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.

```
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.

```
# All the imports for the notebook to work
import pandas as pd
import seaborn as sns
import math
import matplotlib.pyplot as plt
from sklearn.decomposition import PCA
from sklearn.discriminant_analysis import StandardScaler
from sklearn.linear_model import LogisticRegression
from sklearn.model_selection import train_test_split, GridSearchCV
from sklearn.calibration import LabelEncoder
from sklearn.metrics import classification_report
from sklearn.cluster import KMeans
```

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.

```
# Fetching from CSV as it's easier for me
wine_red = pd.read_csv("./data/winequality-red.csv", sep=";")
wine_white = pd.read_csv("./data/winequality-white.csv", sep=";")
```

```
# Adding a color column
wine_red["color"] = "red"
wine_white["color"] = "white"

# Base data should not be modified
base_data = pd.concat([wine_red, wine_white], axis=0, ignore_index=True)

# This is to avoid aving red - white ordered already...
base_data = base_data.sample(frac=1, random_state=42).reset_index(drop=True)
base_data
```

```
      fixed acidity  volatile acidity  citric acid  residual sugar  chlorides  \
0               7.0              0.17         0.74           12.80      0.045
1               7.7              0.64         0.21            2.20      0.077
2               6.8              0.39         0.34            7.40      0.020
3               6.3              0.28         0.47           11.20      0.040
4               7.4              0.35         0.20           13.90      0.054
...             ...               ...          ...             ...        ...
6492            7.6              0.32         0.58           16.75      0.050
6493            5.6              0.28         0.27            3.90      0.043
6494            6.4              0.37         0.20            5.60      0.117
6495            6.5              0.26         0.50            8.00      0.051
6496            7.2              0.62         0.06            2.70      0.077

      free sulfur dioxide  total sulfur dioxide  density    pH  sulphates  \
0                    24.0                 126.0  0.99420  3.26       0.38
1                    32.0                 133.0  0.99560  3.27       0.45
2                    38.0                 133.0  0.99212  3.18       0.44
3                    61.0                 183.0  0.99592  3.12       0.51
4                    63.0                 229.0  0.99888  3.11       0.50
...                   ...                   ...      ...   ...        ...
6492                 43.0                 163.0  0.99990  3.15       0.54
6493                 52.0                 158.0  0.99202  3.35       0.44
6494                 61.0                 183.0  0.99459  3.24       0.43
6495                 46.0                 197.0  0.99536  3.18       0.47
6496                 15.0                  85.0  0.99746  3.51       0.54

      alcohol  quality  color
0        12.2        8  white
1         9.9        5    red
2        12.0        7  white
3         9.5        6  white
4         8.9        6  white
...       ...      ...    ...
6492      9.2        5  white
6493     10.7        7  white
6494      9.5        5  white
6495      9.5        5  white
6496      9.5        5    red

[6497 rows x 13 columns]
```

```
target = "color"
features = [x for x in base_data.columns.values if x != target]
x_base: pd.DataFrame = base_data[features]
y_base: pd.DataFrame = base_data[target]
```

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.

```
# Complete this cell with your code
x_base.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      quality
count  6497.000000  6497.000000  6497.000000  6497.000000
mean      3.218501     0.531268    10.491801     5.818378
std       0.160787     0.148806     1.192712     0.873255
min       2.720000     0.220000     8.000000     3.000000
25%       3.110000     0.430000     9.500000     5.000000
50%       3.210000     0.510000    10.300000     6.000000
75%       3.320000     0.600000    11.300000     6.000000
max       4.010000     2.000000    14.900000     9.000000
```

We can see that there is no 'hole' in the data. No NaN or null values

```
y_base.describe()
```

```
count      6497
unique        2
top       white
freq       4898
Name: color, dtype: object
```

As we can see, the data is unbalanced, as there is way more white than red wine.

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.

```
red_wine = base_data[base_data["color"] == "red"]
white_wine = base_data[base_data["color"] == "white"]
```

```
red_wine.describe()
```

```
       fixed acidity  volatile acidity  citric acid  residual sugar  \
count    1599.000000       1599.000000  1599.000000     1599.000000
mean        8.319637          0.527821     0.270976        2.538806
std         1.741096          0.179060     0.194801        1.409928
min         4.600000          0.120000     0.000000        0.900000
25%         7.100000          0.390000     0.090000        1.900000
50%         7.900000          0.520000     0.260000        2.200000
75%         9.200000          0.640000     0.420000        2.600000
max        15.900000          1.580000     1.000000       15.500000

         chlorides  free sulfur dioxide  total sulfur dioxide      density  \
count  1599.000000          1599.000000           1599.000000  1599.000000
mean      0.087467            15.874922             46.467792     0.996747
std       0.047065            10.460157             32.895324     0.001887
min       0.012000             1.000000              6.000000     0.990070
25%       0.070000             7.000000             22.000000     0.995600
50%       0.079000            14.000000             38.000000     0.996750
75%       0.090000            21.000000             62.000000     0.997835
max       0.611000            72.000000            289.000000     1.003690

                pH    sulphates      alcohol      quality
count  1599.000000  1599.000000  1599.000000  1599.000000
mean      3.311113     0.658149    10.422983     5.636023
std       0.154386     0.169507     1.065668     0.807569
min       2.740000     0.330000     8.400000     3.000000
25%       3.210000     0.550000     9.500000     5.000000
50%       3.310000     0.620000    10.200000     6.000000
75%       3.400000     0.730000    11.100000     6.000000
max       4.010000     2.000000    14.900000     8.000000
```

```
white_wine.describe()
```

```
       fixed acidity  volatile acidity  citric acid  residual sugar  \
count    4898.000000       4898.000000  4898.000000     4898.000000
mean        6.854788          0.278241     0.334192        6.391415
std         0.843868          0.100795     0.121020        5.072058
min         3.800000          0.080000     0.000000        0.600000
25%         6.300000          0.210000     0.270000        1.700000
50%         6.800000          0.260000     0.320000        5.200000
75%         7.300000          0.320000     0.390000        9.900000
max        14.200000          1.100000     1.660000       65.800000

         chlorides  free sulfur dioxide  total sulfur dioxide      density  \
count  4898.000000          4898.000000           4898.000000  4898.000000
mean      0.045772            35.308085            138.360657     0.994027
std       0.021848            17.007137             42.498065     0.002991
min       0.009000             2.000000              9.000000     0.987110
25%       0.036000            23.000000            108.000000     0.991723
50%       0.043000            34.000000            134.000000     0.993740
75%       0.050000            46.000000            167.000000     0.996100
max       0.346000           289.000000            440.000000     1.038980

                pH    sulphates      alcohol      quality
count  4898.000000  4898.000000  4898.000000  4898.000000
mean      3.188267     0.489847    10.514267     5.877909
std       0.151001     0.114126     1.230621     0.885639
```

```
min       2.720000     0.220000     8.000000     3.000000
25%       3.090000     0.410000     9.500000     5.000000
50%       3.180000     0.470000    10.400000     6.000000
75%       3.280000     0.550000    11.400000     6.000000
max       3.820000     1.080000    14.200000     9.000000
```

```
def getSSMD(frame1: pd.DataFrame, frame2: pd.DataFrame):
    ssmd_values = {}
    d1 = frame1.describe()
    d2 = frame2.describe()
    for c in d1.columns.values:
        u1 = d1[c]["mean"]
        u2 = d2[c]["mean"]
        o1 = d1[c]["std"]
        o2 = d2[c]["std"]
        ssmd_values[c] = (u1 - u2) / (math.sqrt(math.pow(o1, 2) + math.pow(o2, 2)))
    return ssmd_values

ssmd = getSSMD(red_wine, white_wine)
ssmd
```

```
{'fixed acidity': 0.7570984913882014,
 'volatile acidity': 1.2146180859422453,
 'citric acid': -0.2756520281549347,
 'residual sugar': -0.7318262377213726,
 'chlorides': 0.8035252800557684,
 'free sulfur dioxide': -0.9732927083649252,
 'total sulfur dioxide': -1.7098935451586068,
 'density': 0.7689026646491103,
 'pH': 0.5688537900809766,
 'sulphates': 0.8236123900161842,
 'alcohol': -0.05607448758109532,
 'quality': -0.20181608588284952}
```

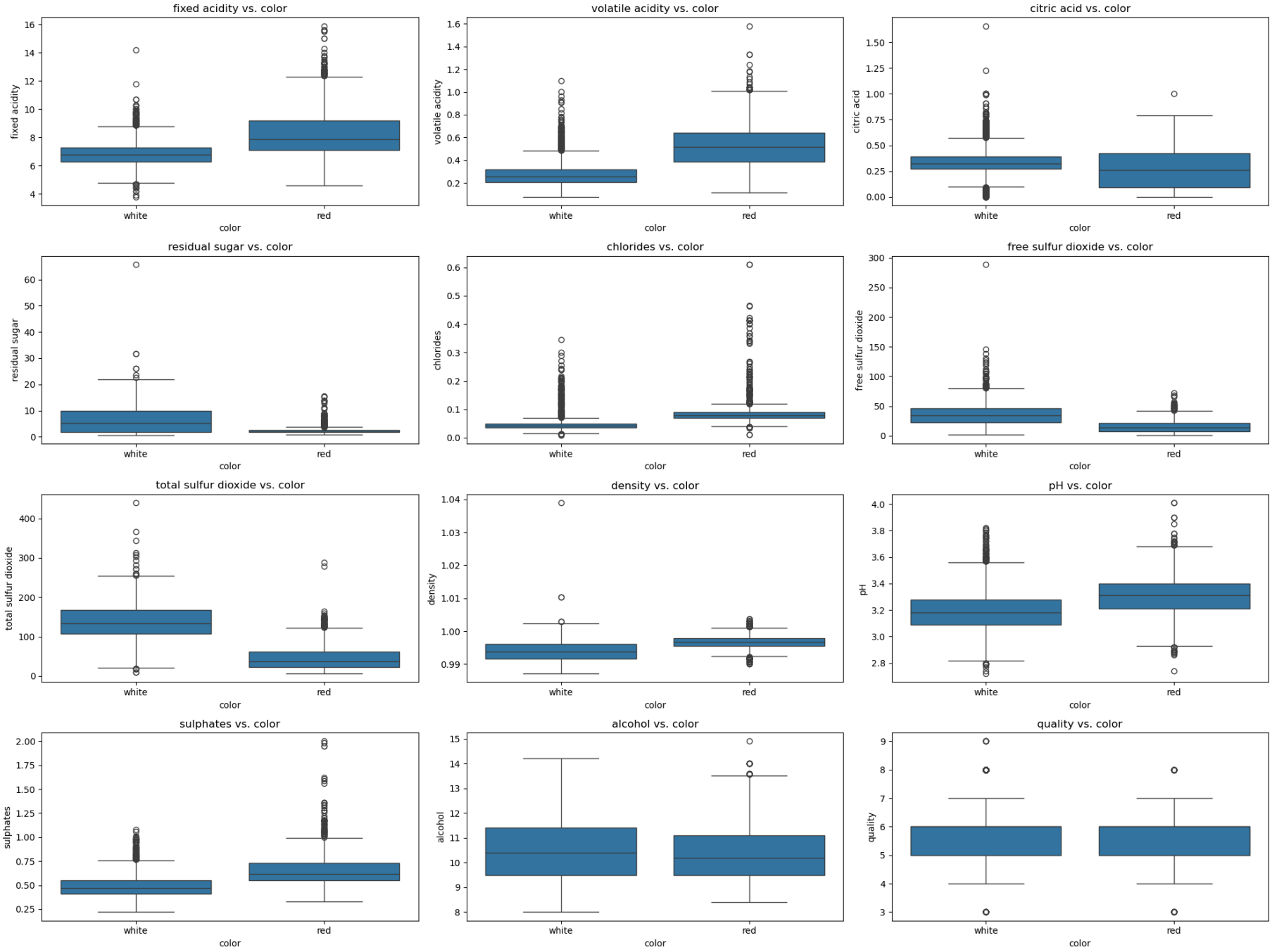
Here, we can already have an idea of which features will be significants to split the data. As the more differences there is the more the data is splittable easily per feature.

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?

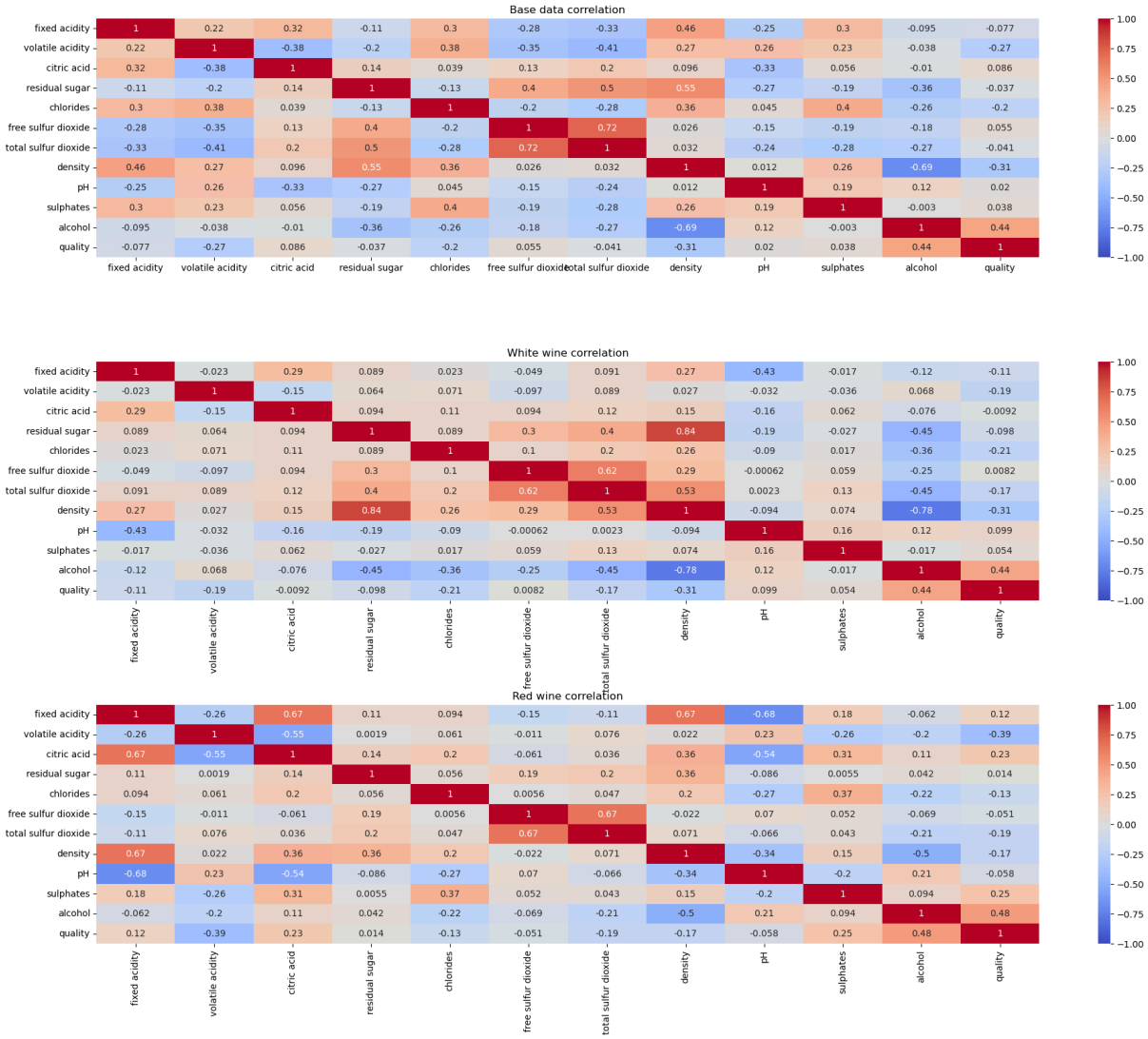
```
# Complete this cell with your code
# Set up the plot
plt.figure(figsize=(20, 15))

# Create violin plots for each feature
for i, feature in enumerate(features, 1):
    plt.subplot(4, 3, i)
    sns.boxplot(x="color", y=feature, data=base_data)
    plt.title(f"{feature} vs. color")
    plt.xlabel("color")
    plt.ylabel(feature)
```

```
plt.tight_layout()
plt.show()
```


fixed acidity vs. color
fixed acidity
color
white
red
volatile acidity vs. color
volatile acidity
citric acid vs. color
citric acid
residual sugar vs. color
residual sugar
chlorides vs. color
chlorides
free sulfur dioxide vs. color
free sulfur dioxide
total sulfur dioxide vs. color
total sulfur dioxide
density vs. color
density
pH vs. color
pH
sulphates vs. color
sulphates
alcohol vs. color
alcohol
quality vs. color
quality

On those graphs, we can see some features that might be used to split the data. We can see some that are unsplittable, as the quality..

```
plt.figure(figsize=(20, 15))


# For base data
plt.subplot(3, 1, 1)
plt.tight_layout()
sns.heatmap(
    base_data[features].corr(),
    annot=True,
    cmap="coolwarm",
    vmin=-1,
    vmax=1,
    center=0,
)
plt.title("Base data correlation")

# For white wine
plt.subplot(3, 1, 2)
plt.tight_layout()
sns.heatmap(
    white_wine[features].corr(),
    annot=True,
    cmap="coolwarm",
    vmin=-1,
    vmax=1,
    center=0,
)
plt.title("White wine correlation")

# For red wine
plt.subplot(3, 1, 3)
plt.tight_layout()
sns.heatmap(
    red_wine[features].corr(),
    annot=True,
    cmap="coolwarm",
    vmin=-1,
    vmax=1,
    center=0,
)
plt.title("Red wine correlation")

# Show the plot
plt.show()
```

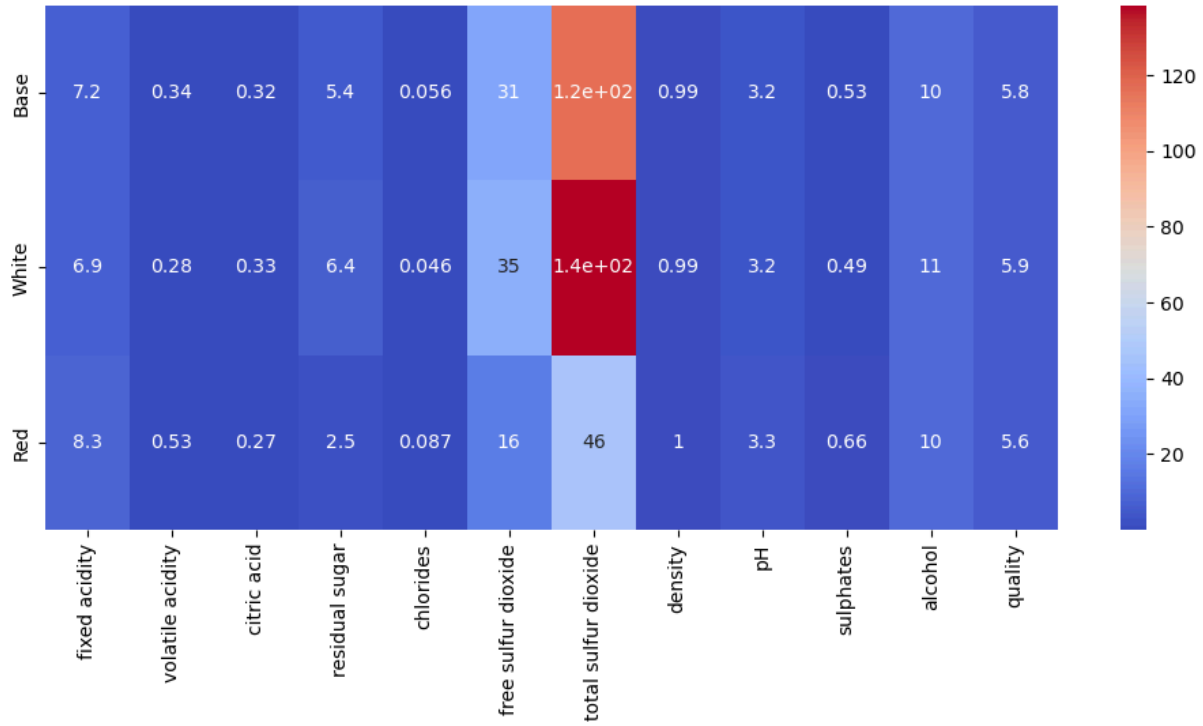


Here, we can observe that some correlations are present in both red and white wines, but not at the same level. and some are completly absent/inverted

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?

