Classification by Wine Type

Wine Data

Data from http://archive.ics.uci.edu/ml/datasets/Wine+Quality (http://archive.ics.uci.edu/ml/datasets/Wine+Quality)

Citations


```
Dua, D. and Karra Taniskidou, E. (2017).
UCI Machine Learning Repository [http://archive.ics.uci.edu/ml/index.php].
Irvine, CA: University of California, School of Information and Computer Science.

P. Cortez, A. Cerdeira, F. Almeida, T. Matos and J. Reis.
Modeling wine preferences by data mining from physicochemical properties.
In Decision Support Systems, Elsevier, 47(4):547-553. ISSN: 0167-9236.
```


Available at:

- @Elsevier (http://dx.doi.org/10.1016/j.dss.2009.05.016)
- Pre-press (pdf) (http://www3.dsi.uminho.pt/pcortez/winequality09.pdf)
- bib (http://www3.dsi.uminho.pt/pcortez/dss09.bib) ## Setup

In [1]:
```
%matplotlib inline

import matplotlib.pyplot as plt
import numpy as np
import pandas as pd
import seaborn as sns
```

Read in the data:

In [2]:
```
red_wine = pd.read_csv('data/winequality-red.csv')
white_wine = pd.read_csv('data/winequality-white.csv', sep=';')
```

EDA

In [3]:
```
white_wine.head()
```

Out[3]:

	fixed acidity	volatile acidity	citric acid	residual sugar	chlorides	free sulfur dioxide	total sulfur dioxide	density	pH	sulphates	alcohol
0	7.0	0.27	0.36	20.7	0.045	45.0	170.0	1.0010	3.00	0.45	8.8
1	6.3	0.30	0.34	1.6	0.049	14.0	132.0	0.9940	3.30	0.49	9.5
2	8.1	0.28	0.40	6.9	0.050	30.0	97.0	0.9951	3.26	0.44	10.1
3	7.2	0.23	0.32	8.5	0.058	47.0	186.0	0.9956	3.19	0.40	9.9
4	7.2	0.23	0.32	8.5	0.058	47.0	186.0	0.9956	3.19	0.40	9.9

In [4]:
```
red_wine.head()
```

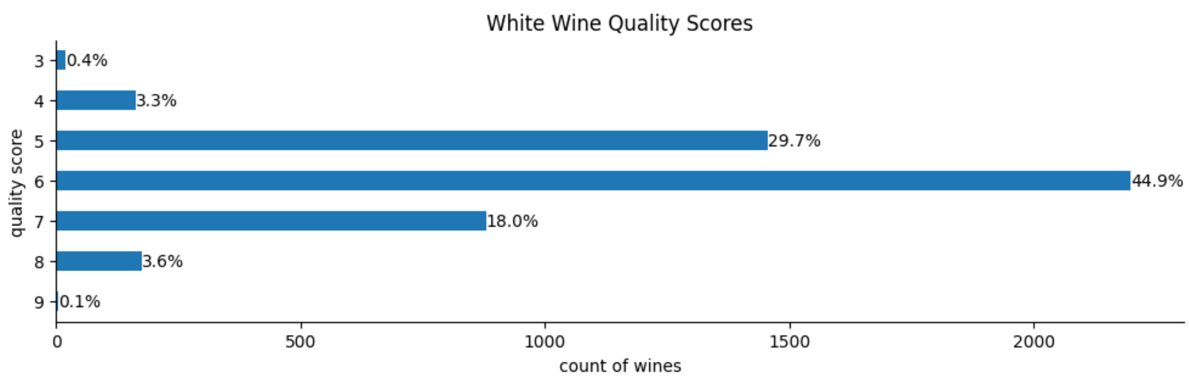
Out[4]:

	fixed acidity	volatile acidity	citric acid	residual sugar	chlorides	free sulfur dioxide	total sulfur dioxide	density	pH	sulphates	alcohol
0	7.4	0.70	0.00	1.9	0.076	11.0	34.0	0.9978	3.51	0.56	9.4
1	7.8	0.88	0.00	2.6	0.098	25.0	67.0	0.9968	3.20	0.68	9.8
2	7.8	0.76	0.04	2.3	0.092	15.0	54.0	0.9970	3.26	0.65	9.8
3	11.2	0.28	0.56	1.9	0.075	17.0	60.0	0.9980	3.16	0.58	9.8
4	7.4	0.70	0.00	1.9	0.076	11.0	34.0	0.9978	3.51	0.56	9.4

