A BINARY CLASSIFIER FOR DEFECT PREDICTION: EXAMPLE USE CASE WITH WINE ID

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1 Executive summary

Given the rising prevalence of data science teams in industry and the widespread adoption of the *Team Data Science Process (TDSP)* methodology, classifier *Machine Learning* (ML) models will see deployment in more and more use cases. Even small teams will be deploying data science tools that are tailored for many different settings throughout various enterprises (Hyatt, 2024).

The concept is explored with a use case that seeks to deploy a binary classifier for a defect prediction application. Using the `wine` data set (Vanschoren, 2014) from `openml.org` we have 14 features for 178 records that include labels on if the sample is wine or not. *Exploratory Data Analysis (EDA)* is conducted with the aim of selecting, training and tuning four models to classify, for now, a sample as wine or not. This would be extended to a model that seeks to predict samples that run a high probability of being defective or non-conforming. Emphasis is on turning this wine classifier deployment into a DRY (*Don't Repeat Yourself*), generic (but still flexible) and easy to deploy tool that data scientists can use to expedite routine data exploration, data wrangling and data mining.

All four models took very little ($<$0.3 seconds) to both fit and predict. This is possibly due, in part, to the small data set. The *RandomForestClassifier* performed the best of the four. The accuracy, precision, recall and f1 scores were 0.96, 0.9, 0.9 and 0.9 respectively.

2 Research design

There are a variety of options for ML binary classifiers (Geron, 2023, ch 3). Is there a particular algorithm that should be considered when the target is conformance vs non-conformance from a quality assurance perspective? What steps should be taken to tune a binary classifier for maximal accuracy, precision and recall? The following is an ML project meant to test some best practices for deploying these classifiers.

The study will create a work flow that mirrors the TDSP ("What is the Team Data Science Process?", 2024). Various stages in the TDSP (which is illustrated in figure 1) are represented by data models and have methods for applying standard work to these structures, moving them along the path to the next stage. The benefits of using customized libraries to conduct ML projects are shortened development cycles, more robust/stable applications, greater interoperability amongst team members and more time to focus on making models that perform better and provide more actionable conclusions (Geron, 2023). The code for the

project (and this paper) can be found in the `GitHub` repository located at `https://github.com/kgeidel/MSDS-422-final-project` (Geidel, 2024).

Performance of four different classifier models and various techniques will be measured and compared. Various transformations and parameters are used. All four trials will be evaluated using the same metrics. Several quantitative performance metrics are industry standards for evaluating ML effectiveness (Powers, 2007). Table 1 lists the metrics used.

After cursory *Exploratory Data Analysis* (EDA) and the creation of three engineered features, a train/test split of 15% is used to prevent target and data leakage. Our target label is separated from features and a preprocessing pipeline is developed. All four models are fit to the cleaned training data. Cross-validation is used to find average performance metrics against other folds of the training data and then the test data itself.

3 Exploratory Data Analysis (EDA)

Listing 1 at the end of the appendix includes the twenty-nine cells of Jupyter notebook code and their output. EDA begins in cell 2 by loading the data set which was downloaded in the `arff` format. There are 178 records with 13 features plus a label, the binary class that I encode to *isWine*. Cell 3 lists the features and their data types. We see *binaryClass* is the only categorical label and all records contain values for all features. In cells 4 and 5 we encode the *binaryClass* into our numeric target *isWine*.

The data set structure is further probed in cell 6, which describes each feature. We see a glimpse at the distribution of each feature. In cell 7 we confirm no missing values which removes the need for an imputer. Visualization begins in cell 8, we create histograms of each feature. Some, particularly *Malic Acid*, *Ash*, *color intensity* and *Proline* seem to have normal distributions (although skewed.) Others appear to have multi-modal distributions (such as *alcohol* and the *OD280/OD315 dilution*.) Numeric descriptions continue in cell 9, finding Pearson correlation coefficients for each variable in relation to our target. The strongest correlation is a negative correlation between *alcohol* and the target at -0.7264. *Color intensity* and *proline* also have strong correlations.

Scatter plots are created in cell 10, showing how each variable moves with the others. A few interesting combinations are chosen for further analysis. *Color intensity* over *Flavanoids* had two very distinct groupings in the scatter plots. *Alcohol* over *Color intensity* has a tightly bound linear section with a positive correlation and then another cluster the appears to be a cluster with zero slope. *Alcohol* over *Flavanoids* has

a hooked shape in the scatter plot with two ostensibly distinct clusters. Cell 11 generates these plots much larger for examination.

Cell 12 compares the distribution of these features but with targets (*isWine* true/false) separated. *Alcohol* is a promising feature, the interquartile ranges of the target true and target false distributions do not over lap at all. The other distributions are interesting but as these features stand on their own do not appear to have much predictive power.