```
# Complete this cell with your code
base_features_means = base_data[features].mean()
white_features_means = white_wine[features].mean()
red_features_means = red_wine[features].mean()
ylbl = ["Base", "White", "Red"]
plt.figure(figsize=(12, 5))
sns.heatmap(
    [base_features_means, white_features_means, red_features_means],
    annot=True,
    cmap="coolwarm",
    xticklabels=features,
    yticklabels=ylbl,
)
plt.show()
```



The easiest way seems to be on the total sulfur dioxide. As the values differenciate greatly between the two

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?

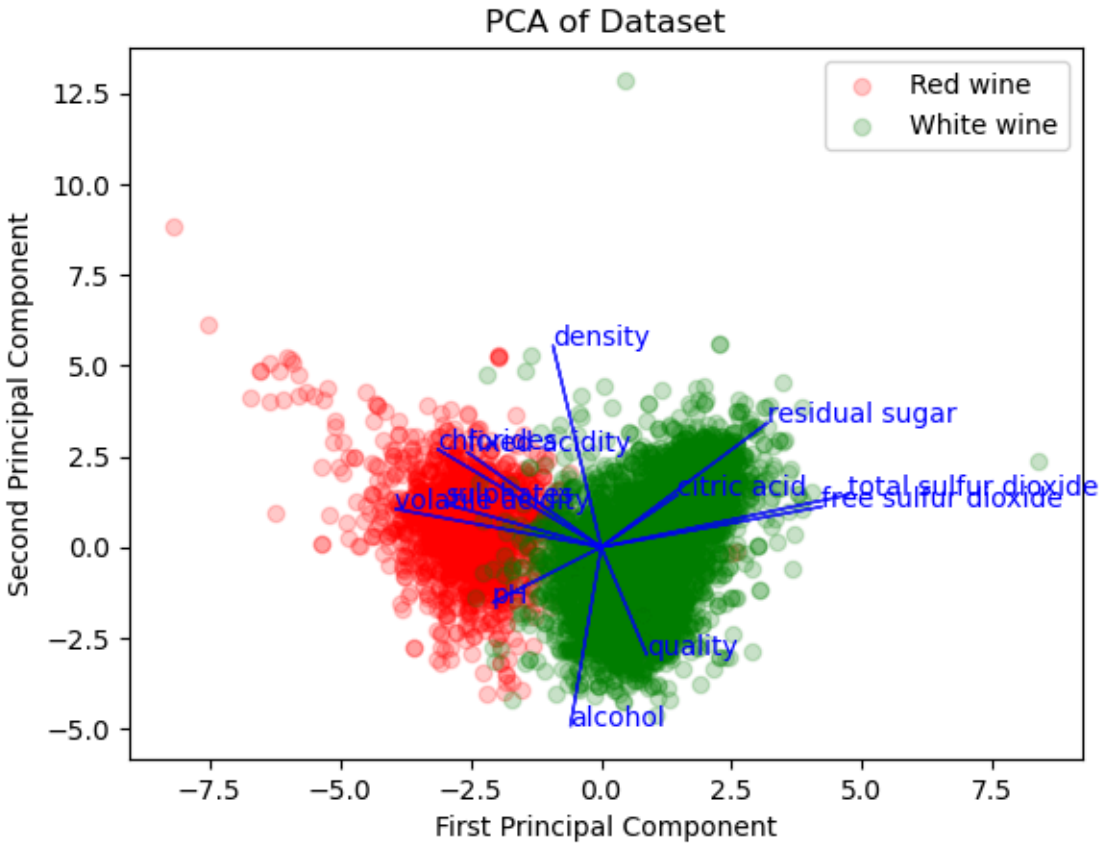
Project the unit vectors that correspond to each vector onto the principal components, using the same transformation. What does it tell you about the relative feature importance? Does it match the observations you made previously?

```
# Complete this cell with your code


scaler = StandardScaler()
x_scaled = scaler.fit_transform(x_base)

pca = PCA(n_components=2)
x_pca = pca.fit_transform(x_scaled)
pca_df = pd.DataFrame(data=x_pca, columns=["PC1", "PC2"])

pca_df["color"] = y_base.reset_index(drop=True)

components = list(zip(pca.components_[0], pca.components_[1]))
components
```

```
[(-0.2569287331108535, 0.26184306204602015),
 (-0.39493117944046174, 0.10519825134119526),
 (0.14646061066301436, 0.1440934849469867),
 (0.3189051914749266, 0.34258496764107266),
 (-0.3134499396675332, 0.26977009551276876),
 (0.4226913715672136, 0.1111787805638863),
 (0.4744196843566576, 0.1439475285736659),
```

```
 (-0.09243753243272002, 0.5549204739711832),
 (-0.20806956645989705, -0.15292185359766805),
 (-0.2998519160898691, 0.11963420329954372),
 (-0.05892408274769738, -0.4927274740495645),
 (0.08747570978774036, -0.2966009063197228)]
```

```
plt.figure()
plt.scatter(
    pca_df[pca_df["color"] == "red"]["PC1"],
    pca_df[pca_df["color"] == "red"]["PC2"],
    c="red",
    alpha=0.2,
)
plt.scatter(
    pca_df[pca_df["color"] == "white"]["PC1"],
    pca_df[pca_df["color"] == "white"]["PC2"],
    c="green",
    alpha=0.2,
)
ARROW_SCALE = 10
for i, (x, y) in enumerate(components):
    currX = x * ARROW_SCALE
    currY = y * ARROW_SCALE
    plt.arrow(0, 0, currX, currY, color="b", alpha=0.8)
    plt.text(currX, currY, base_data.columns.values[i], color="b")
plt.xlabel("First Principal Component")
plt.ylabel("Second Principal Component")
plt.legend(["Red wine", "White wine"])
plt.title("PCA of Dataset")
plt.show()
```



As we can see, the PCA keeps our groups well separated. This means that there is a real separation available in the data.

Cluster the data in 2-dimensional space

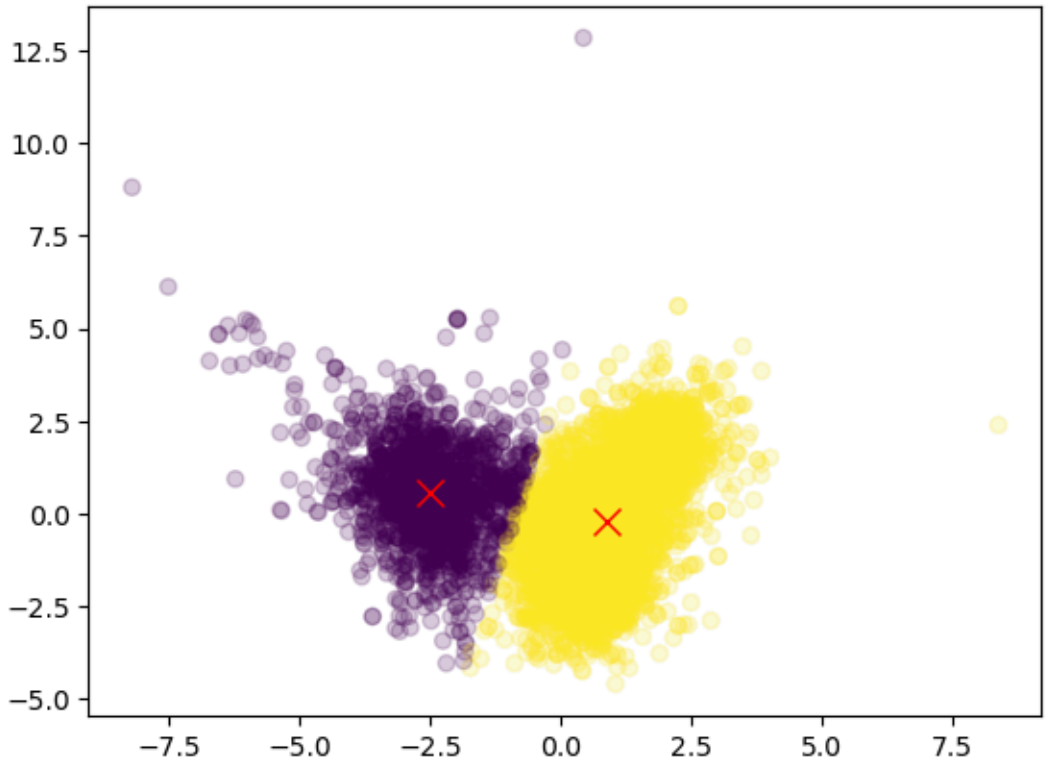
Use k-means to cluster the data into 2 clusters and plot the same view as before, but with a coloring that corresponds to the cluster memberships.

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_pca = KMeans(n_clusters=2, random_state=0)
kmeans_pca.fit(pca_df[["PC1", "PC2"]])
kmeans_pca.labels_
```

```
array([1, 0, 1, ..., 1, 1, 0], dtype=int32)
```

```
plt.scatter(
    pca_df["PC1"], pca_df["PC2"], c=kmeans_pca.labels_, cmap="viridis", alpha=0.2
)
plt.scatter(
    kmeans_pca.cluster_centers_[:, 0],
    kmeans_pca.cluster_centers_[:, 1],
    marker="x",
    s=100,
    linewidths=1,
    color="r",
)
plt.show()
```



As we ca see, the kmeans, wihtout any tweaking, is able so seperate the red from the white wines with a pretty good score.

```
lblEncoder = LabelEncoder()
lblEncoder.fit(["red", "white"])
```

```
# Or we can encore the [0,1,0...] to ["white", "red", "white"..] to match the pca_df
y_pred_pca = lblEncoder.inverse_transform(kmeans_pca.labels_)
print(classification_report(pca_df["color"], y_pred_pca))
```

```
              precision    recall  f1-score   support

         red       0.92      0.98      0.95      1599
       white       0.99      0.97      0.98      4898

    accuracy                           0.98      6497
   macro avg       0.96      0.98      0.97      6497
weighted avg       0.98      0.98      0.98      6497
```

```
kmeans = KMeans(n_clusters=2, random_state=0)
kmeans.fit(x_base)
```

```
y_pred_pca = []
for x in kmeans.labels_:
    if x == 0:
        y_pred_pca.append("red")
    else:
        y_pred_pca.append("white")
print(classification_report(y_base, y_pred_pca))
```

```
              precision    recall  f1-score   support

         red       0.54      0.95      0.69      1599
```

```
       white       0.98      0.74      0.84      4898

    accuracy                           0.79      6497
   macro avg       0.76      0.84      0.77      6497
weighted avg       0.87      0.79      0.80      6497
```

We can see that the KMeans works better after the PCA, as the non important features have been removed. We can see too that the precision on the red wine is less good. This is probably due to the imbalance of our data

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_base, y_base, train_size=0.8, random_state=42
)
```

```
logreg = LogisticRegression()

paramsGrid = {
    "C": [0.01, 0.1, 1, 10, 50, 75, 100, 200],
}

scaler = StandardScaler()
lblEncoder2 = LabelEncoder()
y_train_encoded = lblEncoder2.fit_transform(y_train)
x_train_scaled = scaler.fit_transform(x_train)

cv = GridSearchCV(logreg, paramsGrid, scoring="f1")
cv.fit(x_train_scaled, y_train_encoded)
print(f"Best params were {cv.best_params_}")
print(f"Best score is {cv.best_score_}")
bestModel = cv.best_estimator_
```

```
Best params were {'C': 50}
Best score is 0.9960368560655614
```

```
y_predict = bestModel.predict(scaler.transform(x_test))

print(
    classification_report(
        y_true=y_test, y_pred=lblEncoder2.inverse_transform(y_predict)
    )
)
```

```
              precision    recall  f1-score   support

         red       0.99      0.98      0.99       309
       white       0.99      1.00      1.00       991

    accuracy                           0.99      1300
```

```
   macro avg       0.99      0.99      0.99      1300
weighted avg       0.99      0.99      0.99      1300
```

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?

```
# Complete this cell with your code
for i, x in enumerate(bestModel.coef_[0]):
    print(f"{features[i]} : {x}")
```

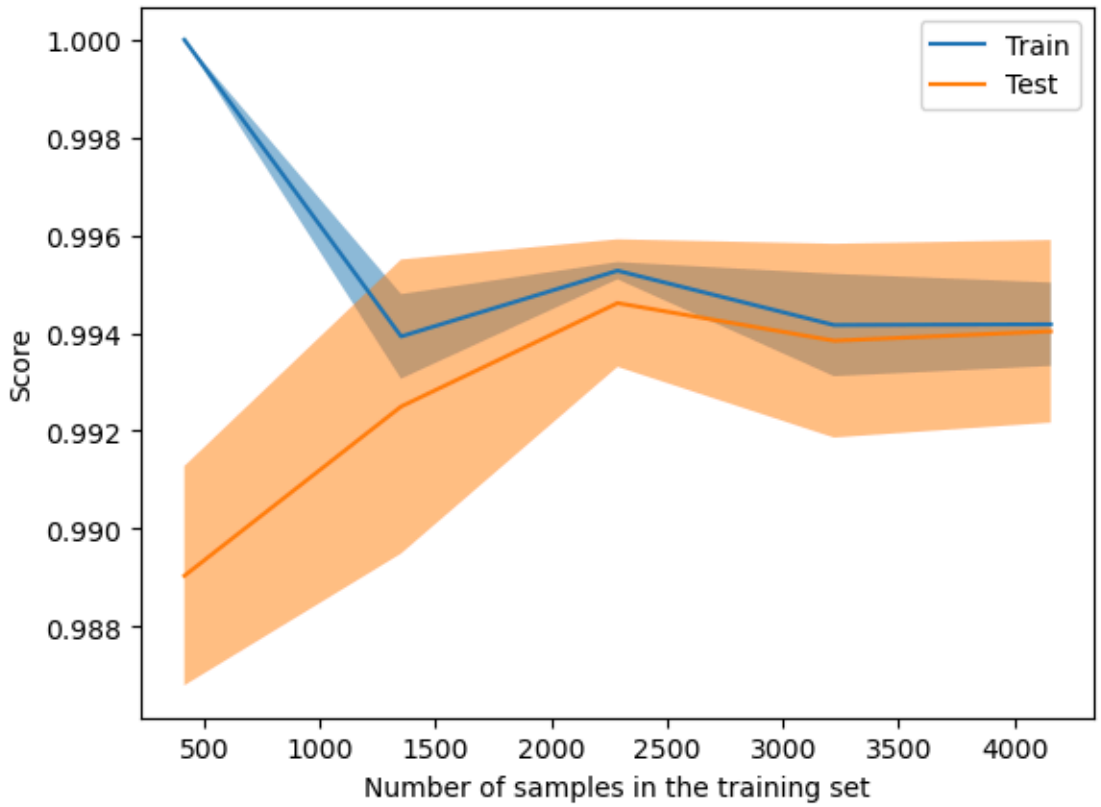
```
fixed acidity : 0.007534354995156941
volatile acidity : -1.269163700765758
citric acid : 0.4314376717282913
residual sugar : 4.9440689288552315
chlorides : -0.8477166330231628
free sulfur dioxide : -0.8990804769560243
total sulfur dioxide : 2.7851187309232572
density : -5.02816765131531
pH : 0.130666048396102
sulphates : -0.5069419267433969
alcohol : -1.7964356607824754
quality : -0.45772261836563544
```

It is compatible with what we saw on the plots on the analysis. The one that suprise me, is the density. It is higher than I expected.

It may be due to the data imbalance in the first place...

```
from sklearn.model_selection import LearningCurveDisplay


LearningCurveDisplay.from_estimator(
    bestModel, x_train_scaled, y_train_encoded, n_jobs=-1
)
```

```
<sklearn.model_selection._plot.LearningCurveDisplay at 0x7f17e78929b0>
```



This graph shows us that we may encounter overfitting, but it's not very clear. As the incertitude is quite big compared to the percentage changes

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?

```
# Complete this cell with your code
def modelWithoutDens():
    features_without_dens = [x for x in features if x != "density"]
    logreg = LogisticRegression()
    paramsGrid = {
        "C": [0.01, 0.1, 1, 10, 50, 75, 100, 200],
    }
    x_train, x_test, y_train, y_test = train_test_split(
        x_base[features_without_dens], y_base, train_size=0.6
    )
    scaler = StandardScaler()
    lblEncoder = LabelEncoder()
    y_train_encoded = lblEncoder.fit_transform(y_train)
    x_train_scaled = scaler.fit_transform(x_train)

    cv = GridSearchCV(logreg, paramsGrid, scoring="f1")
    cv.fit(x_train_scaled, y_train_encoded)
    print(f"Best params were {cv.best_params_}")
    print(f"Best score is {cv.best_score_}")
    bestModel = cv.best_estimator_
    y_predict = lblEncoder.inverse_transform(bestModel.predict(x_test))
```

```
    print(classification_report(y_pred=y_predict, y_true=y_test))


modelWithoutDens()
```

```
Best params were {'C': 0.1}
Best score is 0.9915504920073678
              precision    recall  f1-score   support

         red       0.00      0.00      0.00       652
       white       0.75      1.00      0.86      1947

    accuracy                           0.75      2599
   macro avg       0.37      0.50      0.43      2599
weighted avg       0.56      0.75      0.64      2599
```

As we can see, without the density, our model seems to overfit quite strongly. As we have 0.99 f1-score on the training set, but way less on the test set. With an accuracy that's not that good.

```
def trainL1():
    logreg = LogisticRegression(solver="saga")
    paramsGrid = {
        "C": [0.01, 0.1, 1, 10, 50, 75, 100, 200],
        "penalty": ["l1"],
    }
    x_train, x_test, y_train, y_test = train_test_split(x_base, y_base,
train_size=0.8)
    scaler = StandardScaler()
    lblEncoder = LabelEncoder()
    y_train_encoded = lblEncoder.fit_transform(y_train)
    x_train_scaled = scaler.fit_transform(x_train)

    cv = GridSearchCV(logreg, paramsGrid, scoring="f1")
    cv.fit(x_train_scaled, y_train_encoded)
    print(f"Best params were {cv.best_params_}")
    print(f"Best score is {cv.best_score_}")
    bestModel = cv.best_estimator_
    y_predict = lblEncoder.inverse_transform(bestModel.predict(x_test))
    print(classification_report(y_pred=y_predict, y_true=y_test))


trainL1()
```

```
Best params were {'C': 1, 'penalty': 'l1'}
Best score is 0.9962888532846126
              precision    recall  f1-score   support

         red       0.50      0.00      0.01       308
       white       0.76      1.00      0.87       992

    accuracy                           0.76      1300
   macro avg       0.63      0.50      0.44      1300
weighted avg       0.70      0.76      0.66      1300
```

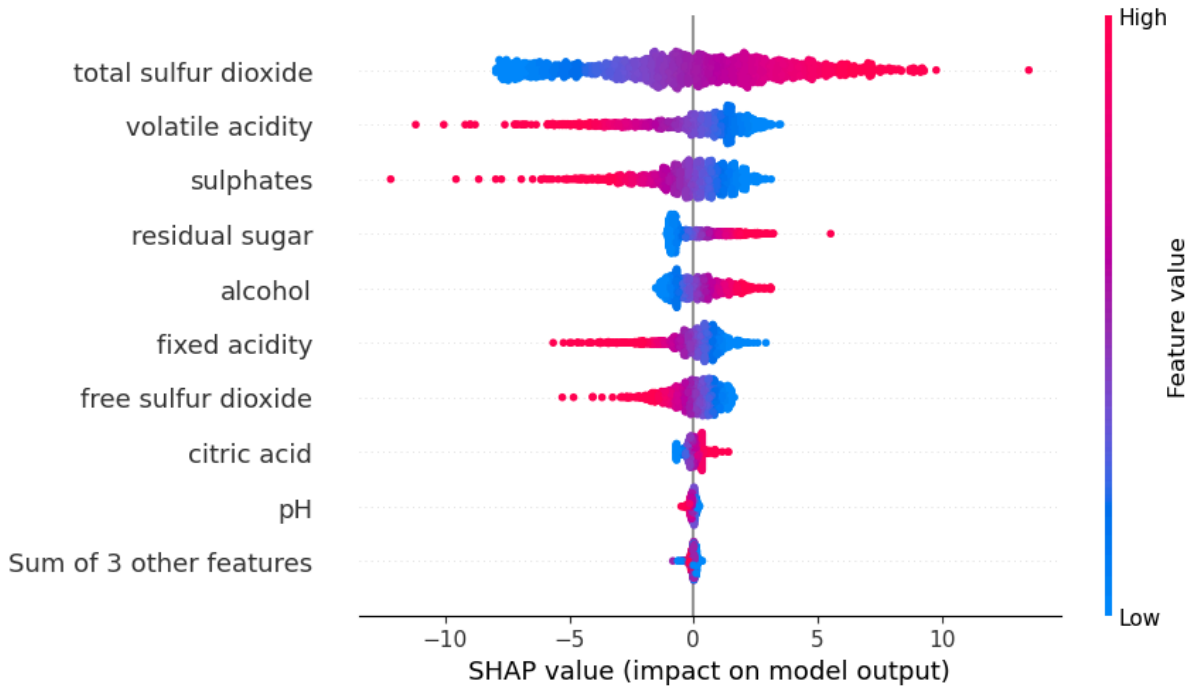
Using Shapley values

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'?

