notebook10

June 2, 2024

```
[1]: # MSDS 422 - Section 55

# Spring '24

# Module 05 - Midpoint check in for final project

# Initial EDA

# Kevin Geidel

import numpy as np
import pandas as pd
import os
import settings # runs commands that sets base paths, configures

→ behavors, etc
import utils # defines functions used throughout
```

EDA: Data source

```
[2]: # Load the dataset

from scipy.io.arff import loadarff

arff_name = 'wine.arff'

raw_data = loadarff(
    os.path.join(settings.DATA_PATH, arff_name)
)
data = pd.DataFrame(raw_data[0])

data.head()
```

```
[2]:
       Alcohol Malic_acid
                            Ash Alcalinity_of_ash Magnesium Total_phenols \
         14.23
                      1.71 2.43
                                              15.6
                                                                        2.80
    0
                                                        127.0
         13.20
                                              11.2
                                                                       2.65
    1
                      1.78 2.14
                                                        100.0
         13.16
                      2.36 2.67
                                              18.6
                                                                       2.80
                                                        101.0
    3
         14.37
                      1.95 2.50
                                              16.8
                                                        113.0
                                                                       3.85
         13.24
                      2.59 2.87
                                              21.0
                                                        118.0
                                                                       2.80
```

```
Flavanoids Nonflavanoid_phenols Proanthocyanins Color_intensity Hue \0 3.06 0.28 2.29 5.64 1.04
```

```
2.76
     1
                                    0.26
                                                      1.28
                                                                       4.38 1.05
     2
              3.24
                                    0.30
                                                                       5.68 1.03
                                                      2.81
     3
              3.49
                                    0.24
                                                      2.18
                                                                       7.80 0.86
     4
              2.69
                                                                       4.32 1.04
                                    0.39
                                                      1.82
        OD280/OD315_of_diluted_wines Proline binaryClass
     0
                                3.92
                                       1065.0
     1
                                3.40
                                       1050.0
                                                      b'N'
     2
                                3.17
                                       1185.0
                                                      b'N'
     3
                                3.45
                                       1480.0
                                                      b'N'
     4
                                2.93
                                        735.0
                                                      b'N'
[3]: # Examine the dataset
     data.info()
    <class 'pandas.core.frame.DataFrame'>
    RangeIndex: 178 entries, 0 to 177
    Data columns (total 14 columns):
     #
         Column
                                        Non-Null Count
                                                        Dtype
         ____
                                        _____
                                                        ____
     0
         Alcohol
                                        178 non-null
                                                        float64
                                        178 non-null
                                                        float64
     1
         Malic_acid
     2
                                        178 non-null
                                                        float64
         Ash
     3
         Alcalinity_of_ash
                                        178 non-null
                                                        float64
     4
         Magnesium
                                        178 non-null
                                                        float64
     5
         Total_phenols
                                        178 non-null
                                                        float64
         Flavanoids
     6
                                        178 non-null
                                                        float64
     7
         Nonflavanoid_phenols
                                        178 non-null
                                                        float64
         Proanthocyanins
                                        178 non-null
                                                        float64
     9
         Color_intensity
                                        178 non-null
                                                        float64
     10 Hue
                                        178 non-null
                                                        float64
         OD280/OD315_of_diluted_wines 178 non-null
                                                        float64
     12 Proline
                                        178 non-null
                                                        float64
     13 binaryClass
                                        178 non-null
                                                        object
    dtypes: float64(13), object(1)
    memory usage: 19.6+ KB
```

```
[4]: # The target (binaryClass) happens to be the only caterorical (in this case boolean) variable

# but still, we look at each one

data.select_dtypes(include=[object]).value_counts()
```

