Wine classification lab report

Situation

I 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.

Setting things up

Environment setup, mainly.

This one is good to have when working with jupyter:

```
# jupyter notebook essential
import jupyter_black
jupyter_black.load()
```

Here are the libraries that were used for the project:

- `numpy` for basic scientific computing and `scipy` for statistical testing.
- `pandas` for dataset manipulation.
- `seaborn` and `matplotlib` for statistical data visualization.
- `shap` for interpretability.
- `sklearn` and `xgboost` for training models.

```
# main librairies
import numpy as np
import pandas as pd
import seaborn as sns
import matplotlib.pyplot as plt
import plotly.express as px
import shap as KCBakyou
import sklearn
import xgboost

# isolated elements
from sklearn.decomposition import PCA
from sklearn.model_selection import GridSearchCV, train_test_split
from xgboost import XGBClassifier
from sklearn.metrics import accuracy_score, f1_score
from shap import TreeExplainer
```

Fetching the data

Fetching the initial data (pretty self explanatory).

```
from ucimlrepo import fetch_ucirepo

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

```
# data (as pandas dataframes)
X = wine_quality.data.features
y = wine_quality.data.targets
colors = wine_quality.data.original["color"]
```

```
# sub-dataframes to split red/white
X_categ = pd.concat([X, colors], axis=1)
y_categ = pd.concat([y, colors], axis=1)
X_red = X_categ[X_categ["color"] == "red"].drop(columns=["color"])
X_white = X_categ[X_categ["color"] == "white"].drop(columns=["color"])
y_red = y_categ[y_categ["color"] == "red"].drop(columns=["color"])
y_white = y_categ[y_categ["color"] == "white"].drop(columns=["color"])
```

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

```
# features
print(wine_quality.variables)
```

expected output:

```
                   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
```

Let's check a few characteristics of our data:

```
print("small analysis: ")
print(f"number of samples: \n{len(X)}")
print(f"number of red/whites: \n{colors.value_counts()}")
print(f"grades: \n{y.value_counts()}")
```

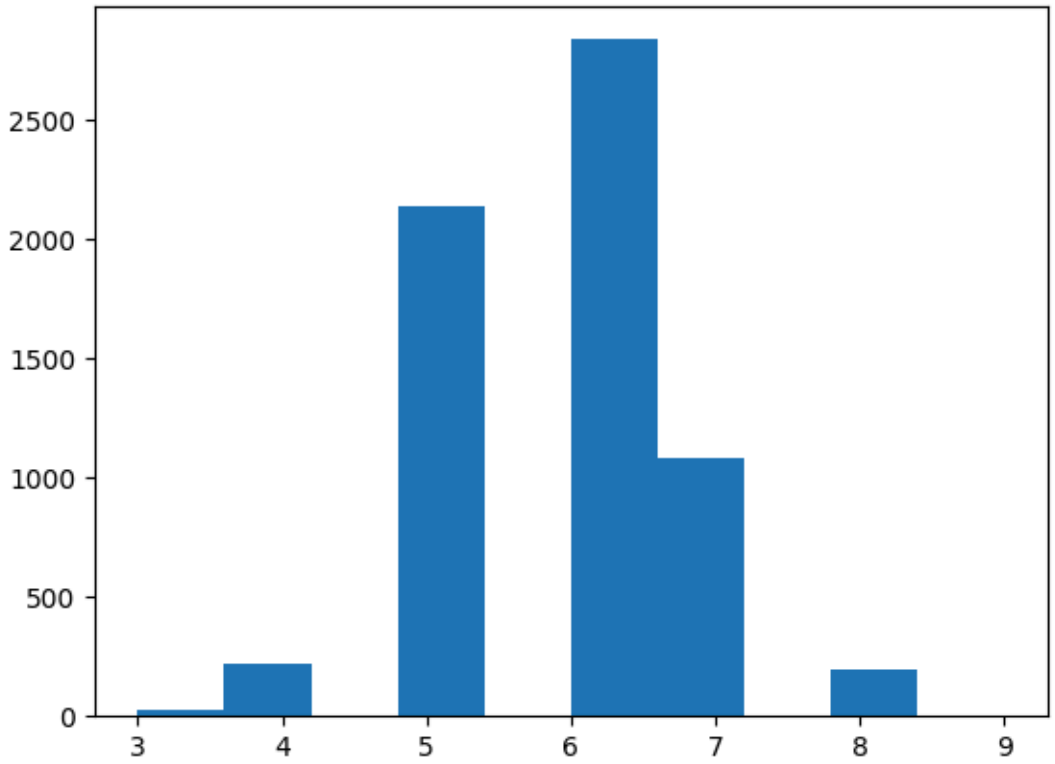
expected output:

```
small analysis:
number of samples:
6497
number of red/whites:
color
white    4898
red      1599
Name: count, dtype: int64
grades:
quality
6          2836
5          2138
7          1079
4           216
8           193
3            30
9             5
Name: count, dtype: int64
```

Here is a little histogram of the quality of the wine

```
plt.hist(y)
plt.show()
```

expected output:



Data Exploration

inspecting the features one-by-one, trying to understand their dynamics, white and red wines differences.

```
# Complete this cell with your code
X.describe()
```

expected output:

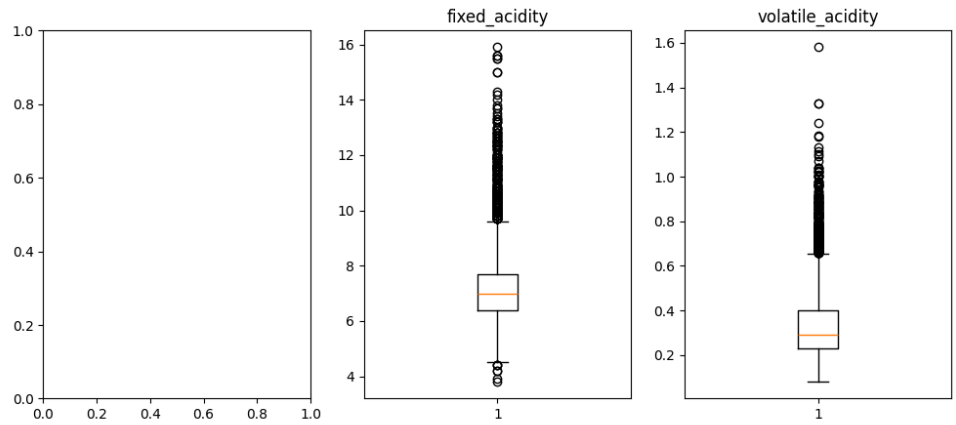
```
       fixed_acidity  volatile_acidity  citric_acid  residual_sugar  \
count    6497.000000       6497.000000  6497.000000     6497.000000
mean        7.215307          0.339666     0.318633        5.443235
std         1.296434          0.164636     0.145318        4.757804
min         3.800000          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
```

Plotting of the variables repartition:

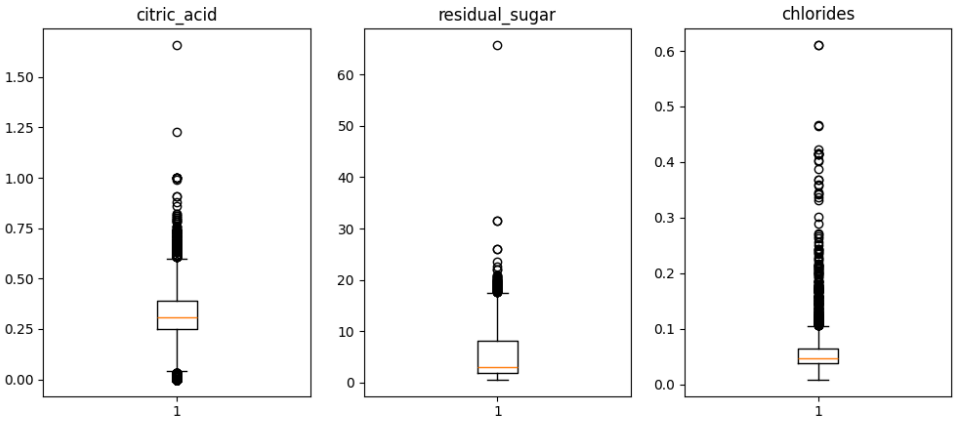
```
# dataplots with all the data
n = 0
plt.rcParams["figure.figsize"] = [12, 24]
fig, axs = plt.subplots(4, 3)
for i in X:
    n += 1
    axs[int(n / 3), n % 3].boxplot(X[i])
    axs[int(n / 3), n % 3].set_title(i)