```
import shap


def getShapBeeswarmGraph():
    lg = LogisticRegression(C=50)
    x_train, x_test, y_train, y_test = train_test_split(x_base, y_base,
train_size=0.8)
    lg.fit(x_train, y_train)

    explainer = shap.Explainer(lg, x_train, feature_names=feature)
    shap_values = explainer(x_test)

    shap.plots.beeswarm(shap_values)


getShapBeeswarmGraph()
```



We can see in this graph that there are some features that are pretty determinant on that makes a wine red or white.

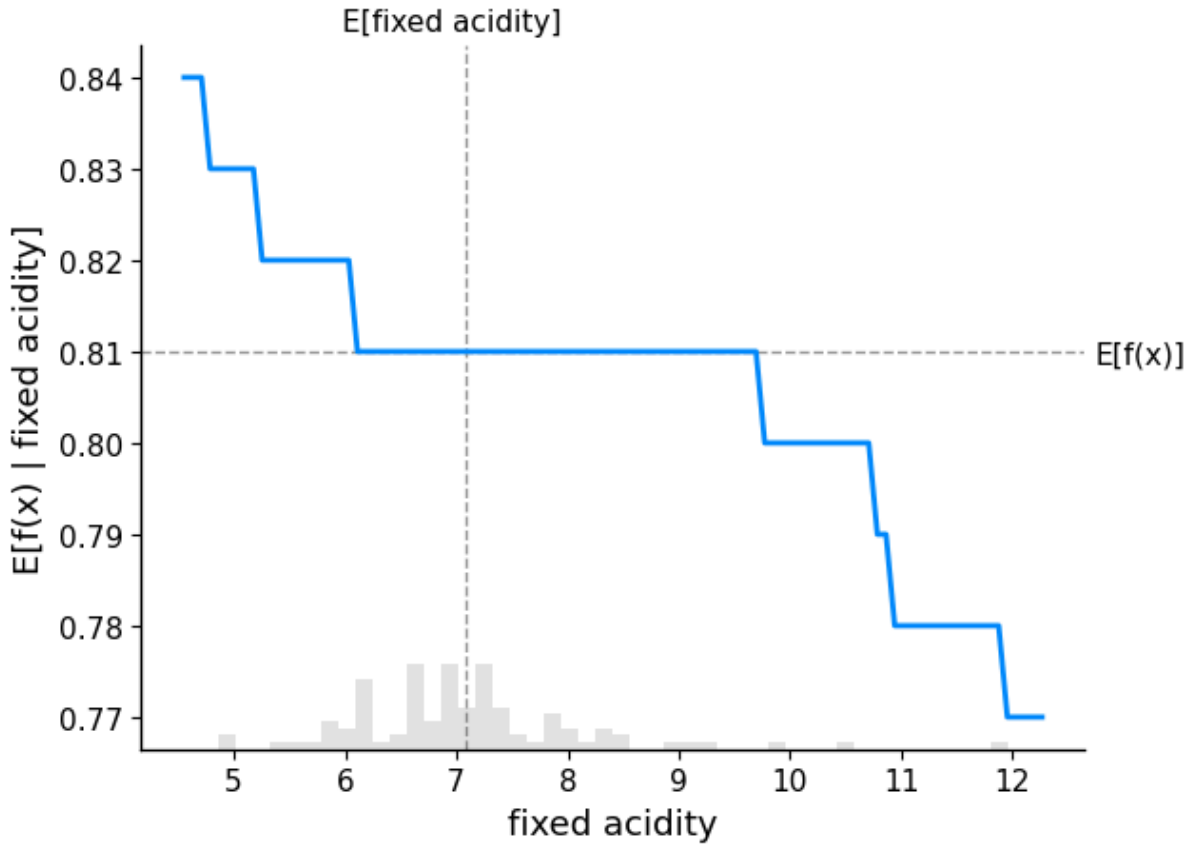
For example, the total sulfur dioxide, aor the volatile acidity. Etc...

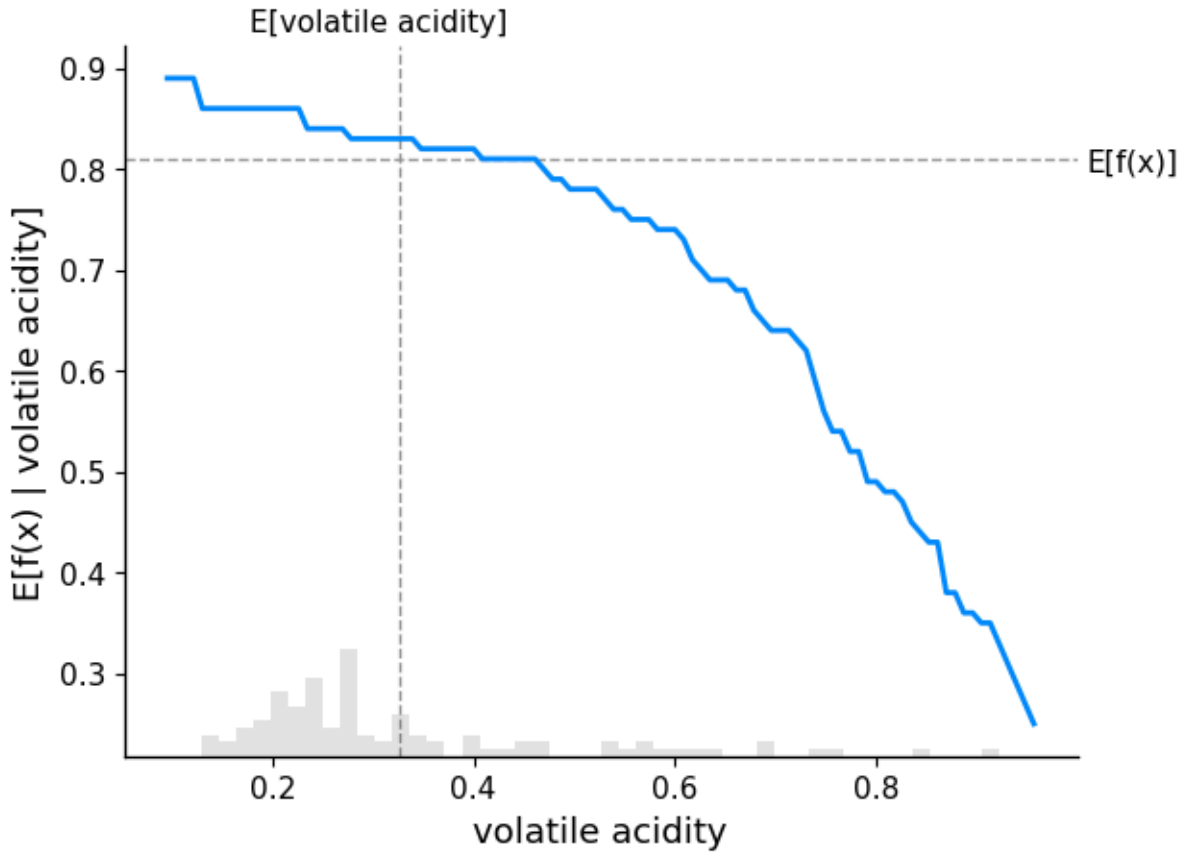
- Now use Partial Dependence Plots to see how the expected model output varies with the variation of each feature.

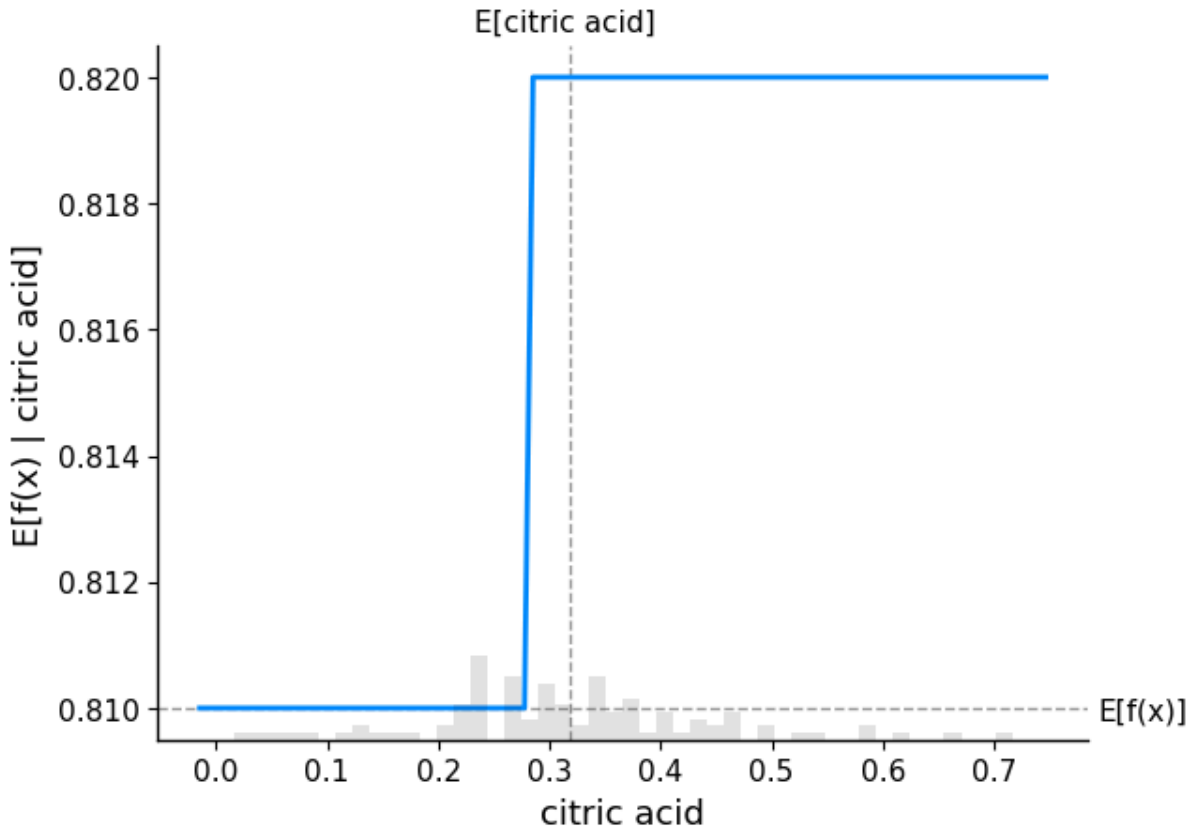
```
def getShapPartialDependencePlot():
    lg = LogisticRegression(C=50)
    x_train, x_test, y_train, y_test = train_test_split(x_base, y_base,
train_size=0.8)
    lblEncoder = LabelEncoder()
    y_train = lblEncoder.fit_transform(y_train)
    lg.fit(x_train, y_train)

    explainer = shap.Explainer(lg, x_train, feature_names=feature)
```

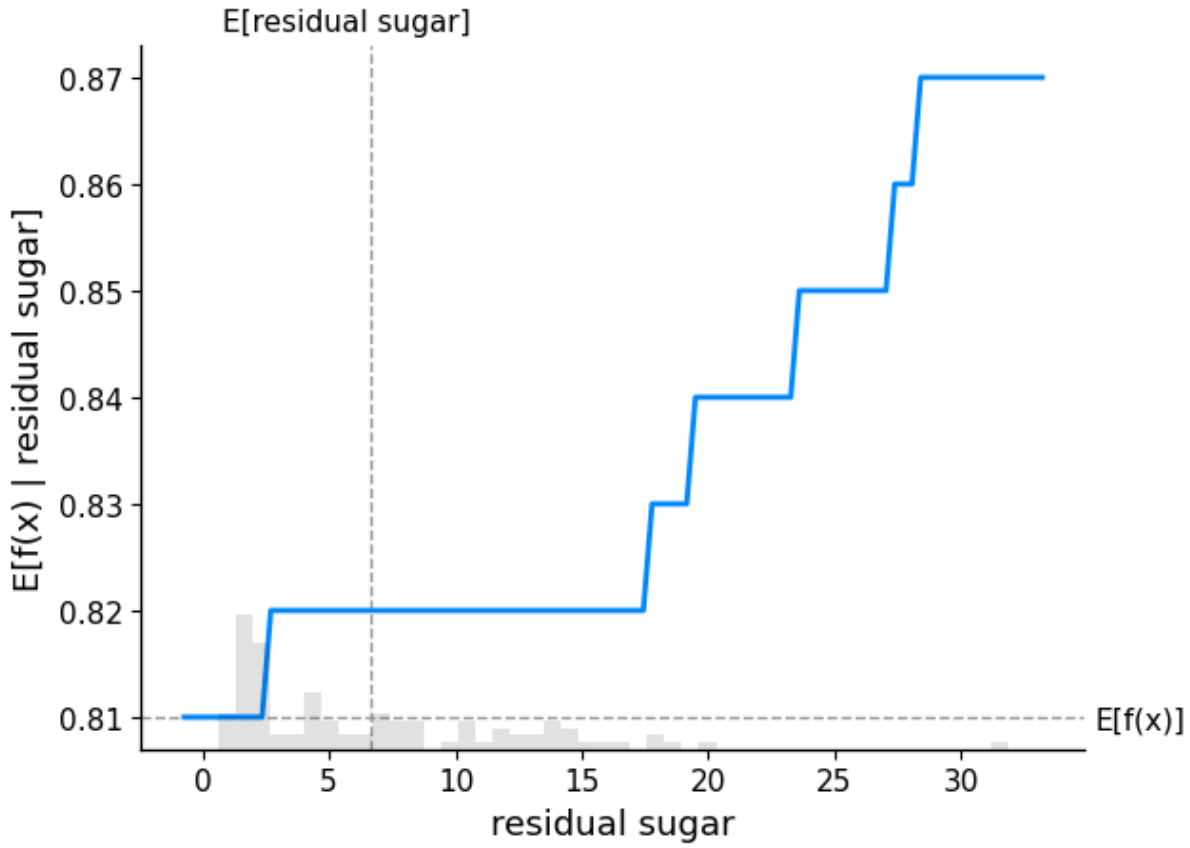
```
    X100 = shap.utils.sample(x_train, 100)
    for f in features:
        shap.partial_dependence_plot(
            f,
            lg.predict,
            X100,
            ice=False,
            model_expected_value=True,
            feature_expected_value=True,
        )
```

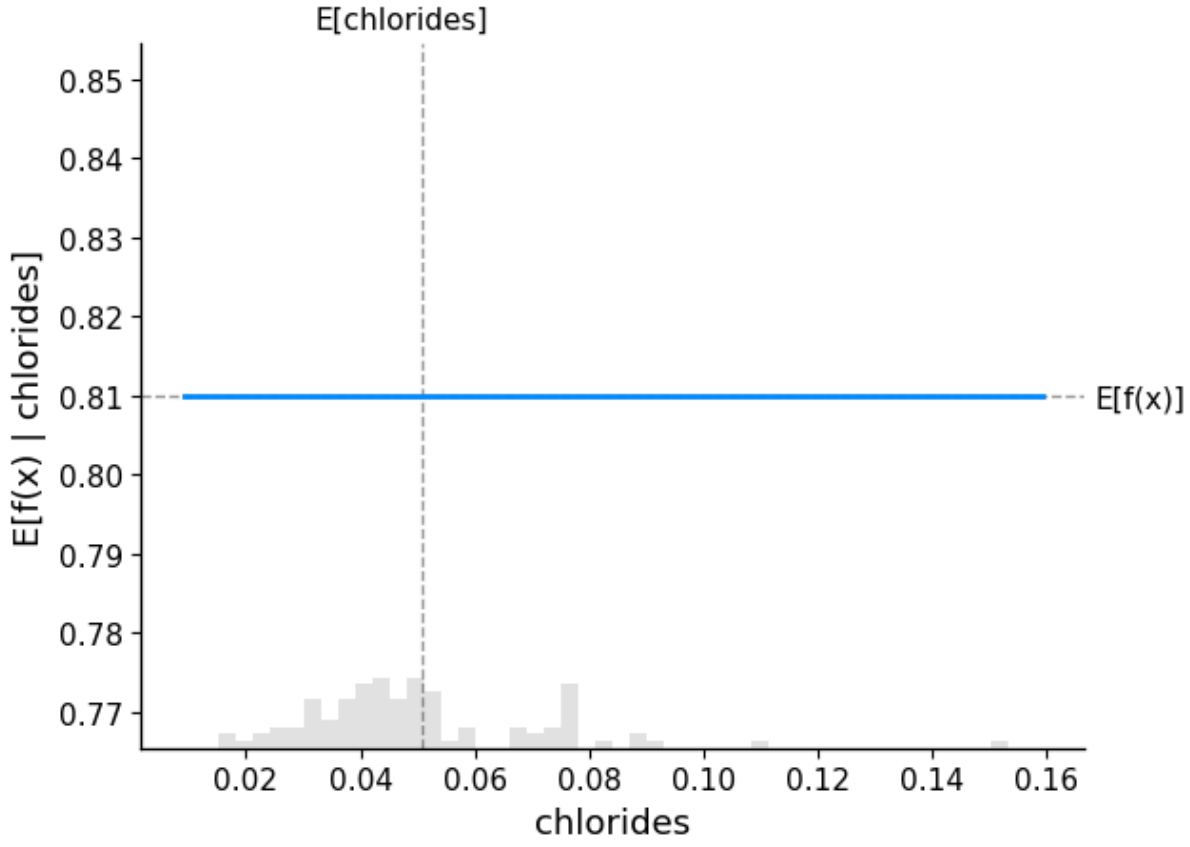
```
getShapPartialDependencePlot()
```

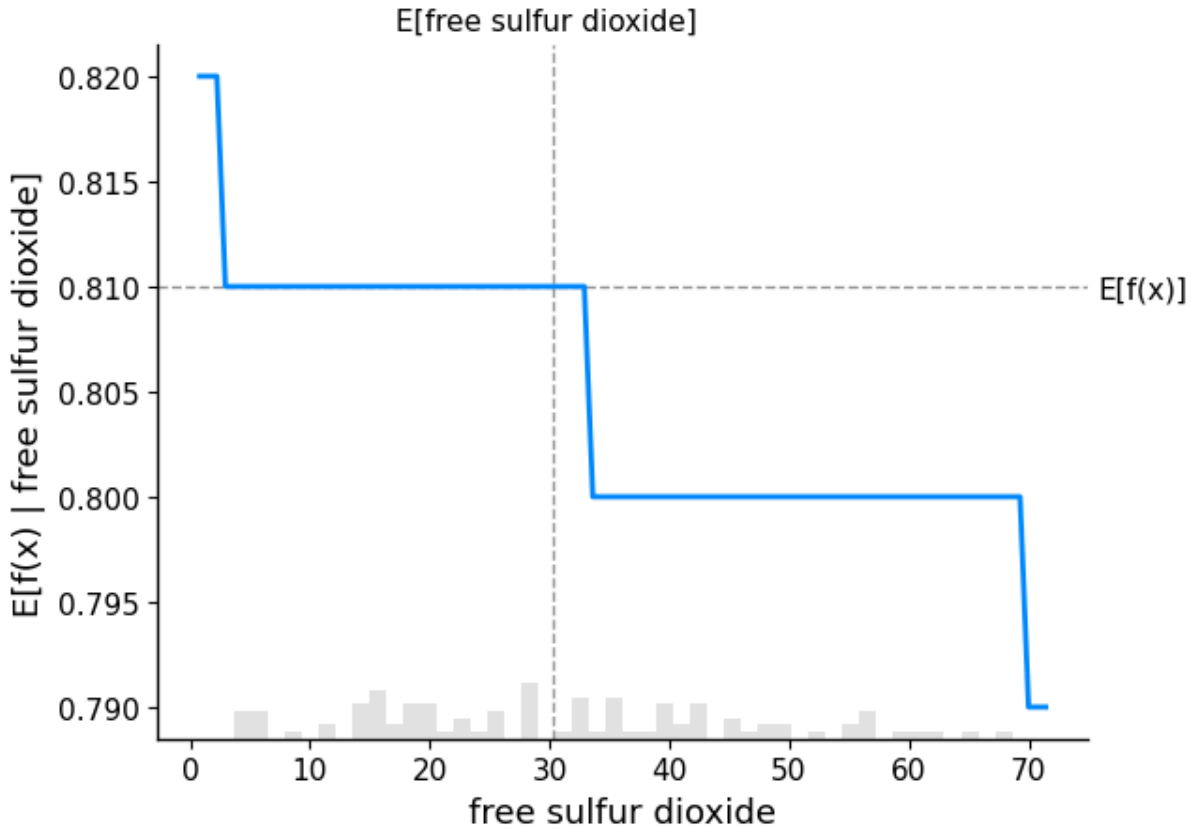


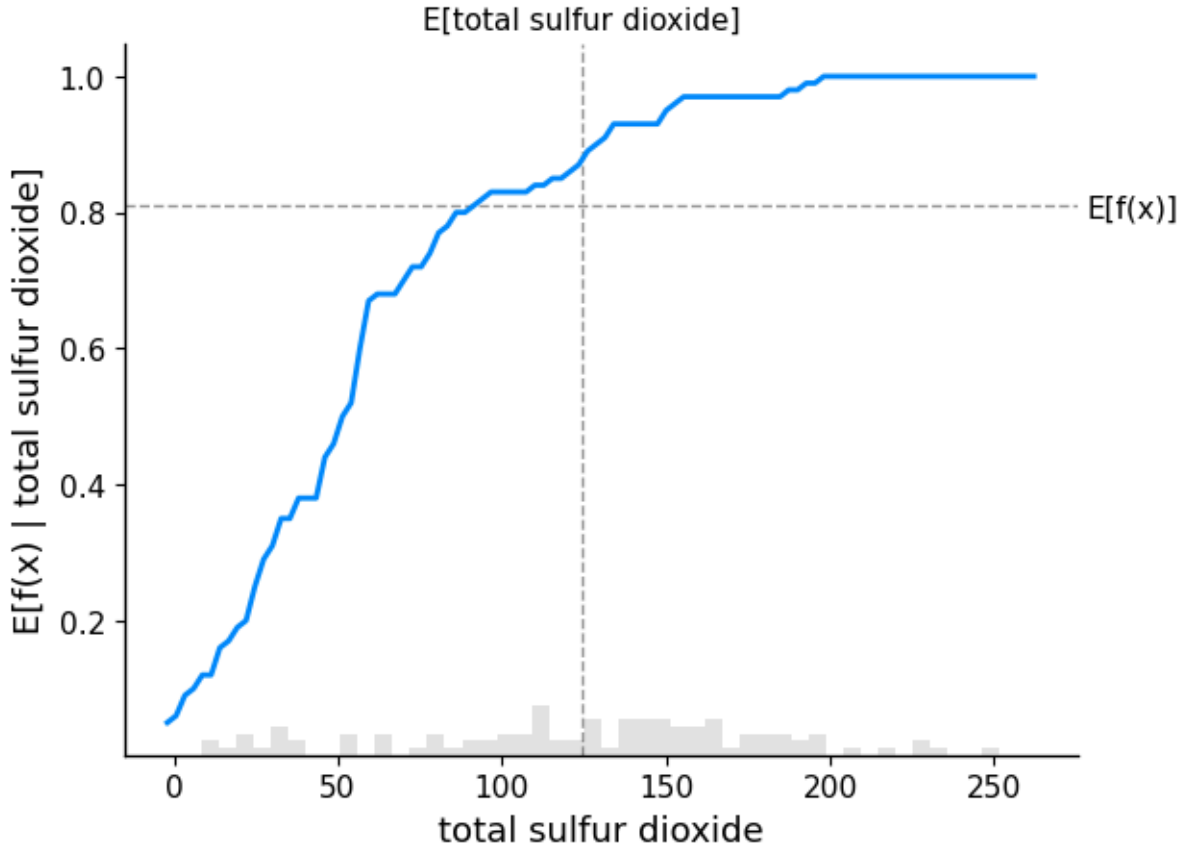

E[volatile acidity]
E[f(x)]
E[f(x) | volatile acidity]
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.4
0.6
0.8
volatile acidity

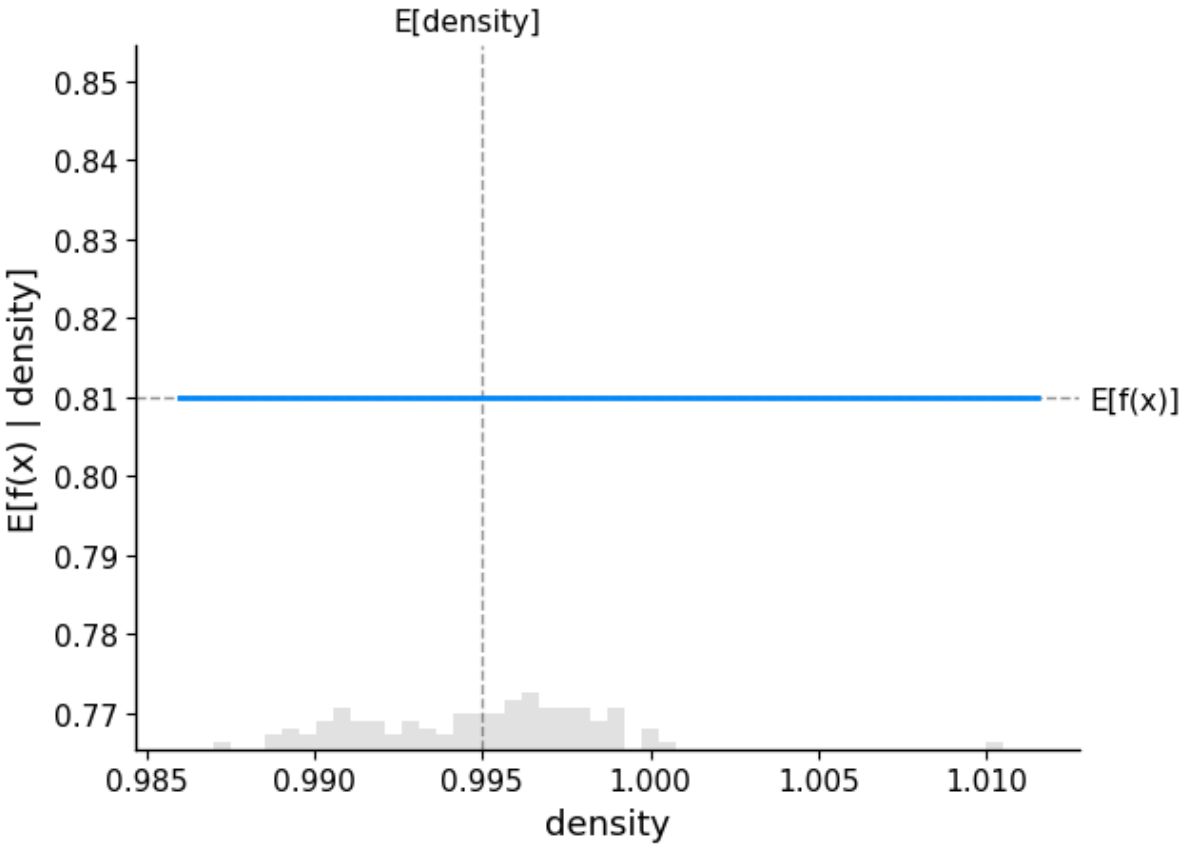

E[citric acid]
E[f(x)]
E[f(x) | citric acid]
0.820
0.818
0.816
0.814
0.812
0.810
0.0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
citric acid

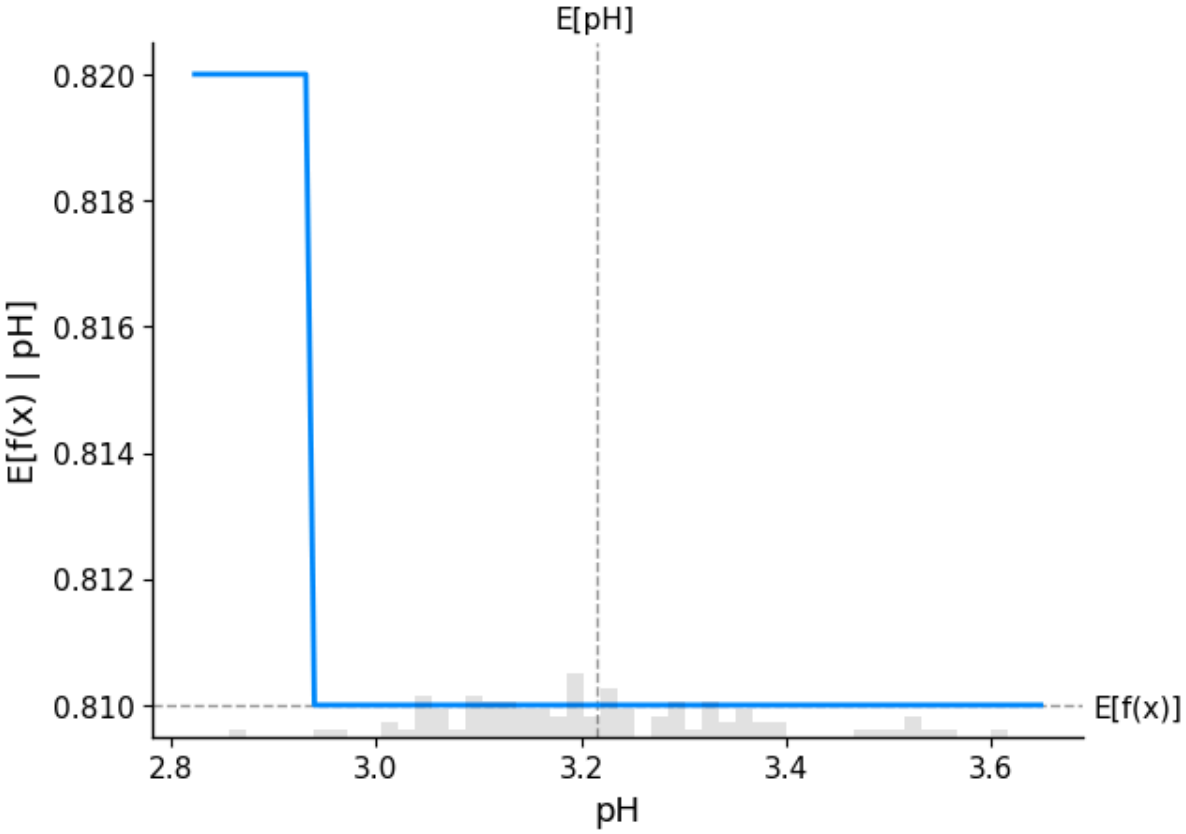

E[residual sugar]
0.87
0.86
0.85
0.84
0.83
0.82
0.81
E[f(x) | residual sugar]
E[f(x)]
0
5
10
15
20
25
30
residual sugar

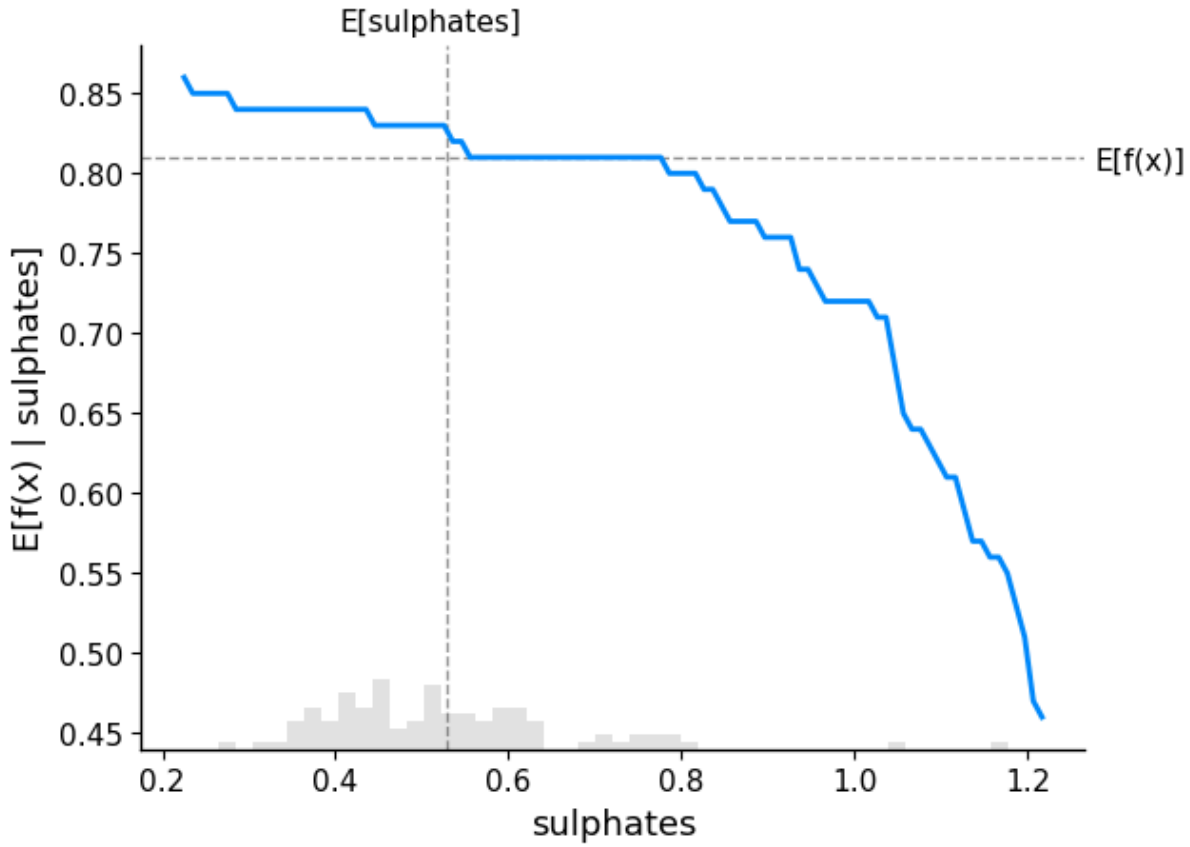

E[chlorides]
0.85
0.84
0.83
0.82
0.81
0.80
0.79
0.78
0.77
E[f(x) | chlorides]
E[f(x)]
0.02
0.04
0.06
0.08
0.10
0.12
0.14
0.16
chlorides

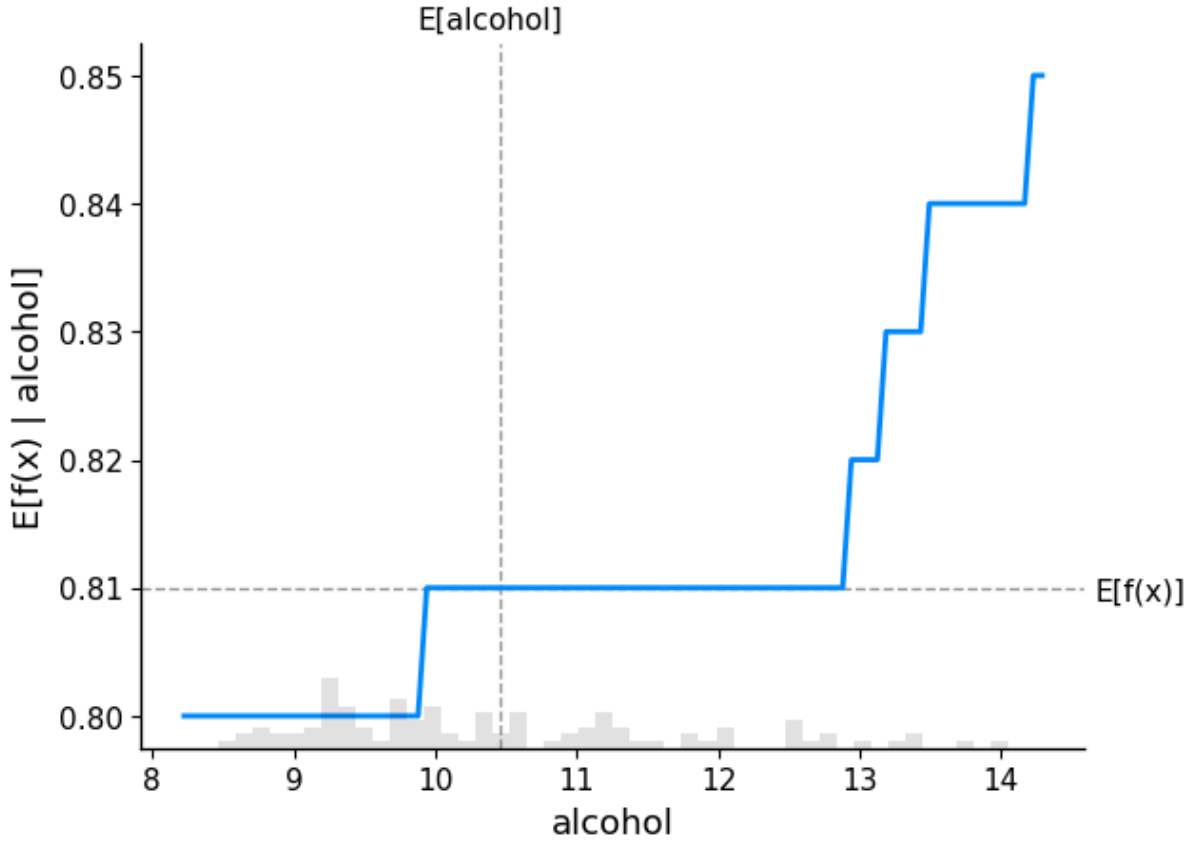

E[free sulfur dioxide]
0.820
0.815
0.810
0.805
0.800
0.795
0.790
E[f(x) | free sulfur dioxide]
E[f(x)]
0
10
20
30
40
50
60
70
free sulfur dioxide

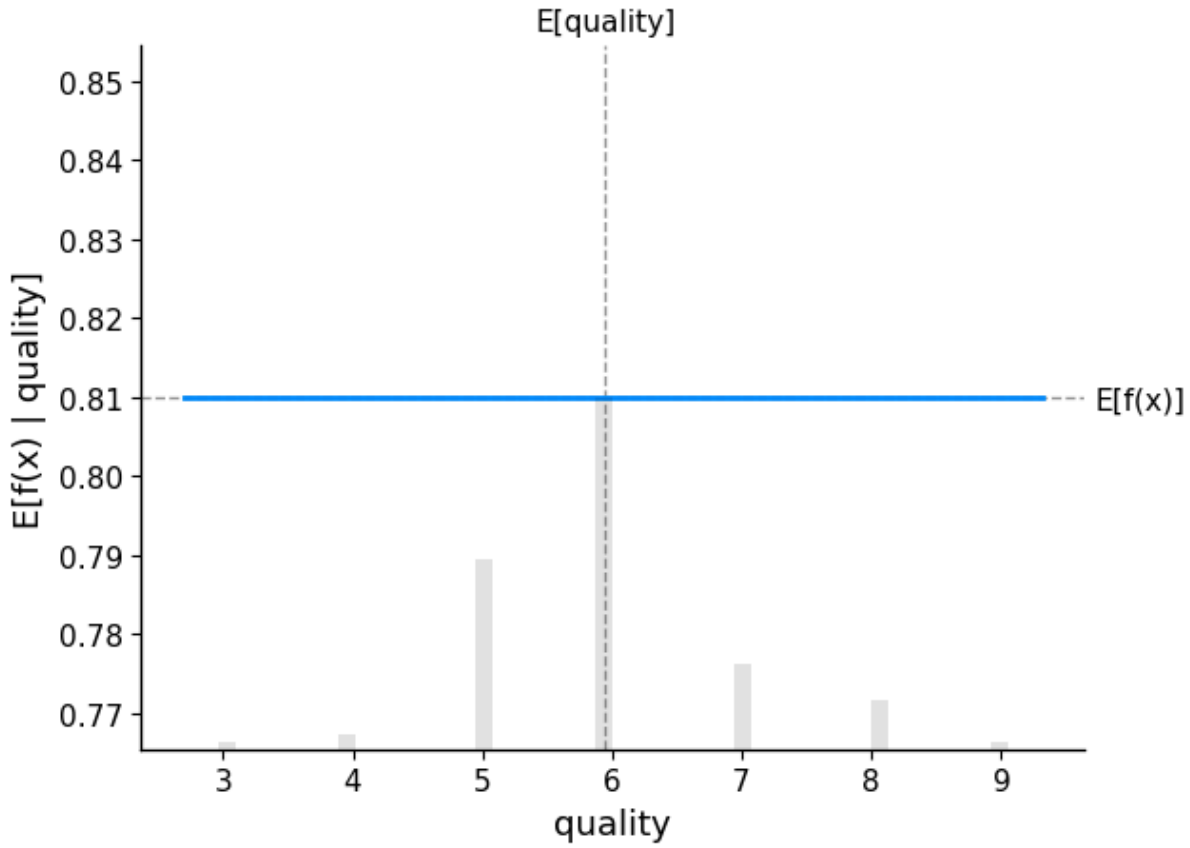

E[total sulfur dioxide]
1.0
0.8
0.6
0.4
0.2
E[f(x) | total sulfur dioxide]
E[f(x)]
0
50
100
150
200
250
total sulfur dioxide


E[density]
0.85
0.84
0.83
0.82
0.81
0.80
0.79
0.78
0.77
E[f(x) | density]
E[f(x)]
0.985
0.990
0.995
1.000
1.005
1.010
density


E[pH]
0.820
0.818
0.816
0.814
0.812
0.810
E[f(x) | pH]
E[f(x)]
2.8
3.0
3.2
3.4
3.6
pH

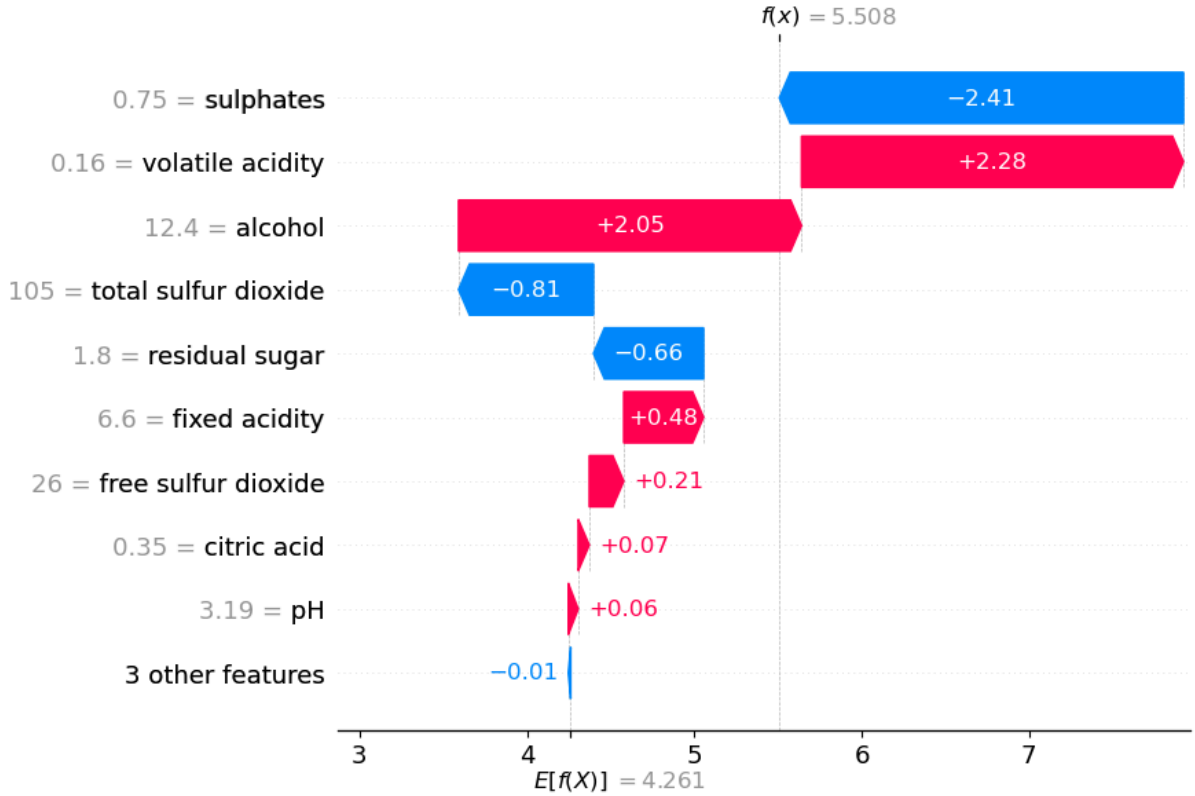

E[sulphates]
E[f(x)]
E[f(x) | sulphates]
0.85
0.80
0.75
0.70
0.65
0.60
0.55
0.50
0.45
0.2
0.4
0.6
0.8
1.0
1.2
sulphates

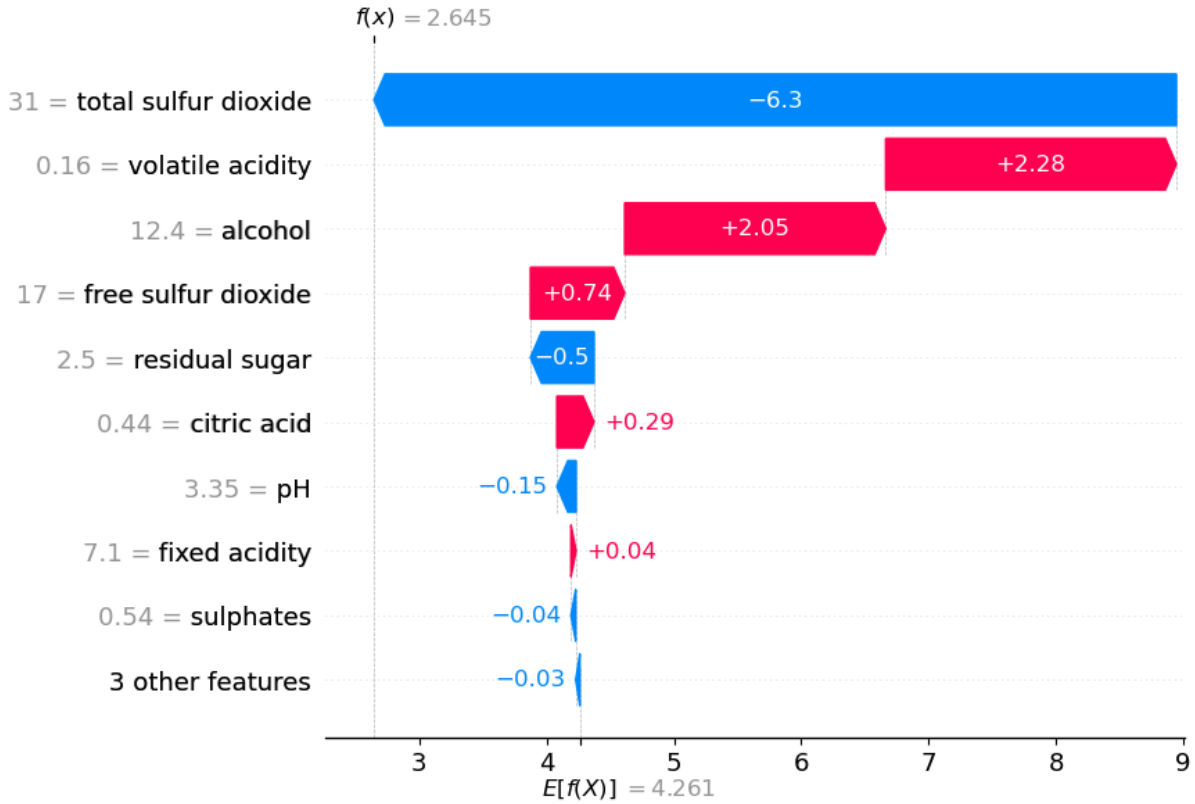

E[alcohol]
E[f(x)]
E[f(x) | alcohol]
0.85
0.84
0.83
0.82
0.81
0.80
8
9
10
11
12
13
14
alcohol



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

```
def shapWaterfall(index):
    lg = LogisticRegression(C=50)
    x_train, x_test, y_train, y_test = train_test_split(
        x_base, y_base, train_size=0.8, random_state=42
    )
    lg.fit(x_train, y_train)
    explainer = shap.Explainer(lg, x_train, feature_names=feature)
    shap_values = explainer(x_test)
    y_predicted = lg.predict(x_test)
    shap.plots.waterfall(shap_values[index])
    # for x, y in enumerate(y_predicted):
    #     if y_test.iloc[x]
    falses = [x for x, y in enumerate(y_predicted) if y_test.iloc[x] != y]
    shap.plots.waterfall(shap_values[falses[0]])

shapWaterfall(5)
```





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.

```
# Complete this cell with your code
target = "quality"


def replaceGoodBad(x):
    if x > 6:
        return "good"
    else:
        return "bad"


features = [x for x in base_data.columns.values if x != target]
x_base = base_data[features]
y_base = base_data[target].map(replaceGoodBad)
```

```
x_base
```

```
      fixed acidity  volatile acidity  citric acid  residual sugar  chlorides  \
0               7.0              0.17         0.74           12.80      0.045
1               7.7              0.64         0.21            2.20      0.077
2               6.8              0.39         0.34            7.40      0.020
3               6.3              0.28         0.47           11.20      0.040
4               7.4              0.35         0.20           13.90      0.054
...             ...               ...          ...             ...        ...
6492            7.6              0.32         0.58           16.75      0.050
6493            5.6              0.28         0.27            3.90      0.043
6494            6.4              0.37         0.20            5.60      0.117
6495            6.5              0.26         0.50            8.00      0.051
6496            7.2              0.62         0.06            2.70      0.077

      free sulfur dioxide  total sulfur dioxide  density    pH  sulphates  \
0                    24.0                 126.0  0.99420  3.26       0.38
1                    32.0                 133.0  0.99560  3.27       0.45
2                    38.0                 133.0  0.99212  3.18       0.44
3                    61.0                 183.0  0.99592  3.12       0.51
4                    63.0                 229.0  0.99888  3.11       0.50
...                   ...                   ...      ...   ...        ...
6492                 43.0                 163.0  0.99990  3.15       0.54
6493                 52.0                 158.0  0.99202  3.35       0.44
6494                 61.0                 183.0  0.99459  3.24       0.43
6495                 46.0                 197.0  0.99536  3.18       0.47
6496                 15.0                  85.0  0.99746  3.51       0.54

      alcohol  color
0        12.2  white
1         9.9    red
2        12.0  white
3         9.5  white
4         8.9  white
...       ...    ...
6492      9.2  white
6493     10.7  white
6494      9.5  white
6495      9.5  white
6496      9.5    red
```

```
[6497 rows x 12 columns]
```

```
y_base
```

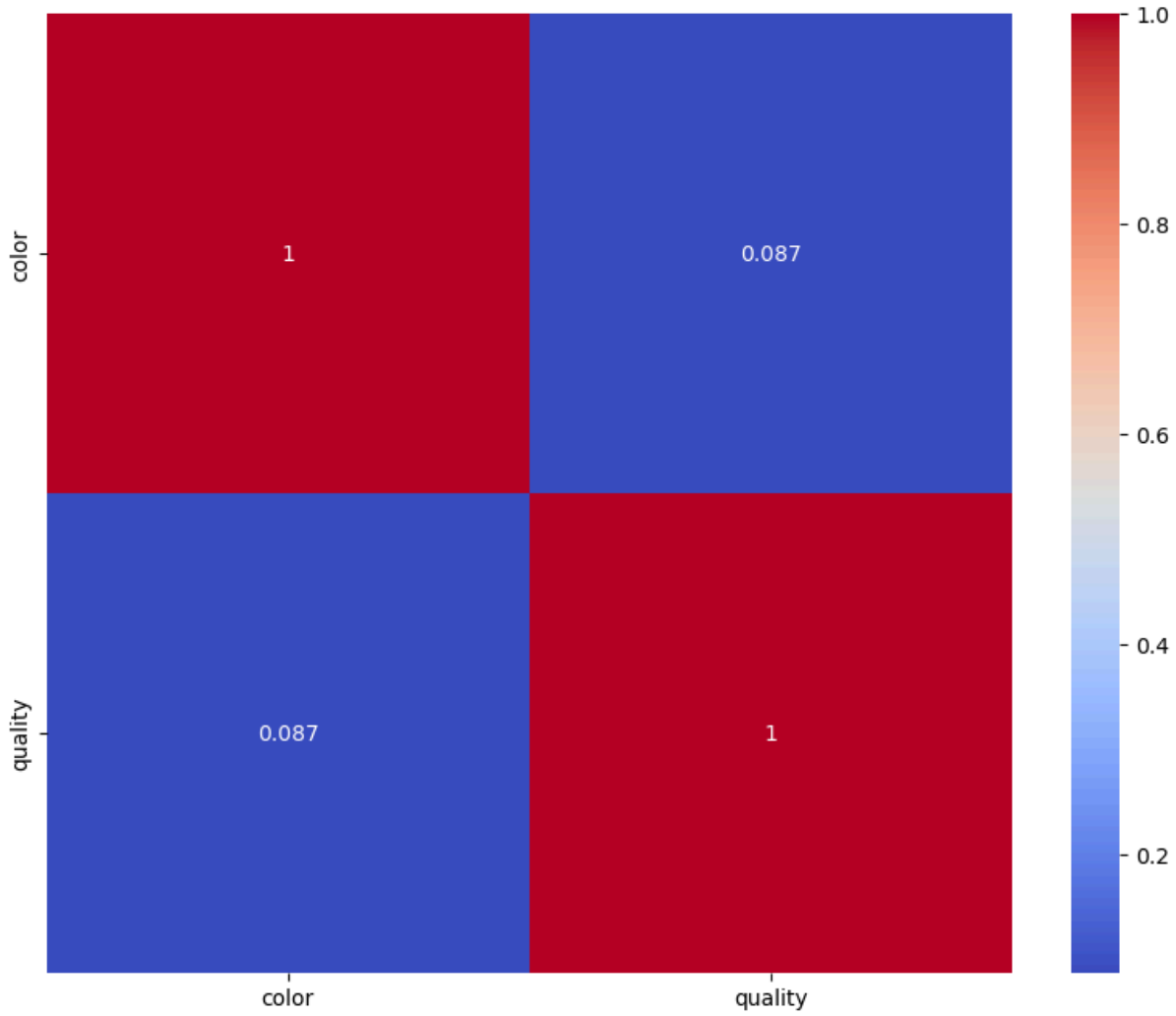
```
0       good
1        bad
2       good
3        bad
4        bad
        ...
6492     bad
6493    good
6494     bad
6495     bad
6496     bad
Name: quality, Length: 6497, dtype: object
```

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?

```
def getQualityCorrMatrix():
    df = pd.DataFrame()
    lblEncoder = LabelEncoder()
    lblEncoder2 = LabelEncoder()
    df["color"] = lblEncoder.fit_transform(x_base["color"])
    df[target] = lblEncoder2.fit_transform(y_base)
    plt.figure(figsize=(10, 8))
    sns.heatmap(df.corr(), annot=True, cmap="coolwarm")
    plt.show()


getQualityCorrMatrix()
```



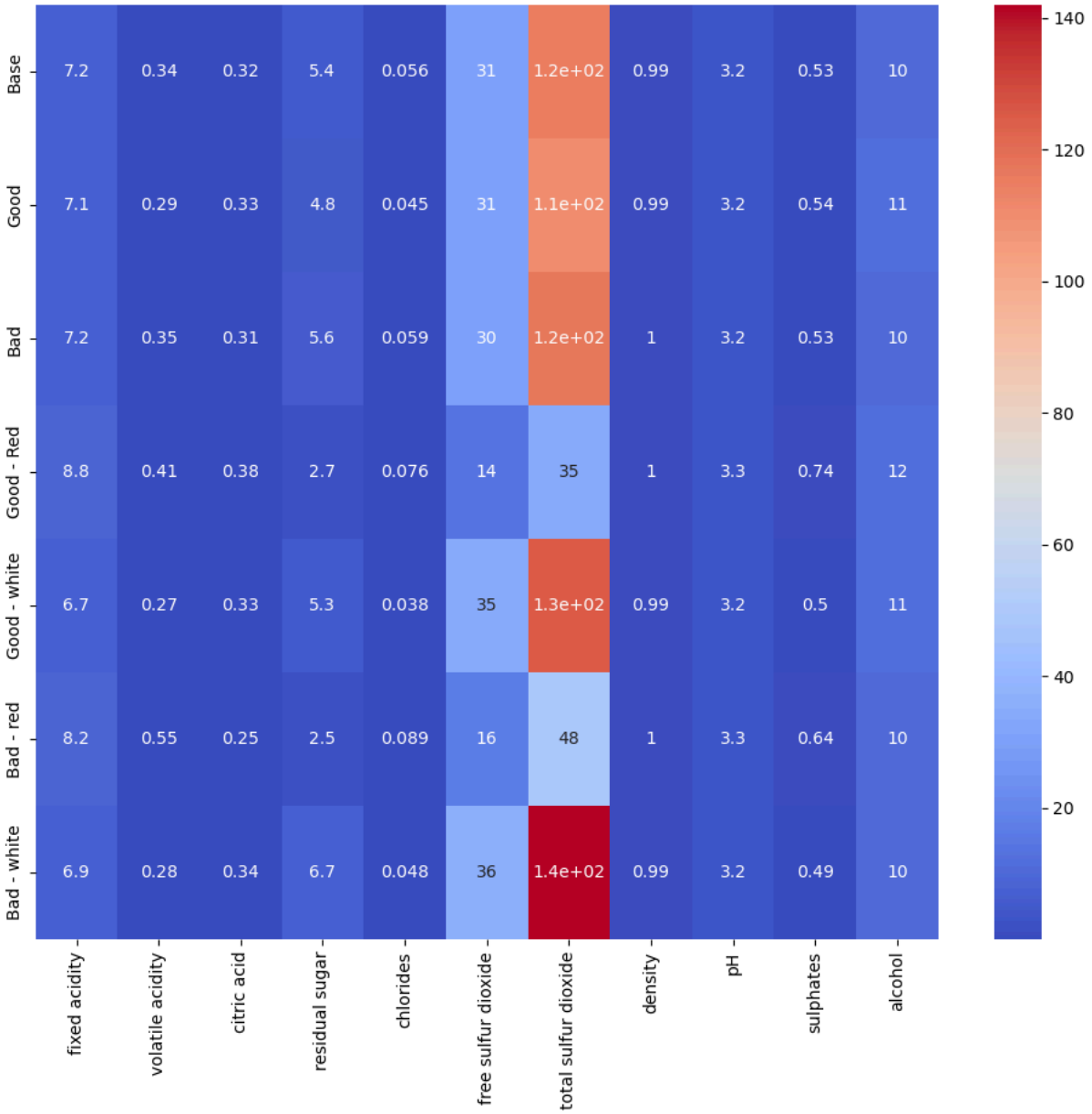
If it turns out that there are significantly more bad red wines than bad white wines or vice versa, what are the implications for your analysis?

- 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?

```
num_features = [x for x in features if x != "color"]
good_wines = x_base[y_base == "good"]
bad_wines = x_base[y_base == "bad"]
```

```
def showFeatureAvgHeatmap():
    base_features_means = base_data[num_features].mean()
    good_wines_means = good_wines[num_features].mean()
    bad_wines_means = bad_wines[num_features].mean()
    good_red_wines = good_wines[good_wines["color"] == "red"][num_features].mean()
    good_white_wines = good_wines[good_wines["color"] == "white"]
[num_features].mean()
    bad_red_wines = bad_wines[bad_wines["color"] == "red"][num_features].mean()
    bad_white_wines = bad_wines[bad_wines["color"] == "white"][num_features].mean()
    plt.figure(figsize=(12, 10))
    sns.heatmap(
        [
```

```
            base_features_means,
            good_wines_means,
            bad_wines_means,
            good_red_wines,
            good_white_wines,
            bad_red_wines,
            bad_white_wines,
        ],
        annot=True,
        cmap="coolwarm",
        xticklabels=num_features,
        yticklabels=[
            "Base",
            "Good",
            "Bad",
            "Good - Red",
            "Good - white",
            "Bad - red",
            "Bad - white",
        ],
    )
    plt.show()


showFeatureAvgHeatmap()
```



As we can see, there is no visible difference between good and bad wine. This won't be this easy

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
}
```

From now on, we will focus only on the white wines for our analysis

```
from sklearn.preprocessing import OneHotEncoder
from xgboost import XGBClassifier

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
}

model = XGBClassifier()
# onehotEncoder = OneHotEncoder(sparse_output=False)
# x_encoded = x_base[num_features].copy(deep=True)
# encoded_data = onehotEncoder.fit_transform(x_base[["color"]])
# encoded_df = pd.DataFrame(
#     encoded_data, columns=onehotEncoder.get_feature_names_out(["color"])
# )
# for c in encoded_df.columns.values:
#     x_encoded[c] = encoded_df[c]
lblEncoder = LabelEncoder()
y_encoded = lblEncoder.fit_transform(y_base[x_base["color"] == "white"])
x_train, x_test, y_train, y_test = train_test_split(
    x_base[x_base["color"] == "white"][num_features], y_encoded, train_size=0.8
)

cv = GridSearchCV(model, param_grid, scoring="f1", n_jobs=-1)

cv.fit(x_train, y_train)

print(f"Best params were : {cv.best_params_}")
print(f"Best score is : {cv.best_score_}")
bestModel = cv.best_estimator_
```

```
Best params were : {'colsample_bytree': 1.0, 'gamma': 0.1, 'learning_rate': 0.1,
'max_depth': 5, 'min_child_weight': 1, 'n_estimators': 100, 'subsample': 0.7}
Best score is : 0.6095181175313442
```

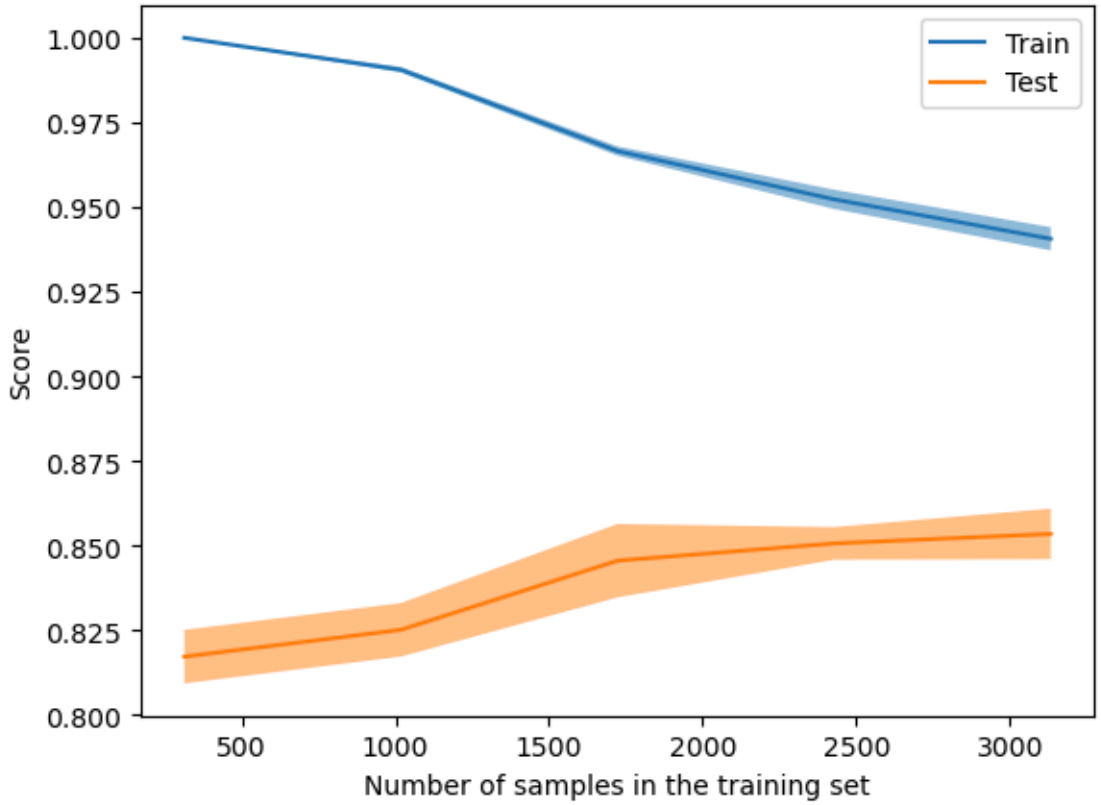
- Analyze the results (test and train), validate whether there is overfitting.

```
y_pred = bestModel.predict(x_test)
print(classification_report(y_test, y_pred))
```

```
              precision    recall  f1-score   support

           0       0.87      0.96      0.91       754
           1       0.79      0.50      0.62       226

    accuracy                           0.86       980
   macro avg       0.83      0.73      0.76       980
weighted avg       0.85      0.86      0.84       980
```

```
LearningCurveDisplay.from_estimator(bestModel, x_train, y_train, n_jobs=-1)
```

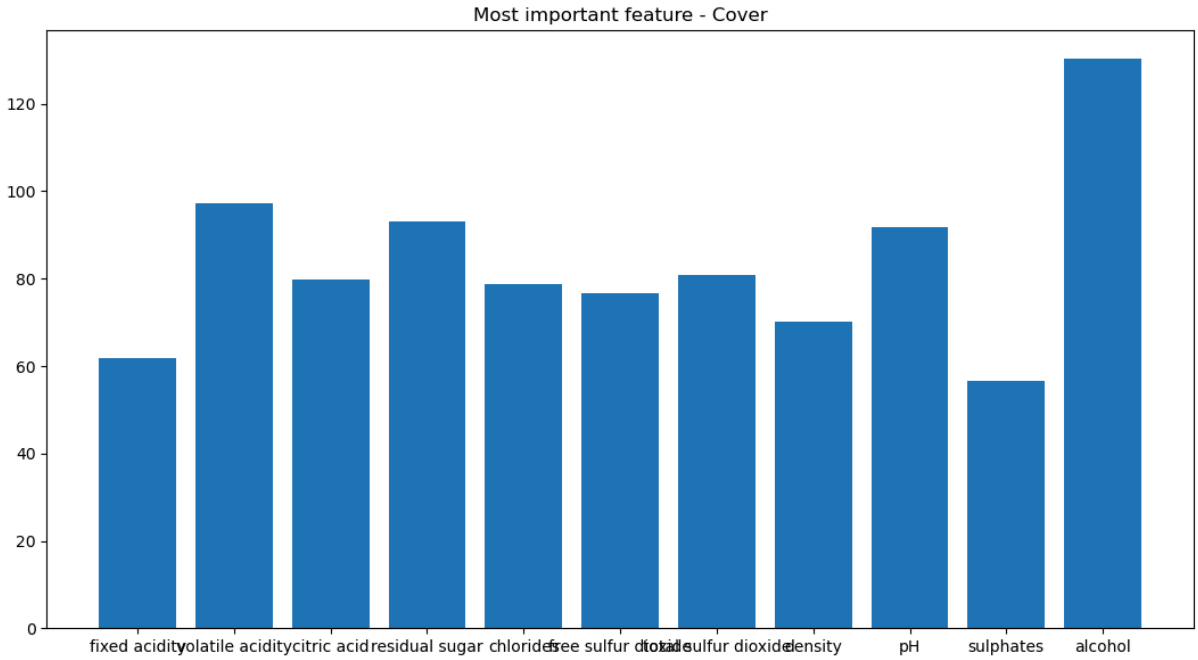
```
<sklearn.model_selection._plot.LearningCurveDisplay at 0x7f17e6d1b7c0>
```

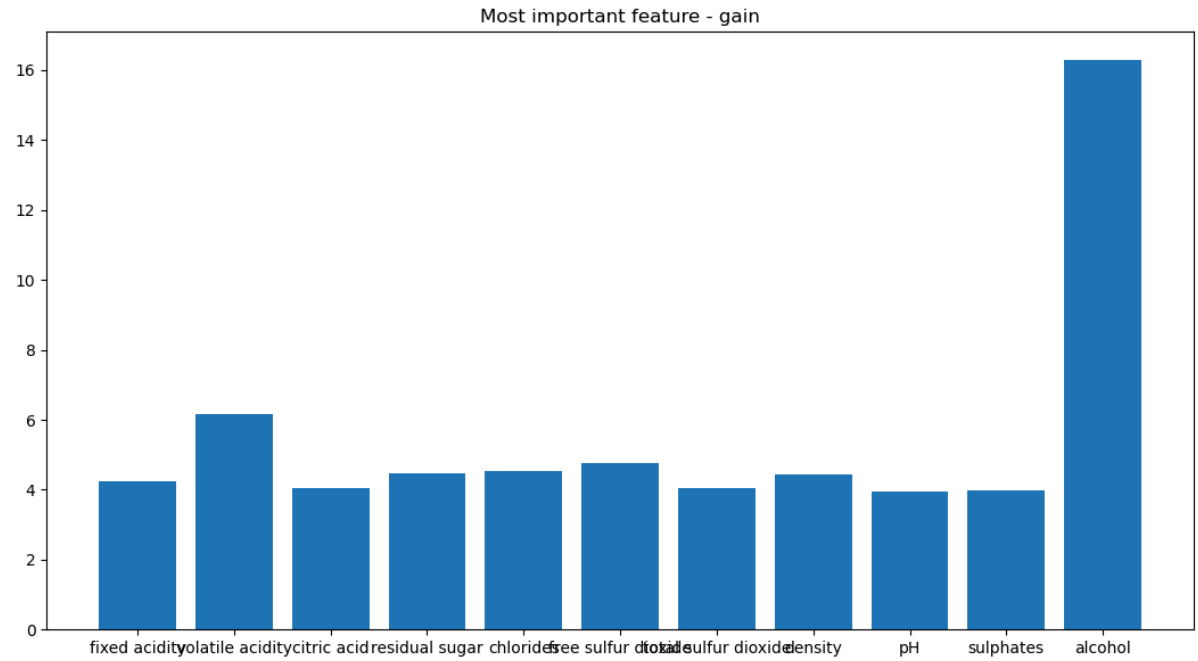


Interpretability with SHAP (2h)

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

```
# Complete this cell with your code
import xgboost as xgb

# Set feature names

cover = bestModel.get_booster().get_score(importance_type="cover")
gain = bestModel.get_booster().get_score(importance_type="gain")

# Plot feature importance
plt.figure(figsize=(13, 15))
plt.subplot(2, 1, 1)
plt.bar(cover.keys(), cover.values())
plt.title("Most important feature - Cover")
plt.subplot(2, 1, 2)
plt.bar(gain.keys(), gain.values())
plt.title("Most important feature - gain")
plt.show()
```



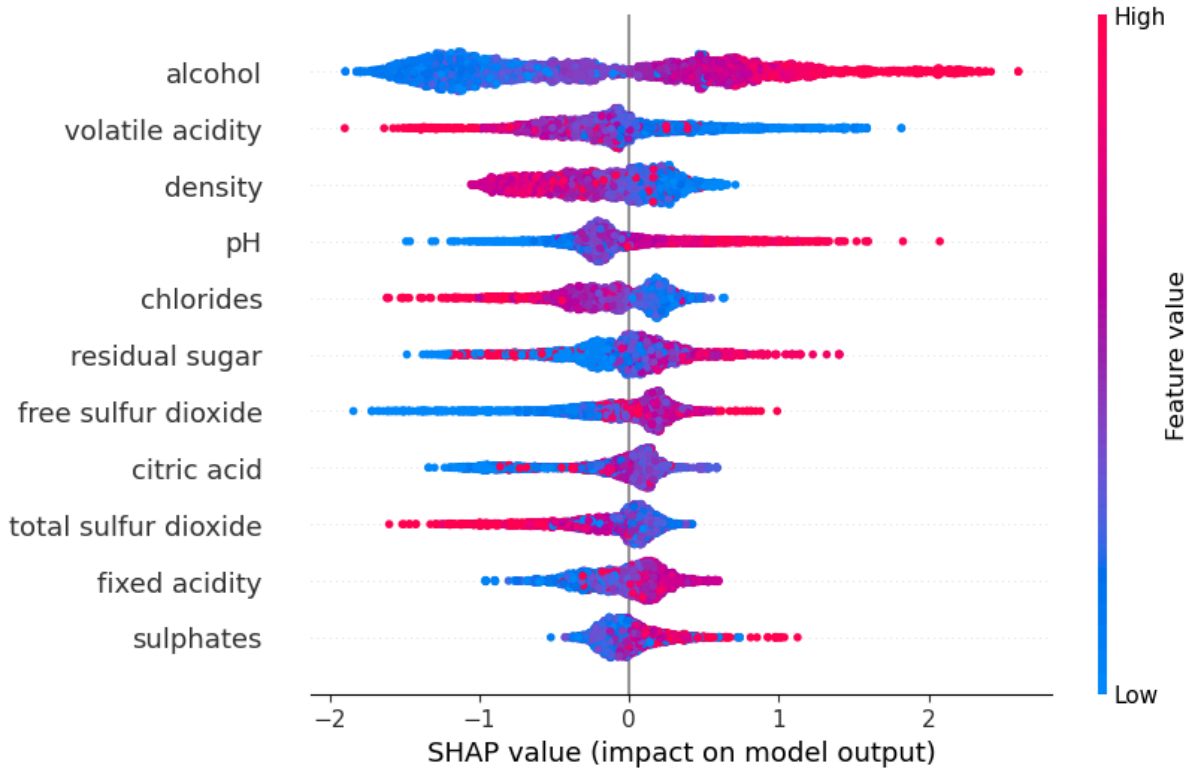


- Use SHAP's `TreeExplainer` to compute feature importance (Shapley values). Do you see any difference with XGBoost's feature importances?
- Produce different plots to analyze Shapley values:
  - A bar plot that summarizes the mean absolute value of each feature.
  - A beeswarm plot that shows the shapley 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'?

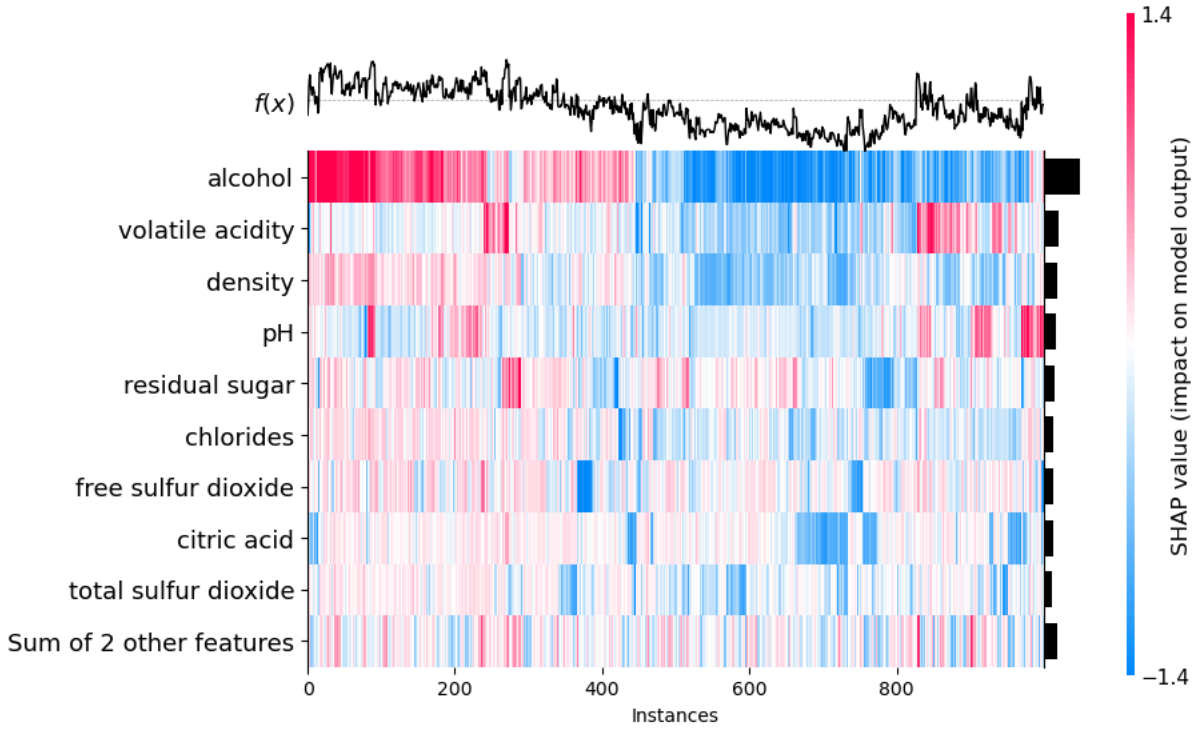
```
from shap import TreeExplainer


explainer = TreeExplainer(bestModel)
```

```
shap_values = explainer(x_train)
```

```
shap.plots.beeswarm(shap_values, max_display=20)
```




```
shap.plots.heatmap(shap_values[:1000])
```

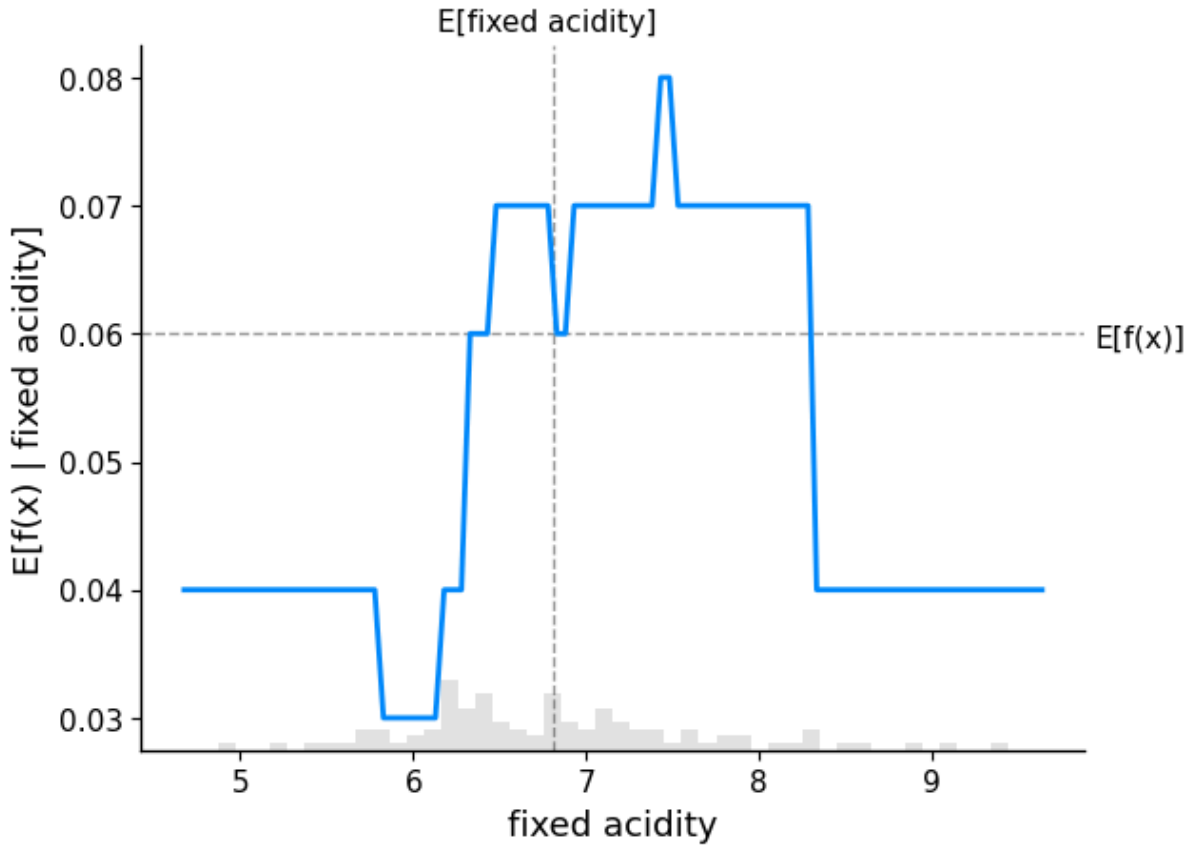


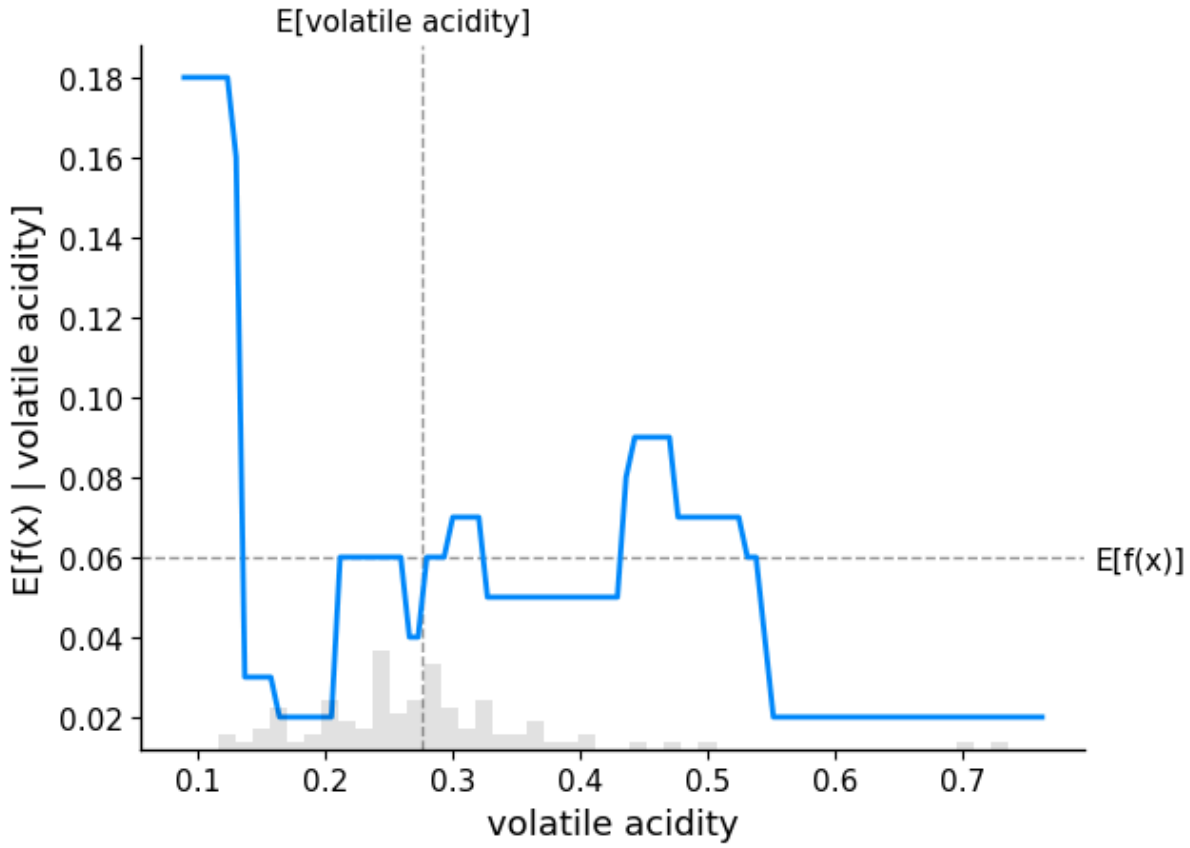

```
<Axes: xlabel='Instances'>
```

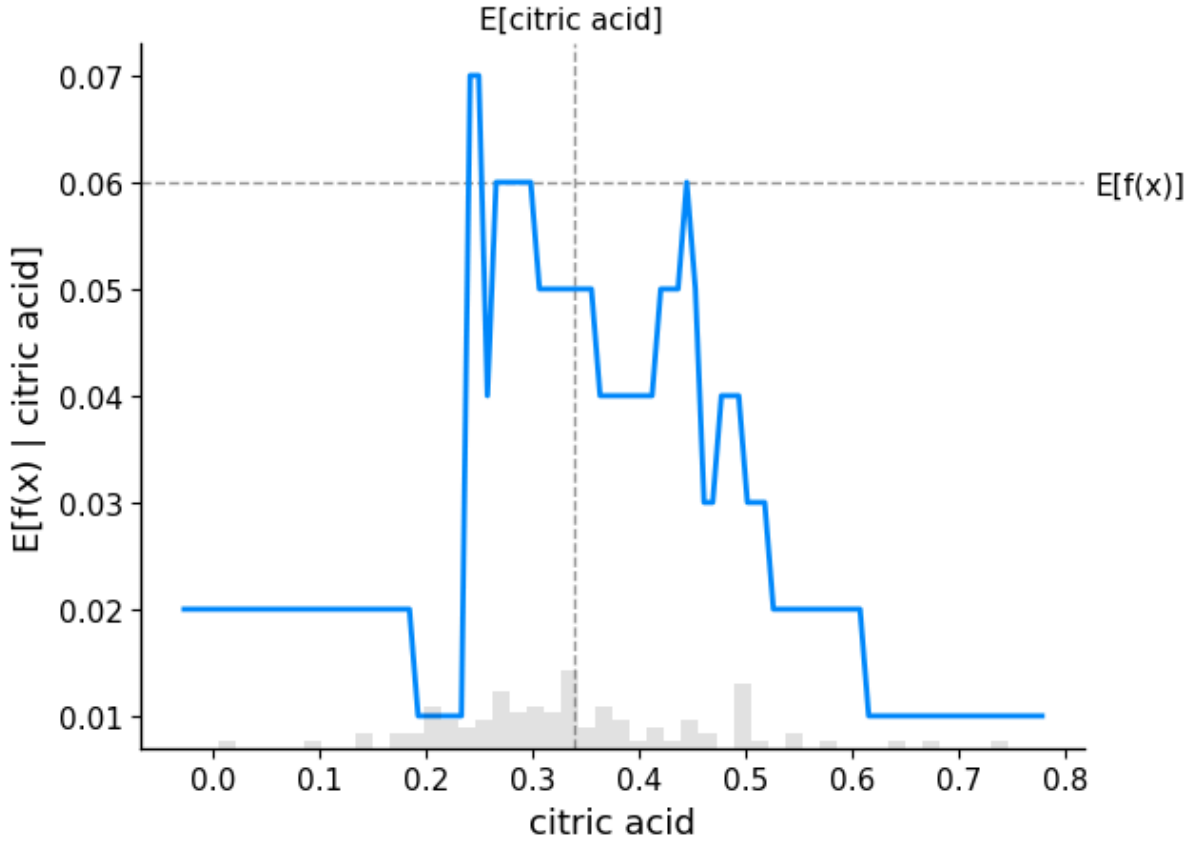
- Now use Partial Dependence Plots to see how the expected model output varies with the variation of each feature.
- How does that modify your perspective on what makes a good or bad wine?

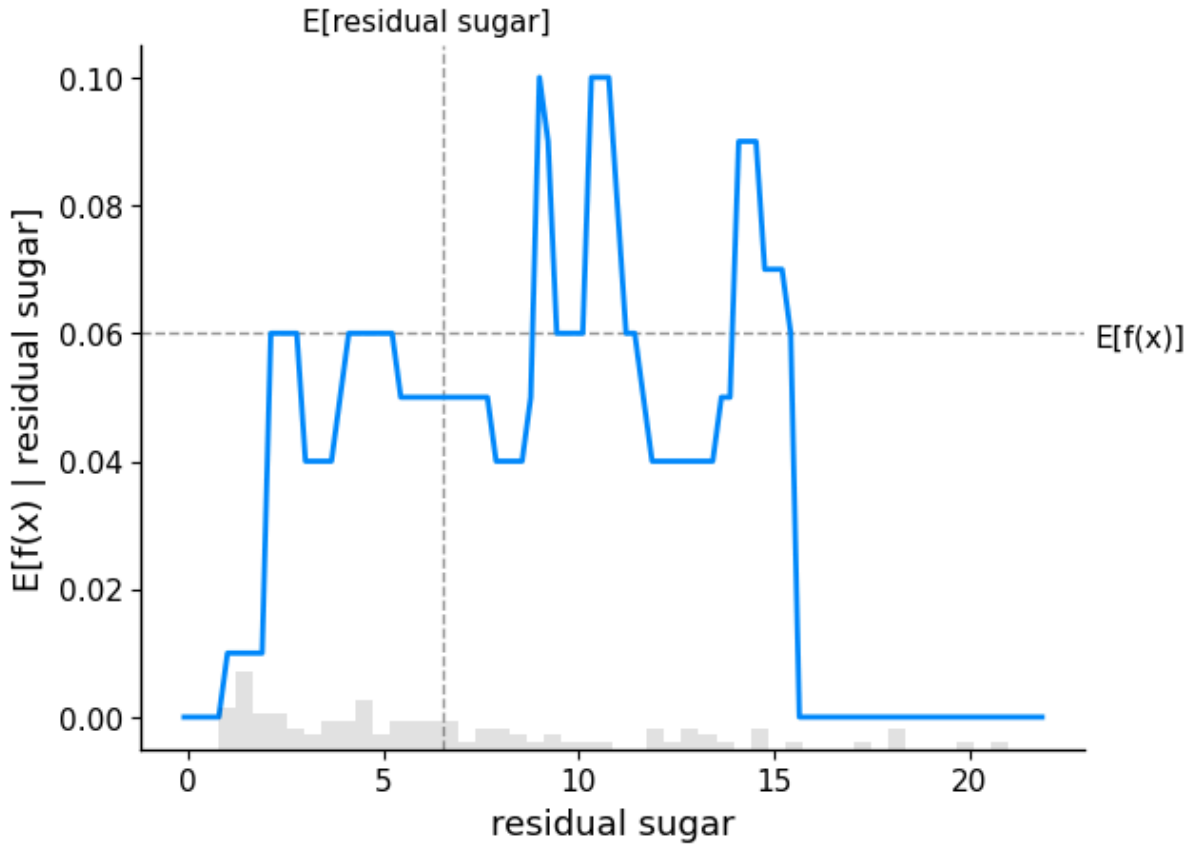
```
def getShapPartialDependencePlot():
    X100 = shap.utils.sample(x_train, 100)
    for f in num_features:
        shap.partial_dependence_plot(
            f,
            bestModel.predict,
            X100,
            ice=False,
            model_expected_value=True,
            feature_expected_value=True,
        )
```

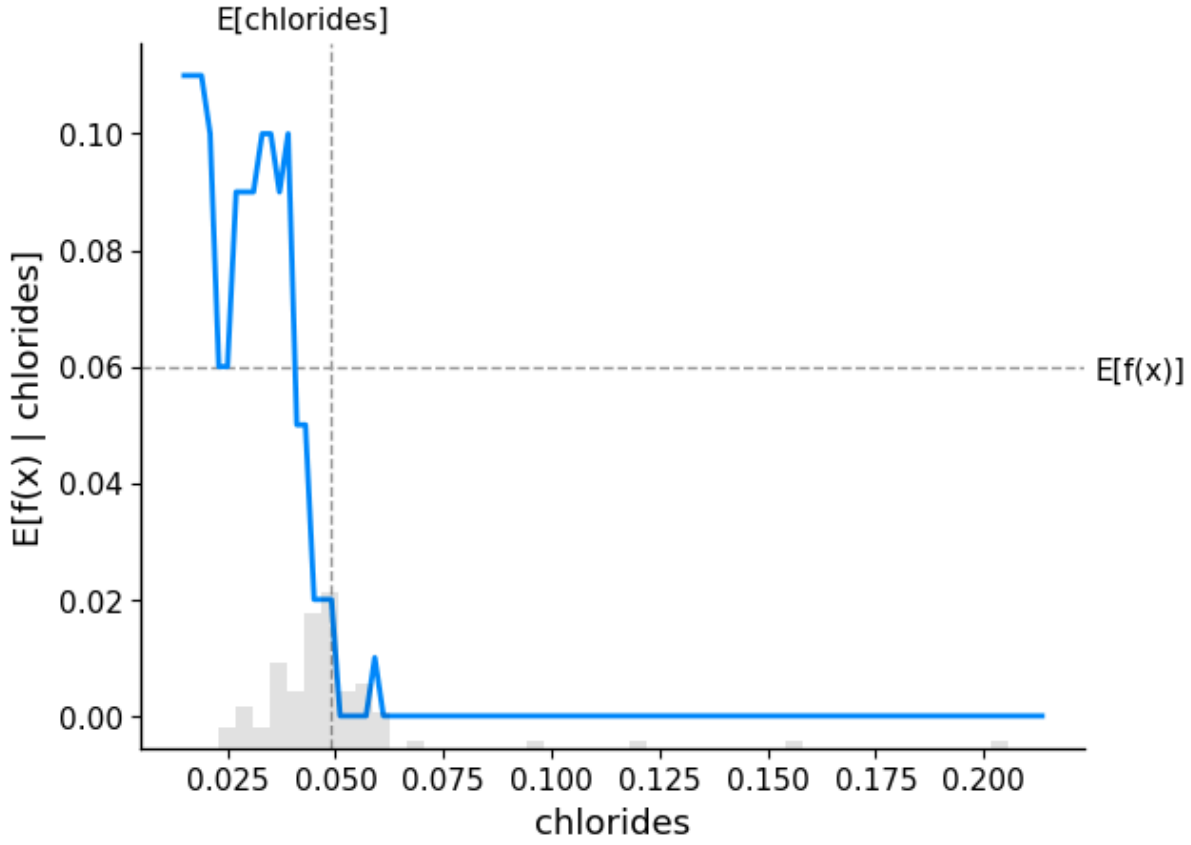
```
getShapPartialDependencePlot()
```

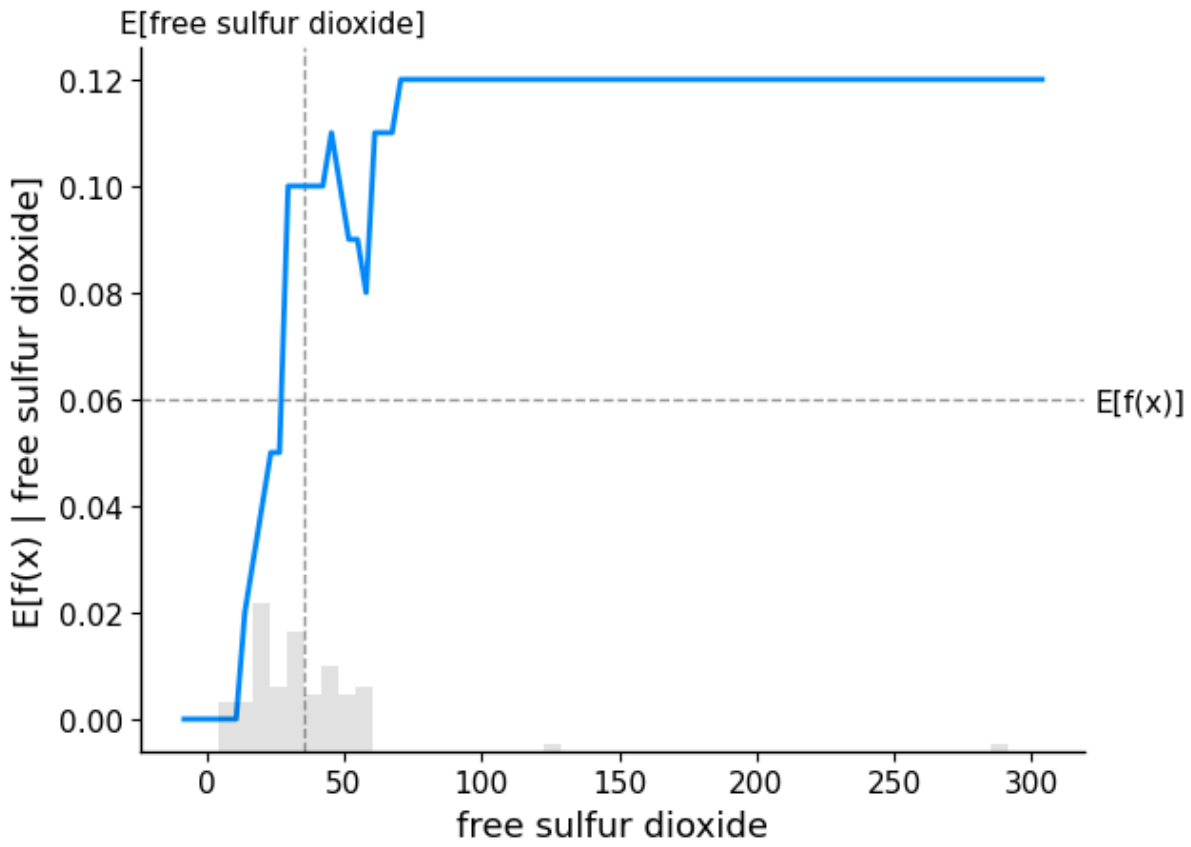


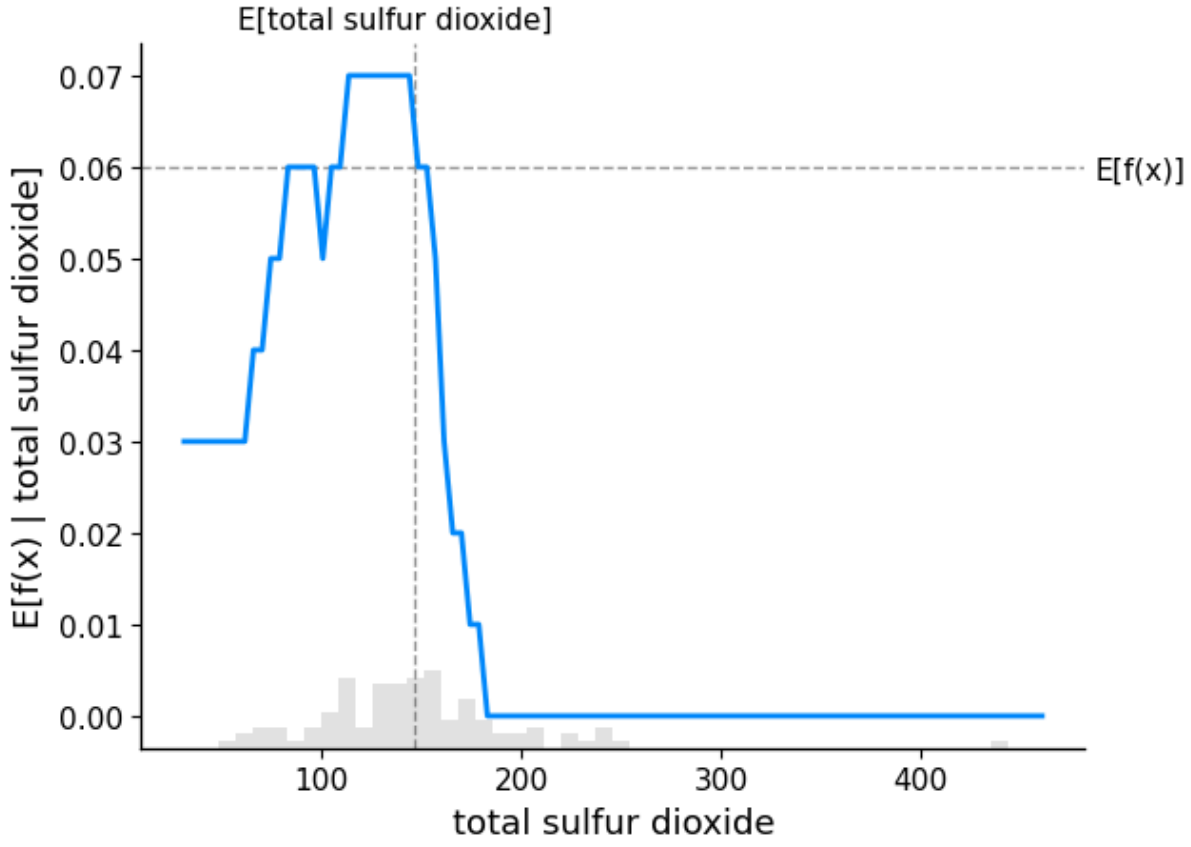

E[volatile acidity]
0.18
0.16
0.14
0.12
0.10
0.08
0.06
0.04
0.02
E[f(x) | volatile acidity]
E[f(x)]
0.1
0.2
0.3
0.4
0.5
0.6
0.7
volatile acidity

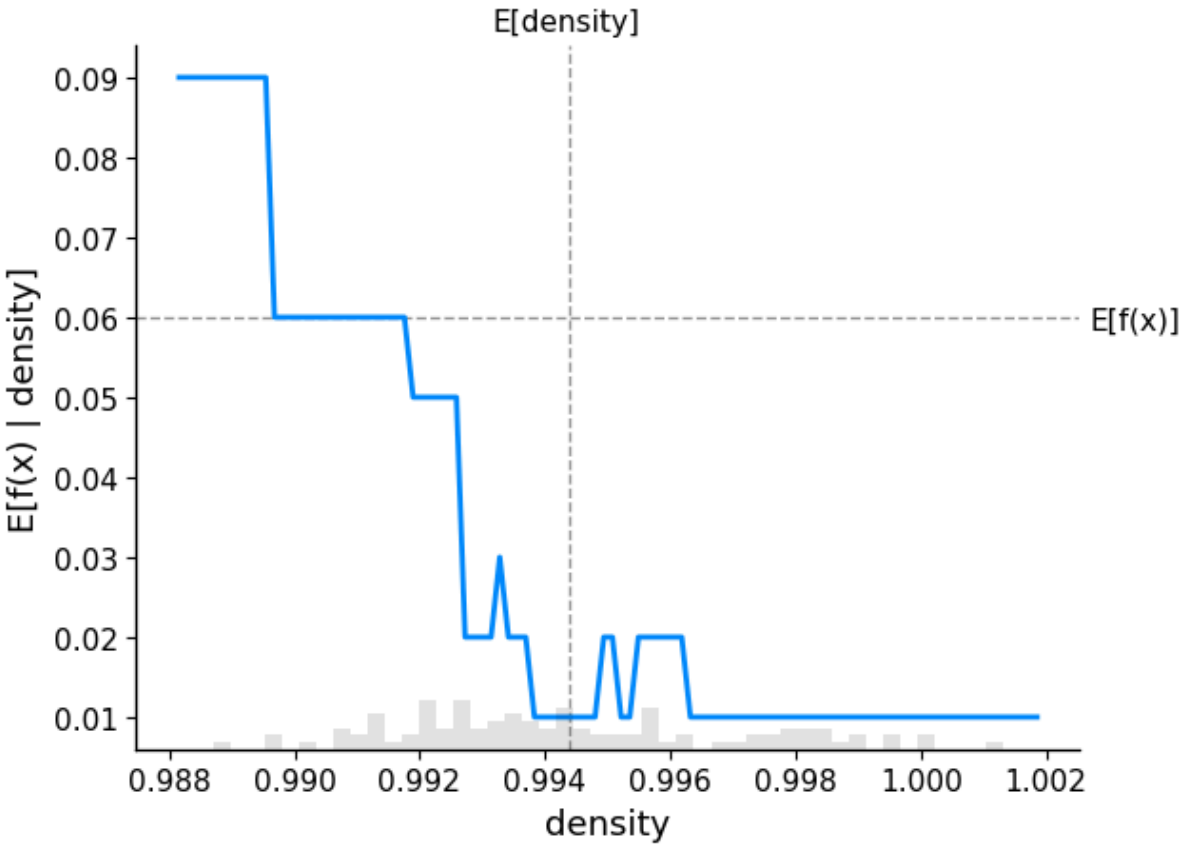

E[citric acid]
0.07
0.06
0.05
0.04
0.03
0.02
0.01
E[f(x) | citric acid]
E[f(x)]
0.0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
citric acid

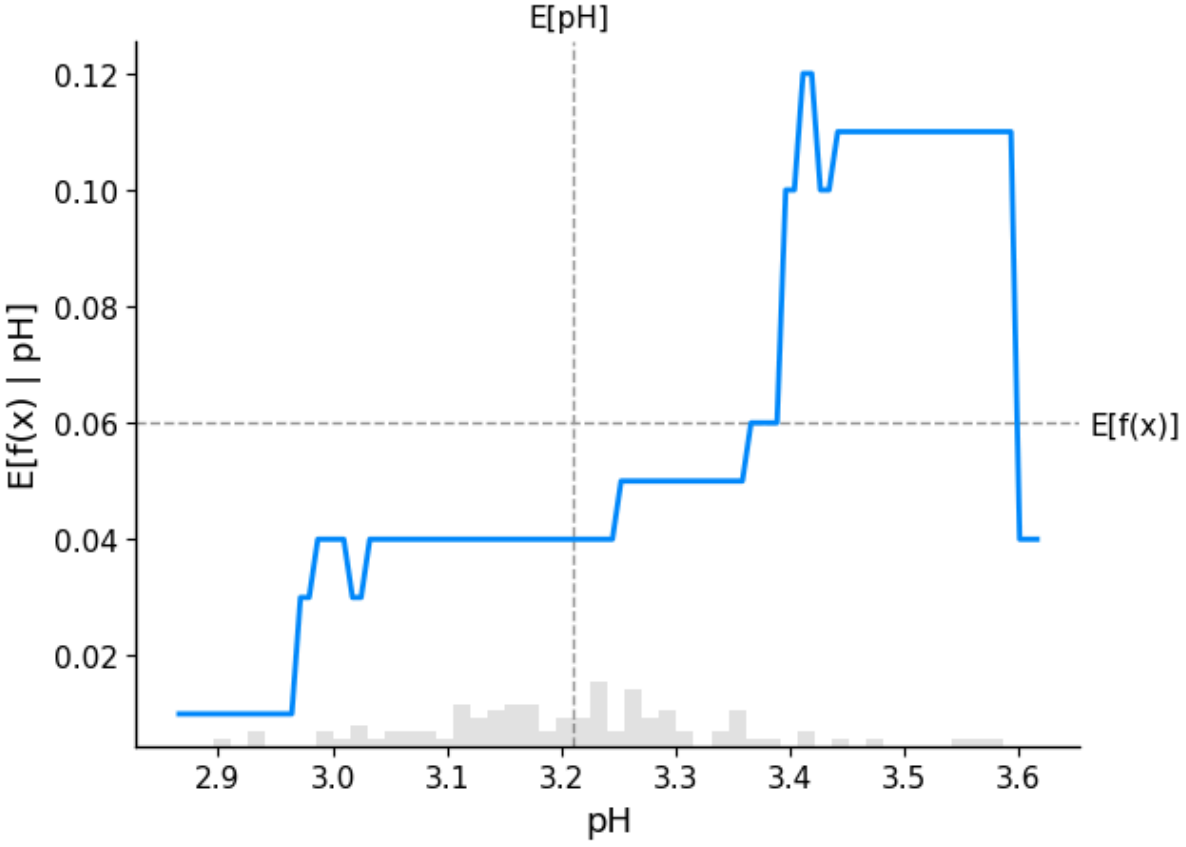

E[residual sugar]
E[f(x) | residual sugar]
0.10
0.08
0.06
0.04
0.02
0.00
E[f(x)]
0
5
10
15
20
residual sugar

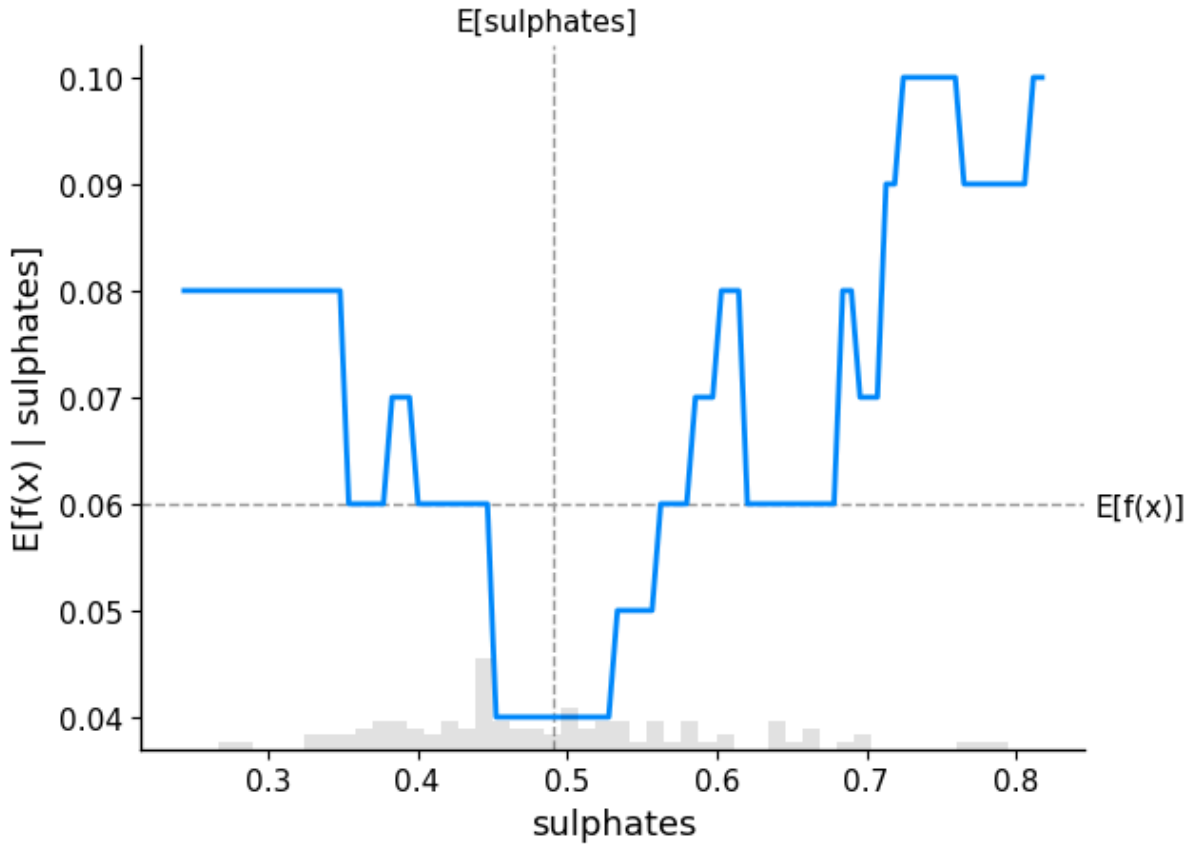

E[chlorides]
E[f(x) | chlorides]
0.10
0.08
0.06
0.04
0.02
0.00
E[f(x)]
0.025
0.050
0.075
0.100
0.125
0.150
0.175
0.200
chlorides

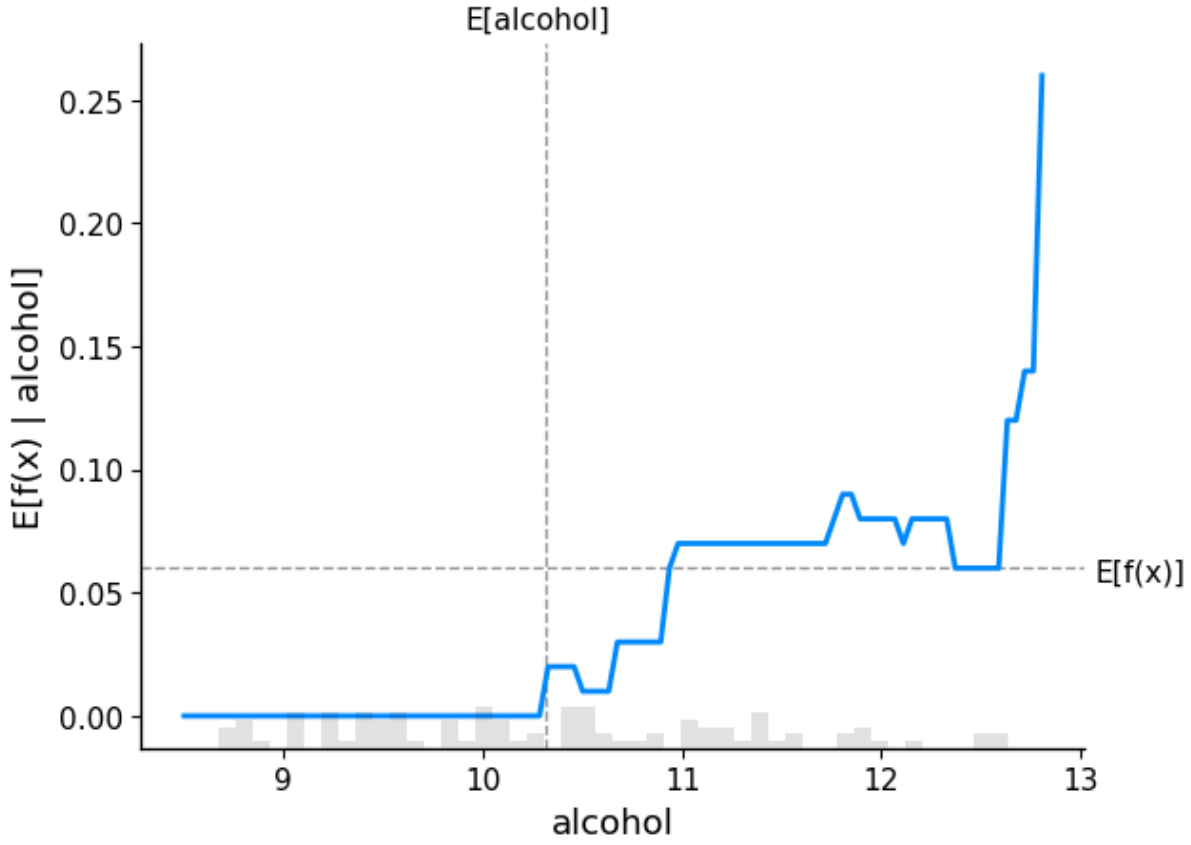

E[free sulfur dioxide]
0.12
0.10
0.08
0.06
0.04
0.02
0.00
E[f(x) | free sulfur dioxide]
E[f(x)]
0
50
100
150
200
250
300
free sulfur dioxide


E[total sulfur dioxide]
0.07
0.06
0.05
0.04
0.03
0.02
0.01
0.00
E[f(x) | total sulfur dioxide]
E[f(x)]
100
200
300
400
total sulfur dioxide


E[density]
E[f(x) | density]
E[f(x)]
0.09
0.08
0.07
0.06
0.05
0.04
0.03
0.02
0.01
0.988
0.990
0.992
0.994
0.996
0.998
1.000
1.002
density


E[pH]
E[f(x) | pH]
E[f(x)]
0.12
0.10
0.08
0.06
0.04
0.02
2.9
3.0
3.1
3.2
3.3
3.4
3.5
3.6
pH





We can see that for certain features, it's quite messy. And for other, it may indicate a sweeetspot.

For example, for the chlorides. Here it is clear that the value have a range considered as good. And everything outside of this is bad. It is even clearer with the `total sulfur dioxide`, everything greater than ~150 is considered bad.

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

After some searching, some findings that I got are quite well aligned with the resources I found. For example, the chlorides. Apprently, you want to keep the chlorides as low as possible to get a good white wine.

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?

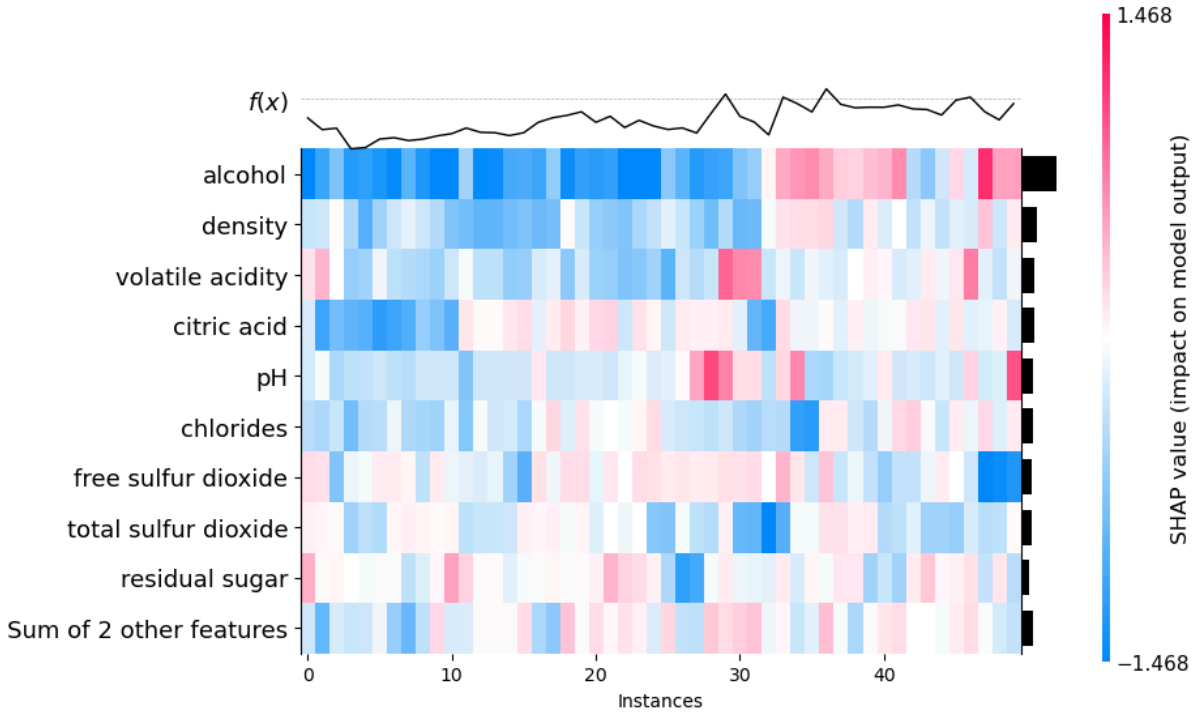
```
from shap import TreeExplainer


explainer = TreeExplainer(bestModel)
encoded = lblEncoder.transform(["bad"])[0]
mask = y_train == encoded

shap_values = explainer(x_train[mask])
```

```
x_train[mask]
```

```
      fixed acidity  volatile acidity  citric acid  residual sugar  chlorides  \
303             6.8              0.22         0.30            10.6      0.070
4671            7.3              0.17         0.23             6.3      0.051
2836            6.2              0.24         0.25            12.5      0.055
3862            8.9              0.33         0.32             1.5      0.047
500             6.6              0.32         0.27            10.9      0.041
...             ...               ...          ...             ...        ...
1112            8.1              0.26         0.37             1.9      0.072
5170            6.3              0.31         0.30            10.0      0.046
2453            7.6              0.29         0.29             4.4      0.051
3001            6.6              0.38         0.36             9.2      0.061
2665            8.3              0.16         0.48             1.7      0.057

      free sulfur dioxide  total sulfur dioxide  density    pH  sulphates  \
303                  67.0                 194.0  0.99654  2.89       0.42
4671                 35.0                 240.0  0.99630  3.36       0.54
2836                 47.0                 134.0  0.99758  3.30       0.51
3862                 11.0                 200.0  0.99540  3.19       0.46
500                  37.0                 146.0  0.99630  3.24       0.47
...                   ...                   ...      ...   ...        ...
1112                 48.0                 159.0  0.99490  3.37       0.70
5170                 49.0                 212.0  0.99620  3.74       0.55
2453                 26.0                 146.0  0.99390  3.16       0.39
3001                 42.0                 214.0  0.99760  3.31       0.56
2665                 31.0                  98.0  0.99430  3.15       0.41

      alcohol
303       9.0
4671     10.0
2836      9.0
```

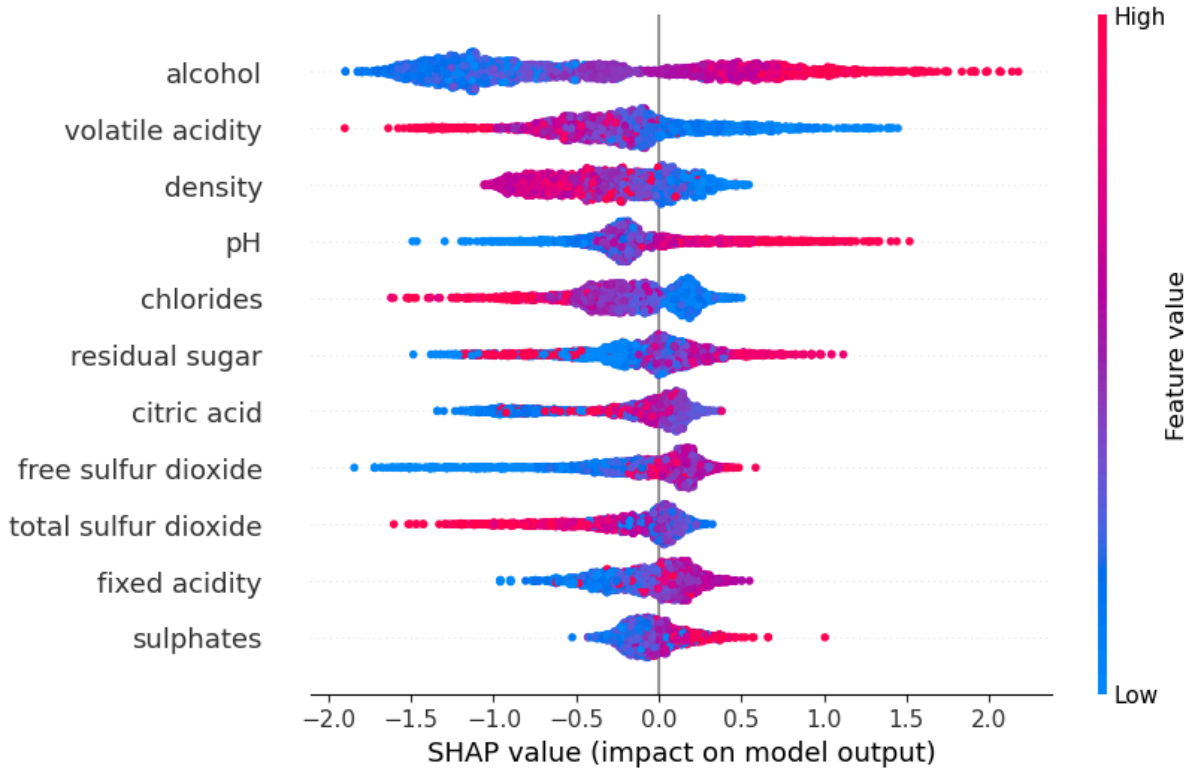
```
3862      9.4
500      10.0
...       ...
1112     10.9
5170     11.9
2453     10.2
3001      9.4
2665     10.3

[3084 rows x 11 columns]
```

```
shap.plots.heatmap(shap_values[:50])
```




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

```
shap.plots.beeswarm(shap_values, max_display=12)
```



As we can see, our model saw some good wines with great content in alcohol. So our model has a great weight on the alcohol feature. And this causes some missclassification. But one feature that seems to be quite correct is the chlorides. The lowest the better

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.

The limitations of our model are pretty clear. It will only see correlations between features and target. As so, the correlation might be founded, or not.

In our case, a correlation that is incorrect (but works well with our dataset) is that the higher the alcohol, the higher the quality. We as humans, know it's false. But our model saw this correlation, and putted a great weight on it.

But, for correlations that are founded, our model is really handy in predicting the quality of a wine. For example, our model showed that a higher rate of chlorides is really not good for a white wine. As no entries with a high rate of chlorides got a positive quality.

Our model doesn't understand the relations between chemicals either. For example, a wine with a greater sugar rate, but a greater acidity might be good, as the acidity will balance out the sugar. But if there is no acidity, the wine might not be good. Those relations, if rare, are very hard for our model to catch.

After thos considerations, we can analyse a bit more what our model tells us.

First, the volatile acidity. A lower volatile acidity seems to be better for a white wine. There is a zone which is quite neutral, but too high, and the quality of the wine drops.

It’s quite the same for some features. For example total sulfur dioxide. Those feature are quite neutral, or quite bad. But doesn’t pull the quality up. It means that our model didn’t see a clear causality between those feature and a good wine, but found that if those values outside of a certain range, the quality drops.

For others, like citric acid, we can see that our model can’t really tell anything with it. Are some low value are considered good and bad. So it didn’t found any correlation betweem them and the quality of the wine.

And finally, features like sulphates seems to almost only have a positive impact on the wine.

Tips on improving wine quality

After those observations, we know that we can focus on some wine feature, to avoid a drop in wine quality.

For example, you could try to keep the total sulfur dioxide rate low by :

- Minimizing oxidation early, by limiting the grape exposure to oxygen
- Keeping fermentation temperature cool (around 15-18℃)

Or you could try to keep the chlorides level low by :

- Using low-chloride water during all the winemaking preprocess
- Avoid using fertilizers or pesticides that contains chlorides