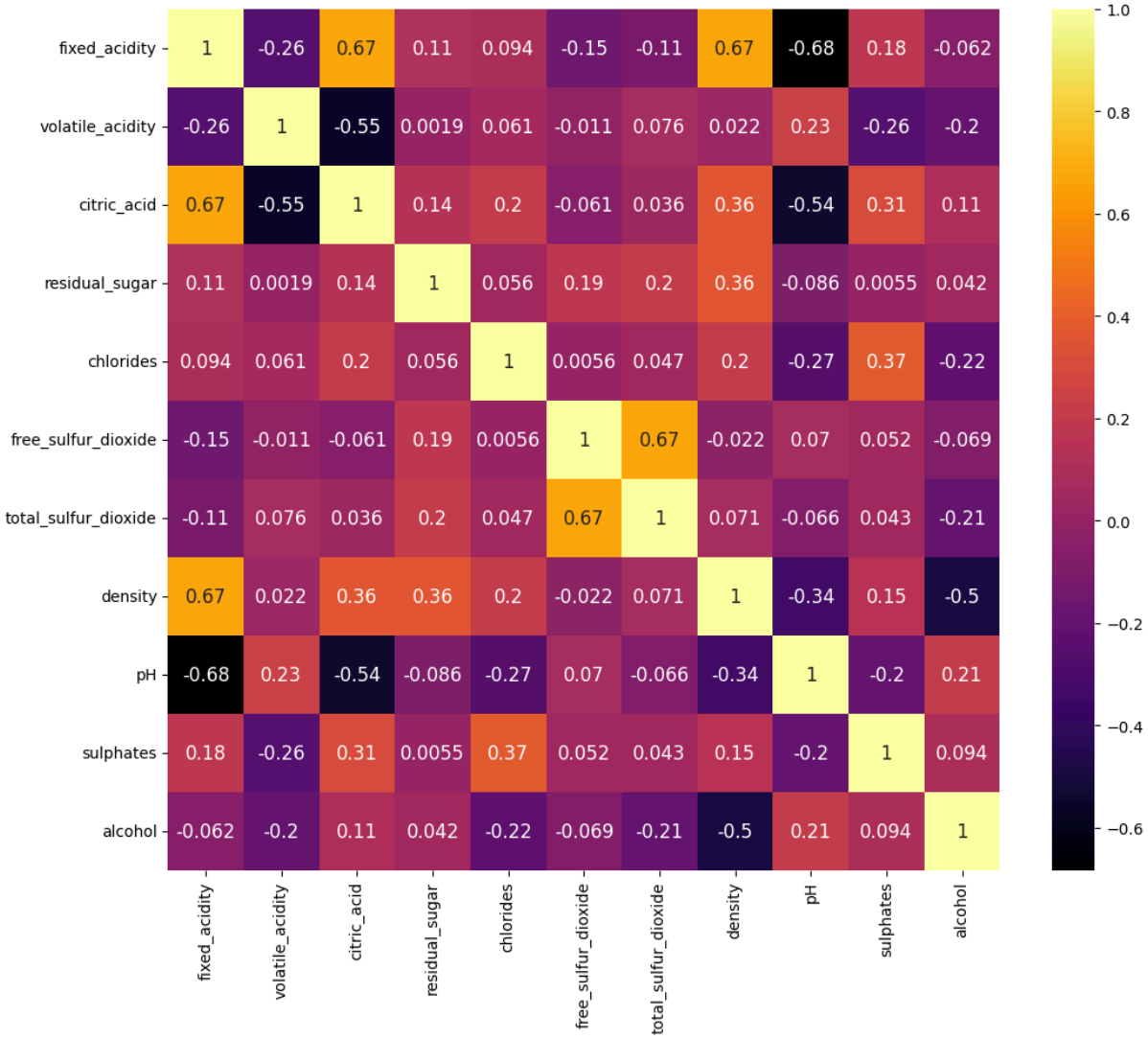


- Fixed acidity, volatile acidity, and citric acid show a higher range of values for red wines, while white wines have narrower distributions.
- Residual sugar and total sulfur dioxide are significantly higher in white wines, indicating a broader range and more outliers.
- Chlorides, free sulfur dioxide, and alcohol also have wider distributions in white wines, suggesting more variability.
- Most features, like pH and density, show similar medians but different spreads, with some having distinct multimodal shapes (e.g., alcohol).

```
# Set up figure for Histograms
plt.figure(figsize=(15, 10))
for i, feature in enumerate(numeric_features, 1):
    plt.subplot(4, 3, i)
    sns.histplot(
        data=df,
        x=feature,  # we use multiple feature
        hue="color",  # use to determine the color of plot
        element="step",
        stat="density",
        common_norm=False,
        palette="Set2",
    )
    plt.title(f"Histogram of {feature} for Red and White Wines")
plt.tight_layout()
plt.show()
```

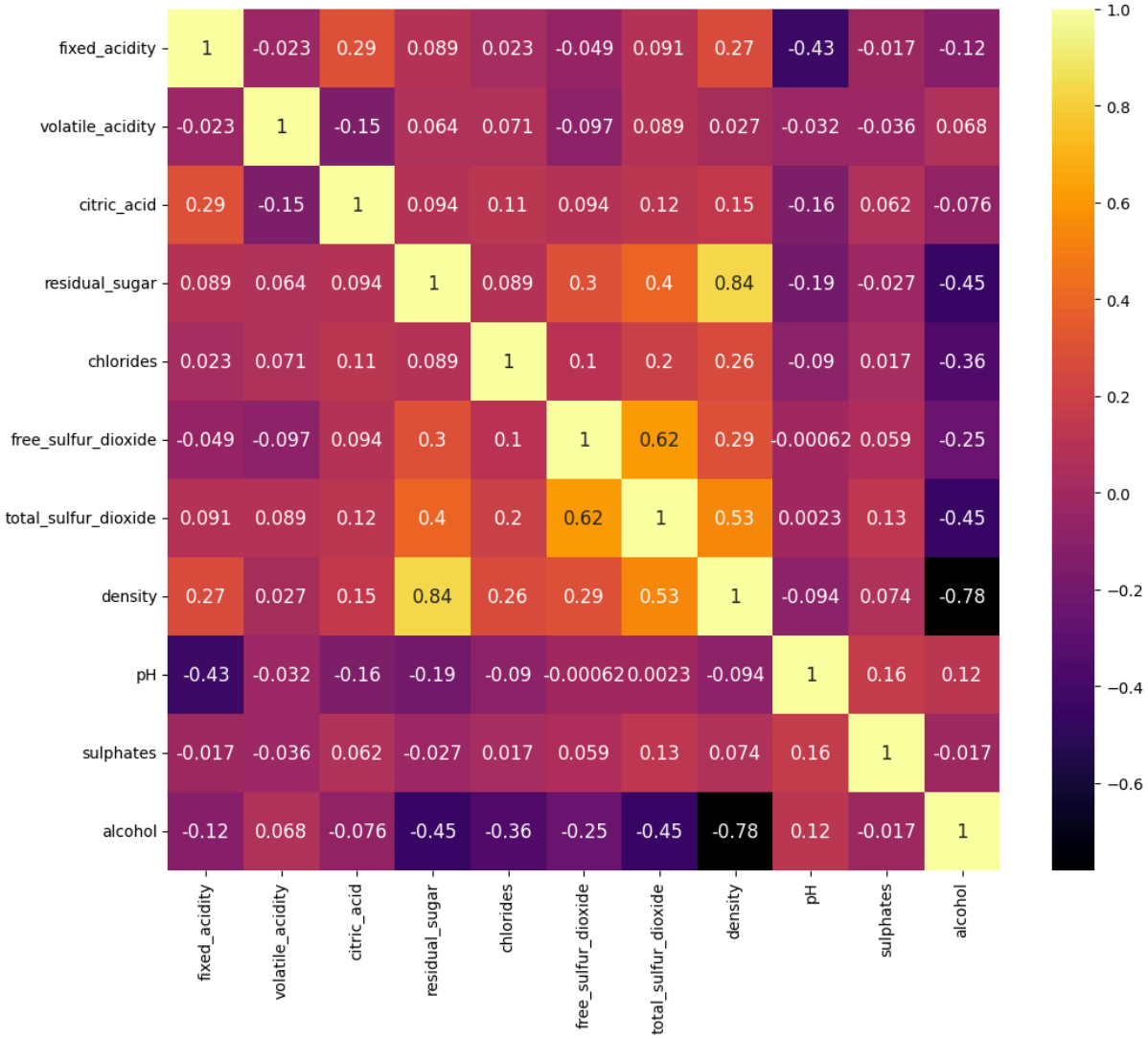



```
corr_matrix = df_red.drop(
    columns=["color", "quality"]
).corr()  # Taking without color and score
fig, ax = plt.subplots(figsize=(12, 10))
sns.heatmap(corr_matrix, annot=True, cmap="inferno", annot_kws={"size": 12})
plt.show()
```



Fixed acidity and citric acid : higher fixed acidity also tend to have higher citric acid content
Fixed acidity and density : wines with more fixed acidity tend to have higher density **Free sulfur dioxide and total sulfur dioxide :** they're linked so normal

```
corr_matrix = df_white.drop(
    columns=["color", "quality"]
).corr()  # Taking without color and score
fig, ax = plt.subplots(figsize=(12, 10))
sns.heatmap(corr_matrix, annot=True, cmap="inferno", annot_kws={"size": 12})
plt.show()
```



Residual sugar and density : residual sugar increases the density of the wine **Free sulfur dioxide and total sulfur dioxide :** Naturally, if free sulfur dioxide increases, total sulfur dioxide will also increase **Residual sugar and total sulfur dioxide :** Wines with higher sugar content often need more sulfur dioxide to preserve them

General information

Alcohol and density: Alcohol is less dense than water, so it makes sense that wines with higher alcohol content tend to have lower density

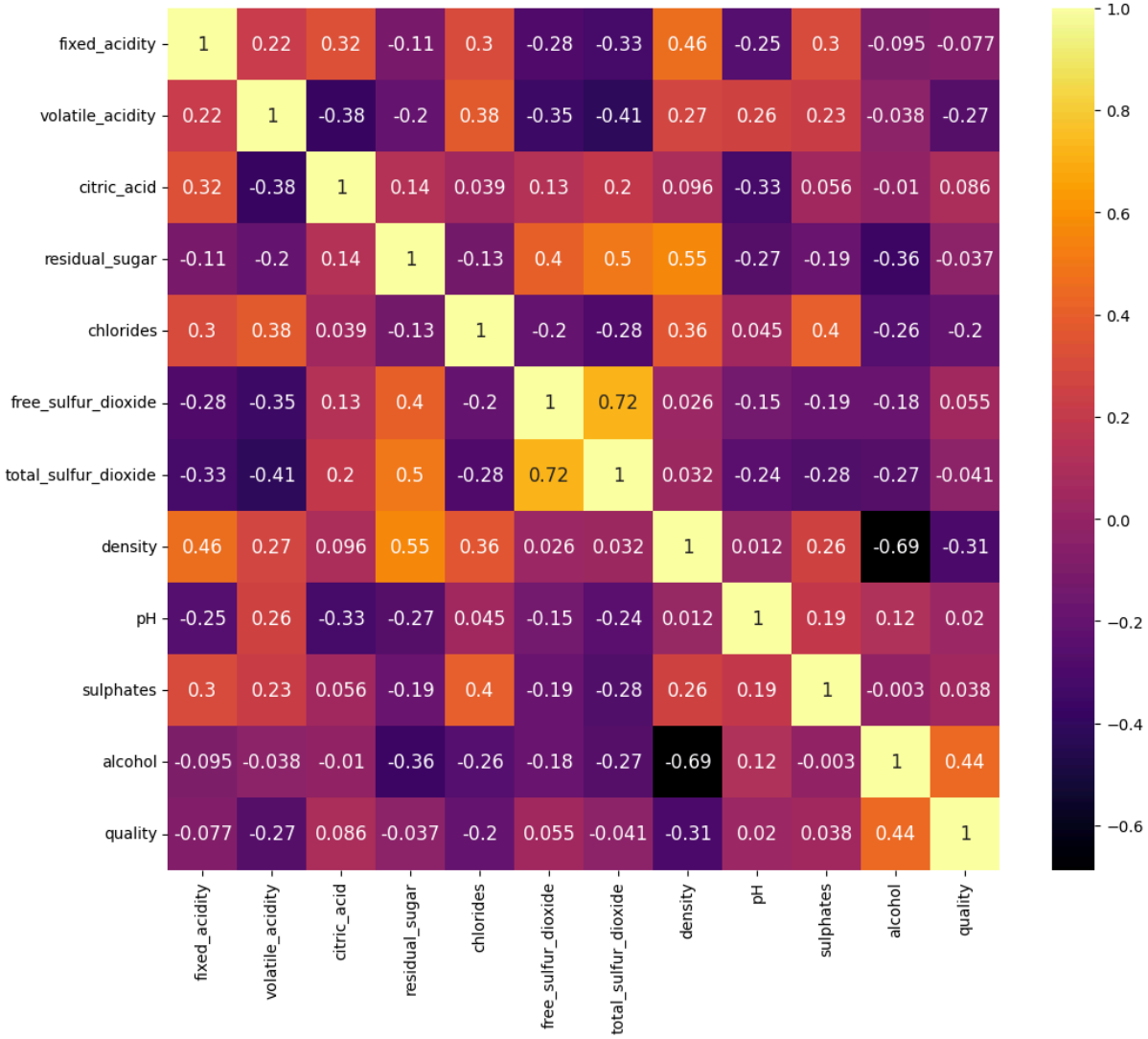
pH and fixed acidity : pH measures the acidity of the wine, and higher fixed acidity corresponds to lower pH

Feature correlation with label

Cheking if one of ours features is correlated with the label it can be interesting. Regareding the output, we can see that the volume of alcohol is a little bit correlated with the score! Isn't it interesting?

```
df2 = df[
    [
        "fixed_acidity",
        "volatile_acidity",
```