Looking at quality scores

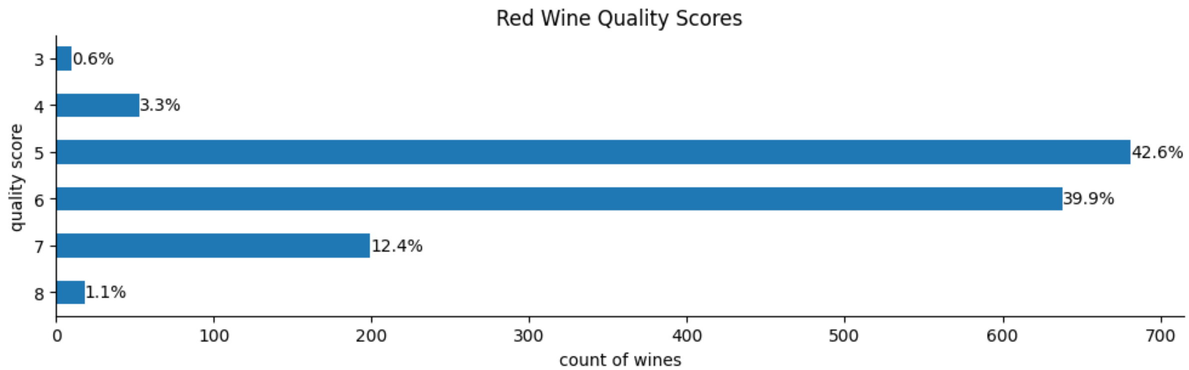
In [5]:
```
def plot_quality_scores(df, kind):
    ax = df.quality.value_counts().sort_index().plot.barh(
        title=f'{kind.title()} Wine Quality Scores', figsize=(12, 3)
    )
    ax.axes.invert_yaxis()
    for bar in ax.patches:
        ax.text(
            bar.get_width(),
            bar.get_y() + bar.get_height()/2,
            f'{bar.get_width()/df.shape[0]:.1%}',
            verticalalignment='center'
        )
    plt.xlabel('count of wines')
    plt.ylabel('quality score')

    for spine in ['top', 'right']:
        ax.spines[spine].set_visible(False)

    return ax

plot_quality_scores(white_wine, 'white')
```

Out[5]:
```
<AxesSubplot:title={'center':'White Wine Quality Scores'}, xlabel='count of w
ines', ylabel='quality score'>
```



In [6]:
```
plot_quality_scores(red_wine, 'red')
```

Out[6]:
```
<AxesSubplot:title={'center':'Red Wine Quality Scores'}, xlabel='count of win
es', ylabel='quality score'>
```



Combining red and white wine data

In [7]:
```
wine = pd.concat([
    white_wine.assign(kind='white'), red_wine.assign(kind='red')
])
wine.sample(5, random_state=10)
```

Out[7]:

	fixed acidity	volatile acidity	citric acid	residual sugar	chlorides	free sulfur dioxide	total sulfur dioxide	density	pH	sulphates	alcol
848	6.4	0.64	0.21	1.8	0.081	14.0	31.0	0.99689	3.59	0.66	
2529	6.6	0.42	0.13	12.8	0.044	26.0	158.0	0.99772	3.24	0.47	
131	5.6	0.50	0.09	2.3	0.049	17.0	99.0	0.99370	3.63	0.63	1
244	15.0	0.21	0.44	2.2	0.075	10.0	24.0	1.00005	3.07	0.84	
1551	6.6	0.19	0.99	1.2	0.122	45.0	129.0	0.99360	3.09	0.31	

No null data:

In [8]:
```
wine.info()
```

```
<class 'pandas.core.frame.DataFrame'>
Int64Index: 6497 entries, 0 to 1598
Data columns (total 13 columns):
 #   Column                Non-Null Count  Dtype  
---  ------                --------------  -----  
 0   fixed acidity         6497 non-null   float64
 1   volatile acidity      6497 non-null   float64
 2   citric acid           6497 non-null   float64
 3   residual sugar        6497 non-null   float64
 4   chlorides             6497 non-null   float64
 5   free sulfur dioxide   6497 non-null   float64
 6   total sulfur dioxide  6497 non-null   float64
 7   density               6497 non-null   float64
 8   pH                    6497 non-null   float64
 9   sulphates             6497 non-null   float64
 10  alcohol               6497 non-null   float64
 11  quality               6497 non-null   int64  
 12  kind                  6497 non-null   object 
dtypes: float64(11), int64(1), object(1)
memory usage: 710.6+ KB
```

We have more whites than reds:

In [9]:
```
wine.kind.value_counts()
```

Out[9]:
```
white    4898
red      1599
Name: kind, dtype: int64
```

We want to understand if chemical properties can be used to determine wine type. Unfortunately, `describe()` gives a very long output, so we need a visualization to compare the wines this way:

In [10]:
```
wine.drop(columns='quality').groupby('kind').describe()
```

Out[10]:

	fixed acidity								volatile acidity		...	sulphates	
	count	mean	std	min	25%	50%	75%	max	count	mean	...	75%	max
kind													
red	1599.0	8.319637	1.741096	4.6	7.1	7.9	9.2	15.9	1599.0	0.527821	...	0.73	2.00
white	4898.0	6.854788	0.843868	3.8	6.3	6.8	7.3	14.2	4898.0	0.278241	...	0.55	1.08