[4]: binaryClass
b'N' 107
b'P' 71

Name: count, dtype: int64

```
[5]: # We are going to encode the boolean values later anyways
     # let's address this now so we can use the target in the rest of the EDA
     data['isWine'] = data['binaryClass'].replace({b'N': 0, b'P': 1})
     data.head()
[5]:
        Alcohol Malic_acid
                              Ash Alcalinity_of_ash Magnesium Total_phenols \
          14.23
                       1.71 2.43
     0
                                                15.6
                                                           127.0
                                                                           2.80
     1
          13.20
                       1.78 2.14
                                                11.2
                                                           100.0
                                                                           2.65
          13.16
                                                18.6
                       2.36 2.67
                                                           101.0
                                                                           2.80
     3
       14.37
                       1.95 2.50
                                                16.8
                                                                           3.85
                                                           113.0
          13.24
                       2.59 2.87
                                                21.0
                                                           118.0
                                                                           2.80
        Flavanoids Nonflavanoid_phenols Proanthocyanins Color_intensity
                                                                              Hue
     0
              3.06
                                    0.28
                                                     2.29
                                                                       5.64 1.04
              2.76
                                    0.26
     1
                                                     1.28
                                                                       4.38 1.05
              3.24
                                    0.30
                                                     2.81
                                                                       5.68 1.03
     3
              3.49
                                    0.24
                                                     2.18
                                                                       7.80 0.86
     4
              2.69
                                    0.39
                                                     1.82
                                                                       4.32 1.04
        OD280/OD315_of_diluted_wines Proline binaryClass
     0
                                3.92
                                       1065.0
                                                     b'N'
                                                                 0
                                3.40
                                                                 0
     1
                                       1050.0
                                                     b'N'
     2
                                3.17
                                                     b'N'
                                                                 0
                                       1185.0
     3
                                3.45
                                       1480.0
                                                     b'N'
                                                                 0
                                2.93
                                        735.0
                                                     b'N'
    EDA: Basic data structure
[6]: # Descriptive stats of numerical columns
     data.describe()
[6]:
               Alcohol Malic_acid
                                                                     Magnesium \
                                           Ash Alcalinity_of_ash
```

```
count 178.000000 178.000000 178.000000
                                                   178.000000 178.000000
mean
        13.000618
                     2.336348
                                 2.366517
                                                    19.494944
                                                               99.741573
std
         0.811827
                     1.117146
                                 0.274344
                                                     3.339564
                                                                14.282484
                     0.740000
                                                                70.000000
min
        11.030000
                                 1.360000
                                                    10.600000
25%
        12.362500
                     1.602500
                                 2.210000
                                                    17.200000
                                                                88.000000
50%
        13.050000
                     1.865000
                                 2.360000
                                                    19.500000
                                                                98.000000
75%
        13.677500
                     3.082500
                                 2.557500
                                                    21.500000
                                                               107.000000
max
        14.830000
                     5.800000
                                 3.230000
                                                    30.000000
                                                               162.000000
```

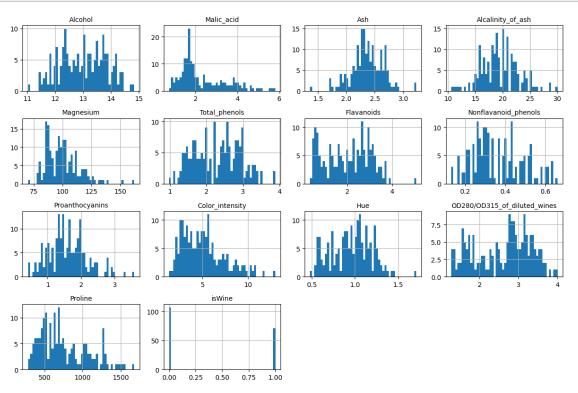
Total_phenols Flavanoids Nonflavanoid_phenols Proanthocyanins \

```
178.000000
                            178.000000
                                                    178.000000
                                                                      178.000000
     count
                  2.295112
                               2.029270
                                                      0.361854
                                                                         1.590899
     mean
     std
                  0.625851
                               0.998859
                                                      0.124453
                                                                        0.572359
     min
                  0.980000
                               0.340000
                                                      0.130000
                                                                        0.410000
     25%
                  1.742500
                               1.205000
                                                      0.270000
                                                                        1.250000
     50%
                  2.355000
                               2.135000
                                                      0.340000
                                                                         1.555000
     75%
                  2.800000
                               2.875000
                                                      0.437500
                                                                        1.950000
     max
                  3.880000
                               5.080000
                                                      0.660000
                                                                        3.580000
            Color_intensity
                                           OD280/OD315_of_diluted_wines
                                                                                Proline \
                                      Hue
                  178.000000
                                                                             178.000000
     count
                               178.000000
                                                               178.000000
     mean
                    5.058090
                                 0.957449
                                                                 2.611685
                                                                             746.893258
     std
                    2.318286
                                 0.228572
                                                                 0.709990
                                                                             314.907474
     min
                    1.280000
                                 0.480000
                                                                 1.270000
                                                                             278.000000
     25%
                                 0.782500
                                                                             500.500000
                    3.220000
                                                                 1.937500
     50%
                                                                             673.500000
                    4.690000
                                 0.965000
                                                                 2.780000
     75%
                    6.200000
                                 1.120000
                                                                 3.170000
                                                                             985.000000
                   13.000000
                                 1.710000
                                                                 4.000000
                                                                            1680.000000
     max
                 isWine
            178.000000
     count
               0.398876
     mean
     std
               0.491049
               0.000000
     min
     25%
               0.000000
     50%
               0.00000
     75%
               1.000000
     max
               1.000000
[7]: # Get null counts
     pd.DataFrame(
         [(col, data[col].isnull().sum()) for col in data.columns],
         columns = ['Columns Name', 'Null Count']
     )
[7]:
                          Columns Name
                                         Null Count
     0
                                Alcohol
                                                   0
     1
                            Malic_acid
                                                   0
     2
                                    Ash
                                                   0
     3
                     Alcalinity_of_ash
                                                   0
     4
                                                   0
                             Magnesium
     5
                                                   0
                         Total_phenols
                                                   0
     6
                            Flavanoids
     7
                  Nonflavanoid_phenols
                                                   0
     8
                       Proanthocyanins
                                                   0
     9
                       Color_intensity
                                                   0
```

```
10 Hue 0
11 0D280/0D315_of_diluted_wines 0
12 Proline 0
13 binaryClass 0
14 isWine 0
```