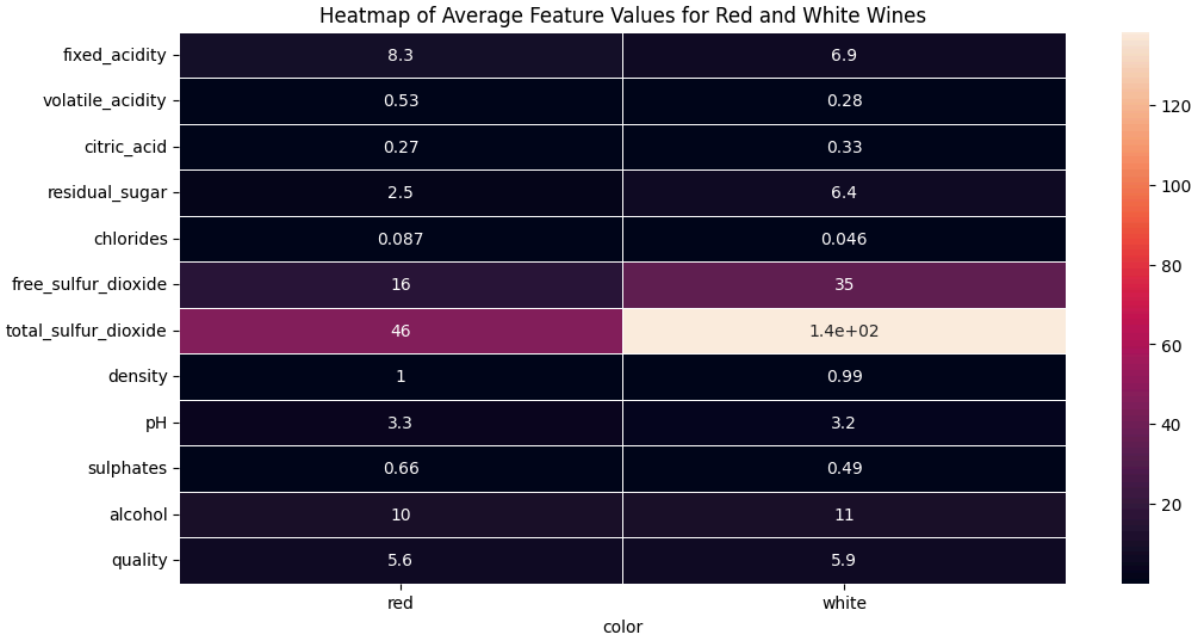
```
        "citric_acid",
        "residual_sugar",
        "chlorides",
        "free_sulfur_dioxide",
        "total_sulfur_dioxide",
        "density",
        "pH",
        "sulphates",
        "alcohol",
        "quality",
    ]
]
corr_matrix = df2.corr()  # Taking without color and score
fig, ax = plt.subplots(figsize=(12, 10))
sns.heatmap(corr_matrix, annot=True, cmap="inferno", annot_kws={"size": 12})
plt.show()
```



Data Exploration using Unsupervised Learning (3h)

We first explore the data in an unsupervised fashion. Start by creating a heatmap of the average feature value for red and white wines. Can you spot an easy way to differentiate between reds and whites?

```
# heatmap
# Calculate the mean values for red and white wines
mean_values = df.groupby("color").mean()

# Create a heatmap of the average feature values
plt.figure(figsize=(12, 6))
sns.heatmap(mean_values.T, annot=True, linewidths=0.5)
plt.title("Heatmap of Average Feature Values for Red and White Wines")
plt.show()
```



Analyse

White wines tend to have more sulfur dioxide for preservation and more residual sugar, making them lighter and often sweeter than red wines. Red wines, on the other hand, have higher acidity and volatile components, which contribute to their richer and more complex flavors.

Using PCA to reduce the dimensionality

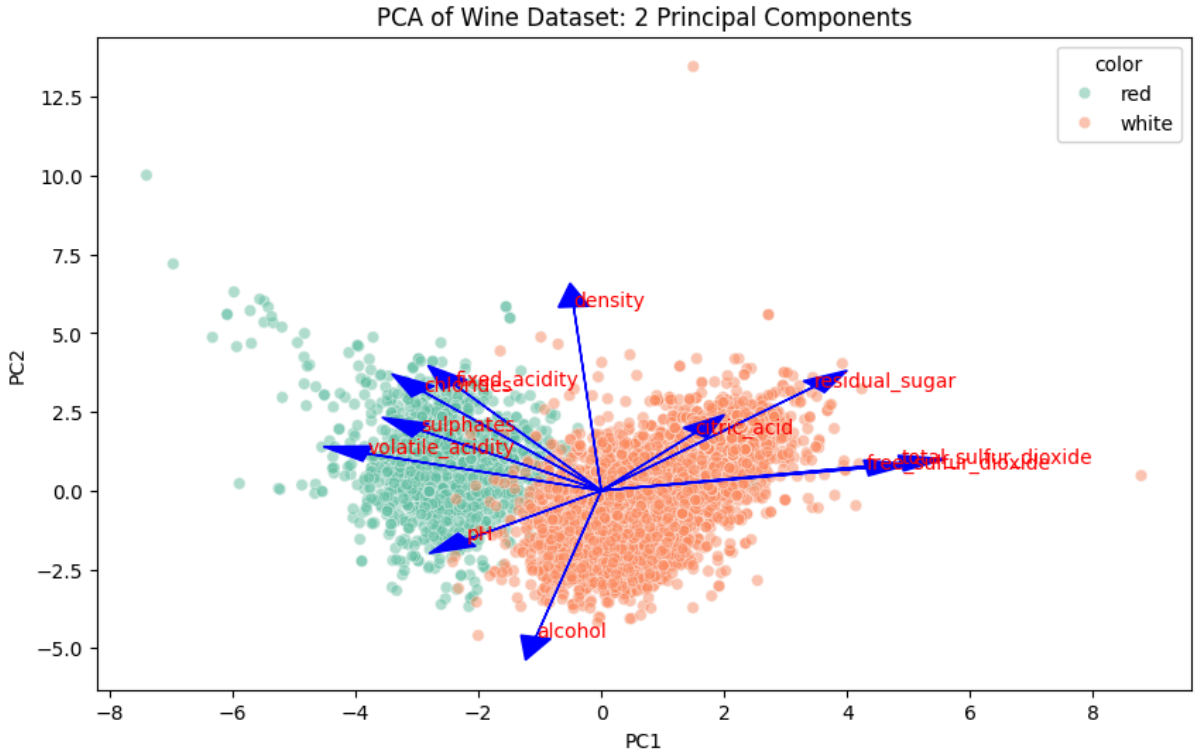
Use PCA to reduce the dimensionality of data. Do not forget that it requires data normalization (centering on the mean and scaling to unit variance). Plot the whole dataset onto the two principal components and color it by wine color. What does it tell you?

- We can see that it separates quite well by wine.

Project the unit vectors that correspond to each vector onto the principal components, using the same transformation. What does it tell you about the relative feature importance? Does it match the observations you made previously? response under the graph

```
# scale standart scaler to normalize data
scaler = StandardScaler()
df_normalized = scaler.fit_transform(X[numeric_features])

# Project unit vectors (feature importance) onto the principal components
# Stack overflow --> https://stackoverflow.com/questions/50796024/feature-variable-importance-after-a-pca-analysis
# Use the components_ attribute from PCA to get the feature importance for each principal component
```

```
scaleFactor = 10  # using a scale factor to make it bigger
# Perform PCA and reduce the data to 2 components
pca = PCA(n_components=2)
pca_result = pca.fit_transform(df_normalized)

# Create a new DataFrame to store the PCA results
pca_df = pd.DataFrame(data=pca_result, columns=["PC1", "PC2"])
# adding color to the df
pca_df["color"] = df["color"]


# Plot the PCA results, coloring by wine type (red or white)
plt.figure(figsize=(10, 6))

sns.scatterplot(x="PC1", y="PC2", hue="color", data=pca_df, palette="Set2",
alpha=0.5)
for i, feature in enumerate(numeric_features):
    plt.arrow(
        0,
        0,
        pca.components_[0, i] * scaleFactor,  # we give the dx
        pca.components_[1, i] * scaleFactor,  # give the dy
        color="blue",
        head_width=0.05 * scaleFactor,
    )
    plt.text(
        pca.components_[0, i] * scaleFactor,
        pca.components_[1, i] * scaleFactor,
        feature,  # just taking the feature
        color="red",  # adding the component name
    )
plt.title("PCA of Wine Dataset: 2 Principal Components")
plt.show()
```



Analyse

It helps us to see the features that influence our pca shape, we can see that for white whine citric acid, residual sugar help a lot to shape this PCA. Red whine volatile acidity, sulphates are the main features that help to shape them. For both wines we can see that alcohol and density give balances to center our PCA

```
print(pca.transform(np.eye(X.shape[1])))  # USing teacher method
```

```
[[-0.2387989   0.33635454]
 [-0.3807575   0.11754972]
 [ 0.15238844  0.1832994 ]
 [ 0.34591993  0.32991418]
 [-0.29011259  0.31525799]
 [ 0.43091401  0.0719326 ]
 [ 0.48741806  0.08726628]
 [-0.04493664  0.58403734]
 [-0.21868644 -0.155869  ]
 [-0.29413517  0.19171577]
 [-0.10643712 -0.46505769]]
```

Cluster the data in 2-dimensional space

Use k-means to cluster the data into 2 clusters and plot the same view as before, but with a coloring that corresponds to the cluster memberships.

Assuming that the cluster assignments are predictions of a model, what is the performance you can achieve in terms of mutual information score, accuracy, and f1 score?

```
kmeans = KMeans(n_clusters=2, random_state=42)
y_kmeans = kmeans.fit_predict(df_normalized)
```

```
plt.figure(figsize=(8, 6))
sns.scatterplot(x="PC1", y="PC2", hue=y_kmeans, data=pca_df, palette="Set2",
alpha=0.5)
```

```
plt.title("K-Means Clustering of Wine Data (2 Clusters)")
plt.xlabel("PCA Component 1")
plt.ylabel("PCA Component 2")
plt.show()
```


```
# Mutual Information Score If it's near 0 it tels that th'eyre independant
mi_score = mutual_info_score(df["color"], y_kmeans)
print(f"Mutual Information Score: {mi_score:.4f}")
```

```
Mutual Information Score: 0.4911
```

```
label_mapping = {"red": 0, "white": 1}
df["color_num"] = df["color"].map(label_mapping)

# Swap y_kmeans labels if accuracy is below 0.5
if accuracy_score(df["color_num"], y_kmeans) < 0.5:
    y_kmeans = 1 - y_kmeans

# Calculate accuracy and F1 score
accuracy = accuracy_score(df["color_num"], y_kmeans)
f1 = f1_score(df["color_num"], y_kmeans, average="weighted")

print(f"Accuracy: {accuracy:.4f}")
print(f"F1 Score: {f1:.4f}")
```

```
Accuracy: 0.9858
F1 Score: 0.9859
```

Why is it so good

Algorithm performed remarkably well in distinguishing red wines from white wines, demonstrating that the chemical composition of the *wines provides a clear separation* between the two types.

Mutual information : KMeans algorithm is somewhat effective at identifying clusters related to the actual wine color regarding its score.

Now, we are going to train a **supervised** linear classification model using `sklearn`, and compare the results with the approach using clustering.

- Set up a train/test dataset using `sklearn.model_selection.train_test_split`.
- Use `GridSearchCV` to perform a cross-validation of the model's regularization `C`.
- Compare the test and train performance at the end. Does the model suffer from any overfitting?
- Analyze the test performance specifically. What can you conclude about this general problem of recognizing white vs red wines?

```
X_train, X_test, y_train, y_test = train_test_split(X, wineColor, test_size=0.25)
```

```
pipe = make_pipeline(StandardScaler(), LogisticRegression(max_iter=1000))
```

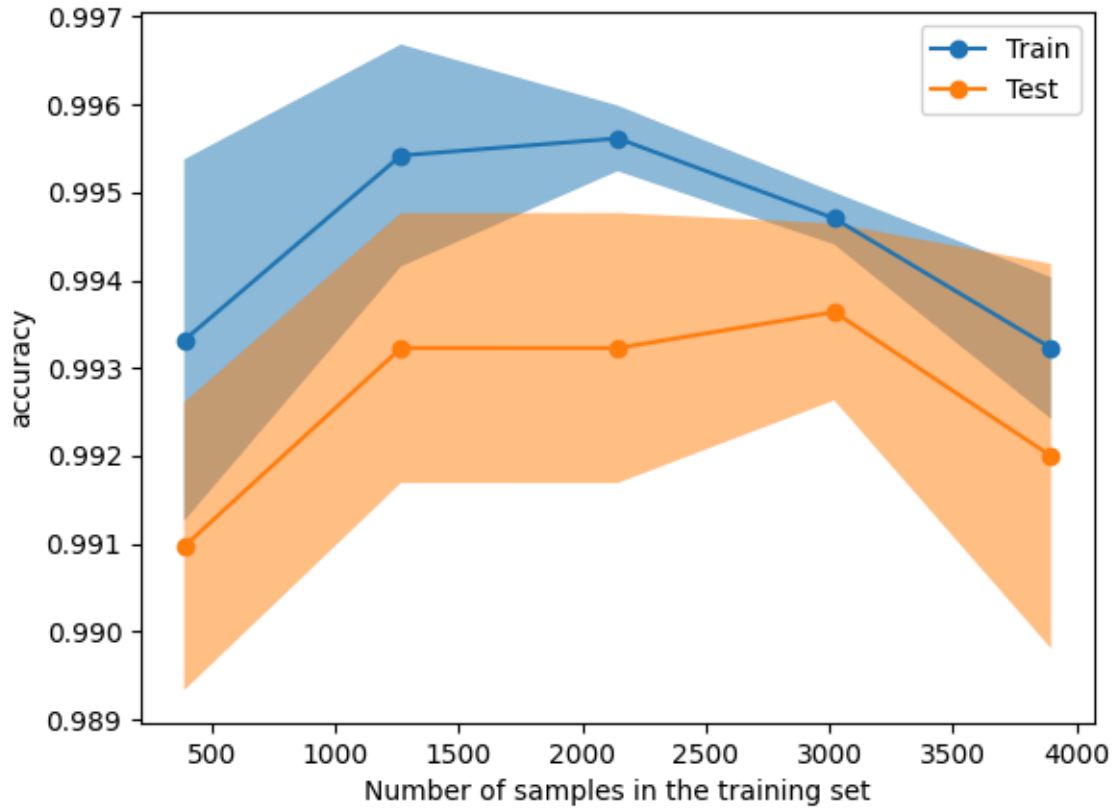
```
# Grid search to find the best parametres
# Create a parameter grid
param_grid = {
    "logisticregression__C": [0.1, 1, 10, 100],
}
```

```
# Fit the model
gs = GridSearchCV(estimator=pipe, param_grid=param_grid, scoring="accuracy")
gs.fit(X_train, y_train)
```

```
GridSearchCV(estimator=Pipeline(steps=[('standardscaler', StandardScaler()),
                                       ('logisticregression',
                                        LogisticRegression(max_iter=1000))]),
             param_grid={'logisticregression__C': [0.1, 1, 10, 100]},
             scoring='accuracy')
```

```
from sklearn.model_selection import LearningCurveDisplay


# Plot the learning curve using LearningCurveDisplay
LearningCurveDisplay.from_estimator(
    gs.best_estimator_,
    X_train,
    y_train,
    scoring="accuracy",
    score_name="accuracy",
    line_kw={"marker": "o"},
    n_jobs=-1,
)
```