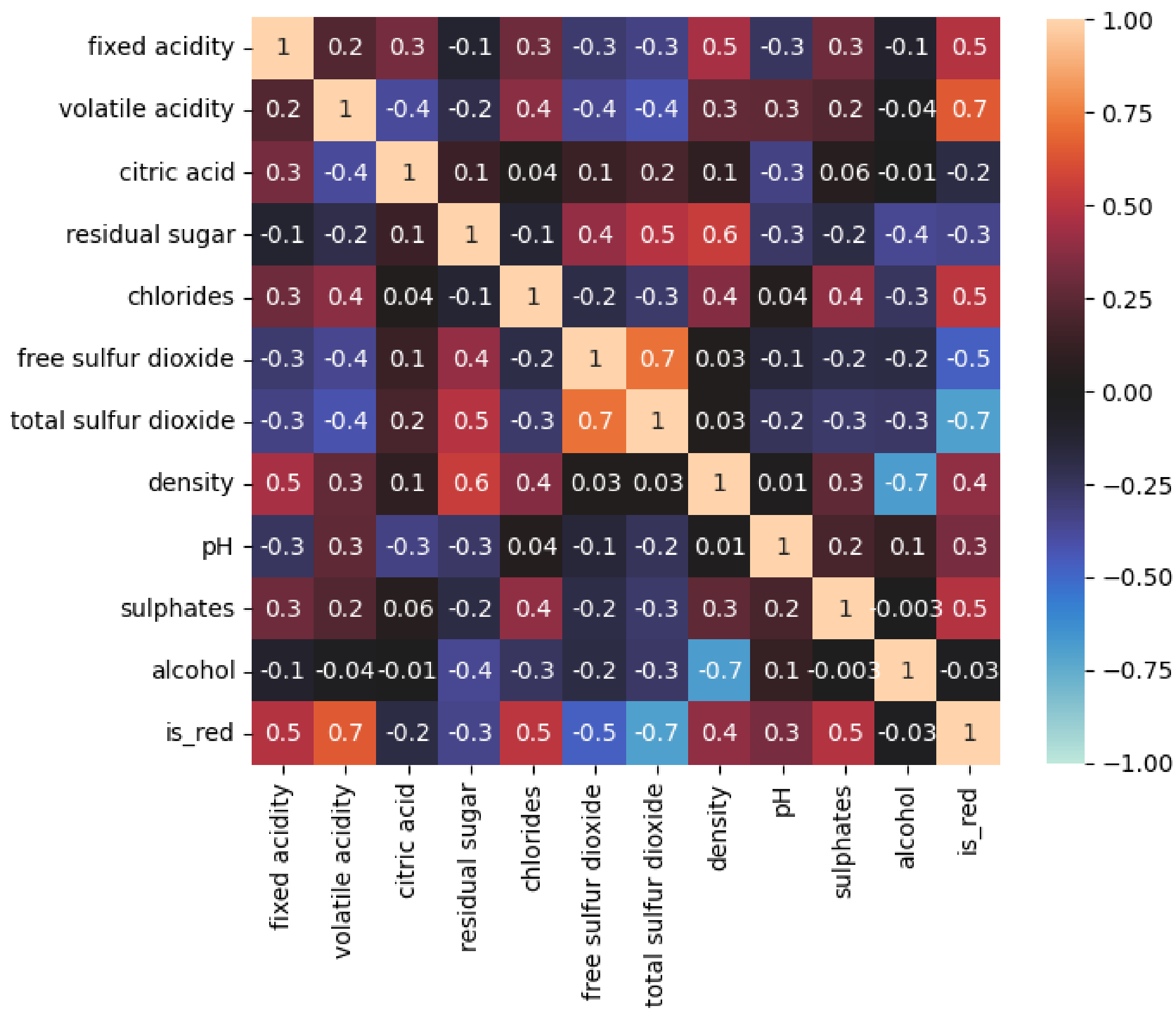
2 rows × 88 columns

How do chemical properties of the wine correlate to each other and the wine type?

It's important to perform an in-depth exploration of the data before modeling. This includes consulting domain experts, looking for correlations between variables, examining distributions, etc. The visualizations covered in chapters 5 and 6 will prove indispensible for this process. One such visualization is the heatmap. In order to predict if the wine is red or white, we would look for correlations between chemical properties and wine type. We would also try to see if there is a difference in the distribution of our variables for white versus red wines. Some other helpful plot types include box plots, pair plots, and the scatter matrix.