EDA: Initial visualizations

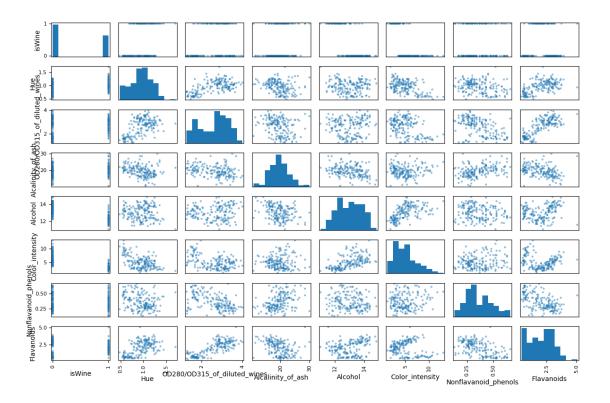
```
[8]: # Make historgrams of the numeric variables for initial visualization
import matplotlib.pyplot as plt
data.hist(bins=50, figsize=(12, 8))
utils.save_fig("attribute_histogram_plots")
plt.show()
```

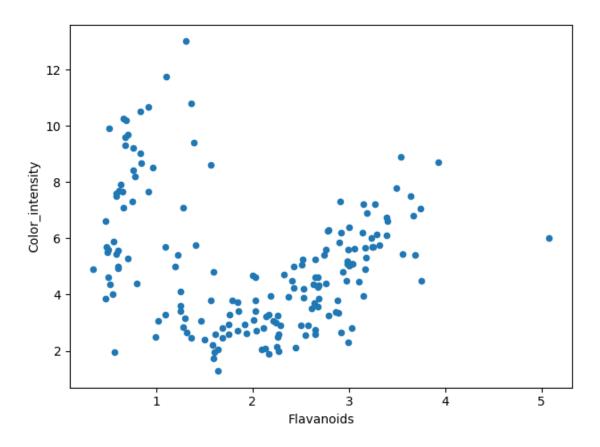


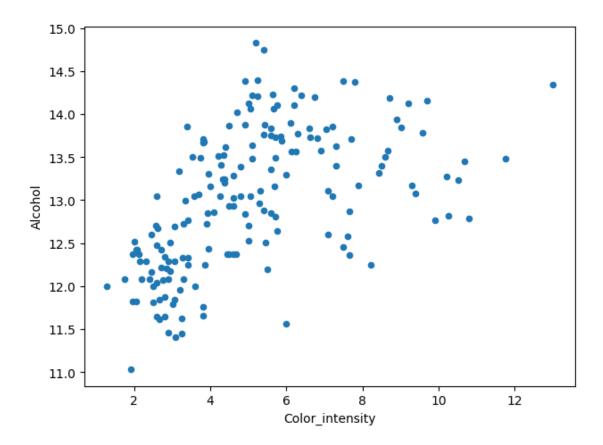
```
[9]: # Check for linear correlations

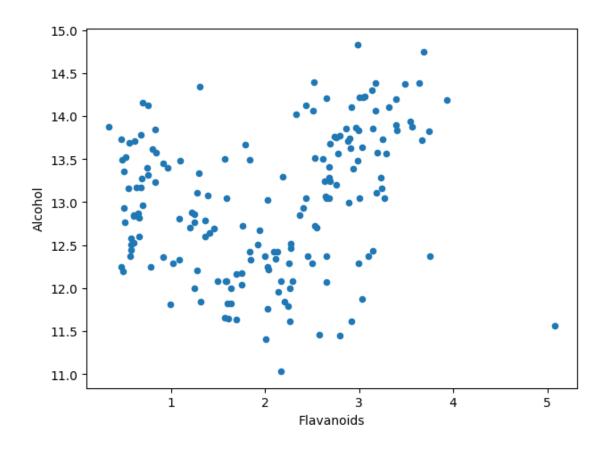
correlations = data.corr(numeric_only=True)
correlations["isWine"].sort_values(ascending=False)
```

```
[9]: isWine
                                      1.000000
     Hue
                                      0.353213
      OD280/OD315_of_diluted_wines
                                      0.199813
      Alcalinity_of_ash
                                      0.181764
     Proanthocyanins
                                      0.056208
     Flavanoids
                                      0.042179
      Nonflavanoid_phenols
                                      0.011868
     Total_phenols
                                     -0.047301
     Malic_acid
                                     -0.295175
     Magnesium
                                     -0.296972
     Ash
                                     -0.362457
                                     -0.589850
     Proline
      Color_intensity
                                     -0.694679
                                     -0.726383
      Alcohol