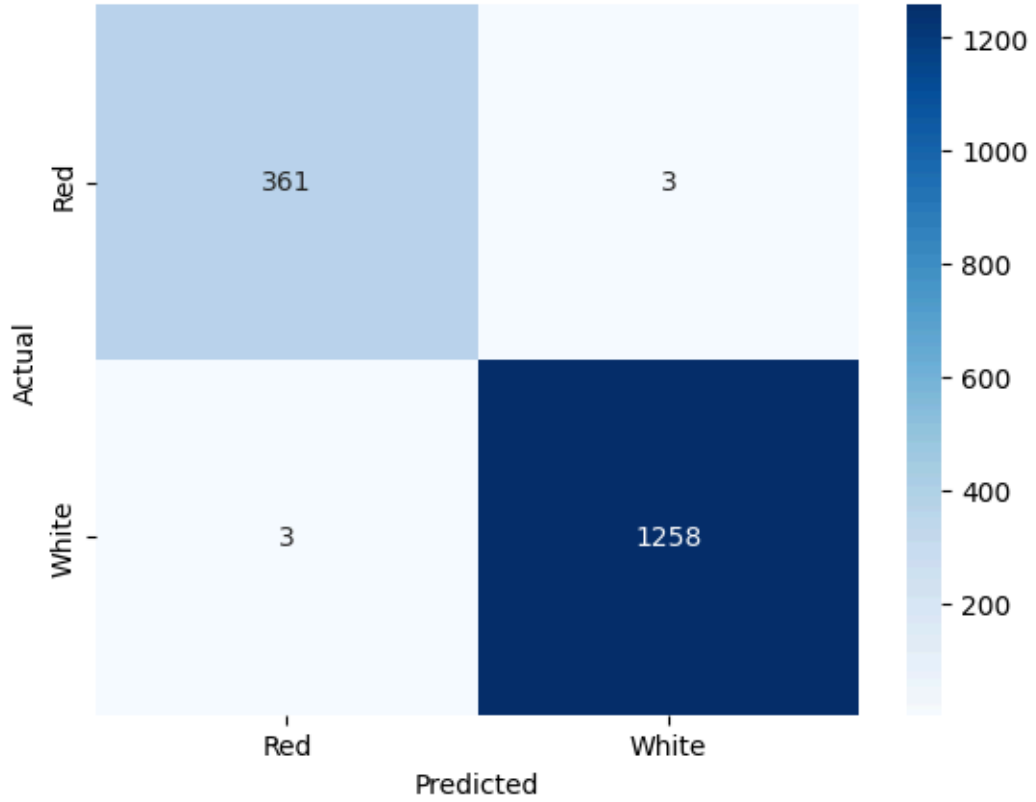
```
<sklearn.model_selection._plot.LearningCurveDisplay at 0x7f8e2fbba690>
```




```
best_model = gs.best_estimator_

# Training and test set accuracy
train_accuracy = best_model.score(X_train, y_train)
test_accuracy = best_model.score(X_test, y_test)

print("Training Accuracy:", train_accuracy)
print("Test Accuracy:", test_accuracy)
```

```
Training Accuracy: 0.9938423645320197
Test Accuracy: 0.9963076923076923
```

```
# Predict on the test set
y_pred = best_model.predict(X_test)

# Confusion matrix
cm = confusion_matrix(y_test, y_pred)
sns.heatmap(
    cm,
    annot=True,
    fmt="d",
    cmap="Blues",
    xticklabels=["Red", "White"],
    yticklabels=["Red", "White"],
)
plt.xlabel("Predicted")
plt.ylabel("Actual")
plt.show()

# Classification report
print(classification_report(y_test, y_pred, target_names=["Red", "White"]))
```



	precision	recall	f1-score	support
Red	0.99	0.99	0.99	364
White	1.00	1.00	1.00	1261
accuracy			1.00	1625
macro avg	0.99	0.99	0.99	1625
weighted avg	1.00	1.00	1.00	1625

Results

Learning Curve: The increase in confidence intervals as the number of training samples grows indicates that the model's performance becomes less consistent with more data, possibly due to increasing variability in the training data.

High Accuracy on Both Training and Test Sets. model performs extremely well on this classification task.

Basic model interpretability: inspecting the model

As a first step towards intepretability of the model predictions, let's take a look at the coefficients of the model. What is the most important feature from this perspective? How do you interpret positive or negative coefficients?

Is it compatible with what you have seen so far? Do you have an explanation why that might be?

```
log_reg_model = gs.best_estimator_.named_steps["logisticregression"]
# Get the feature names (if using a pandas DataFrame, X.columns would provide them)
feature_names = (
    X.columns if hasattr(X, "columns") else [f"Feature {i}" for i in
range(X.shape[1])]
)
```

```
# Get the coefficients from the model
coefficients = log_reg_model.coef_[0]

# Combine feature names and their corresponding coefficients
coeffs_with_features = sorted(
    zip(feature_names, coefficients), key=lambda x: abs(x[1]), reverse=True
)

# Print feature importance
print("Feature importance in descending order:")
for feature, coeff in coeffs_with_features:
    print(f"{feature}: {coeff:.4f}")
```

```
Feature importance in descending order:
density: -4.7294
residual_sugar: 4.3144
total_sulfur_dioxide: 2.7134
alcohol: -1.9171
free_sulfur_dioxide: -1.0631
volatile_acidity: -1.0136
chlorides: -0.8437
sulphates: -0.4917
fixed_acidity: 0.3207
citric_acid: 0.3174
pH: 0.0870
```

Analyse

The higher density and alcohol content in red wines versus the higher sulfur dioxide and residual sugar in white wines are key distinguishing factors.

direction of the coefficients also makes sense based on the chemistry and production processes of different wine types.

Removing features to test their importance

- What happens if you re-train a model, but remove the most important feature in the list?
- What happens if you re-train the model with a `l1` penalty and you use more regularization?
- Interpret the results you obtained above from the perspective of the business problem. What does it tell you about the key differences between a red and white wine?

```
numeric_features
```

```
['fixed_acidity',
 'volatile_acidity',
 'citric_acid',
 'residual_sugar',
 'chlorides',
 'free_sulfur_dioxide',
 'total_sulfur_dioxide',
 'density',
 'pH',
 'sulphates',
 'alcohol']
```

```
param_grid_stronger_regularization = {
    "logisticregression__C": [0.01, 0.1, 1],
    "logisticregression__penalty": ["l1"],
```

```
    "logisticregression__solver": ["liblinear"],
}
```

```
features_to_drop = [
    "total_sulfur_dioxide",
    "alcohol",
    "free_sulfur_dioxide",
    "volatile_acidity",
    "fixed_acidity",
]
X_train_reduced = X_train.drop(columns=features_to_drop)
X_test_reduced = X_test.drop(columns=features_to_drop)
```

```
X_train_reduced.head()
```

	citric_acid	residual_sugar	chlorides	density	pH	sulphates
1952	0.40	6.85	0.038	0.99200	3.03	0.30
2371	0.60	1.10	0.135	0.99270	3.12	0.39
2997	0.36	13.10	0.050	0.99860	3.04	0.46
5801	0.31	2.30	0.044	0.99013	3.29	0.46
1613	0.62	19.25	0.040	1.00020	2.98	0.67

```
X_test_reduced.head()
```

	citric_acid	residual_sugar	chlorides	density	pH	sulphates
6043	0.25	7.80	0.031	0.99241	3.39	0.40
4627	0.37	6.20	0.050	0.99546	3.20	0.55
2755	0.29	16.85	0.054	0.99980	3.16	0.38
2226	0.24	6.20	0.048	0.99570	3.23	0.62
2553	0.34	9.70	0.035	0.99650	3.08	0.49

```
y_train.head()
```

```
1952    white
2371    white
2997    white
5801    white
1613    white
Name: color, dtype: object
```

```
gs_reduced = GridSearchCV(
    estimator=pipe, param_grid=param_grid_stronger_regularization, scoring="accuracy"
)
gs_reduced.fit(X_train_reduced, y_train)
```

```
GridSearchCV(estimator=Pipeline(steps=[('standardscaler', StandardScaler()),
                                       ('logisticregression',
                                        LogisticRegression(max_iter=1000))]),
             param_grid={'logisticregression__C': [0.01, 0.1, 1],
                         'logisticregression__penalty': ['l1'],
                         'logisticregression__solver': ['liblinear']},
             scoring='accuracy')
```

```
# Accuracy
train_accuracy_reduced = gs_reduced.best_estimator_.score(X_train_reduced, y_train)
test_accuracy_reduced = gs_reduced.best_estimator_.score(X_test_reduced, y_test)
```

```
print(f"Training Accuracy (without density): {train_accuracy_reduced}")
print(f"Test Accuracy (without density): {test_accuracy_reduced}")
```

```
Training Accuracy (without density): 0.9630541871921182
Test Accuracy (without density): 0.9624615384615385
```

Analyse

Removing one feature lead me to a very good model it performs less better but it has not a big gap, when removing other good features it starts decreasing. This could prove that my idea about predict a white from a red whine is quite easy from the chemical composition.

Using Shapley values

Now, use SHAP to explore how the model perceives a 'red' and 'white' wine.

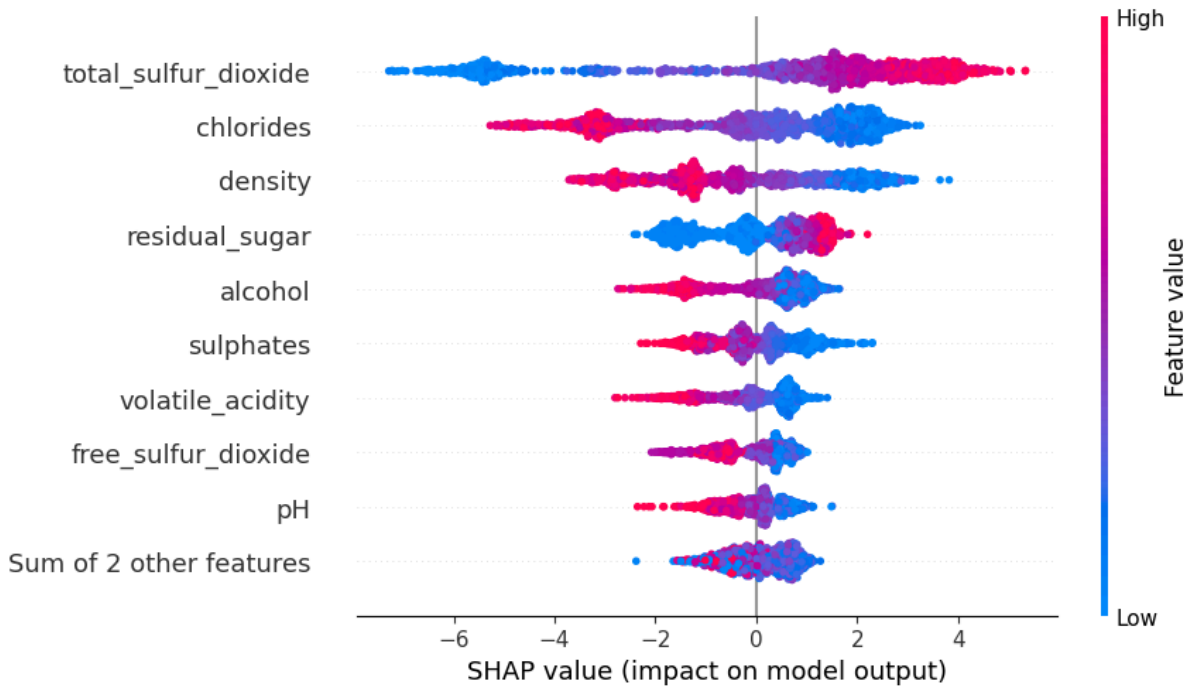
- Use a `beeswarm` plot to analyze the influence of each feature on the model's output.
- What does the plot tell us about what makes a white wine 'white' and a red wine 'red'?

```
label_mapping = {"red": 0, "white": 1}
y_train = y_train.map(label_mapping)
```

```
y_train.head()
```

```
1952    1
2371    1
2997    1
5801    1
1613    1
Name: color, dtype: int64
```

```
# Train the XGBoost classifier
model = xgb.XGBClassifier().fit(X_train, y_train)

# Create the SHAP explainer
explainer = shap.Explainer(model, X_test)

# Calculate SHAP values for the test set
shap_values = explainer(X_test)

# Generate a beeswarm plot to visualize feature impact
shap.plots.beeswarm(shap_values)
```