In [11]:
```
fig = plt.figure(figsize=(7, 7))
sns.heatmap(
    wine.drop(columns='quality').assign(
        is_red=lambda x: np.where(x.kind == 'red', 1, 0)
    ).corr(),
    cbar_kws={'shrink': 0.8},
    center=0, vmin=-1, vmax=1,
    square=True, annot=True, fmt='.1g'
)
```

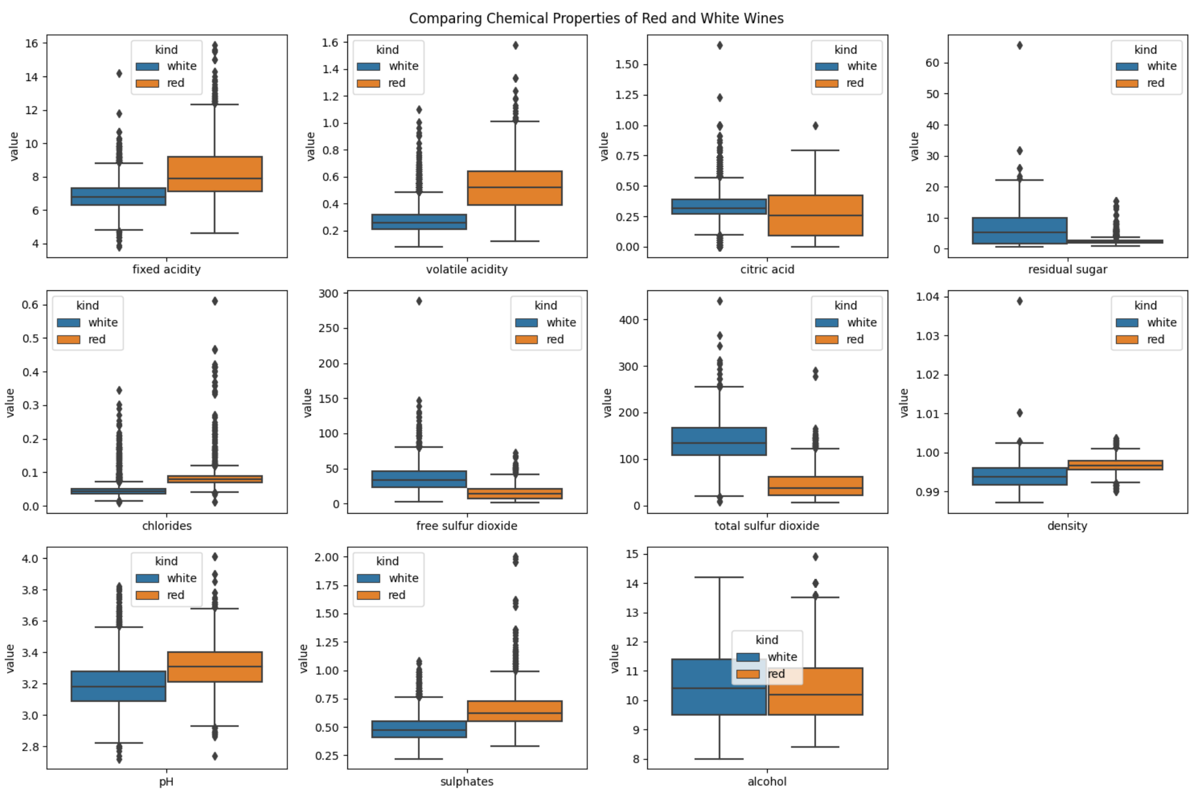
Out[11]: <AxesSubplot:>



Comparison of Red and White Wines by Their Chemical Properties

This visualization will be easier to digest than the output of `describe()` :

In [17]:
```
import math

chemical_properties = [col for col in wine.columns if col not in ['quality',
'kind']]
melted = wine.drop(columns='quality').melt(id_vars=['kind'])

fig, axes = plt.subplots(math.ceil(len(chemical_properties) / 4), 4, figsize=
(15, 10))
axes = axes.flatten()

for prop, ax in zip(chemical_properties, axes):
    sns.boxplot(
        data=melted[melted.variable.isin([prop])],
        x='variable', y='value', hue='kind', ax=ax
    ).set_xlabel('')

# remove the extra subplots
for ax in axes[len(chemical_properties):]:
    ax.remove()

plt.suptitle('Comparing Chemical Properties of Red and White Wines')
plt.tight_layout()
```



Classification of Red and White Wines

1. separate x and y
2. get the training and testing set

In [18]:
```
from sklearn.model_selection import train_test_split

# 1
wine_y = np.where(wine.kind == 'red', 1, 0)
wine_X = wine.drop(columns=['quality', 'kind'])

# 2
w_X_train, w_X_test, w_y_train, w_y_test = train_test_split(
    wine_X, wine_y, test_size=0.25, random_state=0, stratify=wine_y
)
```

1. build a pipeline with standard scaler followed by logistic regression and fit the model

In [19]:
```
from sklearn.linear_model import LogisticRegression
from sklearn.pipeline import Pipeline
from sklearn.preprocessing import StandardScaler

white_or_red = Pipeline([
    ('scale', StandardScaler()),
    ('lr', LogisticRegression(random_state=0))
]).fit(w_X_train, w_y_train)
```