      Name: isWine, dtype: float64
[10]: | # plot scatter plots for interesting columns with promising coefficieients
      from pandas.plotting import scatter_matrix
      scatter_plot_cols = [
          'isWine', 'Hue', 'OD280/OD315_of_diluted_wines', 'Alcalinity_of_ash',
          'Alcohol', 'Color_intensity', 'Nonflavanoid_phenols', 'Flavanoids'
      ]
      scatter_matrix(data[scatter_plot_cols], figsize=(12, 8))
      utils.save_fig("scatter_matrix_plot")
      plt.show()
```



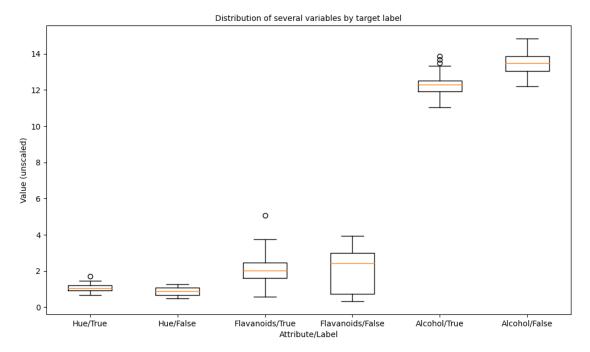






```
[12]: # The scatter plots over the dependent variable were odd (it is a binary target)
      # Lets use box plots to prob those relationships instead
      fig, ax1 = plt.subplots(figsize=(10, 6))
      bp = ax1.boxplot(
          data.Hue[data["isWine"] == True],
              data.Hue[data["isWine"] == False],
              data.Flavanoids[data["isWine"]==True],
              data.Flavanoids[data["isWine"] == False],
              data.Alcohol[data["isWine"] == True],
              data.Alcohol[data["isWine"] == False],
          ],
          notch=False, vert=True, whis=1.5
      ax1\_conf = ax1.set(
          axisbelow=True,
          title='Distribution of several variables by target label',
```

```
xlabel='Attribute/Label',
ylabel='Value (unscaled)',
xticklabels=[
    'Hue/True',
    'Hue/False',
    'Flavanoids/True',
    'Flavanoids/False',
    'Alcohol/True',
    'Alcohol/False',
]
)
utils.save_fig('box_plots')
```



EDA: Engineering features

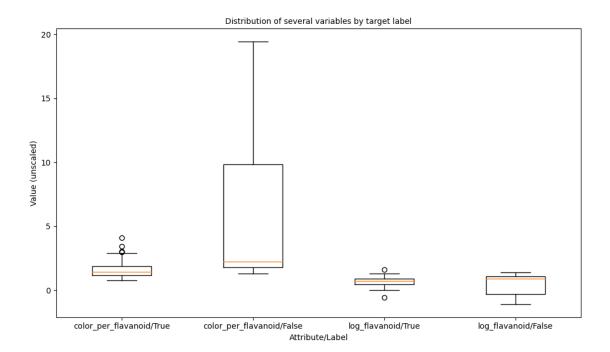
```
[13]: # The scatter plot for Color_intensity over Flavanoids seemed to have two trends_
→ present.

# I wonder what the distributions over their ratio looks like for each
# value of the target (isWine)

data['color_per_flavanoid'] = data['Color_intensity'] / data['Flavanoids']

# Checking out the original histograms diplayed above we can see the_
→ distributions
# of Flavanoids have the same range for isWine == True and isWine == False
```

```
# but the variablity is quite differenent. Let's see if log(Flavanoid) gives
# us anything interesting.
data['log_flavanoid'] = np.log(data['Flavanoids'])
fig, ax1 = plt.subplots(figsize=(10, 6))
bp = ax1.boxplot(
    Γ
        data.color_per_flavanoid[data["isWine"] == True],
        data.color_per_flavanoid[data["isWine"] == False],
        data.log_flavanoid[data["isWine"] == True],
        data.log_flavanoid[data["isWine"] == False],
    ],
   notch=False, vert=True, whis=1.5
ax1\_conf = ax1.set(
    axisbelow=True,
    title='Distribution of several variables by target label',
    xlabel='Attribute/Label',
    ylabel='Value (unscaled)',
    xticklabels=[
        'color_per_flavanoid/True',
        'color_per_flavanoid/False',
        'log_flavanoid/True',
        'log_flavanoid/False',
    ]
utils.save_fig('box_plots_new_features')
plt.show()
print(
    data[['color_per_flavanoid', 'log_flavanoid', 'isWine']].corr()['isWine'].
→sort_values(ascending=False)
)
```



isWine 1.000000 log_flavanoid 0.172148 color_per_flavanoid -0.467811 Name: isWine, dtype: float64

ML Pipeline: Data preparation

```
[14]: # Create a Test Set
      from sklearn.model_selection import train_test_split
                               # Let's set aside 15% of the records for testing
      test_ratio = 0.15
                               # To prevent data leakage I will set a seed while
      random_seed = 1
       \rightarrow developing
                               # so random_seed = 1 will give me the same train/test_
       \rightarrowsplit over and over
      # random_seed = None
                               # but use a fresh seed (seed=None) when its time tou
       \rightarrow submit
      # Set some test_data aside (and not look at it until very end!)
      training_data, test_data = train_test_split(data, test_size=test_ratio,_
       →random_state=random_seed)
      # Take labels off training_data
      x_training = training_data.drop(['isWine', 'binaryClass'], axis=1)
```

```
training_labels = training_data['isWine'].copy()
x_training
```

[14]:		Alcohol	Malic_acid	Ash	Alcalinit	y_of_ash	Magnesium	Total_phen	ols	\
	29	14.02	1.68	2.21		16.0	96.0	2	.65	
	16	14.30	1.92	2.72		20.0	120.0	2	2.80	
	147	12.87	4.61	2.48		21.5	86.0	1	1.70	
	97	12.29	1.41	1.98		16.0	85.0	2	2.55	
	159	13.48	1.67	2.64		22.5	89.0	2	2.60	
	133	12.70	3.55	2.36		21.5	106.0	1	1.70	
	137	12.53	5.51	2.64		25.0	96.0	1	1.79	
	72	13.49	1.66	2.24		24.0	87.0	1	1.88	
	140	12.93	2.81	2.70		21.0	96.0	1	1.54	
	37	13.05	1.65	2.55		18.0	98.0	2.45		
		Flavanoi	ds Nonflava	noid_pl	nenols Pr	oanthocya	nins Color	_intensity	Hue	e \
	29		33	0.26		v	1.98	4.70	1.04	1
	16	3.	14	0.33			1.97	6.20	1.07	7
	147	0.	65	0.47			0.86	7.65	0.54	1
	97	2.	50	0.29			1.77	2.90	1.23	3
	159	1.	10	0.52			2.29	11.75	0.57	7
										•
	133	1.	20	0.17			0.84	5.00	0.78	3
	137	0.	60	0.63			1.10	5.00	0.82	2
	72	1.	84	0.27			1.03		0.98	3
	140	0.	50	0.53			0.75	4.60	0.77	7
	37	2.	43		0.29		1.44	4.25	1.12	2
		OD280/OD	315_of_dilut	ed_wine	es Prolin	e color_	per_flavano	id log_fla	log_flavanoid	
	29			3.5	59 1035.	0	2.0171	67 0.	84586	88
	16			2.6	2.65 1280.0 1.97		1.9745	22 1.	2 1.144223	
	147			1.8	36 625.	0	11.7692	31 -0.	-0.430783	
	97			2.7	2.74 428.		1.1600	00 0.	0.916291	
	159			1.7	1.78 620.0		10.6818	18 0.	0.095310	
	133			1.2			4.1666	67 0.182322		
	137			1.6	69 515.	0	8.333333 -0.51083		26	
	72			2.7	78 472.0 2.032609 0		60976	66		
	140			2.3	31 600.	0	9.2000	00 -0.	69314	17
	37			2.5	51 1105.	0	1.7489	71 0.	88789	91

[151 rows x 15 columns]

```
[15]: # Cleaning begins with null/missing values
      null_rows_idx = x_training.isnull().any(axis=1)
      # We confirm what we discovered above, no missing values in this dataset
      # (For when we move to abstraction later, I will still include an imputer)
      print(
          null_rows_idx[null_rows_idx==True].shape
     (0,)
[16]: # lets build the preprocessing pipeline for numerical features
      from sklearn.pipeline import Pipeline, make_pipeline
      from sklearn.preprocessing import StandardScaler
      from sklearn.impute import SimpleImputer
      numeric_pipeline = Pipeline([
          ("impute", SimpleImputer(strategy="median")),
          ("standardize", StandardScaler()),
      ])
[17]: # this example use case is not using caterorical features
      # but this is how we could construct the pipline for those:
      from sklearn.impute import SimpleImputer
      from sklearn.preprocessing import OneHotEncoder, OrdinalEncoder
      categoric_pipeline = Pipeline([
          ("ordinal_encoder", OrdinalEncoder()),
          ("impute", SimpleImputer(strategy="most_frequent")),
          ("encode", OneHotEncoder(handle_unknown="ignore")),
      ])
[18]: # A ColumnTransformer can make a single pipeline
      from sklearn.compose import make_column_selector, make_column_transformer
      preprocessing = make_column_transformer(
          (numeric_pipeline, make_column_selector(dtype_include=np.number)),
          (categoric_pipeline, make_column_selector(dtype_include=object)),
      preprocessing
```

```
[18]: ColumnTransformer(transformers=[('pipeline-1',
                                        Pipeline(steps=[('impute',
      SimpleImputer(strategy='median')),
                                                        ('standardize',
                                                         StandardScaler())]),
      <sklearn.compose._column_transformer.make_column_selector object at</pre>
      0x7f47ba6daf10>),
                                       ('pipeline-2',
                                        Pipeline(steps=[('ordinal_encoder',
                                                         OrdinalEncoder()),
                                                        ('impute',
      SimpleImputer(strategy='most_frequent')),
                                                        ('encode',
      OneHotEncoder(handle_unknown='ignore'))]),
      <sklearn.compose._column_transformer.make_column_selector object at</pre>
      0x7f47b89370d0>)])
[19]: # We can test our preprocessing pipeline on our training data.
      training_data_cleaned = preprocessing.fit_transform(x_training)
      training_data_cleaned_df = pd.DataFrame(
          training_data_cleaned,
          columns=preprocessing.get_feature_names_out(),
          index=training_data.index
      )
      training_data_cleaned_df.head()
[19]:
           pipeline-1__Alcohol pipeline-1__Malic_acid pipeline-1__Ash \
                      1.259587
                                              -0.619230
                                                                -0.535083
      29
                                                                1.316905
      16
                      1.603015
                                              -0.410962
      147
                     -0.150920
                                               1.923377
                                                                0.445381
      97
                     -0.862306
                                              -0.853531
                                                                -1.370293
      159
                      0.597262
                                              -0.627908
                                                                 1.026397
           pipeline-1__Alcalinity_of_ash pipeline-1__Magnesium \
      29
                                -1.063608
                                                       -0.207330
                                                        1.535977
      16
                                 0.151484
      147
                                 0.607144
                                                       -0.933709
      97
                                -1.063608
                                                       -1.006346
      159
                                 0.910916
                                                       -0.715795
           pipeline-1__Total_phenols pipeline-1__Flavanoids \
      29
                            0.589146
                                                     0.337732
      16
                            0.827519
                                                     1.147851
      147
                           -0.920554
                                                    -1.342516
```

```
97
                            0.430230
                                                     0.507757
      159
                            0.509688
                                                    -0.892449
           pipeline-1__Nonflavanoid_phenols pipeline-1__Proanthocyanins \
      29
                                  -0.874546
                                                                 0.710735
                                  -0.286882
                                                                 0.693358
      16
      147
                                   0.888445
                                                                -1.235501
      97
                                  -0.622690
                                                                 0.345816
      159
                                    1.308205
                                                                 1.249426
           pipeline-1__Color_intensity pipeline-1__Hue \
      29
                             -0.165290
                                                0.365559
      16
                              0.455370
                                                0.494389
      147
                              1.055342
                                               -1.781607
      97
                             -0.910082
                                                1.181482
      159
                              2.751813
                                               -1.652777
           pipeline-1__OD280/OD315_of_diluted_wines pipeline-1__Proline \
      29
                                            1.405185
                                                                 0.963100
      16
                                            0.085971
                                                                 1.769644
      147
                                           -1.022730
                                                                -0.386627
      97
                                            0.212279
                                                                -1.035154
      159
                                           -1.135004
                                                                -0.403087
           pipeline-1__color_per_flavanoid pipeline-1__log_flavanoid
      29
                                 -0.498390
                                                              0.515697
                                                              0.992637
      16
                                 -0.508292
      147
                                  1.766075
                                                             -1.525116
      97
                                 -0.697428
                                                              0.628272
      159
                                                             -0.684120
                                  1.513574
     Deployment: Model selection & evaluation
[20]: # Model number 1 is an SGDClassifier
      from sklearn.linear_model import SGDClassifier
      sgd_clf = SGDClassifier(random_state=422)
      sgd_clf.fit(training_data_cleaned_df, training_labels)
[20]: SGDClassifier(random_state=422)
[21]: # Model number 2 will be a RandomForestClassifier
```

from sklearn.ensemble import RandomForestClassifier

forest_clf = RandomForestClassifier(random_state=422)

```
forest_clf.fit(training_data_cleaned_df, training_labels)
[21]: RandomForestClassifier(random_state=422)
[22]: # Model number 3 will be a SVM
      from sklearn.svm import SVC
      svm_clf = SVC(random_state=422)
      svm_clf.fit(training_data_cleaned_df, training_labels)
[22]: SVC(random_state=422)
[23]: # Model number 4 will be a K-Neighbors Classifier
      from sklearn.neighbors import KNeighborsClassifier
      knn_clf = KNeighborsClassifier(n_neighbors=5)
      knn_clf.fit(training_data_cleaned_df, training_labels)
[23]: KNeighborsClassifier()
[24]: # Let's evaluate our four models on the test data.
      test_y = test_data['isWine']
      test_x = preprocessing.fit_transform(test_data.drop(['isWine', 'binaryClass'],_
      →axis=1))
      test_x = pd.DataFrame(
          test_x,
          columns=preprocessing.get_feature_names_out(),
          index=test_data.index
      test_x.head()
[24]:
           pipeline-1__Alcohol pipeline-1__Malic_acid pipeline-1__Ash \
      161
                      0.834735
                                              1.561867
                                                                0.475048
      117
                     -0.803677
                                             -0.510235
                                                              -0.885316
      19
                      0.770231
                                              1.360936
                                                               0.552783
      69
                     -1.074596
                                             -1.037679
                                                              -2.595489
      53
                      0.937942
                                             -0.146047
                                                               1.019194
           pipeline-1__Alcalinity_of_ash pipeline-1__Magnesium \
      161
                                0.152916
                                                       0.145732
      117
                                0.859892
                                                       0.209196
                                                       0.716907
      19
                               -1.204477
      69
                               -0.752013
                                                       2.938144
                               -0.667176
                                                       0.653443
      53
```

```
-0.944096
      161
                                                    -1.767256
      117
                            -0.654237
                                                     -0.153878
      19
                             0.539303
                                                     0.837347
                                                    -1.008019
      69
                            -0.909995
      53
                             1.050820
                                                     0.584268
           pipeline-1__Nonflavanoid_phenols pipeline-1__Proanthocyanins
      161
                                    1.019077
                                                                 -1.702355
      117
                                   -0.059946
                                                                 -0.174009
      19
                                   -1.206407
                                                                 -0.079667
      69
                                   -1.408724
                                                                  1.505284
      53
                                    0.277249
                                                                 -0.041930
           pipeline-1__Color_intensity pipeline-1__Hue \
      161
                                               -0.060025
                               0.665657
      117
                              -1.748403
                                                0.446439
      19
                               0.172734
                                               -0.060025
      69
                              -1.249160
                                                1.560660
      53
                               0.931077
                                                0.800964
           pipeline-1__OD280/OD315_of_diluted_wines pipeline-1__Proline
                                           -1.378083
      161
                                                                 -0.251360
      117
                                            0.329542
                                                                 -1.168856
      19
                                            0.928708
                                                                 0.200541
                                                                 -0.147286
      69
                                            0.494313
      53
                                            0.284604
                                                                  1.652101
           pipeline-1__color_per_flavanoid pipeline-1__log_flavanoid
      161
                                   2.436004
                                                              -2.187141
      117
                                  -0.708457
                                                               0.111771
      19
                                  -0.477928
                                                               0.760081
      69
                                  -0.298338
                                                              -0.744099
      53
                                  -0.287927
                                                               0.616033
[25]: from sklearn.model_selection import cross_val_score
      from sklearn.metrics import precision_score, recall_score, f1_score
      # Evaluate model #1...
      sgd_preds = sgd_clf.predict(test_x)
      sgd_metrics = dict(
          model = 'Stochastic Gradient Descent',
          accuracy = round(np.mean(cross_val_score(
              sgd_clf, test_x, test_y,
```

pipeline-1__Total_phenols pipeline-1__Flavanoids \

```
cv=3, scoring='accuracy'
          )), 2),
          precision = precision_score(test_y, sgd_preds),
          recall = recall_score(test_y, sgd_preds),
          f1 = f1_score(test_y, sgd_preds),
      )
      sgd_metrics
[25]: {'model': 'Stochastic Gradient Descent',
       'accuracy': 0.89,
       'precision': 0.9,
       'recall': 0.9,
       'f1': 0.9}
[26]: # Evaluate model #2...
      forest_preds = forest_clf.predict(test_x)
      forest metrics = dict(
          model = 'Random Forest Classifier',
          accuracy = round(np.mean(cross_val_score(
              forest_clf, test_x, test_y,
              cv=3, scoring='accuracy'
          )), 2),
          precision = precision_score(test_y, forest_preds),
          recall = recall_score(test_y, forest_preds),
          f1 = f1_score(test_y, forest_preds),
      forest_metrics
[26]: {'model': 'Random Forest Classifier',
       'accuracy': 0.96,
       'precision': 1.0,
       'recall': 1.0,
       'f1': 1.0}
[27]: # Evaluate model #3...
      svm_preds = svm_clf.predict(test_x)
      svm_metrics = dict(
          model = 'Support Vector Machine',
          accuracy = round(np.mean(cross_val_score(
              svm_clf, test_x, test_y,
              cv=3, scoring='accuracy'
```

```
)), 2),
          precision = precision_score(test_y, svm_preds),
          recall = recall_score(test_y, svm_preds),
          f1 = f1_score(test_y, svm_preds),
      svm_metrics
[27]: {'model': 'Support Vector Machine',
       'accuracy': 0.89,
       'precision': 1.0,
       'recall': 1.0,
       'f1': 1.0}
[28]: # Evaluate model #4...
      knn_preds = knn_clf.predict(test_x)
      knn_metrics = dict(
          model = 'K-Neighbors Classifier',
          accuracy = round(np.mean(cross_val_score(
              knn_clf, test_x, test_y,
              cv=3, scoring='accuracy'
          precision = precision_score(test_y, knn_preds),
          recall = recall_score(test_y, knn_preds),
          f1 = round(f1_score(test_y, knn_preds), 2),
      )
      knn_metrics
[28]: {'model': 'K-Neighbors Classifier',
       'accuracy': 0.93,
       'precision': 1.0,
       'recall': 0.9,
       'f1': 0.95}
[29]: metrics_df = pd.DataFrame(
          [sgd_metrics, forest_metrics, svm_metrics, knn_metrics]
      )
      metrics_df
[29]:
                               model accuracy precision recall
      O Stochastic Gradient Descent
                                          0.89
                                                      0.9
                                                              0.9 0.90
      1
            Random Forest Classifier
                                          0.96
                                                      1.0
                                                              1.0 1.00
      2
              Support Vector Machine
                                          0.89
                                                      1.0
                                                              1.0 1.00
```

3 K-Neighbors Classifier

0.93

1.0

0.9 0.95