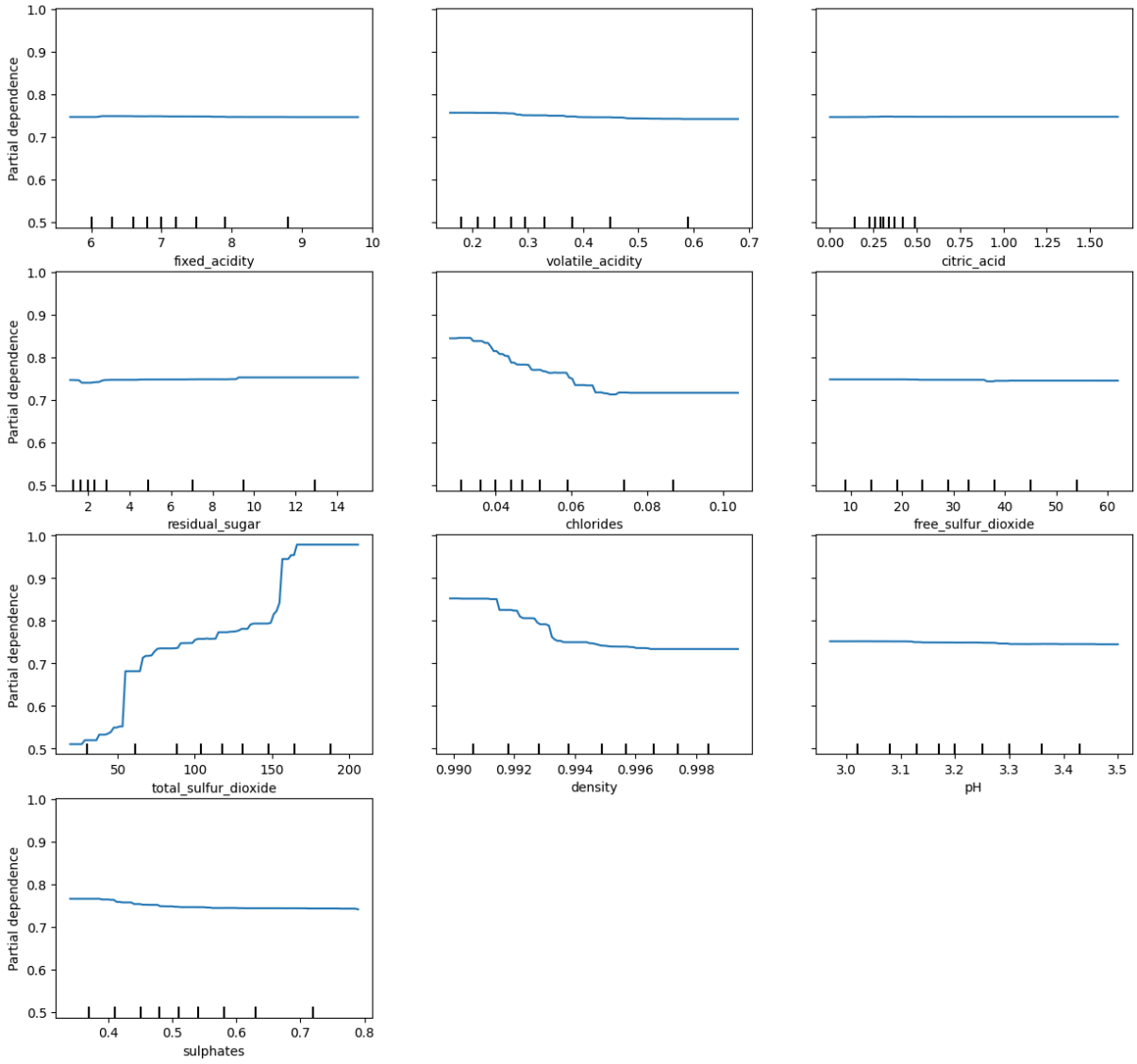
Analyse

Features such as sulfur dioxide, chlorides, residual sugar, alcohol content, and acidity are critical in determining whether the wine is red or white

White wines are associated with higher sulfur dioxide, chlorides, residual sugar, and density, while red wines are linked to higher volatile acidity, alcohol, and fixed acidity.

- Now use Partial Dependence Plots to see how the expected model output varies with the variation of each feature.

```
from sklearn.inspection import PartialDependenceDisplay
import matplotlib.pyplot as plt

features = list(range(X_train.shape[1] - 1))
fig, ax = plt.subplots(figsize=(15, 10))
PartialDependenceDisplay.from_estimator(model, X_train, features, ax=ax)

plt.subplots_adjust(top=1.2)
plt.show()
```



Anylse

Total Sulfur Dioxide: Higher levels of total sulfur dioxide strongly increase the model's predictions.

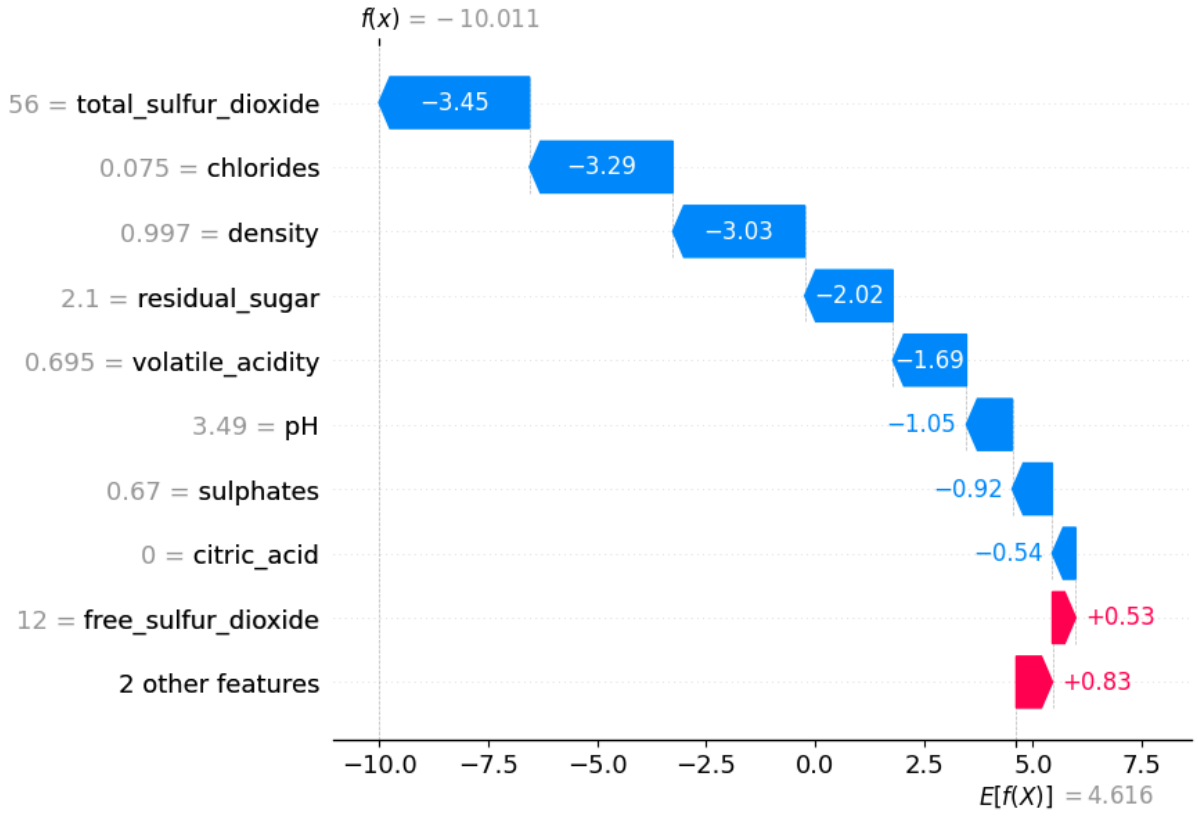
Density: Lower-density wines tend to decrease the prediction, while higher-density wines positively influence the model up to a threshold

Residual Sugar: Higher residual sugar levels significantly increase the model's output, suggesting that sweeter wines are more likely to be classified or scored higher

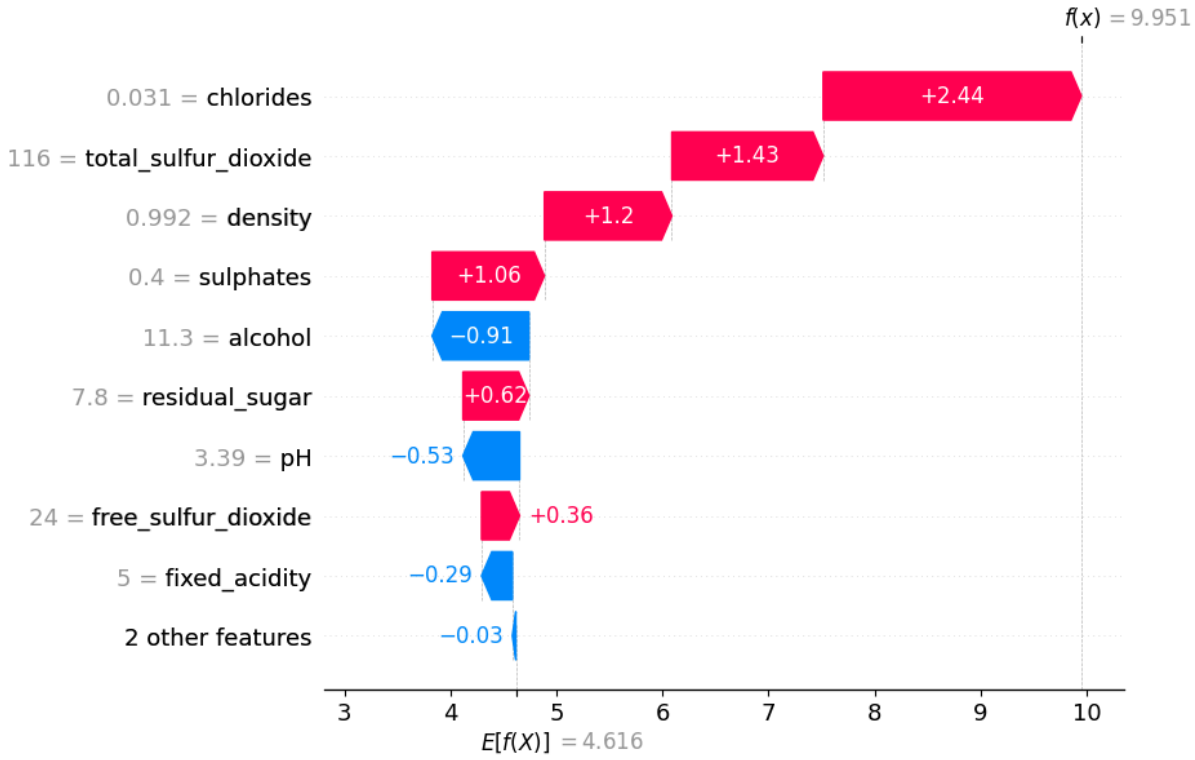
- Now use a waterfall diagram on a specific red and white wine and see how the model has made this specific prediction.

```
# Find the index of the first red wine and white wine in the test set
red_wine_index = list(y_test).index("red")
white_wine_index = list(y_test).index("white")

# Calculate SHAP values for these specific instances
shap_values_red = explainer(X_test[red_wine_index : red_wine_index + 1])
shap_values_white = explainer(X_test[white_wine_index : white_wine_index + 1])

# Step 4: Waterfall plot for red wine
print("Waterfall plot for red wine:")
shap.plots.waterfall(shap_values_red[0])

# Step 5: Waterfall plot for white wine
print("Waterfall plot for white wine:")
shap.plots.waterfall(shap_values_white[0])
```

```
Waterfall plot for red wine:
```




```
Waterfall plot for white wine:
```



Analyse

For the red wine a lower-quality score, with high levels of sulfur dioxide, chlorides, and density negatively impacting the prediction, positive effects from alcohol and free sulfur dioxide

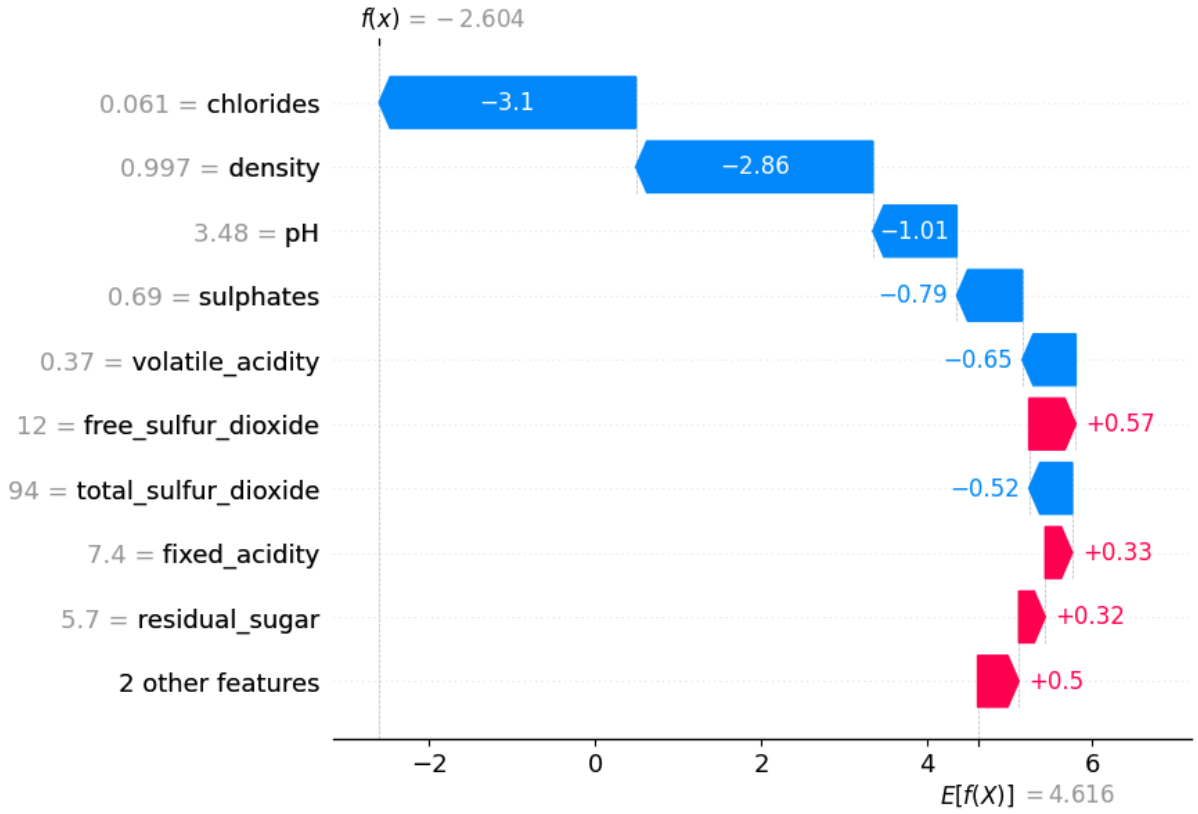
For the white wine a higher quality, driven by positive contributions from chlorides, sulfur dioxide, and density, with slight negative impacts from alcohol and free sulfur dioxide

- Now, let's take an example where the model has made an incorrect prediction, and see how it made this prediction.

```
# Get model predictions on the test set
predictions = model.predict(X_test)

# Convert 'red' and 'white' labels to 0 and 1 in y_test
y_test_numeric = y_test.replace({"red": 0, "white": 1})

# Identify incorrect predictions
incorrect_indices = np.where(predictions != y_test_numeric)[0]

# Check if there are any incorrect predictions
if len(incorrect_indices) > 0:
    print(f"Number of incorrect predictions: {len(incorrect_indices)}")

    # Choose the first incorrect prediction
    incorrect_index = incorrect_indices[0]

    # Print the actual and predicted label
    print(f"Actual label: {y_test_numeric.iloc[incorrect_index]}")  # Now numeric
labels
    print(f"Predicted label: {predictions[incorrect_index]}")

    # Calculate SHAP values for the incorrect prediction
```

```
    shap_values_incorrect = explainer(X_test[incorrect_index : incorrect_index + 1])

    # Waterfall plot to explain the incorrect prediction
    print("Waterfall plot for the incorrect prediction:")
    shap.plots.waterfall(shap_values_incorrect[0])

else:
    print("No incorrect predictions found.")
```

```
Number of incorrect predictions: 5
Actual label: 1
Predicted label: 0
Waterfall plot for the incorrect prediction:
```



Analyse

High sulfur dioxide levels strongly influenced the model towards predicting a higher quality score than expected.