1. make predictions

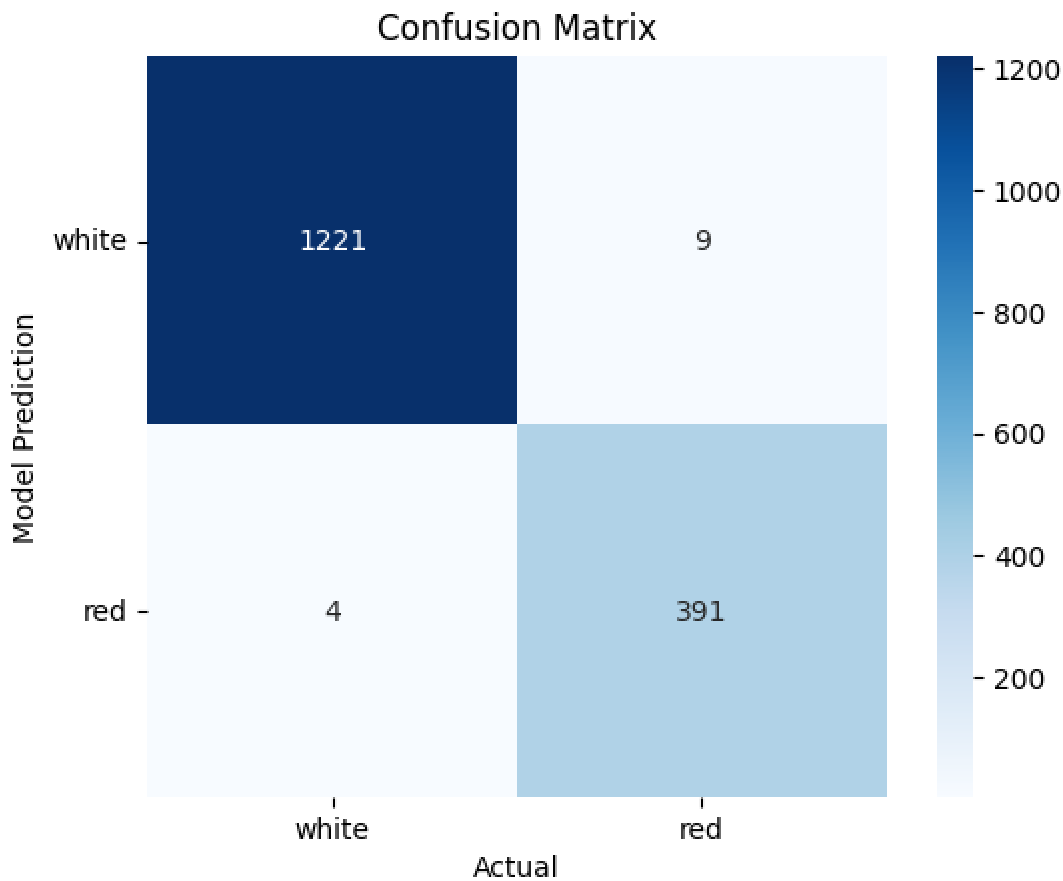
In [20]:
```
kind_preds = white_or_red.predict(w_X_test)
```

1. evaluate predictions

We can use a confusion matrix to see how the model's predictions align with the actual class labels. The model only made 13 incorrect predictions; we will look into these in chapter 10:

In [21]:
```python
from ml_utils.classification import confusion_matrix_visual

confusion_matrix_visual(w_y_test, kind_preds, ['white', 'red'])
```

Out[21]:
```
<AxesSubplot:title={'center':'Confusion Matrix'}, xlabel='Actual', ylabel='Mo
del Prediction'>
```



Precision, recall, and F_1 score all look good with this model:

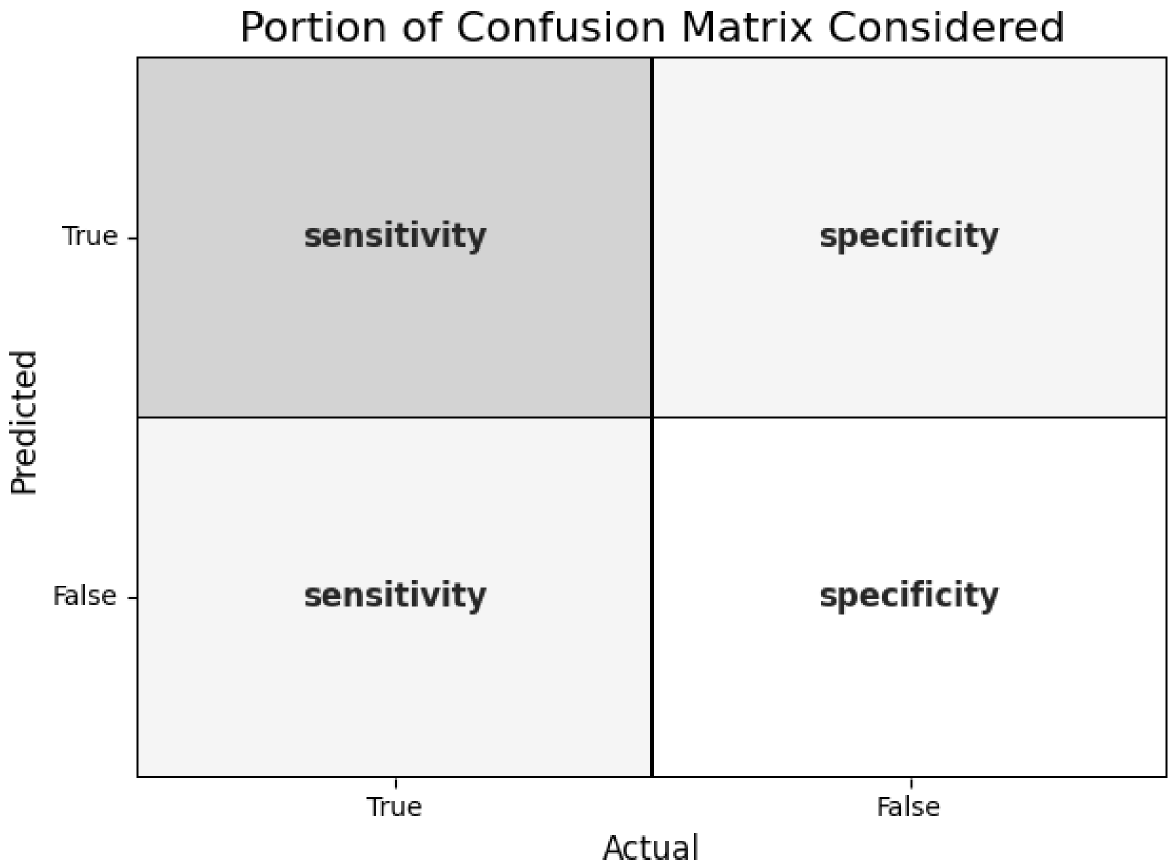
In [22]:
```python
from sklearn.metrics import classification_report
print(classification_report(w_y_test, kind_preds))
```

```
              precision    recall  f1-score   support

           0       0.99      1.00      0.99      1225
           1       0.99      0.98      0.98       400

    accuracy                           0.99      1625
   macro avg       0.99      0.99      0.99      1625
weighted avg       0.99      0.99      0.99      1625
```

Another way to use the confusion matrix is with sensitivity and specificity:

In [23]:
```
from visual_aids import ml_viz
ml_viz.portion_of_confusion_matrix_considered({'sensitivity', 'specificity'})
```

Out[23]: <AxesSubplot:title={'center':'Portion of Confusion Matrix Considered'}, xlabel='Actual', ylabel='Predicted'>



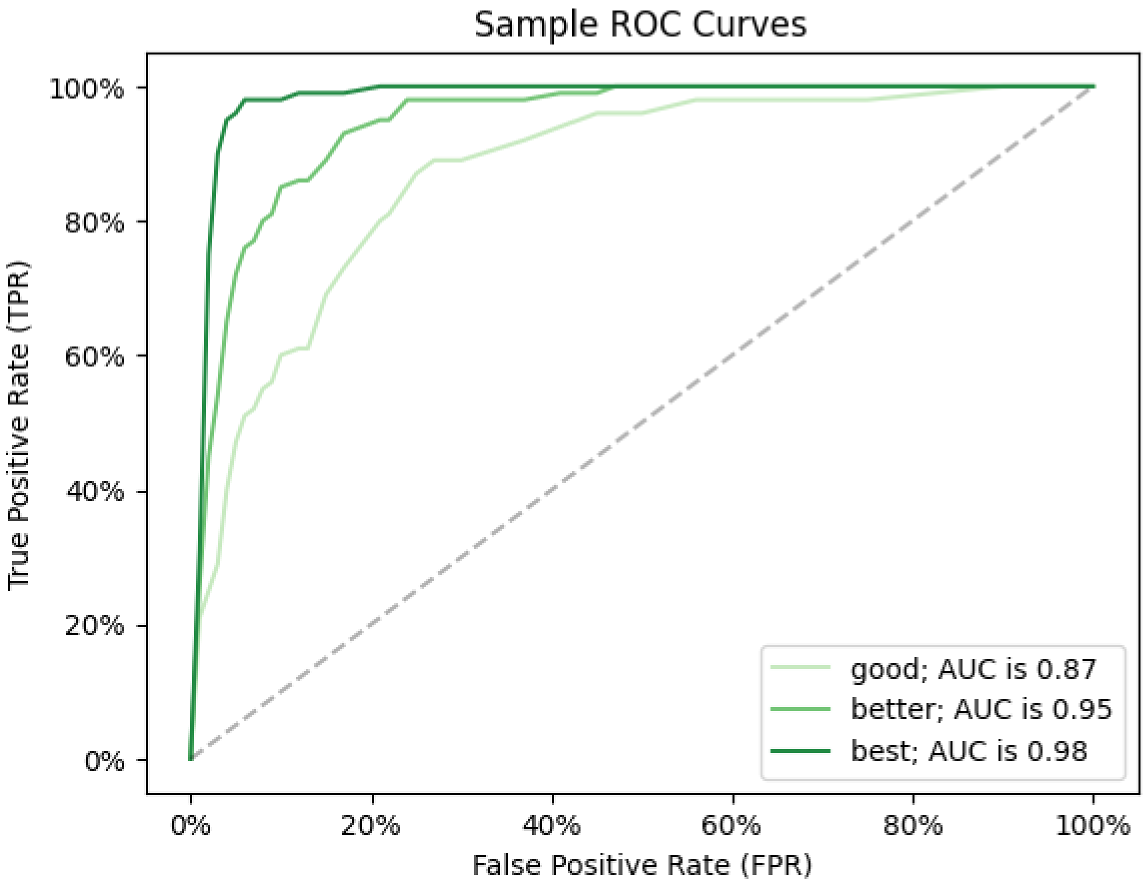
Sensitivity-specificity plots plot sensitivity (TPR) versus 1-specificity (FPR) and are another way to evaluate performance. They include all sections of the confusion matrix, which is why in cases of class balance, they are optimistic of performance. These plots are also called ROC curves.