Two features are engineered in cell 13. *color_per_flavanoid* is defined as the ratio of *color intensity* over *flavanoids*. We also take the natural log of the *flavanoid* attribute. The new features are put into histograms (separated by target.) The ratio *color_per_flavanoid* jumps out as another promising feature as the target true and target false distributions seem distinct.

4 Data pipeline and ML preprocessing

Development of the data pipeline begins in cell 14. The data set is divided into training and test (15%.) Labels are striped from the training features and kept to the side for fitting. Cell 15 is meant to drop records with missing values that could not be imputed. We confirmed above that this does not apply to any records in the data set but a more abstract pipeline would do well to take these steps. In a similar vein, two separate pipelines are created for numeric and categorical features, even though we only require the former in this particular instance. Cell 16 creates the numeric pipeline: a simple imputer utilizing the median strategy and a standard scaler. Cell 17 creates the categorical pipeline: an ordinal encoder, a simple imputer (using "most frequent") and one hot encoding that ignores unknown label values.

In cell 18 these are combined into the preprocessing pipeline. We process the training data in cell 19 and confirm it is ready for model fitting.

5 ML engineering, evaluation and deployment

Four models commonly used for classification are testing and compared. They are the *Stochastic Gradient Descent* (SGD) optimization, the *Random Forest Classifier*, the *Support Vector Machine* (SVM) and the *K-Neighbors Classifier*. Cells 20, 21, 22 and 23 create and fit these four models respectively.

Final evaluation is against the test split of the data set. The target is removed from the test data the features are transformed via the preprocessing pipeline in cell 24. Deployment, in this bench test comparison, entails predicting on the test records and calculating performance metrics (cells 25-28.) Results are outlined in section 6.

6 Findings

The four models tested performed very similarly on the `wine` data set. With only 178 total records (the splits were, obviously, smaller still) time was not a significant factor. All models fit and predicted very quickly. The *RandomForestClassifier* took the "longest" to both fit (0.1 seconds) and predict (0.3 seconds.) Performance against the test data was also similarly impressive across all models.

Cell 29 contains a dataframe that outlines the results. The *RandomForestClassifier* had the best overall performance. The precision, recall and f1 scores were higher for this model. The results were encouraging but may be indicating possible problems with over-fitting or testing bias. This is an issue that additional records and another look at employed techniques would help alleviate.

7 Conclusions

Additional evaluation among folds of the training data would further inform my comparison of the models. This would also hep rule out leakage and bias. Additionally, larger data sets could prove naturally more interesting and require more advanced strategies.

This is a practical choice for deploying classifiers in industry. In fact, this project topic was inspired by a ML tool I developed at my job. We had not performed evaluation on multiple models before selecting a *RandomForestClassifier*. I am relieved to see this model perform well here in this experiment. I got lucky that time, but this type of analysis will be an integral part of my ML deployments in the future.