Alcohol has a large negative effect

residual sugar and density contributed positively

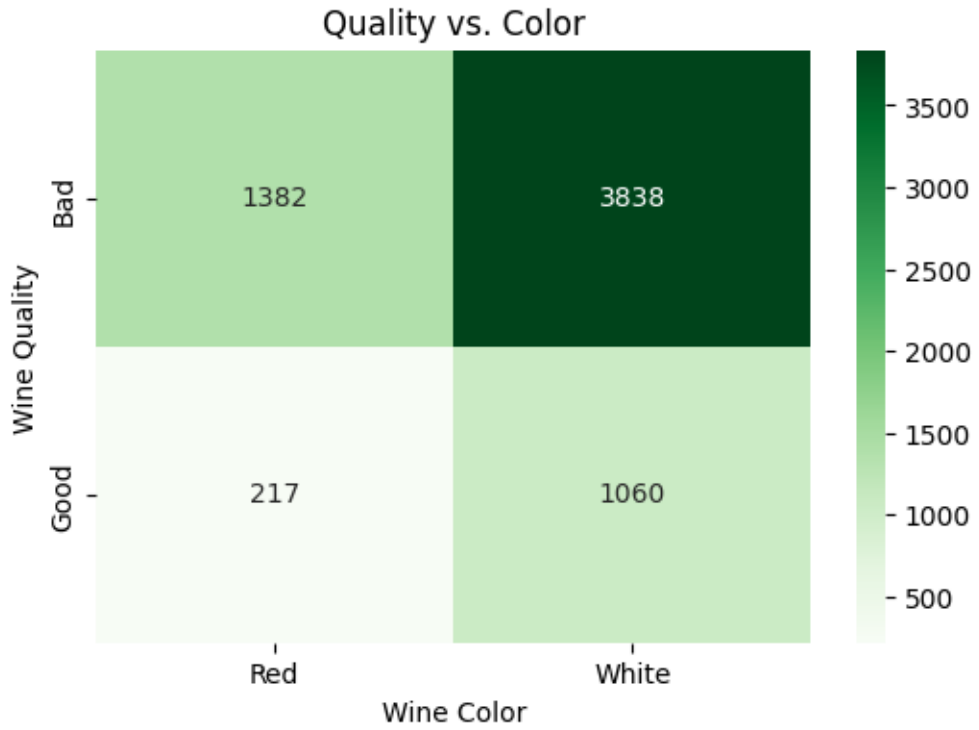
Good vs Bad classification (3h)

We are going to work on a binary classification problem, where all wines with a quality higher than 6 are considered as "good" and other are considered as "bad".

- Prepare a dataset with a new column `binary_quality` that corresponds to the above definition.

```
# Create 'binary_quality' column
df["binary_quality"] = df["quality"].apply(lambda x: 1 if x > 6 else 0)
df["color_label"] = df["color"].map({"red": 0, "white": 1})
```

```
# Confusion matrix between quality and color
cm_quality_color = confusion_matrix(df["binary_quality"], df["color_label"])
plt.figure(figsize=(6, 4))
sns.heatmap(
    cm_quality_color,
    annot=True,
    fmt="d",
    cmap="Greens",
    xticklabels=["Red", "White"],
    yticklabels=["Bad", "Good"],
)
plt.xlabel("Wine Color")
plt.ylabel("Wine Quality")
plt.title("Quality vs. Color")
plt.show()
```



One question that we might ask right away is:

- Is there any correlation of the quality and the color of the wine?

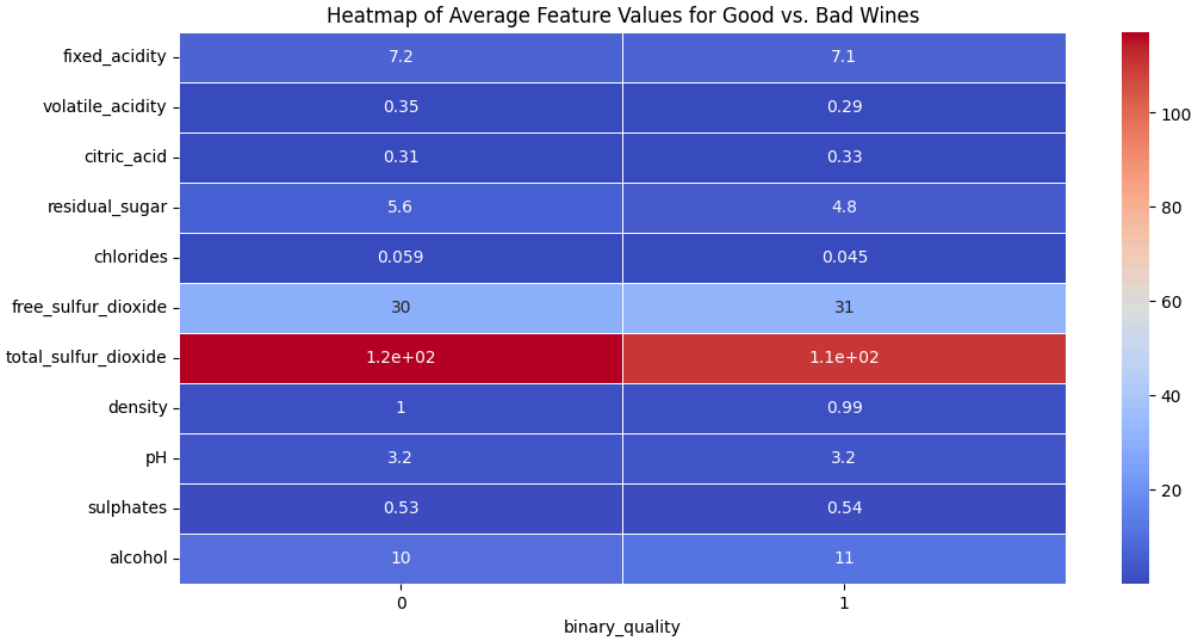
Ideally, there should be almost none. Why could it be a problem otherwise?

Answer : wine quality should not be correlated with color because quality is expected. This imbalance between white and red wines, especially in the "bad" category, could impact your model's performance or cause bias if not accounted for.

If it turns out that there are significantly more bad red wines than bad white wines or vice versa, what are the implications for your analysis?

- Plot a heatmap of the mean feature value for bad and good wines, like we did before for red and white wines.
- Plot two heatmaps, one for red and white wines. How do they differ? What kind of issue can it cause?

```
# Create a heatmap for mean feature values of bad and good wines
good_bad_mean_values = df.groupby("binary_quality")[numeric_features].mean()

plt.figure(figsize=(12, 6))
sns.heatmap(good_bad_mean_values.T, annot=True, cmap="coolwarm", linewidths=0.5)
plt.title("Heatmap of Average Feature Values for Good vs. Bad Wines")
plt.show()
```

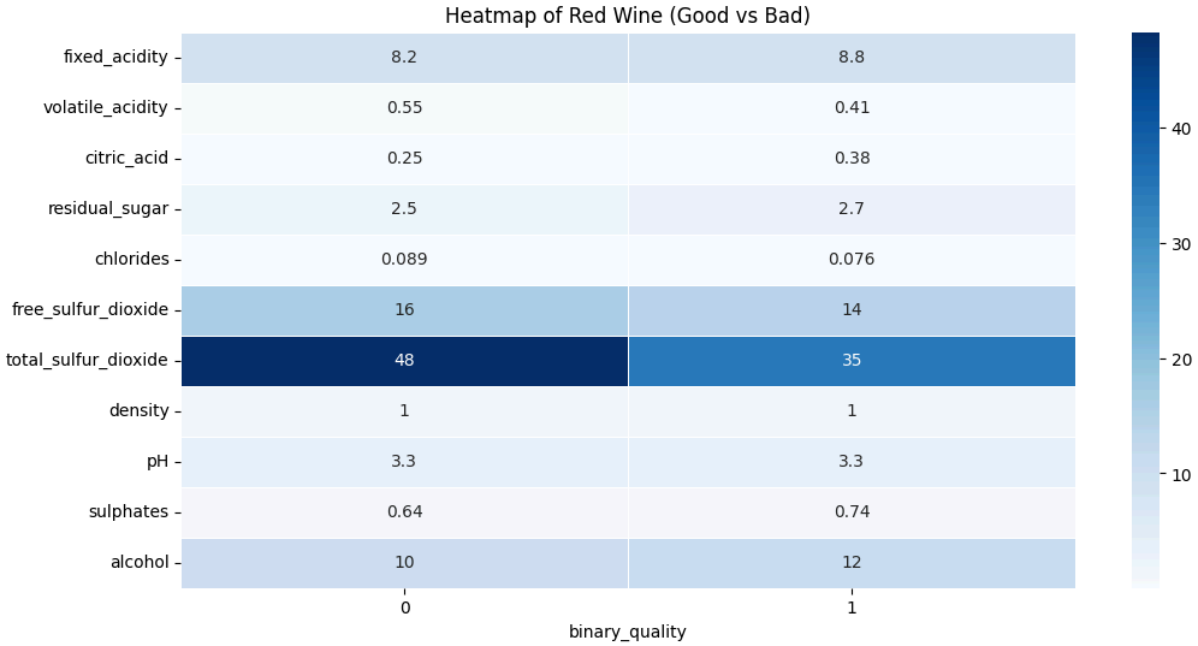


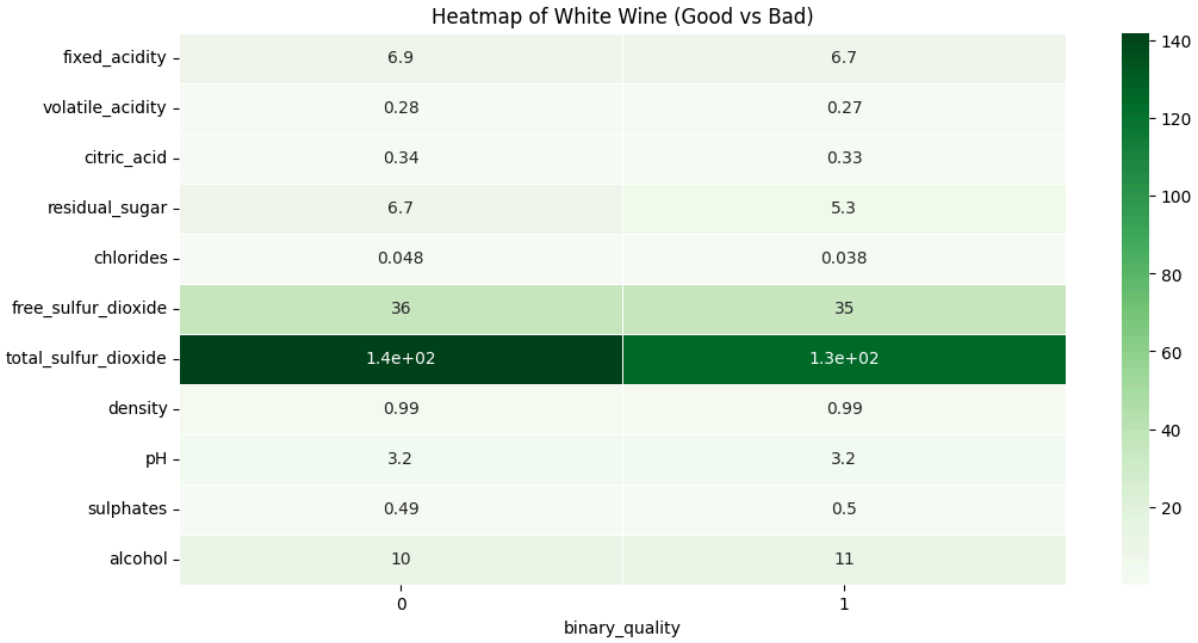
Aalyse Good vs bad

Good wines have higher levels of alcohol, residual sugar, and free sulfur dioxide.

Bad wines, on the other hand, have higher levels of volatile acidity, fixed acidity, and total sulfur dioxide.

```
# Separate red and white wines
df_red = df[df["color_label"] == 0]  # Red wines
df_white = df[df["color_label"] == 1]  # White wines

# Heatmap for red wines
red_good_bad_mean_values = df_red.groupby("binary_quality")[numeric_features].mean()
plt.figure(figsize=(12, 6))
sns.heatmap(red_good_bad_mean_values.T, annot=True, cmap="Blues", linewidths=0.5)
plt.title("Heatmap of Red Wine (Good vs Bad)")
plt.show()

# Heatmap for white wines
white_good_bad_mean_values = df_white.groupby("binary_quality")
[numeric_features].mean()
plt.figure(figsize=(12, 6))
sns.heatmap(white_good_bad_mean_values.T, annot=True, cmap="Greens", linewidths=0.5)
plt.title("Heatmap of White Wine (Good vs Bad)")
plt.show()
```





Analyse white and red good wines

Good red wines show slightly higher levels of alcohol and fixed acidity, while total sulfur dioxide and free sulfur dioxide are generally lower compared to bad wines

Good white wines feature lower total sulfur dioxide levels compared to bad wines, but the difference is less stark than in red wines

It is a lot more difficult now to tell apart good from bad wines. Let's turn to a more complex model, which is a Gradient Boosting Trees. For the sake of interpretability, design your notebook so that you can easily filter on only white and red wines and perform again the entire procedure.

Let's first train a XGBClassifier model to distinguish between good and bad wines. Make sure to use the same best-practices (train/test split, cross-validation) as we did before. Note that the

regularization of the GBTs is a lot more complex than for Logistic Regression. Test the following parameters:

```
param_grid = {
  "max_depth": [3, 4, 5],  # Focus on shallow trees to reduce complexity
  "learning_rate": [0.01, 0.05, 0.1],  # Slower learning rates
  "n_estimators": [50, 100],  # More trees but keep it reasonable
  "min_child_weight": [1, 3],  # Regularization to control split thresholds
  "subsample": [0.7, 0.9],  # Sampling rate for boosting
  "colsample_bytree": [0.7, 1.0],  # Sampling rate for columns
  "gamma": [0, 0.1],  # Regularization to penalize complex trees
}
```

```
features = df[numeric_features + ["color_label"]]
target = df["binary_quality"]

# Split data
X_train_q, X_test_q, y_train_q, y_test_q = train_test_split(
    features, target, test_size=0.25, random_state=42
)
```

```
# Model and grid search
model_xgb_q = xgb.XGBClassifier(use_label_encoder=False, eval_metric="logloss")
grid_search_q = GridSearchCV(
    model_xgb_q, param_grid, cv=5, scoring="accuracy", n_jobs=-1, verbose=1
)
grid_search_q.fit(X_train_q, y_train_q)
```

```
Fitting 5 folds for each of 4 candidates, totalling 20 fits
```

```
GridSearchCV(cv=5,
             estimator=XGBClassifier(base_score=None, booster=None,
                                     callbacks=None, colsample_bylevel=None,
                                     colsample_bynode=None,
                                     colsample_bytree=None, device=None,
                                     early_stopping_rounds=None,
                                     enable_categorical=False,
                                     eval_metric='logloss', feature_types=None,
                                     gamma=None, grow_policy=None,
                                     importance_type=None,
                                     interaction_constraints=None,
                                     learning_rate=...=None,
                                     max_cat_threshold=None,
                                     max_cat_to_onehot=None,
                                     max_delta_step=None, max_depth=None,
                                     max_leaves=None, min_child_weight=None,
                                     missing=nan, monotone_constraints=None,
                                     multi_strategy=None, n_estimators=None,
                                     n_jobs=None, num_parallel_tree=None,
                                     random_state=None, ...),
             n_jobs=-1, param_grid={'logisticregression__C': [0.1, 1, 10, 100]},
             scoring='accuracy', verbose=1)
```

```
print("Best Parameters:", grid_search_q.best_params_)
print("Best Cross-Validation Accuracy:", grid_search_q.best_score_)

# Evaluate on test set
y_pred_q = grid_search_q.predict(X_test_q)
test_accuracy_q = accuracy_score(y_test_q, y_pred_q)
print(f"Test Accuracy: {test_accuracy_q:.4f}")
```

```
Best Parameters: {'logisticregression__C': 0.1}
Best Cross-Validation Accuracy: 0.8641223608697942
Test Accuracy: 0.8825
```

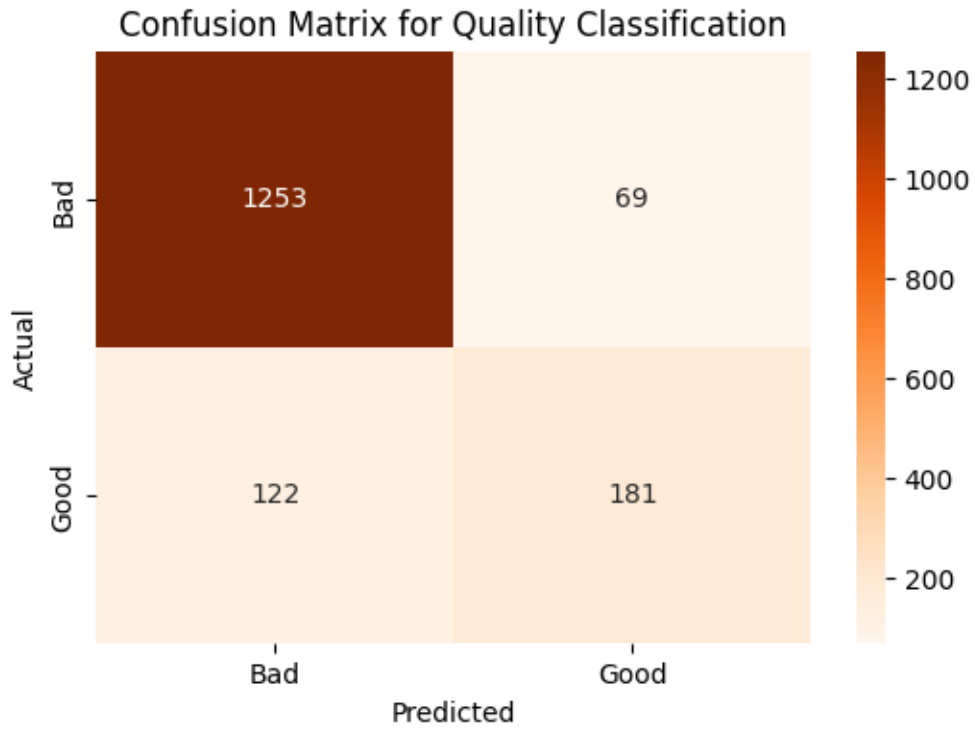
- Analyze the results (test and train), validate whether there is overfitting.

```
# Training accuracy
train_accuracy_q = grid_search_q.score(X_train_q, y_train_q)
print(f"Training Accuracy: {train_accuracy_q:.4f}")

# Compare training and test accuracy
print(f"Training Accuracy: {train_accuracy_q:.4f}")
print(f"Test Accuracy: {test_accuracy_q:.4f}")
```

```
Training Accuracy: 0.9977
Training Accuracy: 0.9977
Test Accuracy: 0.8825
```

```
print("Classification Report:")
print(classification_report(y_test_q, y_pred_q))

# Confusion matrix
cm_q = confusion_matrix(y_test_q, y_pred_q)
plt.figure(figsize=(6, 4))
sns.heatmap(
    cm_q,
    annot=True,
    fmt="d",
    cmap="Oranges",
    xticklabels=["Bad", "Good"],
    yticklabels=["Bad", "Good"],
)
plt.xlabel("Predicted")
plt.ylabel("Actual")
plt.title("Confusion Matrix for Quality Classification")
plt.show()
```

```
Classification Report:
              precision    recall  f1-score   support

           0       0.91      0.95      0.93      1322
           1       0.72      0.60      0.65       303

    accuracy                           0.88      1625
   macro avg       0.82      0.77      0.79      1625
weighted avg       0.88      0.88      0.88      1625
```



Analyse

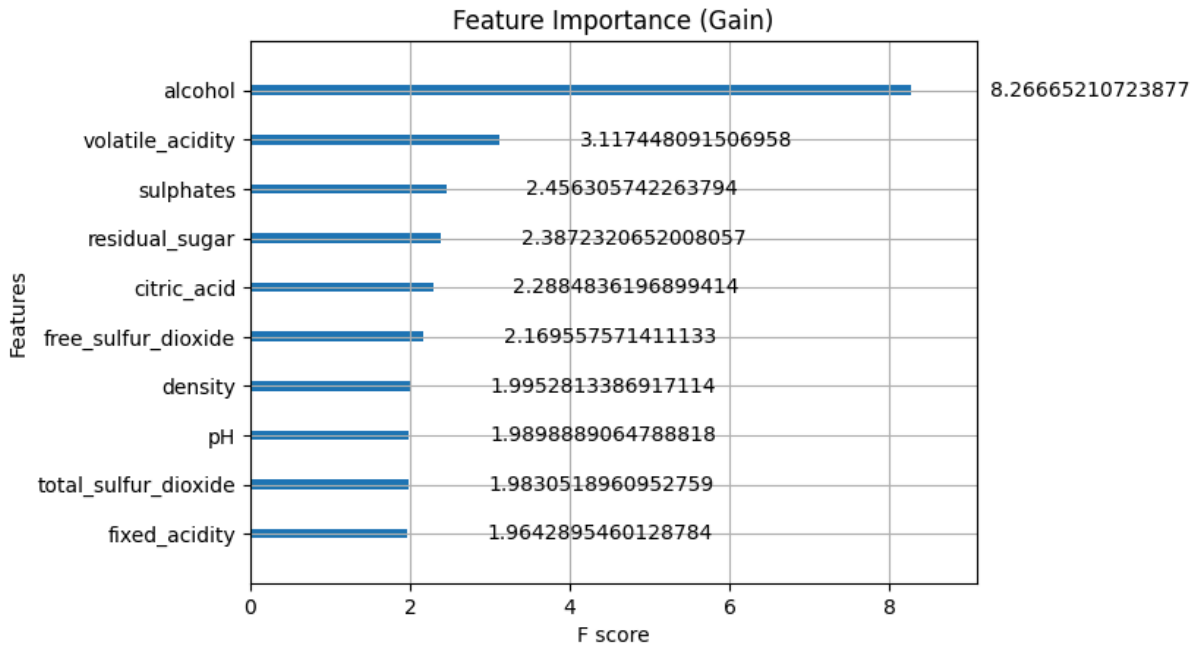
Overfitting, as the model performs much better on the training data than on unseen test data. But the gap is that the training accuracy is 0.99 while the test is 0.88

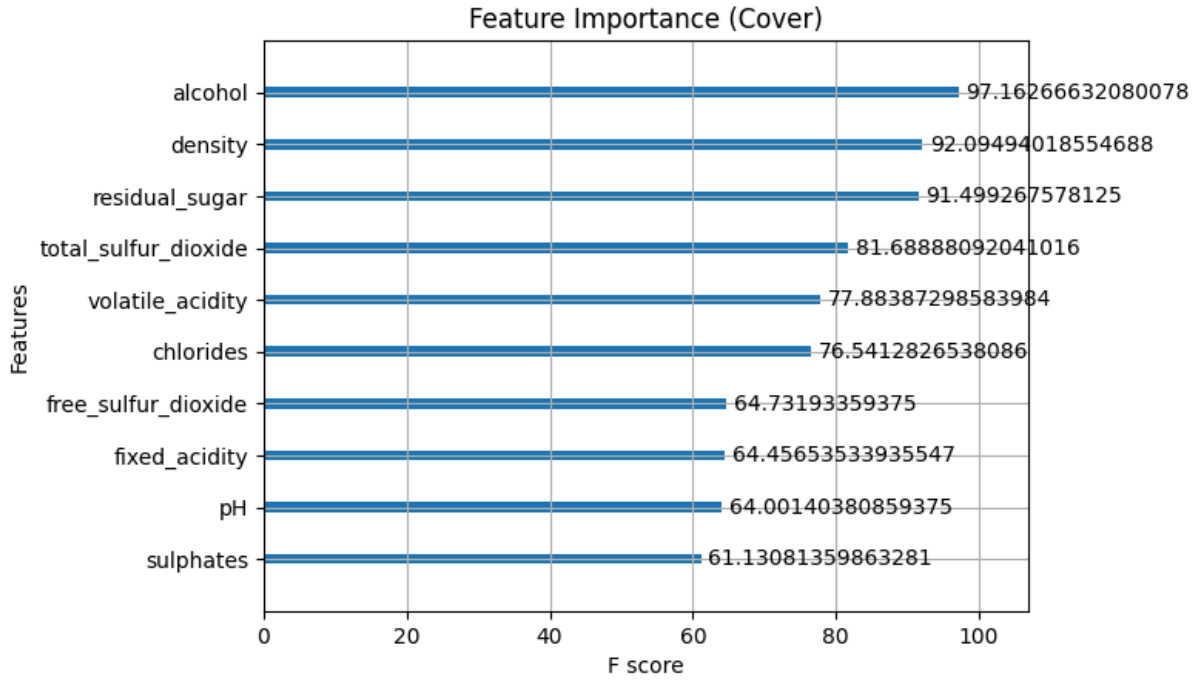
Interpretability with SHAP (2h)

- Plot the feature importance (gain and cover) from the XGBoost model. What can you conclude?

```
# Idea from https://towardsdatascience.com/be-careful-when-interpreting-your-features-importance-in-xgboost-6e16132588e7

# Retrieve feature importance (gain, cover)
importance_gain = grid_search_q.best_estimator_.get_booster().get_score(
    importance_type="gain"
)
importance_cover = grid_search_q.best_estimator_.get_booster().get_score(
    importance_type="cover"
)

# Plot the feature importance based on gain
xgb.plot_importance(
    grid_search_q.best_estimator_,
    importance_type="gain",
    max_num_features=10,
    title="Feature Importance (Gain)",
)
plt.show()

# Plot the feature importance based on cover
xgb.plot_importance(
    grid_search_q.best_estimator_,
    importance_type="cover",
    max_num_features=10,
```

```
    title="Feature Importance (Cover)",
)
plt.show()
```





Volatile_acidity and sulphates follow, but their contributions are much smaller. This suggests that alcohol plays a crucial role in the model's predictive power, while other features like fixed_acidity and total_sulfur_dioxide contribute less.

alcohol, density, and residual_sugar affect a larger portion of the data, while features like sulphates and pH are less commonly used.

Gain: measures the improvement in accuracy or reduction in the loss function brought by a feature. Gain focuses on the quality of a feature's contribution

Cover: measures the number of observations affected by a feature

https://link.springer.com/article/10.1134/S1061934823120171

https://www.sciencehistory.org/stories/magazine/scientia-vitis-decanting-the-chemistry-of-wine-flavor/

https://www.mdpi.com/2306-5710/8/1/1

- Use SHAP's `TreeExplainer` to compute feature importance (Shapley values). Do you see any difference with XGBoost's feature importances?
- Produce different plots to analyze Shapley values:
  - A bar plot that summarizes the mean absolute value of each feature.
  - A beeswarm plot that shows the shapley value for every sample and every feature.
  - A heatmap plot that indicates how different feature patterns influence the model's output.
- Based on the above results, what makes a wine 'good' or 'bad'?
- Following tutorial *

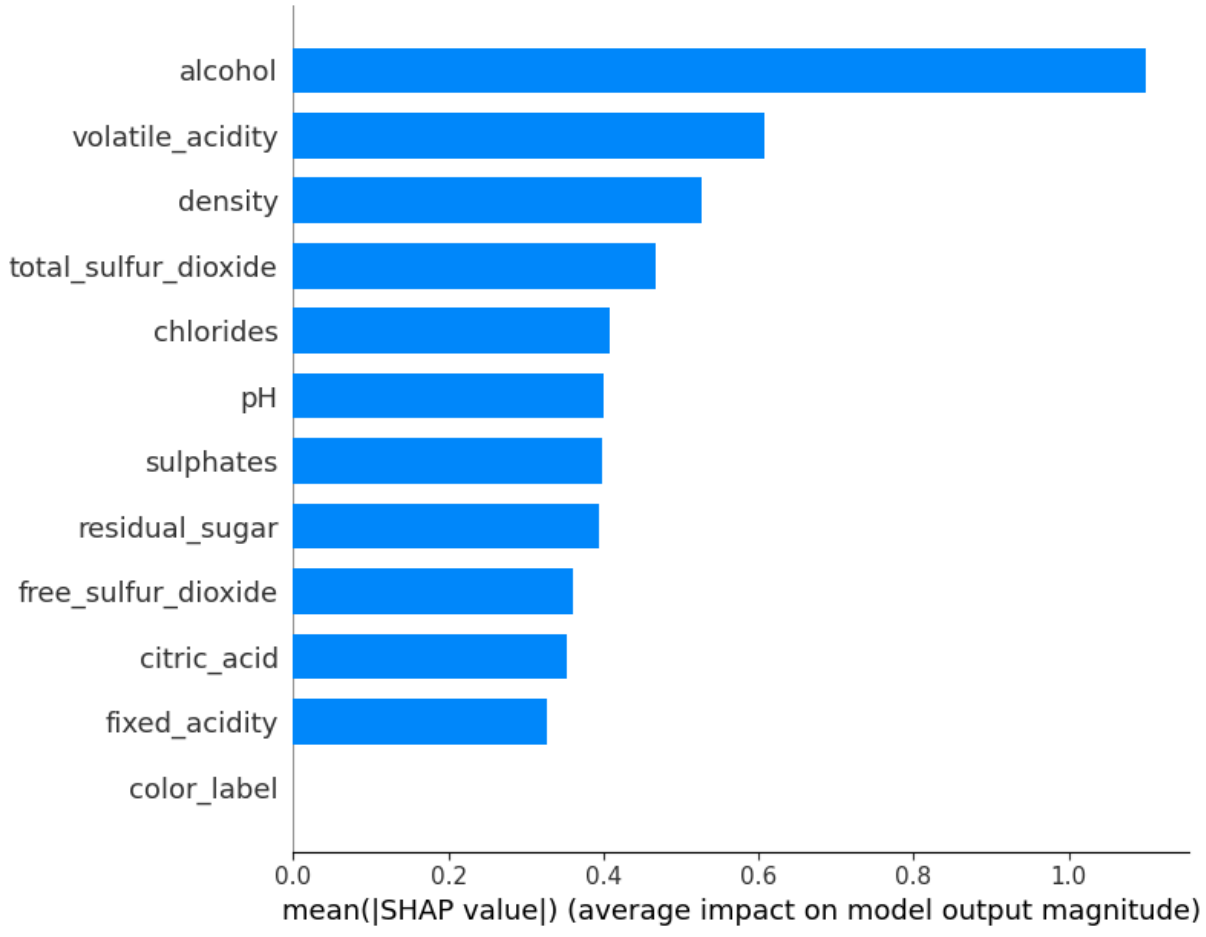
https://medium.com/@emilykmarsh/xgboost-feature-importance-233ee27c33a4

```
shap_object = explainer(X_train_q)
```

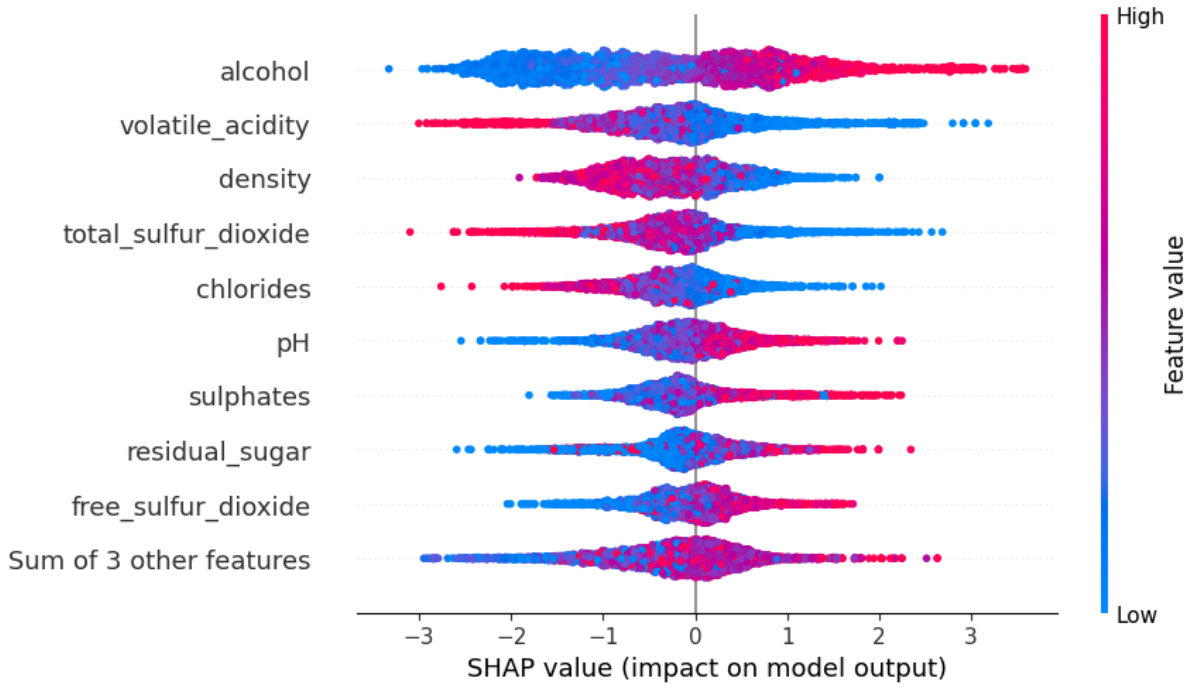
```
# Initialize the SHAP TreeExplainer
explainer = shap.TreeExplainer(grid_search_q.best_estimator_)
```

```
shap_values = explainer.shap_values(X_train_q)
```

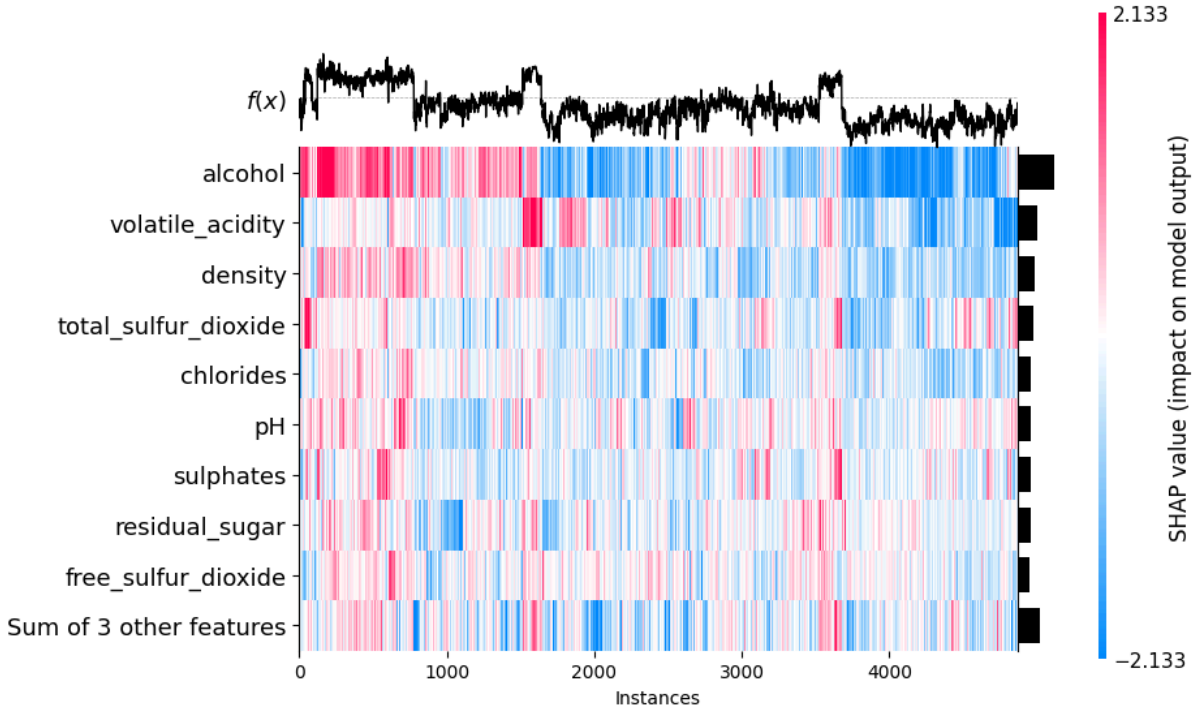
```
shap.summary_plot(shap_values, X_train_q, plot_type="bar")
```



```
shap.plots.beeswarm(shap_object)
```




```
shap.plots.heatmap(shap_object)
```



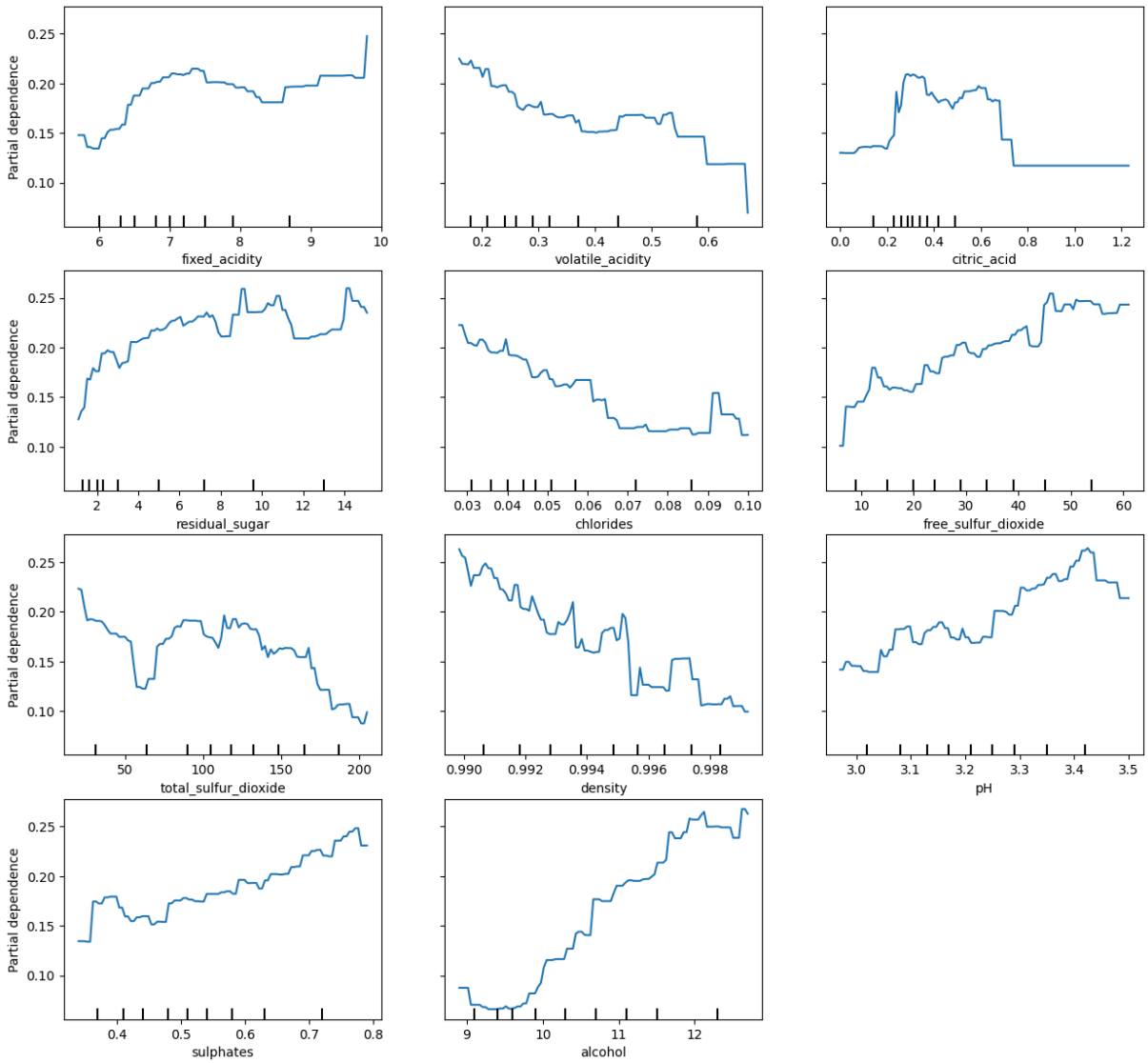

```
<Axes: xlabel='Instances'>
```

- Now use Partial Dependence Plots to see how the expected model output varies with the variation of each feature.
- How does that modify your perspective on what makes a good or bad wine?

```
# Train the_ model with the filtered data
grid_search_q.fit(X_train_q, y_train_q)
```

```
# Generate Partial Dependence Plot
features = list(range(X_train.shape[1]))
fig, ax = plt.subplots(figsize=(15, 10))
PartialDependenceDisplay.from_estimator(
    grid_search_q.best_estimator_, X_train_q, features, ax=ax
)

plt.subplots_adjust(top=1.2)
plt.show()
```

```
Fitting 5 folds for each of 4 candidates, totalling 20 fits
```



- Search for literature or resources that provide indications of the chemical structure of good or poor wines. Do your findings match these resources?

Alcohol: Higher alcohol content generally correlates with better quality, especially in red wines

Volatile Acidity: High levels are undesirable, as they can give the wine a vinegar-like taste, reducing quality(Science History Institute

Total Sulfur Dioxide: High levels preserve the wine but can negatively affect taste if excessive, especially in white wines

Residual Sugar: Affects sweetness; balanced levels enhance wine quality, but too much can make the wine taste overly sweet pH and Acidity: Lower pH (higher acidity) enhances the freshness of the wine, but must be balanced to avoid excessive tartness

Tannins: Provide structure and astringency, especially in red wines; over-extraction leads to bitterness, reducing quality.

Analyze a few bad wines, and try to see how to make them better

Pick some of the worst wines, and try to see what make them so bad. Check out `shap.plots.heatmap` for some visual tool to do this.

How would you go about improving them?

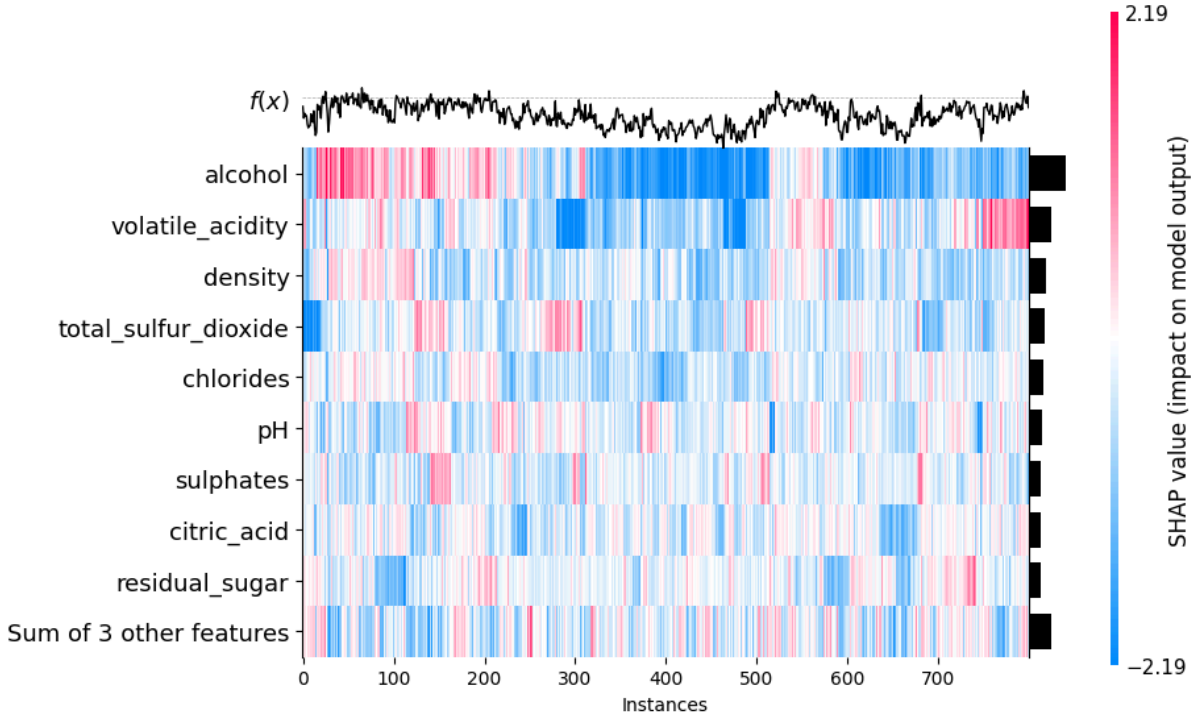
Lets analyse

```
worst_wines = X_train_q[y_train_q == 0]
worst_wines_quality = y_train_q[y_train_q == 0]
# take 10 randomly
random_worst_wines = worst_wines.sample(n=800, random_state=42)
random_worst_wines_quality = worst_wines_quality.loc[random_worst_wines.index]
```

```
# Initialize SHAP TreeExplainer
explainer = shap.TreeExplainer(grid_search_q.best_estimator_)

# Compute SHAP values for the worst wines
shap_values_worst = explainer.shap_values(random_worst_wines)

# Wrap into a SHAP explanation object
shap_values_worst_expl = shap.Explanation(
    shap_values_worst,
    base_values=explainer.expected_value,
    data=random_worst_wines,
    feature_names=worst_wines.columns,
)
```

```
# Create a SHAP heatmap plot for the worst wines
shap.plots.heatmap(shap_values_worst_expl)
```

Worst wines




```
<Axes: xlabel='Instances'>
```

low alcohol content and high volatile acidity are major factors negatively affecting wine quality. Density also contributes negatively for most wines, suggesting an imbalance. Total sulfur dioxide and pH have mixed effects, indicating they need to be optimized for each wine. Increasing alcohol and sulphates, while reducing volatile acidity and density, could improve these wines. Focusing on balancing these key features should lead to higher quality.

```
color = 0  ## use 0 when red 1 when white
random_or_all = False  # takes random n+samples false take all
samples = 15  # number of random sample
good_bad_all = 2  # 0 takes good, 1 bad ,2 all
```

```
if good_bad_all == 0:
    color_wines = X_train_q[y_train_q == 1]
    color_quality = y_train_q[y_train_q == 1]
elif good_bad_all == 1:
    color_wines = X_train_q[y_train_q == 0]
    color_quality = y_train_q[y_train_q == 0]
```

```
# Assuming 'wine_type' is the column that indicates the type of wine (1 for white)
color_wines = X_train_q[X_train_q["color_label"] == color]
color_quality = y_train_q[X_train_q["color_label"] == color]
```

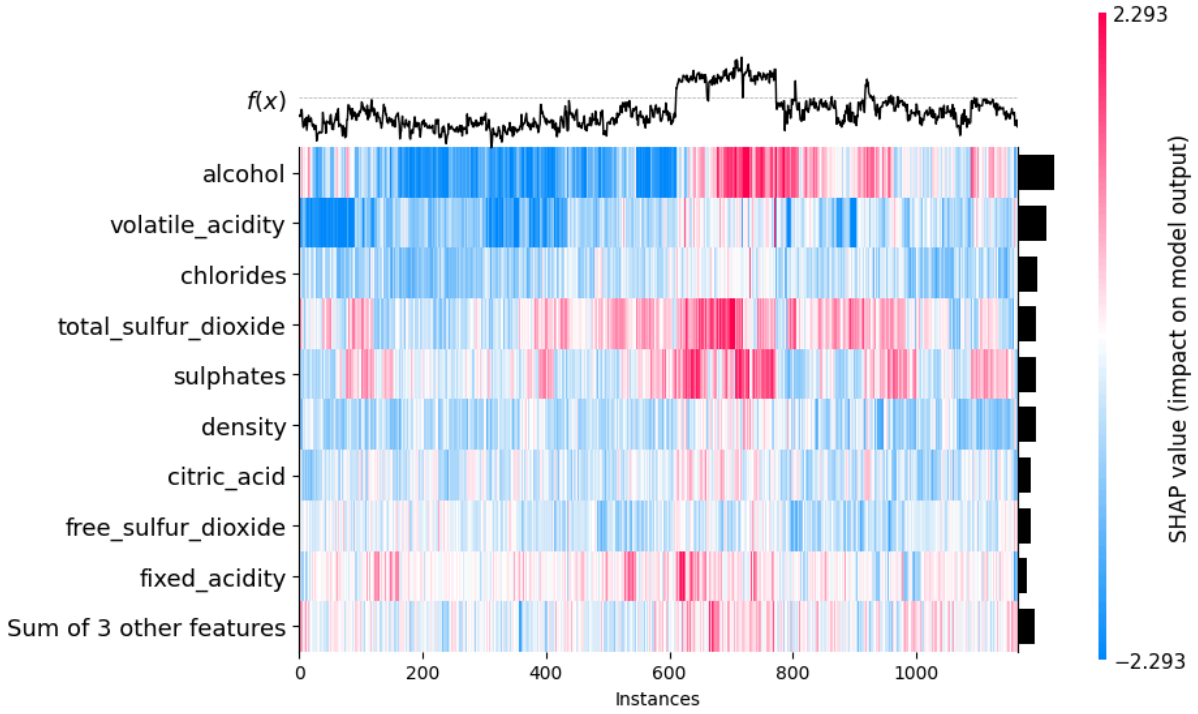
```
if random_or_all:
    color_wines = color_wines.sample(n=samples, random_state=42)
    color_quality = color_quality.loc[color_wines.index]
```

```
len(color_wines)
```

```
1165
```

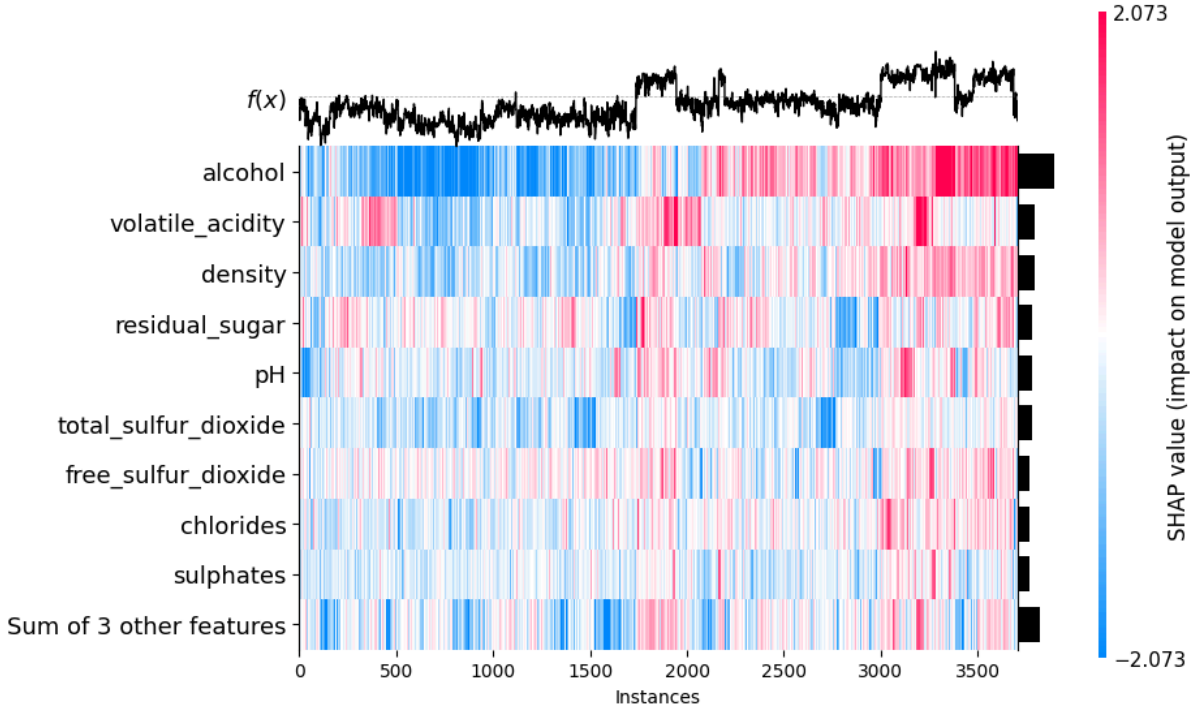
```
# Initialize SHAP TreeExplainer
explainer = shap.TreeExplainer(grid_search_q.best_estimator_)

# Compute SHAP values for the worst wines
shap_values_worst = explainer.shap_values(color_wines)
```

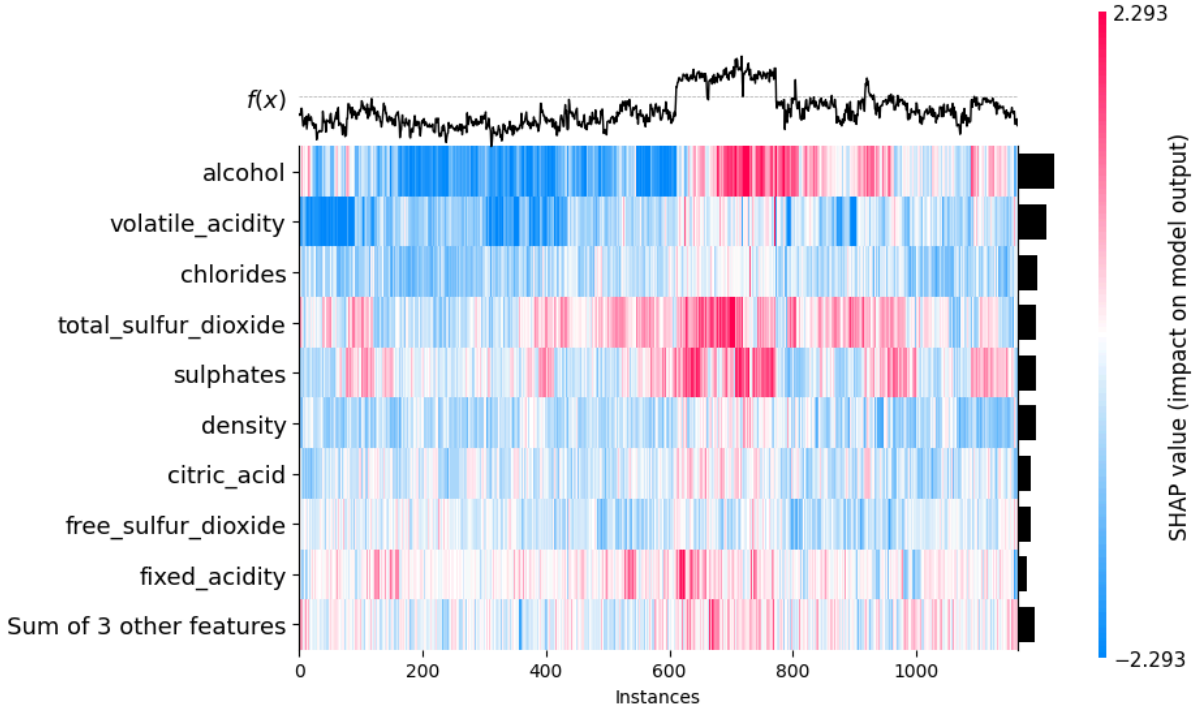
```
# Wrap into a SHAP explanation object
shap_values_worst_expl_white = shap.Explanation(
    shap_values_worst,
    base_values=explainer.expected_value,
    data=color_wines,
    feature_names=color_wines.columns,
)
# Create a SHAP heatmap plot for the worst wines
shap.plots.heatmap(shap_values_worst_expl_white)
```




```
<Axes: xlabel='Instances'>
```

White vs Red





Wrap-up and conclusion

As wrap-up, explain what are your key findings, and make 3 recommendations to the wine maker on how to improve the wines for next year. How confident are you that making these changes will lead to better wines? Explain in simple terms to the winemaker the limitations of your approach in terms of capturing causality.

increasing alcohol content, reducing volatile acidity, and optimizing sulfur dioxide levels can improve wine quality. Alcohol positively impacts both red and white wines, while high volatile

acidity harms red wines. To improve next year's wines, slightly raise alcohol levels, lower volatile acidity, and balance sulfur dioxide

It depends because there is a lot of external elements like weather if there is too much rain and cold whine is gonna be acid.

If there is a lots of sun and warm weather and after lots of rain its gonna be bad.

In a general red wines have a density higher than wite because of the chemical composition.

Conclusion

In conclusion, I identified the key factors that influence wine quality, such as alcohol content, volatile acidity, sulfur dioxide levels, residual sugar, and density. I found that higher alcohol improves both red and white wines, while high volatile acidity negatively impacts red wines. Sulfur dioxide plays a critical role in preserving white wines but needs careful balance to avoid affecting taste. Using clustering and gradient boosting models, I successfully distinguished red from white wines and classified good vs. bad wines based on these features.