ROC Curves

Visualize model performance using true positive rates and false positive rates. The area under the curve is in the range [0, 1] with 1 being the best. This visualization allows us to compare our model to the baseline of random guessing (the diagonal line with AUC of 0.5), as well as, other models:

In [24]:
```
ml_viz.roc_curve()
```

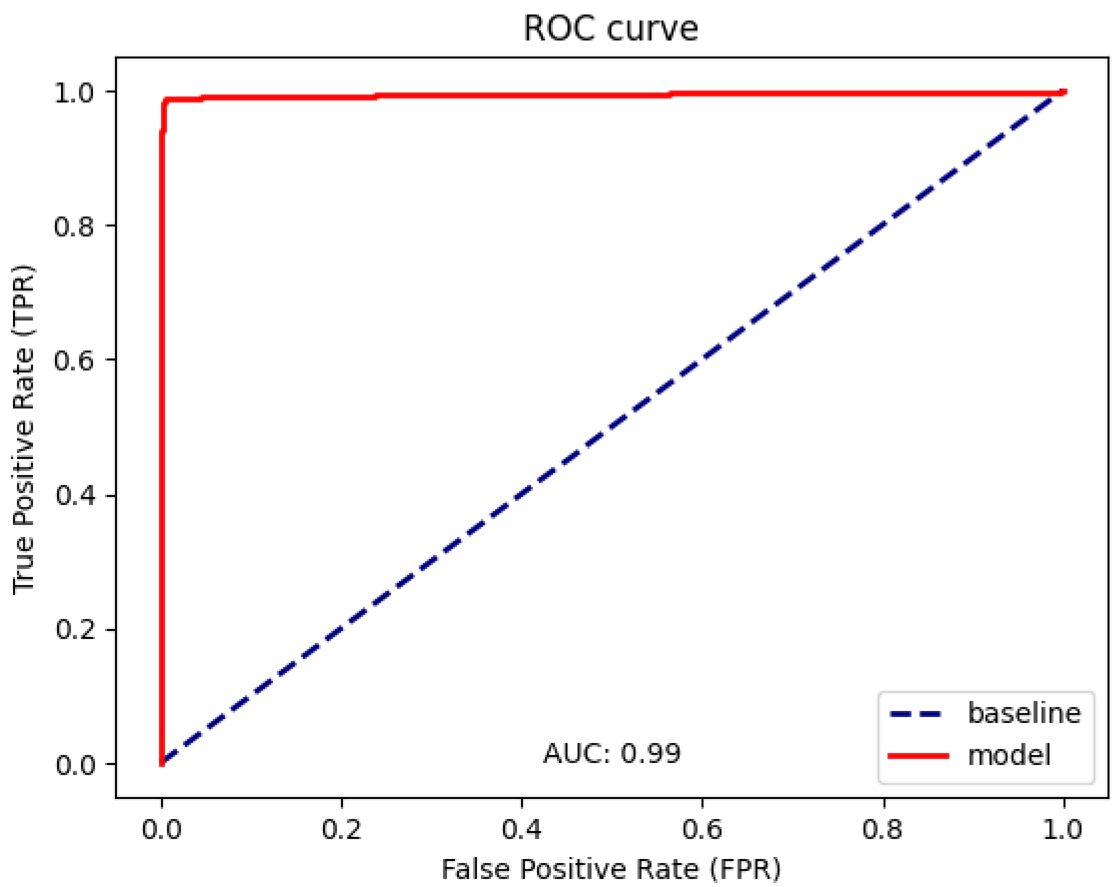
Out[24]: <AxesSubplot:title={'center':'Sample ROC Curves'}, xlabel='False Positive Rate (FPR)', ylabel='True Positive Rate (TPR)'>