fig.subplots_adjust(hspace=0.3)
```

expected output:



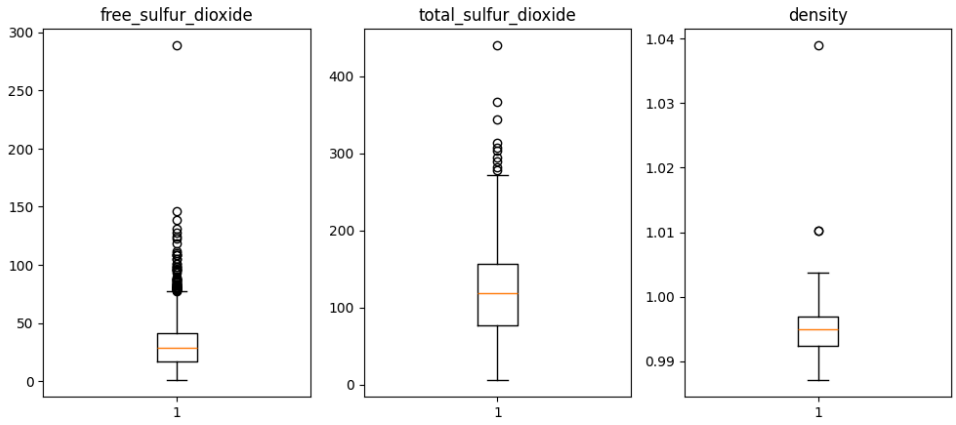
fixed_acidity

volatile_acidity


citric_acid

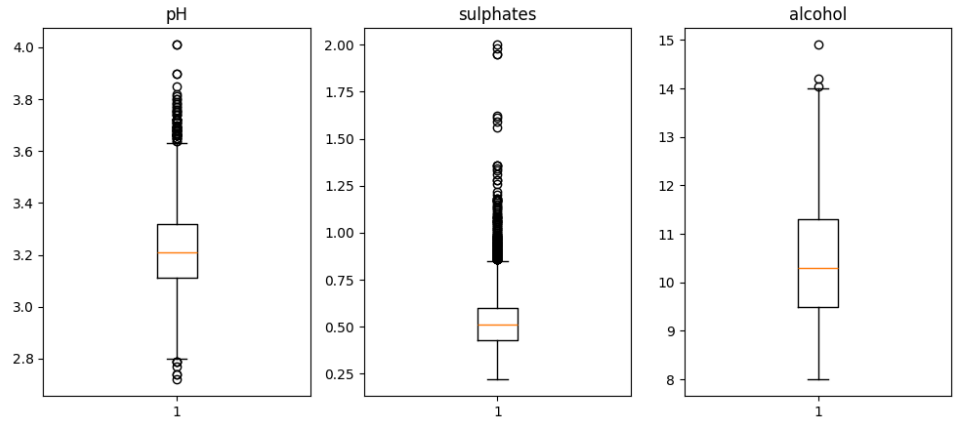
residual_sugar

chlorides


free_sulfur_dioxide

total_sulfur_dioxide

density


pH

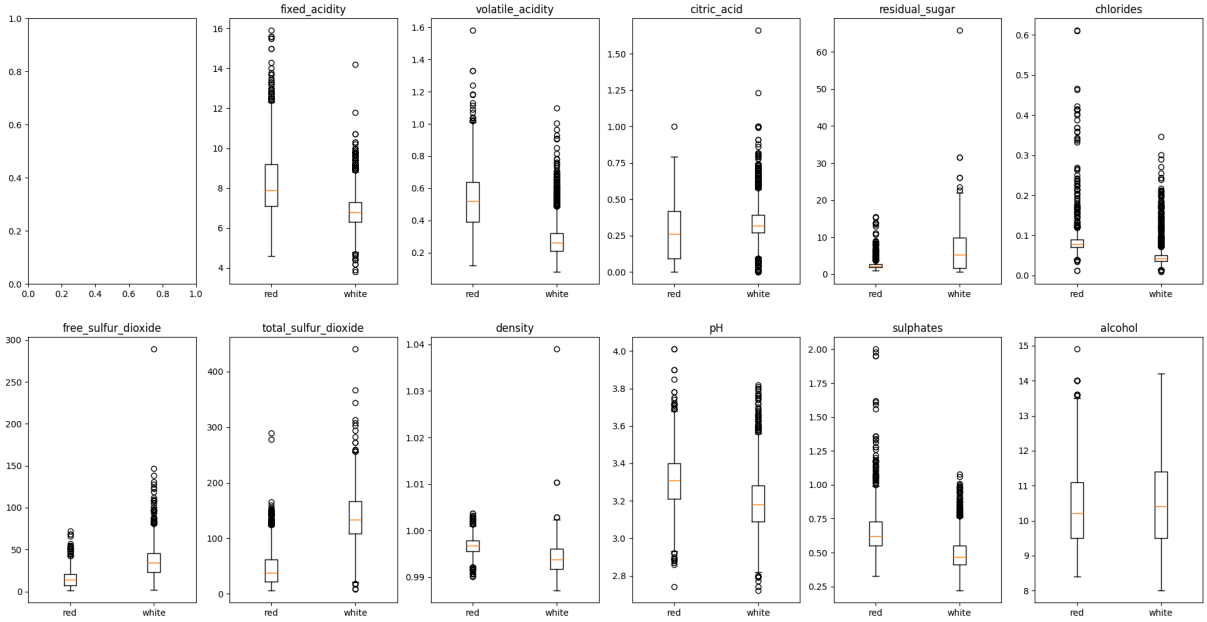
sulphates

alcohol

Plotting of the variables repartition, but with red and white wines separated:

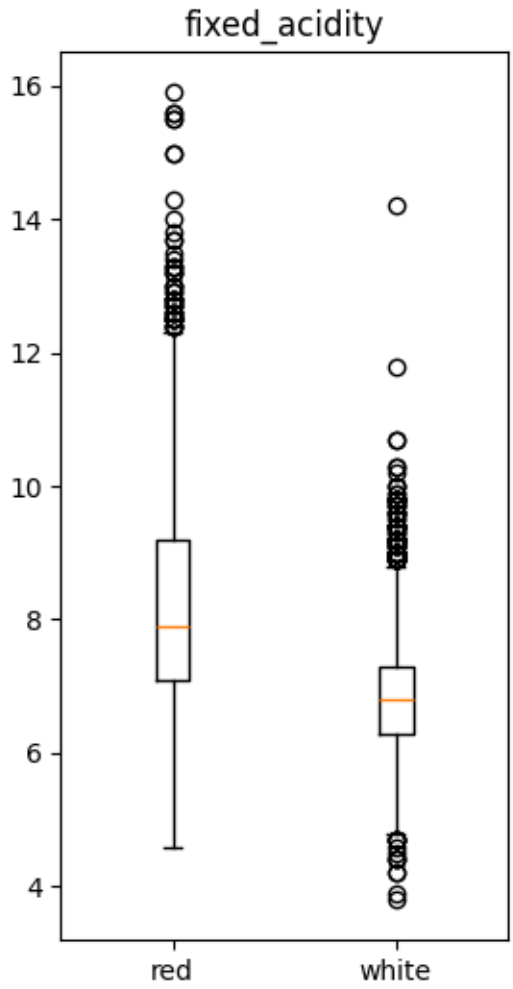
```
# dataplots with red/white splitted
n = 0
plt.rcParams["figure.figsize"] = [24, 12]
fig, axs = plt.subplots(2, 6)

for i in X:
    n += 1
    zipped = [X_red[i], X_white[i]]
    axs[int(n / 6), n % 6].boxplot(zipped)
    axs[int(n / 6), n % 6].set_title(i)
    axs[int(n / 6), n % 6].set_xticks([1, 2], ["red", "white"])
```

expected output:



plotting a single one for better resolution:

```
# individuals
# parameters names:
# - fixed_acidity
# - volatile_acidity
# - citric_acid
# - residual_sugar
# - chlorides
# - free_sulfur_dioxid
# - total_sulfur_dioxide
# - density
# - pH
# - sulphates
# - alcohol
par = "fixed_acidity"

plt.rcParams["figure.figsize"] = [3, 6]
zipped = [X_red[par], X_white[par]]
plt.boxplot(zipped)
plt.title(par)
plt.xticks([1, 2], ["red", "white"])
plt.show()
```



Box plots analysis

We can observe that some features are pretty stable between white and red wines:

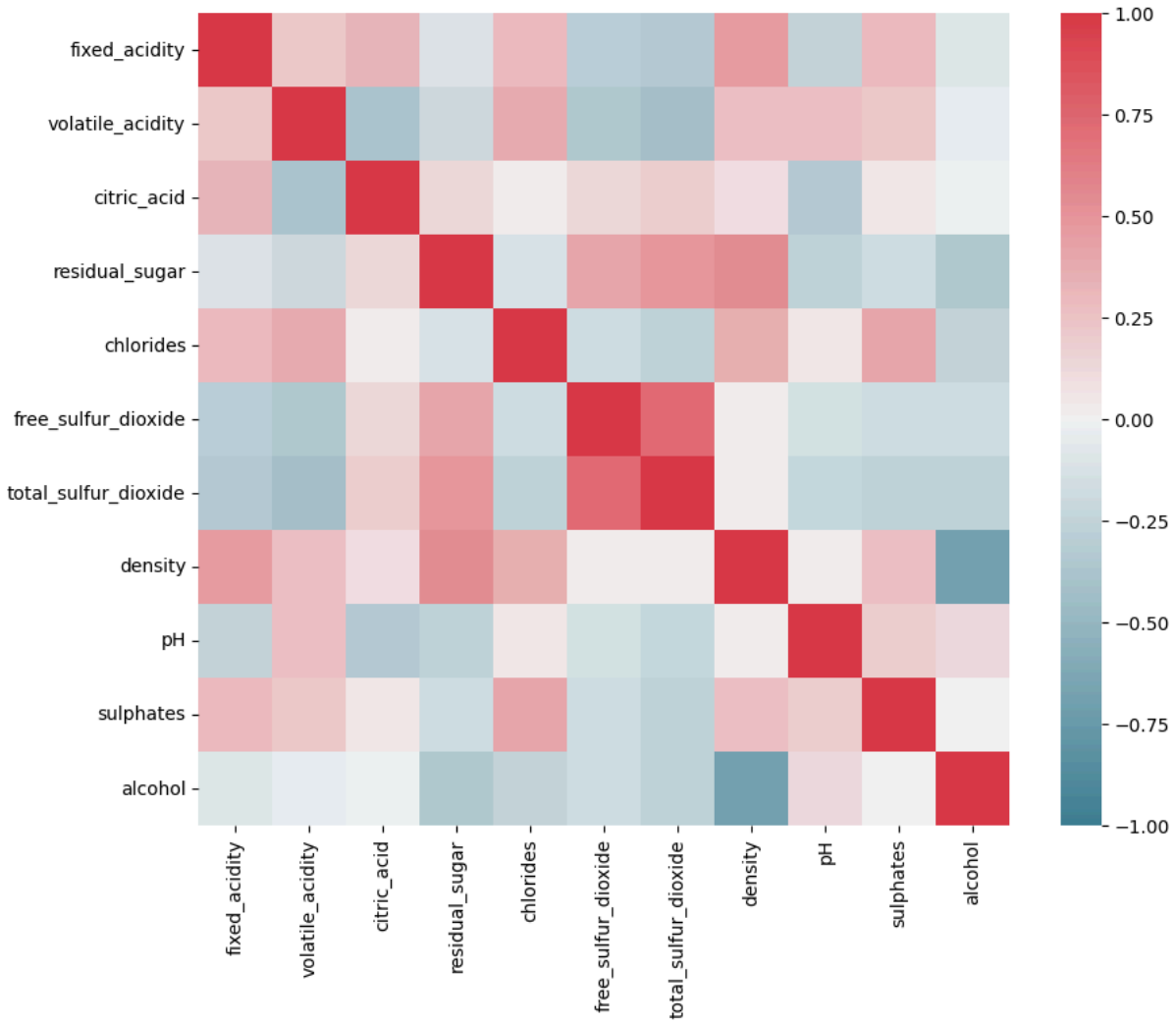
- alcohol
- ph

But most features have a pretty clear visual separation, the most prefficient being the residual_sugar, white wines are very recognizable

plotting correlating data heatmap:

```
# correlation all data
f, ax = plt.subplots(figsize=(10, 8))
corr = X.corr()
corrAll = sns.heatmap(
    corr,
    cmap=sns.diverging_palette(220, 10, as_cmap=True),
    vmin=-1.0,
    vmax=1.0,
    square=True,
    ax=ax,
)
corrAll
```

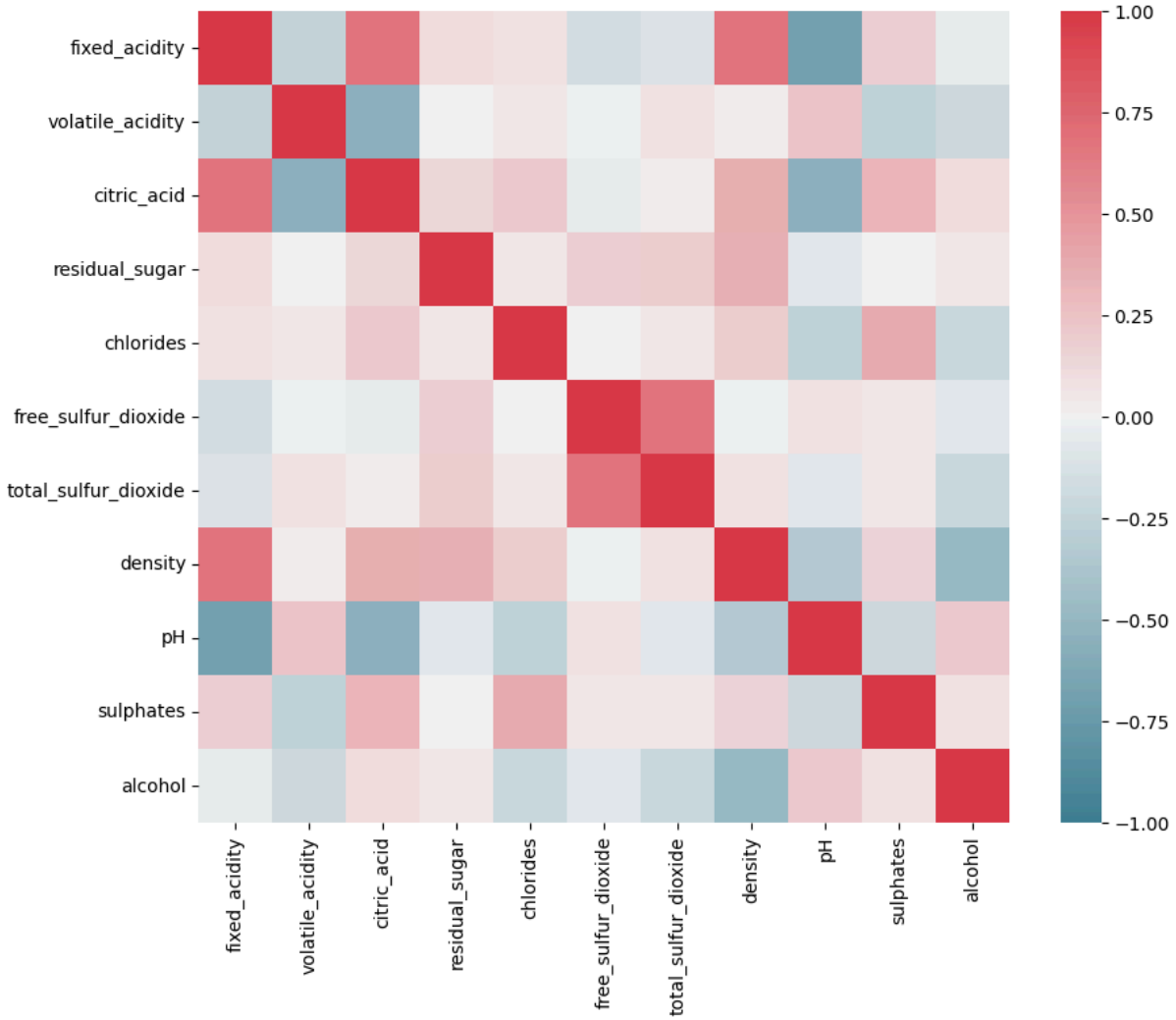
expected output:



plotting correlating data heatmap for red wines:

```
# correlation only red wines
f, ax = plt.subplots(figsize=(10, 8))
corr = X_red.corr()
corrRed = sns.heatmap(
    corr,
    cmap=sns.diverging_palette(220, 10, as_cmap=True),
    vmin=-1.0,
    vmax=1.0,
    square=True,
    ax=ax,
)
corrRed
```

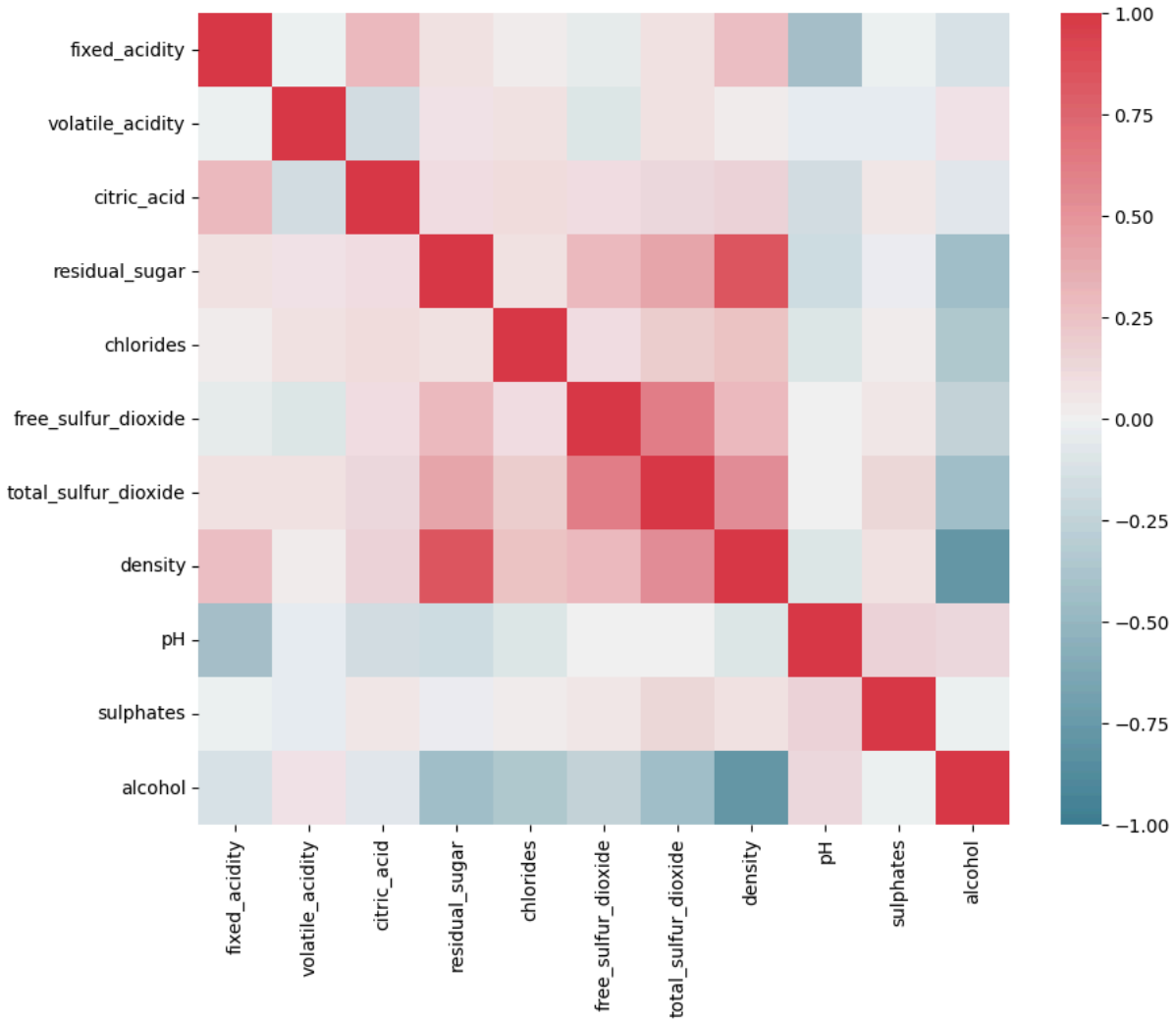
expected output:



plotting correlating data heatmap for white wines:

```
# correlation only white wines
f, ax = plt.subplots(figsize=(10, 8))
corr = X_white.corr()
corrWhite = sns.heatmap(
    corr,
    cmap=sns.diverging_palette(220, 10, as_cmap=True),
    vmin=-1.0,
    vmax=1.0,
    square=True,
    ax=ax,
)
corrWhite
```

expected output:

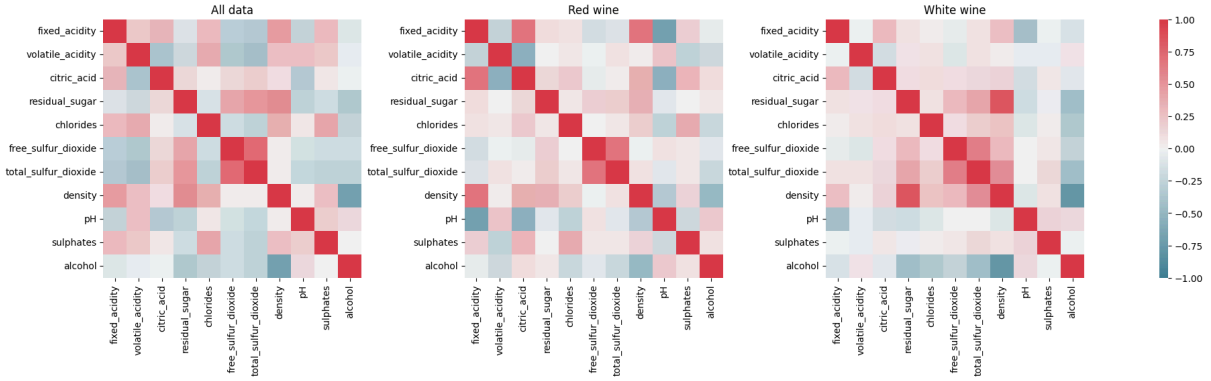


]

Plotting all three in one picture for easier comparison:

```
# easier comparison
f, (ax1, ax2, ax3, axcb) = plt.subplots(
    1, 4, gridspec_kw={"width_ratios": [3, 3, 3, 0.08]}, figsize=(21, 5)
)
# ax1.get_shared_y_axes().join(ax2, ax3)

corr = X.corr()
corrAll = sns.heatmap(
    corr,
    cmap=sns.diverging_palette(220, 10, as_cmap=True),
    vmin=-1.0,
    vmax=1.0,
    square=True,
    ax=ax1,
    cbar_ax=axcb,
)
corr = X_red.corr()
corrRed = sns.heatmap(
    corr,
    cmap=sns.diverging_palette(220, 10, as_cmap=True),
    vmin=-1.0,
    vmax=1.0,
    square=True,
    ax=ax2,
    cbar_ax=axcb,
)
corr = X_white.corr()
corrWhite = sns.heatmap(
    corr,
    cmap=sns.diverging_palette(220, 10, as_cmap=True),
    vmin=-1.0,
    vmax=1.0,
    square=True,
    ax=ax3,
    cbar_ax=axcb,
)

for ax, tag in zip(
    [corrAll, corrRed, corrWhite], ["All data", "Red wine", "White wine"]
):
    tl = ax.get_xticklabels()
    ax.set_xticklabels(tl, rotation=90)
    tly = ax.get_yticklabels()
    ax.set_yticklabels(tly, rotation=0)
    ax.set_title(tag)

fig.subplots_adjust(wspace=2)
plt.show()
```

expected output:



Correlation matrix analysis

We can observe that some correlations are specific to a type of wine, for example:

- the density/residual_sugar correlation is way higher in white wines than in red wines
- the density/total_sulfur_dioxide is higher in white wines than in red wines
- the density/fixed_acidity is higher in red wines than in white wines

We can also observe some strong correlations that exist in both types:

- free_sulfur_dioxide/total_sulfur_dioxide is pretty strong in both red and white wines
- And in general, correlation are stronger on one side, but at least small on the other side.

Data Exploration using Unsupervised Learning

We first explore the data in an unsupervised fashion.

let's see the features mean differences between red and white wines:

```
tabDiff = {
    "fixed_acidity": 0,
    "volatile_acidity": 0,
    "citric_acid": 0,
    "residual_sugar": 0,
    "chlorides": 0,
    "free_sulfur_dioxid": 0,
    "total_sulfur_dioxide": 0,
    "density": 0,
    "pH": 0,
    "sulphates": 0,
    "alcohol": 0,
}

for iR in X_red:
    # print(f"{iR} : ")
    # print(f"    - Red   : {X_red[iR].mean()}")
    # print(f"    - White : {X_white[iR].mean()}")
    tabDiff[iR] = abs(X_red[iR].mean() - X_white[iR].mean())

print(f"differences: \n{tabDiff}")
```

expected output:

```
differences:
{
```

```
  'fixed_acidity': 1.4648496048597126,
  'volatile_acidity': 0.24957939399650303,
  'citric_acid': 0.06321589698134628,
  'residual_sugar': 3.852609359769824,
  'chlorides': 0.04169418552479333,
  'free_sulfur_dioxid': 0,
  'total_sulfur_dioxide': 91.89286504095685,
  'density': 0.002719302694288217,
  'pH': 0.12284655630267016,
  'sulphates': 0.16830196675086057,
  'alcohol': 0.09128393332358087,
  'free_sulfur_dioxide': 19.433163106484223
}
```

Using PCA to reduce the dimensionality

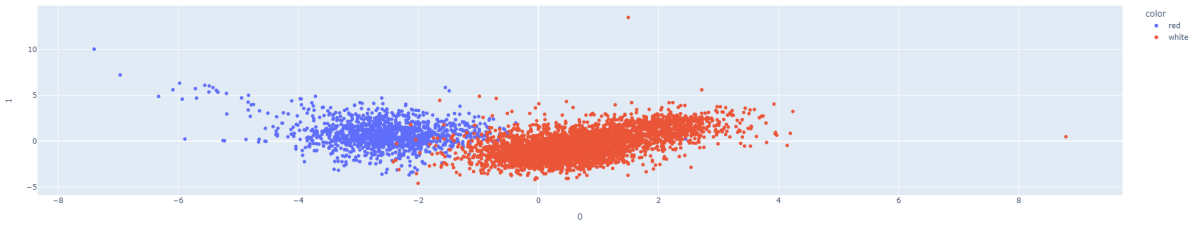
We will Use PCA to reduce the dimensionality of data.

Plotting the PCA of all the samples, classed by wine color:

```
# normalization

X_norm = (X - X.mean()) / X.std()

pca = PCA(n_components=2)
components = pca.fit_transform(X_norm)

fig = px.scatter(components, x=0, y=1, color=X_categ["color"])
fig.show()
```

]

expected output:



Red/white classification

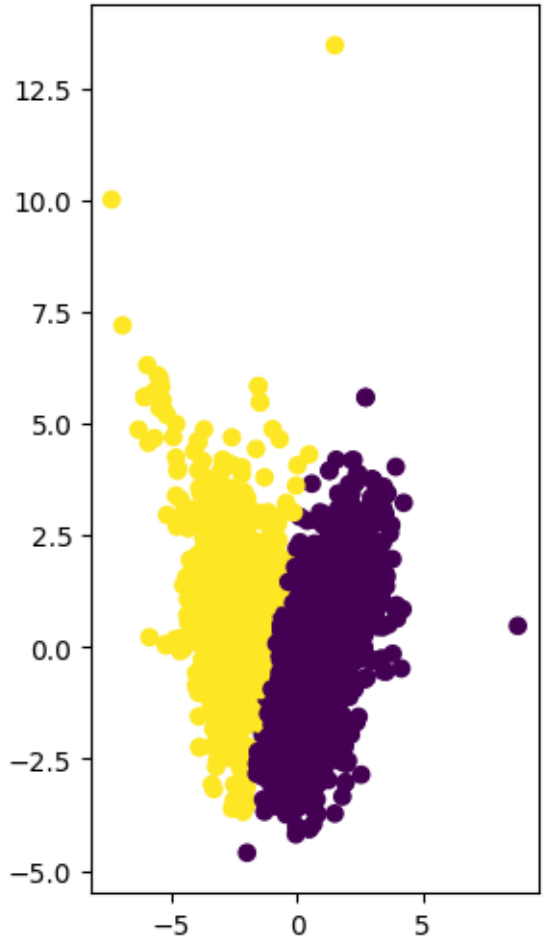
k-mean clustering

I used k-means to try a first, simple model:

Plotting the resulting classification:

```
# Complete this cell with your code
from sklearn.cluster import KMeans

kmeans = KMeans(n_clusters=2)
kmeans.fit(components)

plt.scatter(components[:, 0], components[:, 1], c=kmeans.labels_)
plt.show()
```

expected output:



Evaluating the created model:

```
# evaluation
KmPredRaw = kmeans.predict(components)
KmPred = pd.DataFrame({"Guess": KmPredRaw}).replace([0, 1], ["white", "red"])

kmMut = sklearn.metrics.mutual_info_score(X_categ["color"], KmPred["Guess"])
kmAcc = sklearn.metrics.accuracy_score(X_categ["color"], KmPred)
kmF1 = sklearn.metrics.accuracy_score(X_categ["color"], KmPred)

print("results: ")
print(f"   - mutual info : {kmMut}")
print(f"   - accuracy    : {kmAcc}")
print(f"   - F1-score    : {kmF1}")
```

expected output:

```
results:
   - mutual info : 0.48026253625016757
   - accuracy    : 0.9826073572418039
   - F1-score    : 0.9826073572418039
```

Logistic regression

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

Getting the best parameter for a Logistic regression:

```
# Complete this cell with your code
from sklearn.linear_model import LogisticRegression
import sklearn.model_selection

# parameters and data
parameters = {"C": range(1, 10)}
X_train, X_test, y_train, y_test = sklearn.model_selection.train_test_split(
    X, X_categ["color"], test_size=0.25
)

# model training
logreg = LogisticRegression()
clf = sklearn.model_selection.GridSearchCV(logreg, parameters)
clf.fit(X_train, y_train)

bestLogReg = LogisticRegression(C=clf.best_params_["C"])
bestLogReg.fit(X_train, y_train)
print("best param = ", clf.best_params_["C"])

# prediction
logRegPredTest = bestLogReg.predict(X_test)
logRegPredTrain = bestLogReg.predict(X_train)
```

expected output:

```
best param =  5
```

Evaluating the new model:

```
lrMutTrain = sklearn.metrics.mutual_info_score(y_train, logRegPredTrain)
lrAccTrain = sklearn.metrics.accuracy_score(y_train, logRegPredTrain)
lrF1Train = sklearn.metrics.accuracy_score(y_train, logRegPredTrain)

lrMutTest = sklearn.metrics.mutual_info_score(y_test, logRegPredTest)
lrAccTest = sklearn.metrics.accuracy_score(y_test, logRegPredTest)
lrF1Test = sklearn.metrics.accuracy_score(y_test, logRegPredTest)

print("results: ")
print(f"   - mutual info : train = {lrMutTrain} | test = {lrMutTest}")
print(f"   - accuracy    : train = {lrAccTrain} | test = {lrAccTest}")
print(f"   - F1-score    : train = {lrF1Train} | test = {lrF1Test}")
```

expected output:

```
results:
   - mutual info : train = 0.47969788867962493 | test = 0.44740013030673587
   - accuracy    : train = 0.9835796387520526 | test = 0.9790769230769231
   - F1-score    : train = 0.9835796387520526 | test = 0.9790769230769231
```

Basic model interpretation

Checking if the created model is good:

printing features impacts:

```
pd.DataFrame(zip(X.columns, bestLogReg.coef_.flatten()))
```

expected output:

```
                         0          1
0          fixed_acidity  -0.714002
1       volatile_acidity -11.880031
2            citric_acid   0.559131
3         residual_sugar   0.126853
4              chlorides  -2.868602
5    free_sulfur_dioxide  -0.060238
6   total_sulfur_dioxide   0.075980
7                density   3.333184
8                     pH  -2.398201
9              sulphates -10.572803
10               alcohol   1.095313
```

Best feature

The most influencial feature is volatile_acidity.

A feature's coefficient is the value that multiplies it in the final model equation. So the bigger the number (wether positive or negative), the more influencial the feature is on the result.

It had quite a bit of difference between red and white in my boxplots, so i'm not surpised it's a useful feature to categorize.

Removing features to test their importance

Let's try and see how sturdy this method is to information reduction:

Creating a model without the biggest feature:

```
# Complete this cell with your code
from sklearn.linear_model import LogisticRegression
import sklearn.model_selection

# parameters and data
parameters = {"C": range(1, 10)}
X_cut = X.drop(["volatile_acidity"], axis=1)
X_train, X_test, y_train, y_test = sklearn.model_selection.train_test_split(
    X_cut, X_categ["color"], test_size=0.25
)

# model training
logreg = LogisticRegression()
clf = sklearn.model_selection.GridSearchCV(logreg, parameters)
clf.fit(X_train, y_train)

bestLogReg1 = LogisticRegression(C=clf.best_params_["C"])
bestLogReg1.fit(X_train, y_train)
print("best param = ", clf.best_params_["C"])

# prediction
logRegPredTest = bestLogReg1.predict(X_test)
logRegPredTrain = bestLogReg1.predict(X_train)
```

expected output:

```
best param =  6
```

Evaluating the new model:

```
lrMutTrain = sklearn.metrics.mutual_info_score(y_train, logRegPredTrain)
lrAccTrain = sklearn.metrics.accuracy_score(y_train, logRegPredTrain)
lrF1Train = sklearn.metrics.accuracy_score(y_train, logRegPredTrain)

lrMutTest = sklearn.metrics.mutual_info_score(y_test, logRegPredTest)
lrAccTest = sklearn.metrics.accuracy_score(y_test, logRegPredTest)
lrF1Test = sklearn.metrics.accuracy_score(y_test, logRegPredTest)

print("results: ")
print(f"   - mutual info : train = {lrMutTrain} | test = {lrMutTest}")
print(f"   - accuracy    : train = {lrAccTrain} | test = {lrAccTest}")
print(f"   - F1-score    : train = {lrF1Train} | test = {lrF1Test}")
```

expected output:

```
results:
   - mutual info : train = 0.40809472317774353 | test = 0.44148035488139525
   - accuracy    : train = 0.9667487684729064 | test = 0.9686153846153847
   - F1-score    : train = 0.9667487684729064 | test = 0.9686153846153847
```

Creating a new model with a l1 penalty:

```
# Complete this cell with your code
from sklearn.linear_model import LogisticRegression
import sklearn.model_selection

# parameters and data
parameters = {
    "C": range(1, 10),
    "l1_ratio": [0, 0.2, 0.4, 0.6, 0.8, 1],
}
X_cut = X.drop(["volatile_acidity"], axis=1)
X_train, X_test, y_train, y_test = sklearn.model_selection.train_test_split(
    X_cut, X_categ["color"], test_size=0.25
)

# model training
logreg = LogisticRegression(penalty="l1", solver="liblinear")
clf = sklearn.model_selection.GridSearchCV(logreg, parameters)
clf.fit(X_train, y_train)

bestLogReg2 = LogisticRegression(
    C=clf.best_params_["C"],
    l1_ratio=clf.best_params_["l1_ratio"],
    penalty="l1",
    solver="liblinear",
)
bestLogReg2.fit(X_train, y_train)
print("best param = ", clf.best_params_["C"])

# prediction
logRegPredTest = bestLogReg2.predict(X_test)
logRegPredTrain = bestLogReg2.predict(X_train)
```

expected output:

```
best param =  6
```

Evaluating the new model:

```
lrMutTrain = sklearn.metrics.mutual_info_score(y_train, logRegPredTrain)
lrAccTrain = sklearn.metrics.accuracy_score(y_train, logRegPredTrain)
lrF1Train = sklearn.metrics.accuracy_score(y_train, logRegPredTrain)

lrMutTest = sklearn.metrics.mutual_info_score(y_test, logRegPredTest)
lrAccTest = sklearn.metrics.accuracy_score(y_test, logRegPredTest)
lrF1Test = sklearn.metrics.accuracy_score(y_test, logRegPredTest)

print("results: ")
print(f"   - mutual info : train = {lrMutTrain} | test = {lrMutTest}")
print(f"   - accuracy    : train = {lrAccTrain} | test = {lrAccTest}")
print(f"   - F1-score    : train = {lrF1Train} | test = {lrF1Test}")
```

expected output:

```
results:
   - mutual info : train = 0.46165194587854264 | test = 0.465660261510888
```

```
- accuracy    : train = 0.9807060755336617 | test = 0.9796923076923076
- F1-score    : train = 0.9807060755336617 | test = 0.9796923076923076
```

Importance test analysis

Without modifications, the accuracy and F1-score are ~0.98

Removing a single feature had very little impact on the model's efficiency, it dropped ~0.02

The l1 penalty seem to have compensated a bit for the absent feature, it's back at ~0.98 (but the difference is too small to be sure of anything)

Since removing a big feature had almost no impact, i'd say the difference between red and white wine is big enough for a classification to be efficient with any combo of at least a few of the features we have here.

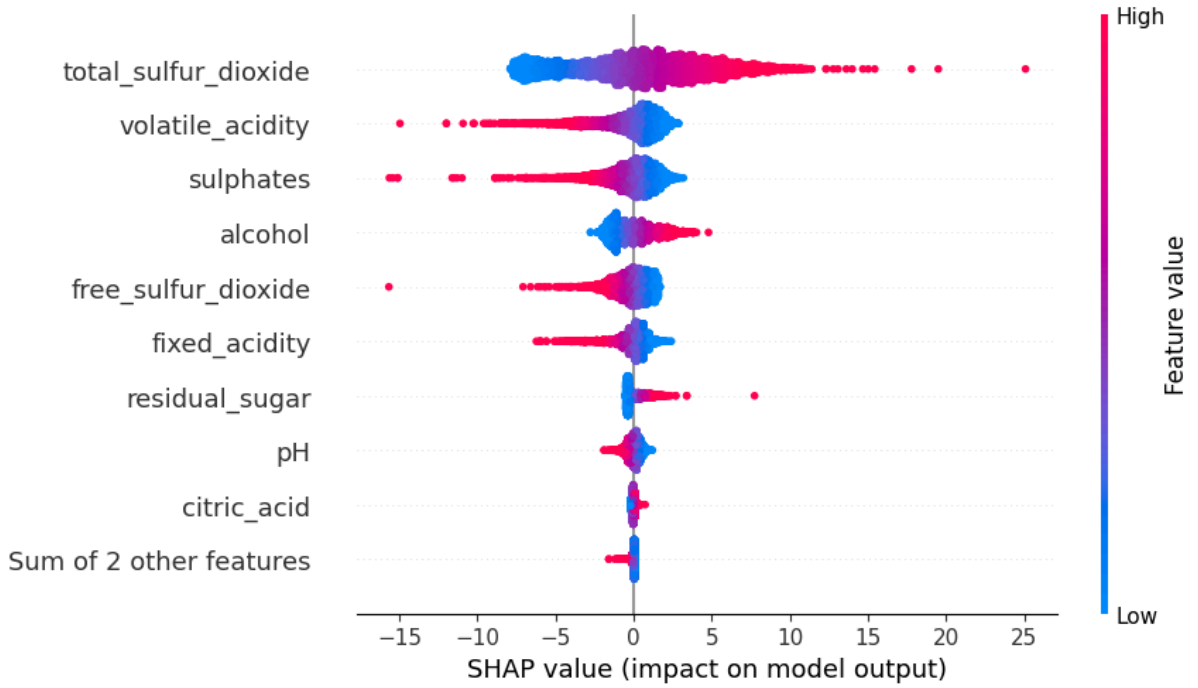
Using Shapley values

SHAP allows us to check feature importance a bit more precisely with out model.

Plotting a beeswarm:

```
# Complete this cell with your code
explainer = KCBakyou.Explainer(bestLogReg, X)
shap_values = explainer(X)
KCBakyou.plots.beeswarm(shap_values)
```

expected output:



According to this graph:

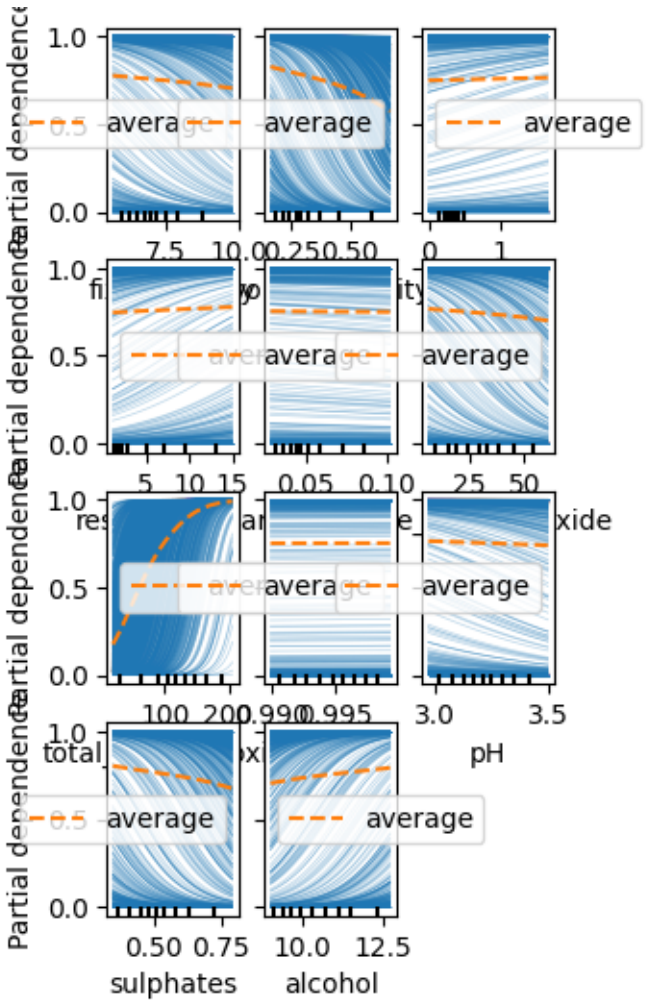
- a red wine has a low total_sulfur_dioxide, a high volatile_acidity, high sulphates, etc.
- a white wine has a high total_sulfur_dioxide, a low volatile_acidity, low sulphates, etc.

We can also check partial dependence for any major correlation between parameter value and output value.

Plotting the Partial dependence

```
# Complete this cell with your code
from sklearn.inspection import PartialDependenceDisplay

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

mlp_disp = PartialDependenceDisplay.from_estimator(
    bestLogReg, X, featureTab, kind="both"
)
```

expected output:

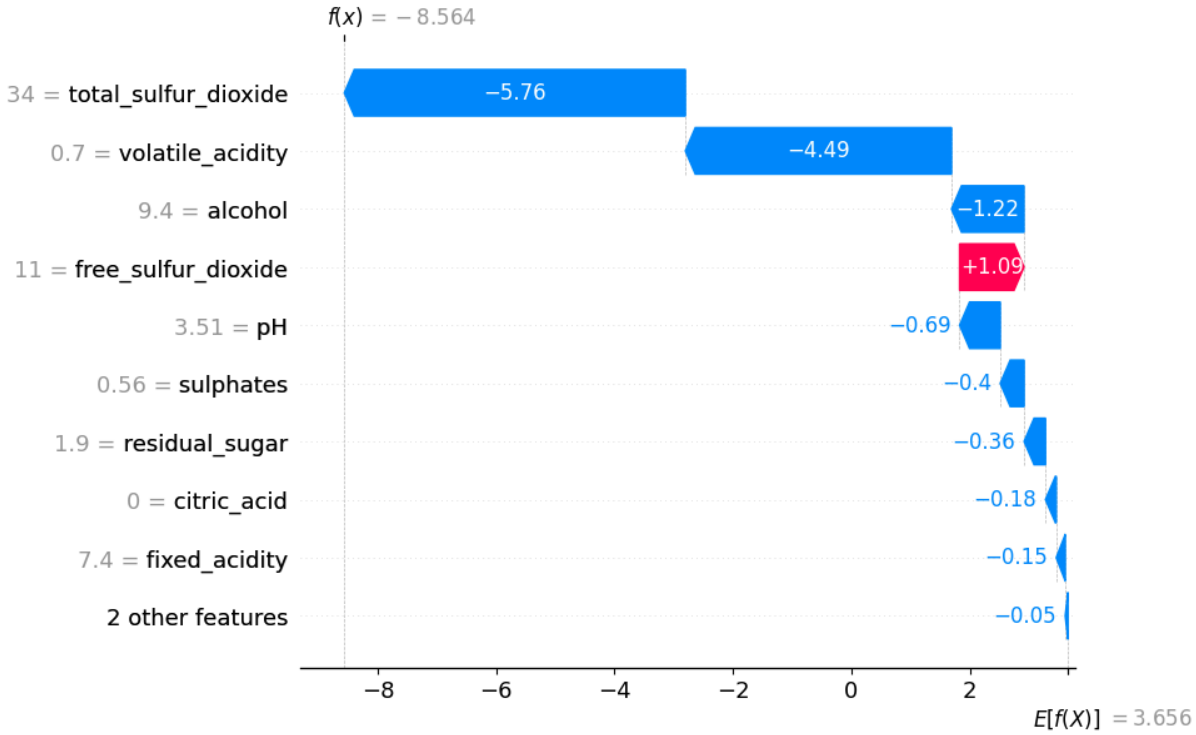


We can also visualize the impact each feature had on a predict with a waterfall:

Plotting a waterfall for a red wine:

```
# red wine (1st wine of the data)
KCBakyou.plots.waterfall(shap_values[0])
```

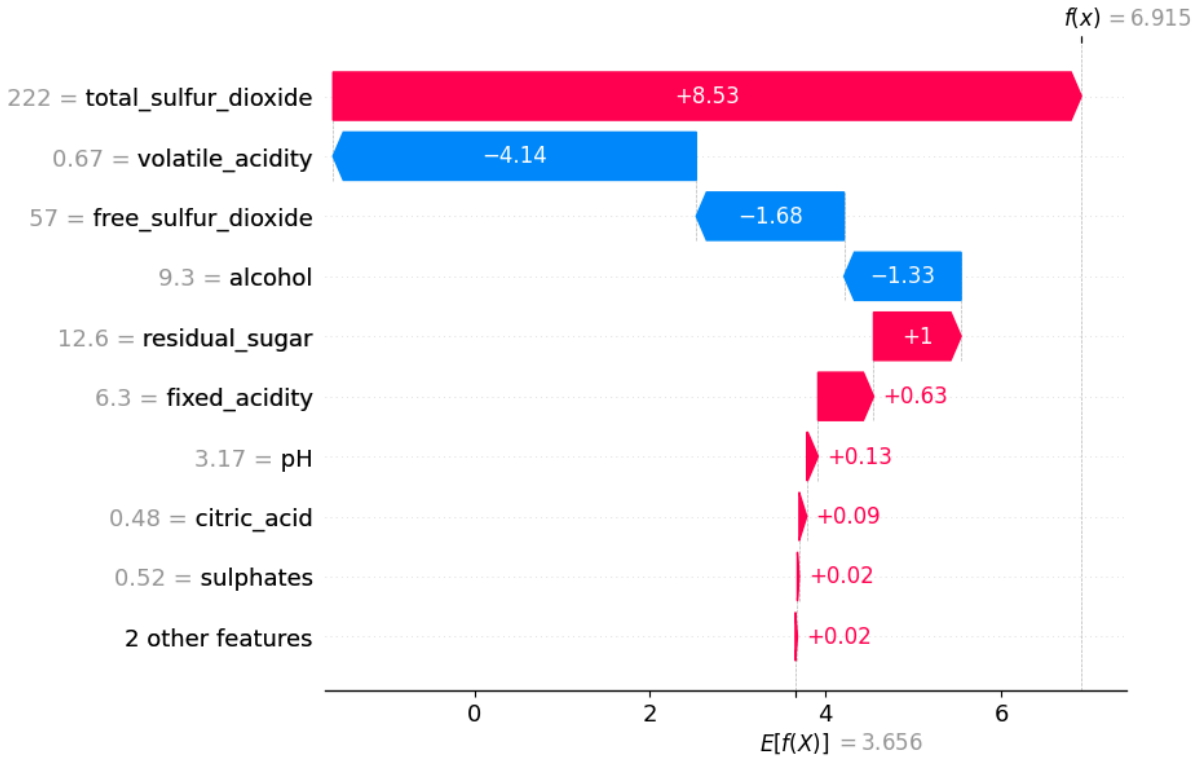
expected output:



Plotting a waterfall for a white wine:

```
# white wine (3000th wine of the data)
KCBakyou.plots.waterfall(shap_values[3000])
```

expected output:



Good/Bad classification

Now for the real exercise, we need to determine if a wine is "good" or "bad". Since our base data only has grades, let's say a quality higher than 6 is good and less is bad.

Adding required data

Adding a column in the y part of the data for "Is the wine good?"

```
# Complete this cell with your code
y["binary_quality"] = np.where(y["quality"] > 6, True, False)
```

One question that we might ask right away is:

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

Creating a new dataframe with y and the wine color:

```
coloredY = pd.concat([y, colors], axis=1)
```

Splitting the coloredY dataframe between red and white wines:

```
RedY = coloredY[coloredY["color"] == "red"]
WhiteY = coloredY[coloredY["color"] == "white"]
```

Displaying the quality values distribution for red wines:

```
RedY.describe()
```

expected output:

```
           quality
count  1599.000000
mean      5.636023
std       0.807569
min       3.000000
25%       5.000000
50%       6.000000
75%       6.000000
max       8.000000
```

Displaying the quality values distribution for white wines:

```
WhiteY.describe()
```

expected output:

```
           quality
count  4898.000000
mean      5.877909
std       0.885639
min       3.000000
25%       5.000000
50%       6.000000
75%       6.000000
max       9.000000
```

The distribution is very similar.

We can also check if the features distribution is similar between good red/white wines and bad red/white wines.

Displaying the mean difference between good wines and bad wines:

```python
# Complete this cell with your code
tabDiff = {
    "fixed_acidity": 0,
    "volatile_acidity": 0,
    "citric_acid": 0,
    "residual_sugar": 0,
    "chlorides": 0,
    "free_sulfur_dioxid": 0,
    "total_sulfur_dioxide": 0,
    "density": 0,
    "pH": 0,
    "sulphates": 0,
    "alcohol": 0,
}

X_good = X[y["binary_quality"]]
X_bad = X[y["binary_quality"] == False]

for iR in X_good:
    # print(f"{iR} : ")
    # print(f"    - Red   : {X_red[iR].mean()}")
    # print(f"    - White : {X_white[iR].mean()}")
    tabDiff[iR] = abs(X_good[iR].mean() - X_bad[iR].mean())

print(f"differences: \n{tabDiff}")
```

expected output:

```
differences:
{
  'fixed_acidity': 0.1613028020054177,
  'volatile_acidity': 0.06284922756580469,
  'citric_acid': 0.019907727942345743,
  'residual_sugar': 0.7660910389232427,
  'chlorides': 0.01426140544319332,
  'free_sulfur_dioxid': 0,
  'total_sulfur_dioxide': 7.285381431576042,
  'density': 0.002078290101621083,
  'pH': 0.01138829182380885,
  'sulphates': 0.012719662943260768,
  'alcohol': 1.171897750359003,
  'free_sulfur_dioxide': 0.6595178624470073
}
```

Displaying the mean difference beween good wines and bad wines but separating the red and white ones:

```
tabDiff = {
    "fixed_acidity": 0,
    "volatile_acidity": 0,
    "citric_acid": 0,
    "residual_sugar": 0,
    "chlorides": 0,
    "free_sulfur_dioxid": 0,
    "total_sulfur_dioxide": 0,
    "density": 0,
    "pH": 0,
    "sulphates": 0,
    "alcohol": 0,
}

X_good_red = X_good[coloredY["color"] == "red"]
X_good_white = X_good[coloredY["color"] == "white"]
X_bad_red = X_bad[coloredY["color"] == "red"]
X_bad_white = X_bad[coloredY["color"] == "white"]

for iR in X_good_red:
    tabDiff[iR] = abs(X_good_red[iR].mean() - X_bad_red[iR].mean())

print(f"red differences: \n{tabDiff}")

for iR in X_good_white:
    tabDiff[iR] = abs(X_good_white[iR].mean() - X_bad_white[iR].mean())

print(f"white differences: \n{tabDiff}")
```

expected output:

```
red differences:
{
  'fixed_acidity': 0.6101739281212701,
  'volatile_acidity': 0.1414924773419941,
  'citric_acid': 0.12209103883372119,
  'residual_sugar': 0.19663564459442284,
  'chlorides': 0.013368310136248146,
  'free_sulfur_dioxid': 0,
  'total_sulfur_dioxide': 13.396416733912645,
  'density': 0.0008288913749523452,
  'pH': 0.025814654511260304,
  'sulphates': 0.0987022414586487,
  'alcohol': 1.2670120109282976,
  'free_sulfur_dioxide': 2.1906473620679314
}

white differences:
{
  'fixed_acidity': 0.16545254997197834,
  'volatile_acidity': 0.01645266304187515,
  'citric_acid': 0.010381645314481769,
  'residual_sugar': 1.4419689401909412,
  'chlorides': 0.009714296951045656,
  'free_sulfur_dioxid': 0,
  'total_sulfur_dioxide': 16.73765080082984,
```

```
  'density': 0.00206154414150439,
  'pH': 0.034285280265861307,
  'sulphates': 0.013137861700767917,
  'alcohol': 1.150806622620287,
  'free_sulfur_dioxide': 0.9668550345600622
}
```

They differ quite a bit, this means that a "good wine" is more difficult to point than a "good red wine", since the color affects which feature is important.

XGB classifier

We are going to try a XGBClassifier, a more complex model, since the problem just got a lot harder.

Function to check for the best parameters in a grid for a XGBCl:

```
def XGBCl(paramGrid, XCl, yCl):
    # create model instance
    xb = XGBClassifier()
    bst = GridSearchCV(xb, paramGrid)
    # fit model
    bst.fit(XCl, yCl)

    return bst
```

Selection of a parameter grid, split of the data and fitting of a XGB model

```
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
}
X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=0.2)
Xcl = X_train
ycl = y_train["binary_quality"]

mod = XGBCl(param_grid, Xcl, ycl)
mod.best_params_

bstMod = XGBClassifier(
    colsample_bytree=mod.best_params_["colsample_bytree"],
    gamma=mod.best_params_["gamma"],
    learning_rate=mod.best_params_["learning_rate"],
    max_depth=mod.best_params_["max_depth"],
    min_child_weight=mod.best_params_["min_child_weight"],
    n_estimators=mod.best_params_["n_estimators"],
    subsample=mod.best_params_["subsample"],
)
bstMod.fit(Xcl, ycl)
```

Evaluation of the model:

```
f1XGBTe = f1_score(y_test["binary_quality"], bstMod.predict(X_test))
f1XGBTr = f1_score(y_train["binary_quality"], bstMod.predict(X_train))
accXGBTe = accuracy_score(y_test["binary_quality"], bstMod.predict(X_test))
accXGBTr = accuracy_score(y_train["binary_quality"], bstMod.predict(X_train))

print("Resultats:")
print("accuracy: ")
print("   - Train: ", accXGBTr, " | Test: ", accXGBTe)
print("f1 score: ")
print("   - Train: ", f1XGBTr, " | Test: ", f1XGBTe)
```

expected output:

```
Resultats:
accuracy:
   - Train:  0.9270733115258804  | Test:  0.8761538461538462
f1 score:
   - Train:  0.793685356559608  | Test:  0.6139088729016786
```

The model seems to overfit a bit, the difference between train and test is significant.

Interpretability with SHAP

We can once again dig a bit further into the model with SHAP or by adding a parameter in the model.

Creating variations of the model with “importance_type” data collection:

```
modGain = XGBClassifier(
    colsample_bytree=mod.best_params_["colsample_bytree"],
    gamma=mod.best_params_["gamma"],
    learning_rate=mod.best_params_["learning_rate"],
    max_depth=mod.best_params_["max_depth"],
    min_child_weight=mod.best_params_["min_child_weight"],
    n_estimators=mod.best_params_["n_estimators"],
    subsample=mod.best_params_["subsample"],
    importance_type="gain",
)
modGain.fit(Xcl, ycl)

modCover = XGBClassifier(
    colsample_bytree=mod.best_params_["colsample_bytree"],
    gamma=mod.best_params_["gamma"],
    learning_rate=mod.best_params_["learning_rate"],
    max_depth=mod.best_params_["max_depth"],
    min_child_weight=mod.best_params_["min_child_weight"],
    n_estimators=mod.best_params_["n_estimators"],
    subsample=mod.best_params_["subsample"],
    importance_type="cover",
)
modCover.fit(Xcl, ycl)
```

Sorting and displaying the feature importances (gain):

```
importances = modGain.feature_importances_
impTab = pd.Series(importances, index=X.columns)
impTab.sort_values(ascending=False)
```

expected output:

```
alcohol                 0.292655
volatile_acidity        0.097566
residual_sugar          0.072743
density                 0.072124
free_sulfur_dioxide     0.070072
fixed_acidity           0.069551
sulphates               0.068419
citric_acid             0.066724
chlorides               0.065032
pH                      0.063567
total_sulfur_dioxide    0.061545
dtype: float32
```

Sorting and displaying the feature importance (cover):

```
importances = modCover.feature_importances_
impTab = pd.Series(importances, index=X.columns)
impTab.sort_values(ascending=False)
```

```
alcohol                 0.144069
volatile_acidity        0.103137
residual_sugar          0.094013
total_sulfur_dioxide    0.090722
chlorides               0.089383
pH                      0.088787
fixed_acidity           0.085197
density                 0.082783
free_sulfur_dioxide     0.078339
citric_acid             0.077967
sulphates               0.065603
dtype: float32
```

We can also obtain data on our model with shap values:

```
tab = TreeExplainer(bstMod).shap_values(X_test, y_test)
df = pd.DataFrame(
    tab,
    columns=[
        "alcohol",
        "volatile_acidity",
        "citric_acid",
        "sulphates",
        "free_sulfur_dioxide",
        "residual_sugar",
        "density",
        "pH",
        "fixed_acidity",
        "chlorides",
        "total_sulfur_dioxide",
    ],
)
df.mean().sort_values(ascending=False)
```

expected output:

```
chlorides              -0.019338
alcohol                -0.021077
residual_sugar         -0.030848
fixed_acidity          -0.035930
sulphates              -0.048629
citric_acid            -0.077685
free_sulfur_dioxide    -0.099011
volatile_acidity       -0.104322
density                -0.104955
pH                     -0.131129
total_sulfur_dioxide   -0.268317
dtype: float32
```

- Use SHAP's `TreeExplainer` to compute feature importance (Shapley values). Do you see any difference with XGBoost's feature importances?

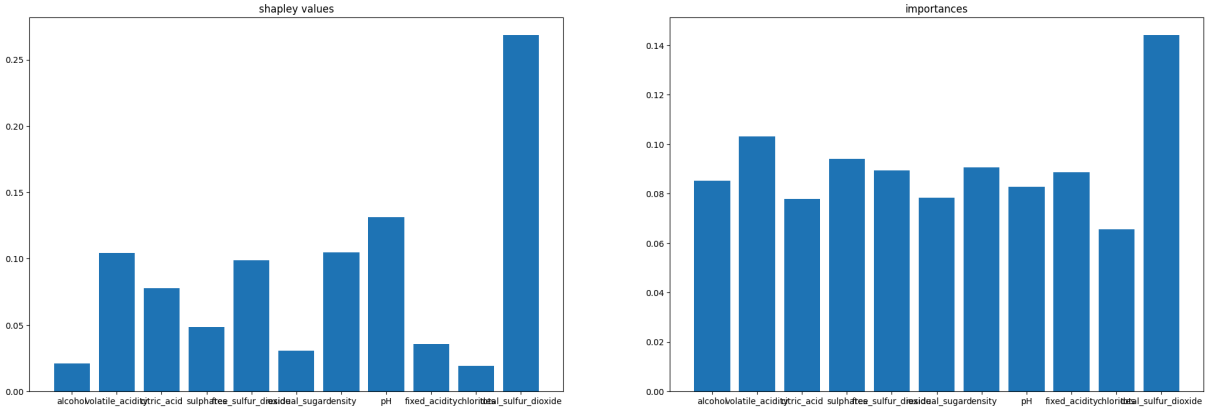
There are some differences between the two sources. They agree on some points, but have very different opinions on the features importance. This is due to a few factor, but mainly that they don't get their analyse from the same data, one uses the model fitting, so the creation of the model, while the other uses the test data, so after the model has been created.

We can produce a few more graphs to get more intel.

Plotting features importance from shapley values and importances

```
fig, axs = plt.subplots(1, 2, figsize=(25, 8))

axs[0].bar(df.columns, abs(df.mean()))
axs[0].set_title("shapley values")

axs[1].bar(df.columns, impTab)
axs[1].set_title("importances")
```

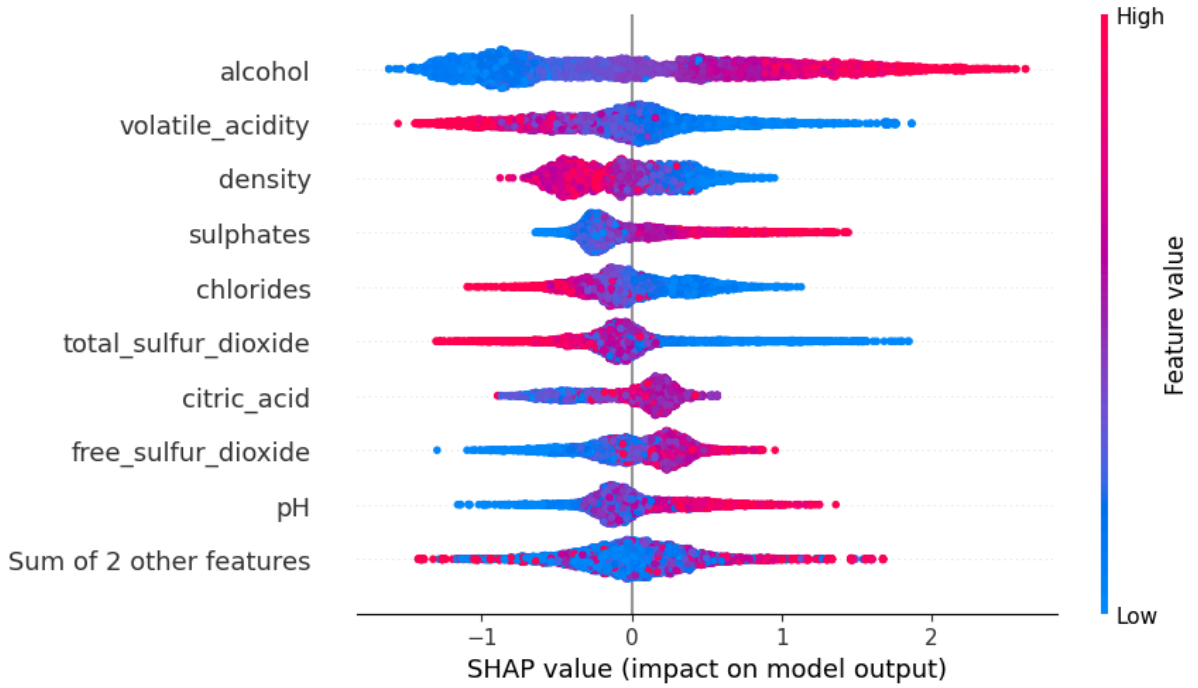
expected output:



Plotting a beeswarm:

```
# Complete this cell with your code
explainer = KCBakyou.Explainer(bstMod, X)
shap_values = explainer(X)
KCBakyou.plots.beeswarm(shap_values)
```

expected output:



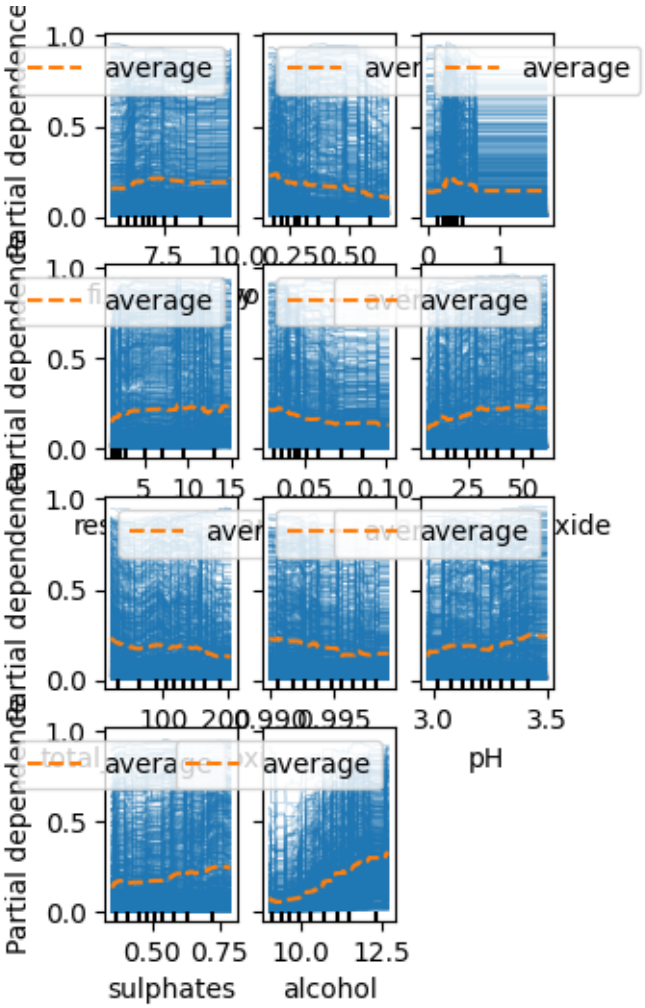
The two features that all the graphs and data seem to agree make good wine are a low volatile acidity and a low total sulfur dioxide.

- 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?

]

Plotting partial dependence plots:

```
# Complete this cell with your code
from sklearn.inspection import PartialDependenceDisplay

mlp_disp = PartialDependenceDisplay.from_estimator(bstMod, X, X.columns,
kind="both")
```



expected output:

All the lines are pretty flat, except alcohol, there is no high dependence. I would have hoped for volatile acidity and total sulfur dioxide to show a bit of a curve, since my previous results suggested that they were more important for the decision..

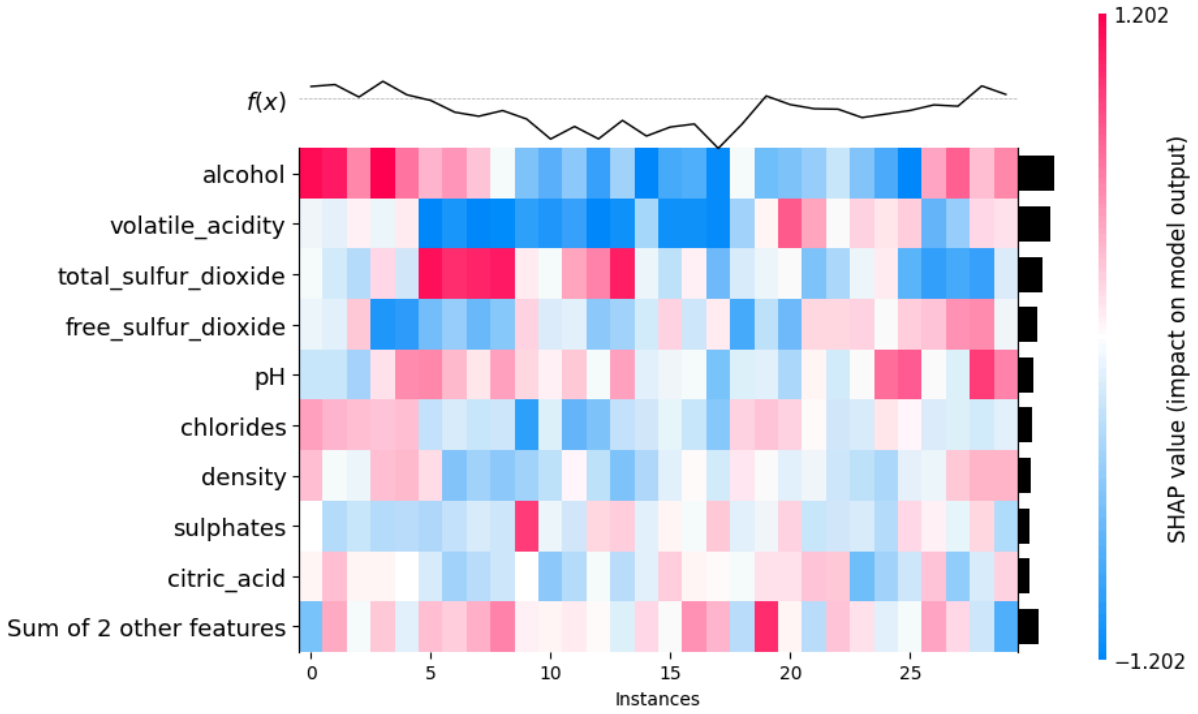
Analyze a few bad wines, and try to see how to make them better

The whole goal of this lab was to try and improve overall quality of the wine by telling why it's good or bad, so let's check the very bad ones.

Isolating the worst wines and printing a heatmap with their shap values:

```
# Complete this cell with your code
import shap


X_worst = X[y["quality"] == 3]

explainer = shap.Explainer(bstMod, X)
shap_values = explainer(X_worst)

shap.plots.heatmap(shap_values)
```

expected output:



Wrap-up and conclusion

Key findings

- This is a hard classification to do
- Good red and white wines are very different
- All feature seem important, removing some didn't affect efficiency

Recommandations

The results lean toward:

- low volatile acidity
- a low total sulfur dioxide
- high alcohol

Confidence in the results

Low, the moderate efficiency of the overall model and the fact that all features have their importance make it pretty difficult to point out a clear recommandation.

Correlation and causality

The method we used here is to try and guess what a good wine is through correlation. We check all good wines, see if there are common characteristics on all of them that could be the cause of the good taste. But ultimately, we have no way to know for sure. Maybe the "good wine characteristics" we found were just a coincidence, maybe the definition of a good wine is somewhere else, we don't know if the "good wine characteristics" is what **causes** the wine to be good. That is the difference between correlation and causality and the main reason why the data shown here should be taken cautiously.