Appendix

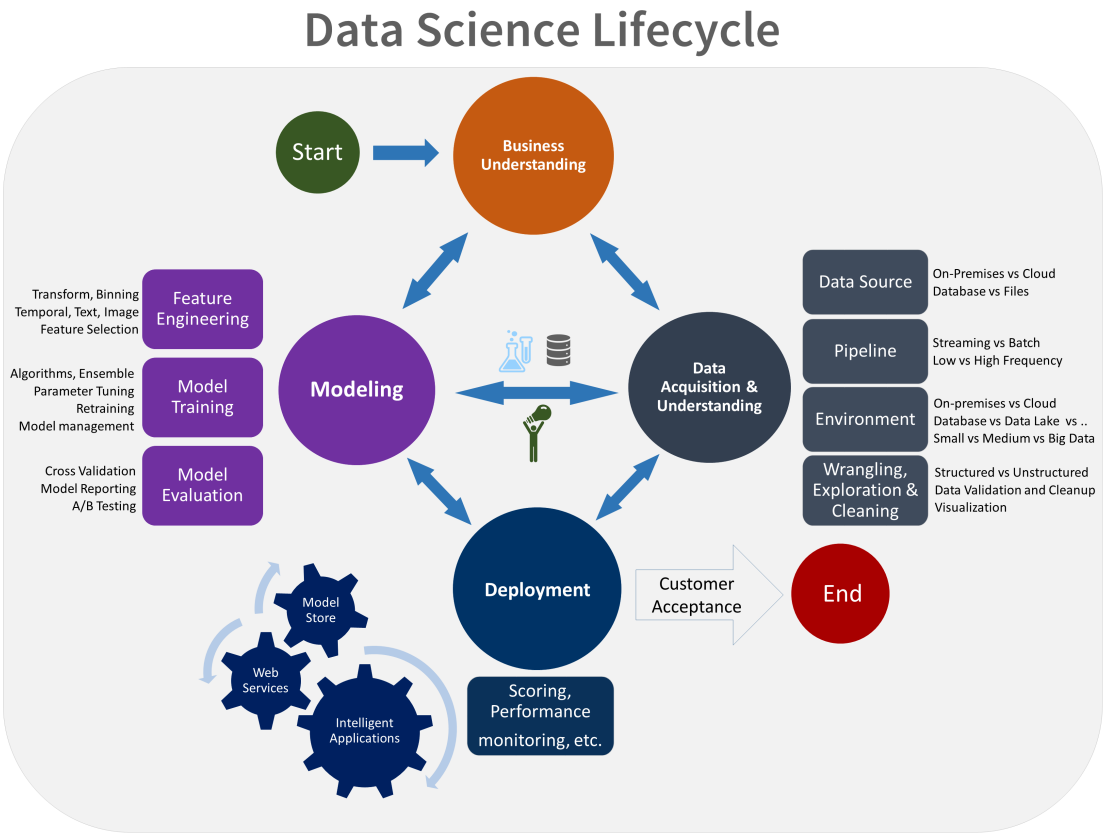


Figure 1: "Data life cycle" ("What is the Team Data Science Process?", 2024)

Metric	Calculations*	Description
Accuracy	$\frac{TP+TN}{TP+TN+FP+FN}$	Fraction of predictions made correctly
Precision	$\frac{TP}{TP+FP}$	Fraction of positive predictions made correctly
Recall	$\frac{TP}{TP+FN}$	Fraction of actual positives correctly identified

*TP=True Positives, TN=True Negatives, FP=False Positives, FN=False Negatives

Table 1: Performance metrics used on each of the four trials.

Listing 1: Python code and output from Module10_Geidel.ipynb

[1]:
```
# MSDS 422 - Section 55
# Spring '24
# Module 10 - Final project

# IsWine Binary Classifier
# 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	\
0	14.23	1.71	2.43	15.6	127.0	2.80	
1	13.20	1.78	2.14	11.2	100.0	2.65	
2	13.16	2.36	2.67	18.6	101.0	2.80	
3	14.37	1.95	2.50	16.8	113.0	3.85	
4	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	
1	2.76	0.26	1.28	4.38	1.05	
2	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'
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
 1   Malic_acid                    178 non-null    float64
 2   Ash                           178 non-null    float64
 3   Alcalinity_of_ash             178 non-null    float64
 4   Magnesium                     178 non-null    float64
 5   Total_phenols                 178 non-null    float64
 6   Flavanoids                    178 non-null    float64
 7   Nonflavanoid_phenols          178 non-null    float64
 8   Proanthocyanins               178 non-null    float64
 9   Color_intensity               178 non-null    float64
 10  Hue                           178 non-null    float64
 11  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
0	14.23	1.71	2.43	15.6	127.0	2.80
1	13.20	1.78	2.14	11.2	100.0	2.65
2	13.16	2.36	2.67	18.6	101.0	2.80
3	14.37	1.95	2.50	16.8	113.0	3.85
4	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
1	2.76	0.26	1.28	4.38	1.05
2	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	isWine
0	3.92	1065.0	b'N'	0
1	3.40	1050.0	b'N'	0
2	3.17	1185.0	b'N'	0
3	3.45	1480.0	b'N'	0
4	2.93	735.0	b'N'	0

EDA: Basic data structure

[6]:
```
# Descriptive stats of numerical columns

data.describe()
```

[6]:

	Alcohol	Malic_acid	Ash	Alcalinity_of_ash	Magnesium
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
min	11.030000	0.740000	1.360000	10.600000	70.000000
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  \
count     178.000000  178.000000            178.000000       178.000000
mean        2.295112    2.029270              0.361854         1.590899
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         Hue  OD280/OD315_of_diluted_wines      Proline  \
count       178.000000  178.000000                   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%           3.220000    0.782500                     1.937500   500.500000
50%           4.690000    0.965000                     2.780000   673.500000
75%           6.200000    1.120000                     3.170000   985.000000
max          13.000000    1.710000                     4.000000  1680.000000

          isWine
count  178.000000
mean     0.398876
std      0.491049
min      0.000000
25%      0.000000
50%      0.000000
75%      1.000000
max      1.000000
```

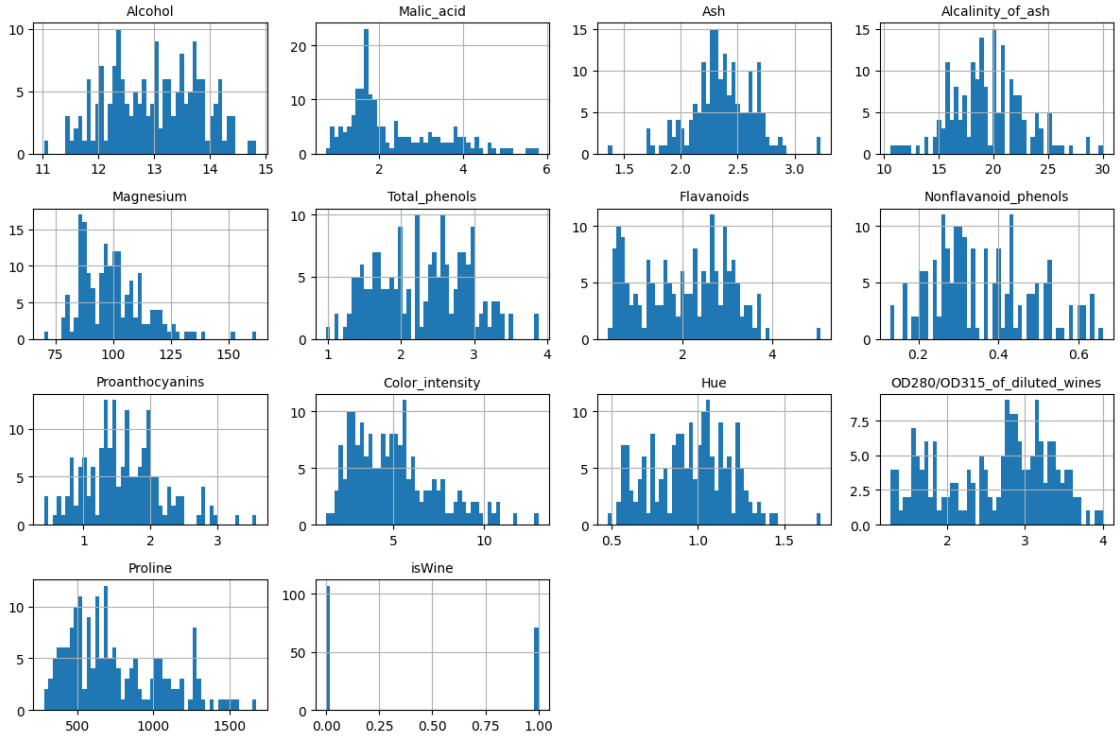
[7]:
```
# Get null counts

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	Magnesium	0
5	Total_phenols	0
6	Flavanoids	0
7	Nonflavanoid_phenols	0
8	Proanthocyanins	0
9	Color_intensity	0
10	Hue	0
11	OD280/OD315_of_diluted_wines	0
12	Proline	0
13	binaryClass	0
14	isWine	0

EDA: Initial visualizations

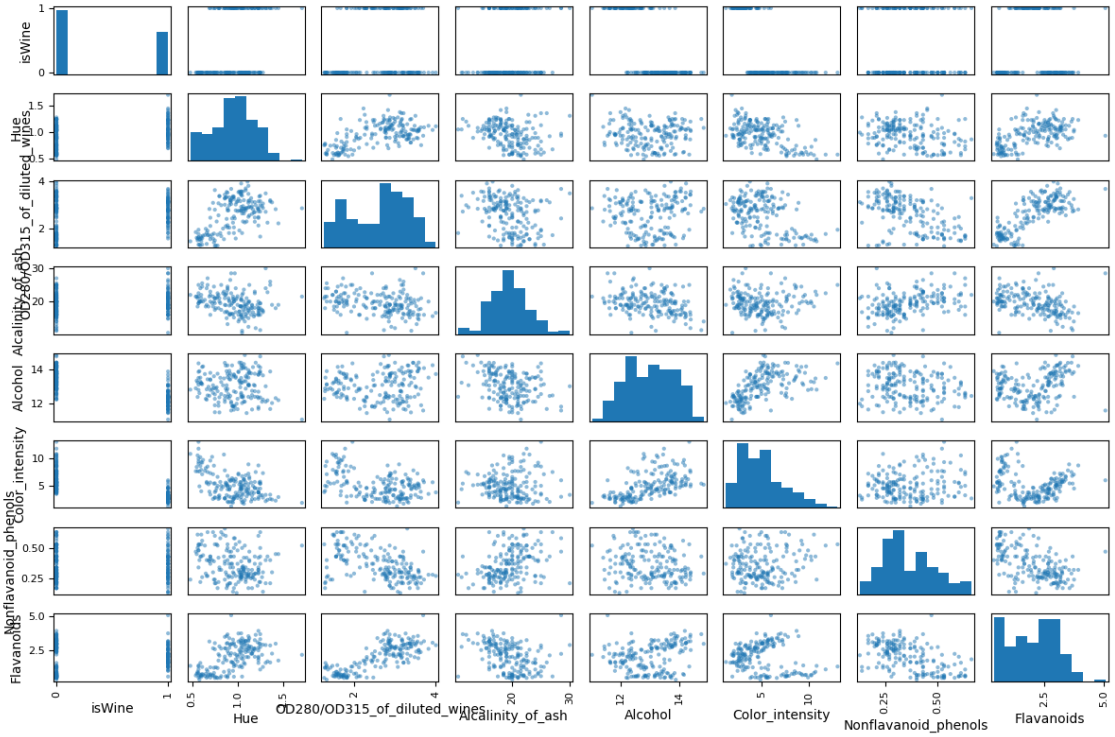
[8]:
```
# Make historgrams of the numeric variables for initial visualization

import matplotlib.pyplot as plt

data.hist(bins=50, figsize=(12, 8))

utils.save_fig("attribute_histogram_plots")
plt.show()
```



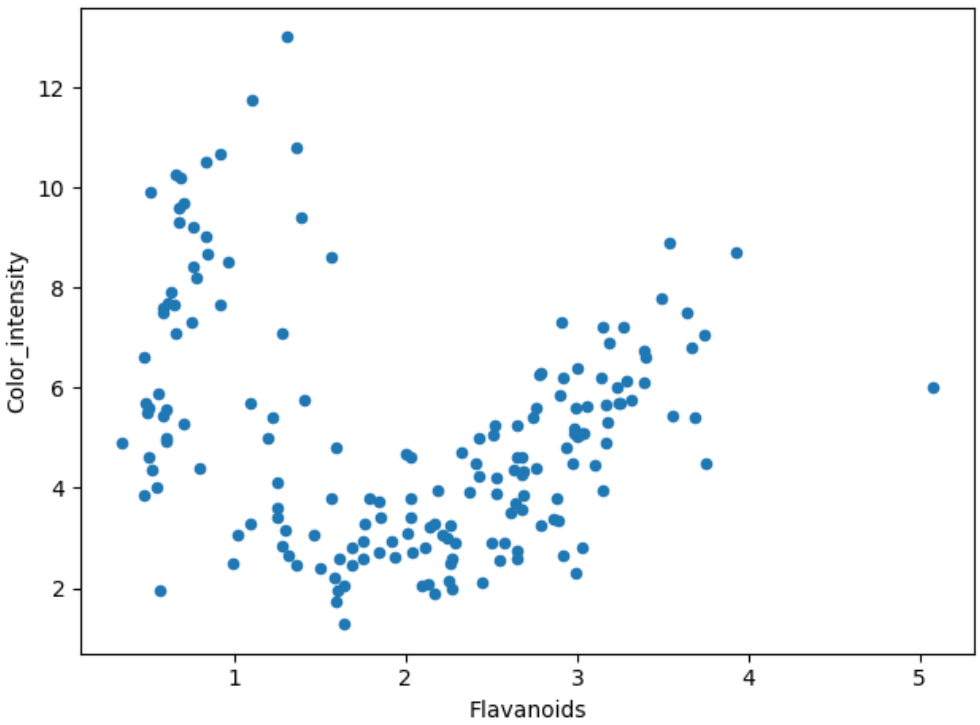
[9]:
```
# Check for linear correlations

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

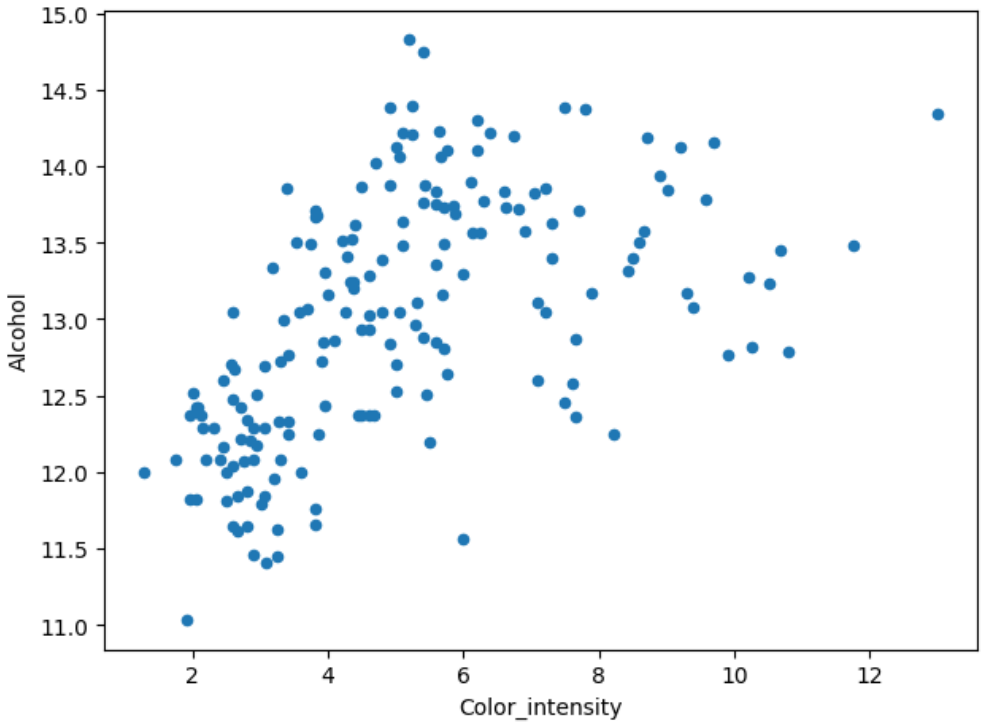
[9]:
```
isWine                          1.000000
Hue                             0.353213
OD280/OD315_of_diluted_wines    0.199813
Alcalinity_of_ash               0.181764
Proanthocyanins                 0.056208
Flavanoids                      0.042179
Nonflavanoid_phenols            0.011868
Total_phenols                  -0.047301
Malic_acid                     -0.295175
Magnesium                      -0.296972
Ash                            -0.362457
Proline                        -0.589850
Color_intensity                -0.694679
Alcohol                        -0.726383
Name: isWine, dtype: float64
```

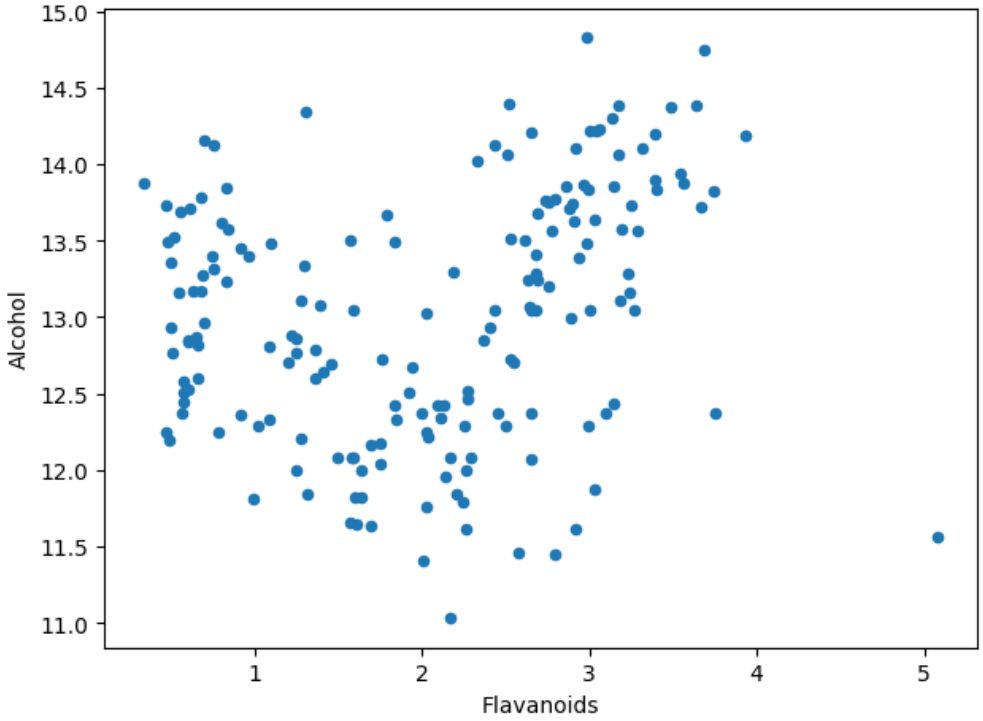
[10]:
```
# plot scatter plots for interesting columns with promising coefficieients

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()
```



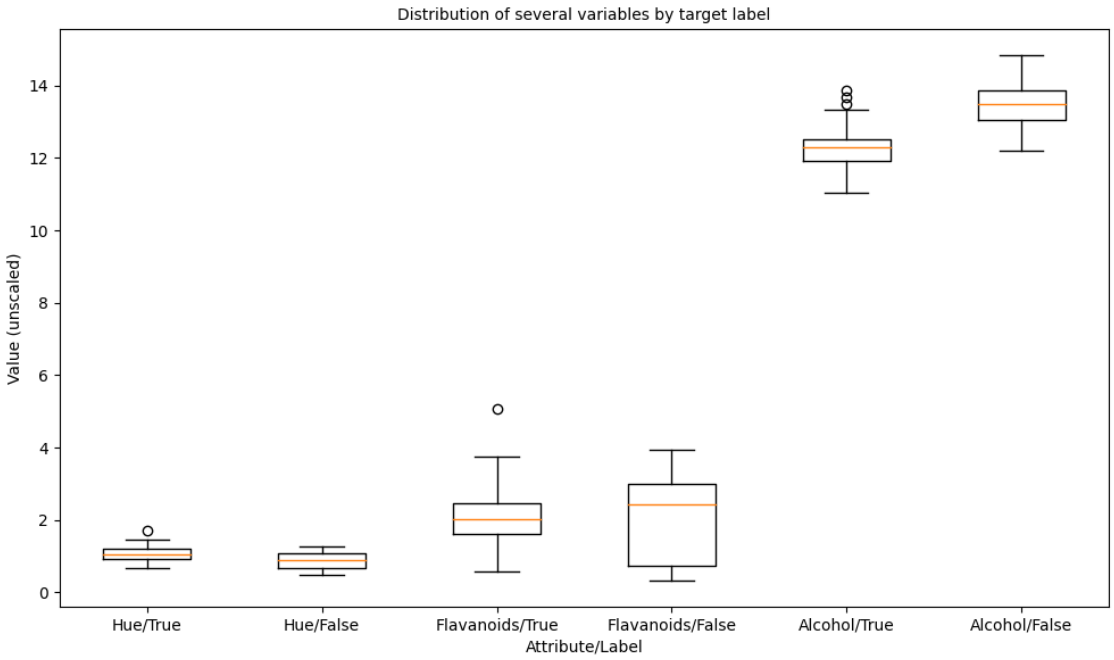
[11]:
```
# lets examine some graphs up close
# we are looking for interesting relationships that may not be linear
# and/or may make for good engineered features.

single_scatter_ls = [
    ('Color_intensity', 'Flavanoids'), # seems to have two distinct groupings
    ('Alcohol', 'Color_intensity'),    # has very curious shape
    ('Alcohol', 'Flavanoids'),         # also has a hook shape w/ ostensibly␣
 ↪distinct clusters
]

for y, x in single_scatter_ls:
    data.plot(kind='scatter', x=x, y=y)
    utils.save_fig(f"scatterplot_{y}_over_{x}")
    plt.show()
```




15.0
14.5
14.0
13.5
13.0
12.5
12.0
11.5
11.0
Alcohol
2
4
6
8
10
12
Color_intensity

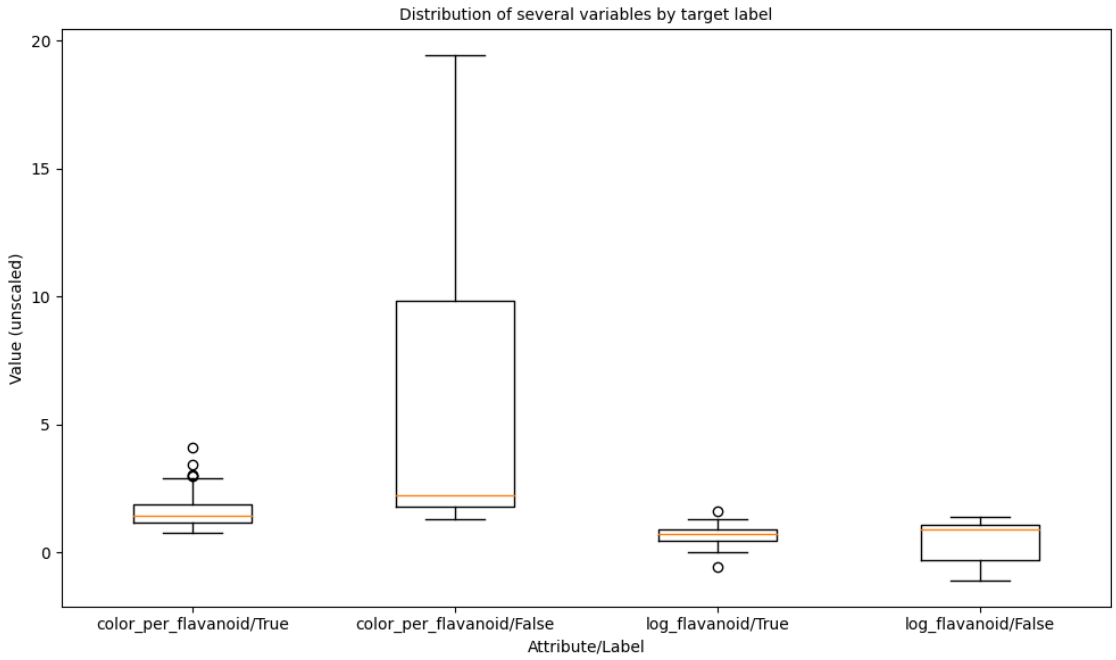

15.0
14.5
14.0
13.5
13.0
12.5
12.0
11.5
11.0
Alcohol
1
2
3
4
5
Flavanoids

[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')
```


Distribution of several variables by target label
Value (unscaled)
0
2
4
6
8
10
12
14
Hue/True
Hue/False
Flavanoids/True
Flavanoids/False
Alcohol/True
Alcohol/False
Attribute/Label

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(
    [
        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

test_ratio = 0.15       # Let's set aside 15% of the records for testing

random_seed = 1         # To prevent data leakage I will set a seed while␣
↪developing
                        # so random_seed = 1 will give me the same train/test␣
↪split over and over
# random_seed = None      # but use a fresh seed (seed=None) when its time to␣
↪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	Alcalinity_of_ash	Magnesium	Total_phenols	\
29	14.02	1.68	2.21	16.0	96.0	2.65	
16	14.30	1.92	2.72	20.0	120.0	2.80	
147	12.87	4.61	2.48	21.5	86.0	1.70	
97	12.29	1.41	1.98	16.0	85.0	2.55	
159	13.48	1.67	2.64	22.5	89.0	2.60	
..	...	...	...	...	...	...	
133	12.70	3.55	2.36	21.5	106.0	1.70	
137	12.53	5.51	2.64	25.0	96.0	1.79	
72	13.49	1.66	2.24	24.0	87.0	1.88	
140	12.93	2.81	2.70	21.0	96.0	1.54	
37	13.05	1.65	2.55	18.0	98.0	2.45	

```
     Flavanoids  Nonflavanoid_phenols  Proanthocyanins  Color_intensity   Hue  \
29         2.33                  0.26             1.98             4.70  1.04
16         3.14                  0.33             1.97             6.20  1.07
147        0.65                  0.47             0.86             7.65  0.54
97         2.50                  0.29             1.77             2.90  1.23
159        1.10                  0.52             2.29            11.75  0.57
..          ...                   ...              ...              ...   ...
133        1.20                  0.17             0.84             5.00  0.78
137        0.60                  0.63             1.10             5.00  0.82
72         1.84                  0.27             1.03             3.74  0.98
140        0.50                  0.53             0.75             4.60  0.77
37         2.43                  0.29             1.44             4.25  1.12

     OD280/OD315_of_diluted_wines  Proline  color_per_flavanoid  log_flavanoid
29                           3.59   1035.0             2.017167       0.845868
16                           2.65   1280.0             1.974522       1.144223
147                          1.86    625.0            11.769231      -0.430783
97                           2.74    428.0             1.160000       0.916291
159                          1.78    620.0            10.681818       0.095310
..                            ...      ...                  ...            ...
133                          1.29    600.0             4.166667       0.182322
137                          1.69    515.0             8.333333      -0.510826
72                           2.78    472.0             2.032609       0.609766
140                          2.31    600.0             9.200000      -0.693147
37                           2.51   1105.0             1.748971       0.887891

[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
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
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	\
29	1.259587	-0.619230	-0.535083	
16	1.603015	-0.410962	1.316905	
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	
16	0.151484	1.535977	
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
16                           -0.286882                     0.693358
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
16                          -0.508292                  0.992637
147                          1.766075                 -1.525116
97                          -0.697428                  0.628272
159                          1.513574                 -0.684120
```

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	pipeline-1__Alcalinity_of_ash	pipeline-1__Magnesium	pipeline-1__Total_phenols	pipeline-1__Flavanoids	pipeline-1__Nonflavanoid_phenols	pipeline-1__Proanthocyanins	pipeline-1__Color_intensity	pipeline-1__Hue
161	0.834735	1.561867	0.475048	0.152916	0.145732	-0.944096	-1.767256	1.019077	-1.702355	0.665657	-0.060025
117	-0.803677	-0.510235	-0.885316	0.859892	0.209196	-0.654237	-0.153878	-0.059946	-0.174009	-1.748403	0.446439
19	0.770231	1.360936	0.552783	-1.204477	0.716907	0.539303	0.837347	-1.206407	-0.079667	0.172734	-0.060025
69	-1.074596	-1.037679	-2.595489	-0.752013	2.938144	-0.909995	-1.008019	-1.408724	1.505284	-1.249160	1.560660
53	0.937942	-0.146047	1.019194	-0.667176	0.653443	1.050820	0.584268	0.277249	-0.041930	0.931077	0.800964

```
     pipeline-1__OD280/OD315_of_diluted_wines  pipeline-1__Proline  \
161                                 -1.378083           -0.251360
117                                  0.329542           -1.168856
19                                   0.928708            0.200541
69                                   0.494313           -0.147286
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,
        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': 0.98,
 'recall': 0.96,
 'f1': 0.94}
```

[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': 0.9,
 'recall': 0.88,
 'f1': 0.86}
```

[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'
    )), 2),
    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': 0.9,
 'recall': 0.9,
 'f1': 0.85}
```

[29]:
```
metrics_df =  pd.DataFrame(
    [sgd_metrics, forest_metrics, svm_metrics, knn_metrics]
)

metrics_df
```

[29]:

	model	accuracy	precision	recall	f1
0	Stochastic Gradient Descent	0.89	0.90	0.90	0.90
1	Random Forest Classifier	0.96	0.98	0.96	0.94
2	Support Vector Machine	0.89	0.90	0.88	0.86
3	K-Neighbors Classifier	0.93	0.90	0.90	0.85

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