This model performs very well, the area under the curve (AUC) is nearly 1:

In [25]:
```
from ml_utils.classification import plot_roc

plot_roc(w_y_test, white_or_red.predict_proba(w_X_test)[:,1])
```

Out[25]:
```
<AxesSubplot:title={'center':'ROC curve'}, xlabel='False Positive Rate (FP
R)', ylabel='True Positive Rate (TPR)'>
```

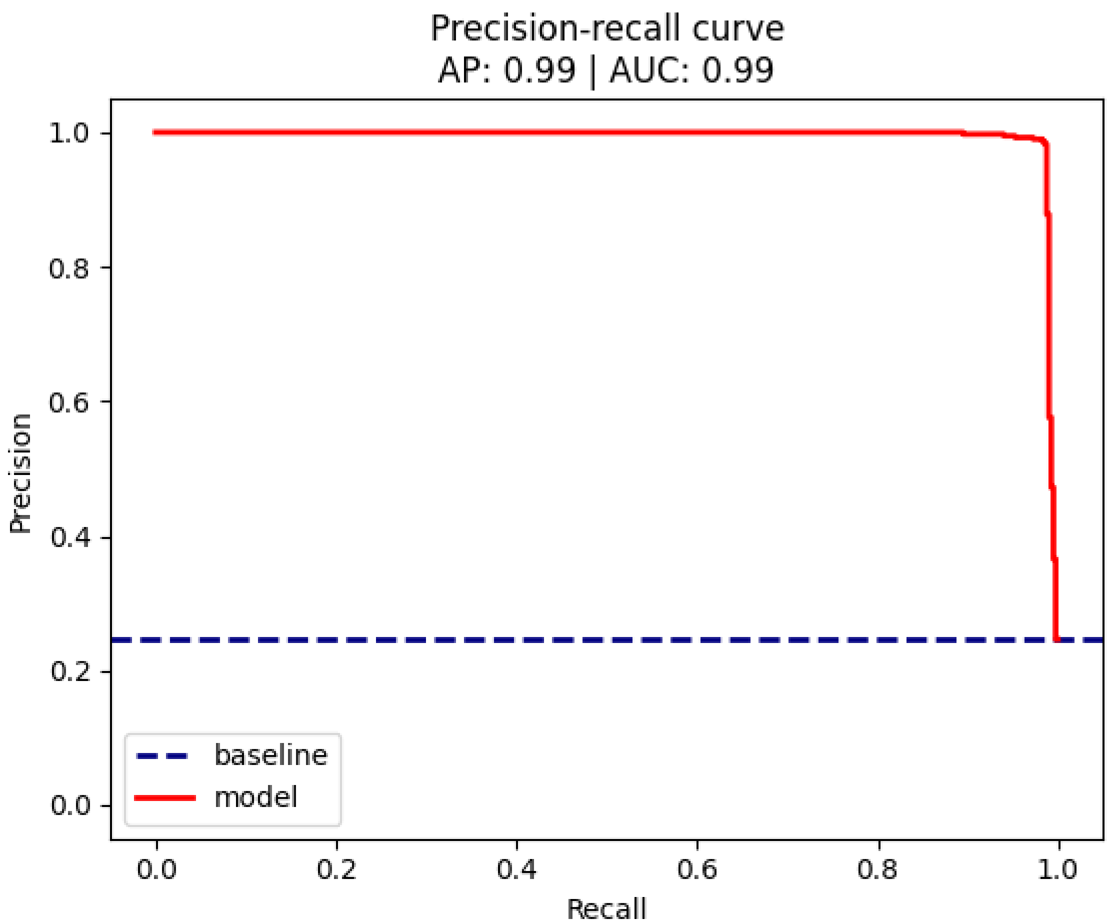


Precision-recall curves

When faced with class imbalance, we use precision-recall curves since ROC curves will be optimistic of model performance. AP is the weighted average precision and AUC is the area under the curve once again in the range [0, 1]. The baseline is now the percentage of observations belonging to the positive class. Values below this line are worse than random:

In [27]:
```
from ml_utils.classification import plot_pr_curve

plot_pr_curve(w_y_test, white_or_red.predict_proba(w_X_test)[:,1])
```

Out[27]:
```
<AxesSubplot:title={'center':'Precision-recall curve\nAP: 0.99 | AUC: 0.99'},
xlabel='Recall', ylabel='Precision'>
```



← Chapter 8 (../../ch_08/anomaly_detection.ipynb) Preprocessing (./preprocessing.ipynb) Planets (./planets_ml.ipynb) Red Wine (./red_wine.ipynb)
</div> Solutions (../../solutions/ch_09/exercise_1.ipynb) Chapter 10 → (../ch_10/red_wine.ipynb)

In [ ]: