[1]:
```python
# 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]:
```python
# 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]:

```python
# 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]:

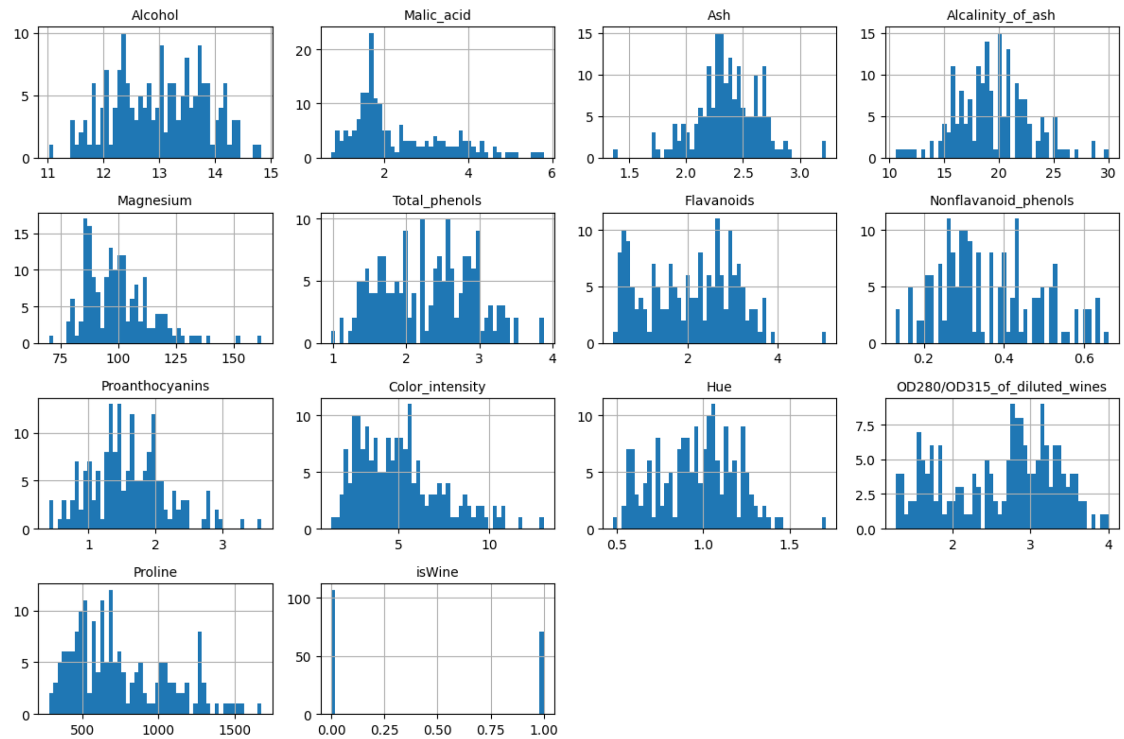
```python
# Get null counts

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]:
```python
# 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()
```

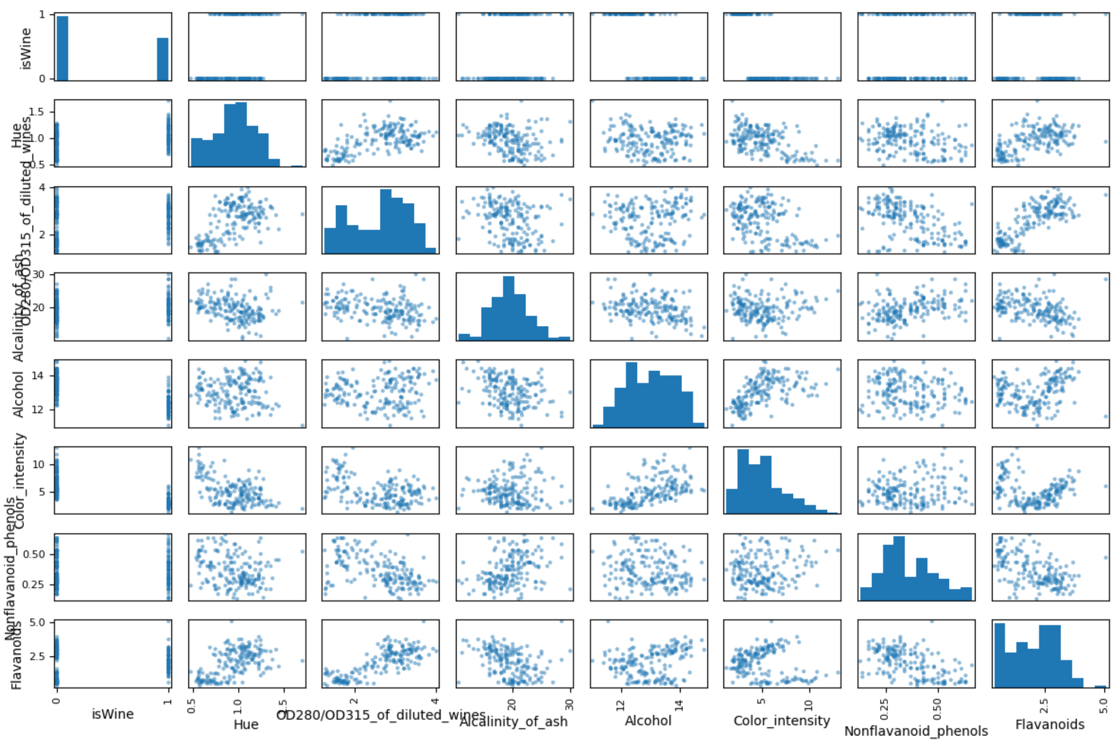


[9]:
```python
# Check for linear correlations

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
```

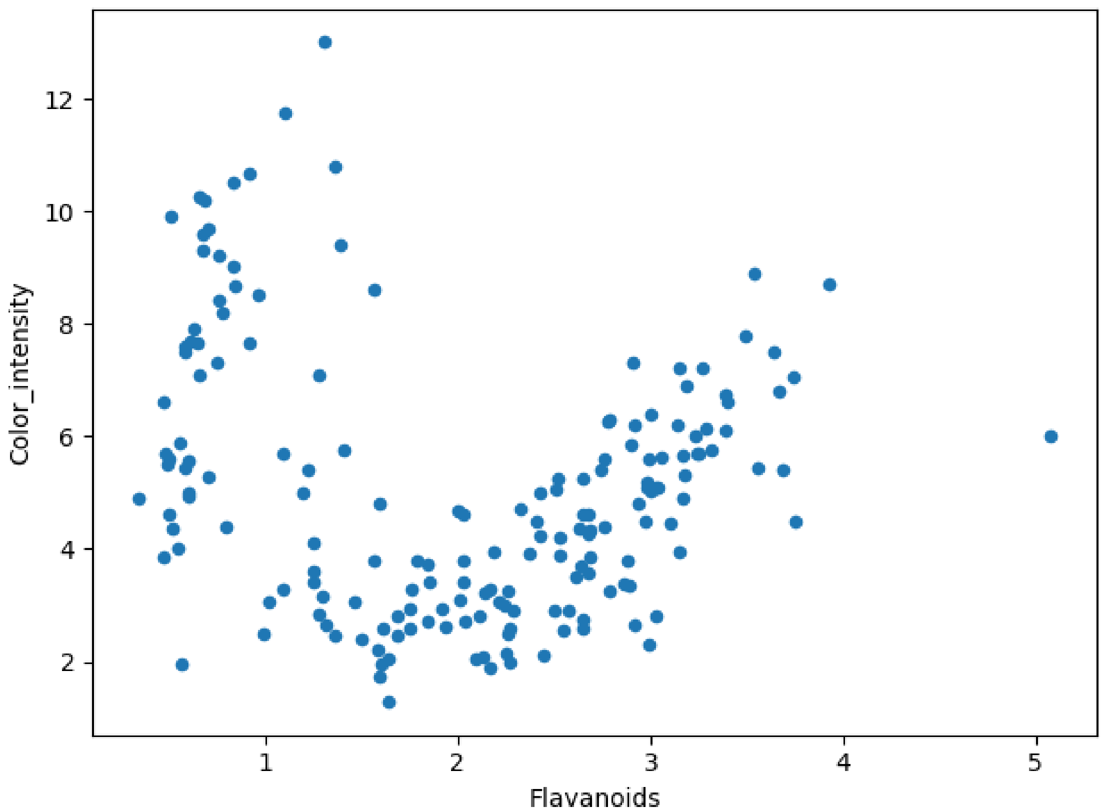
```
Magnesium                         -0.296972
Ash                               -0.362457
Proline                           -0.589850
Color_intensity                   -0.694679
Alcohol                           -0.726383
Name: isWine, dtype: float64
```

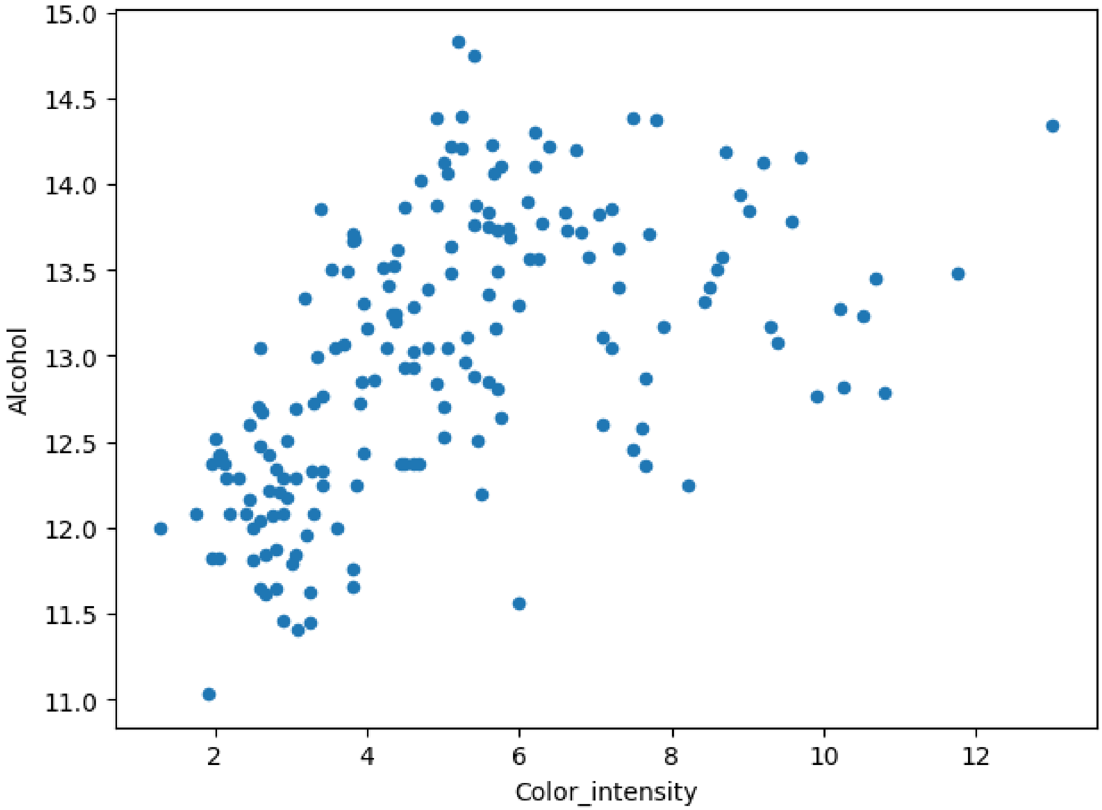
[10]:
```python
# plot scatter plots for interesting columns with promising coefficieients

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()
```

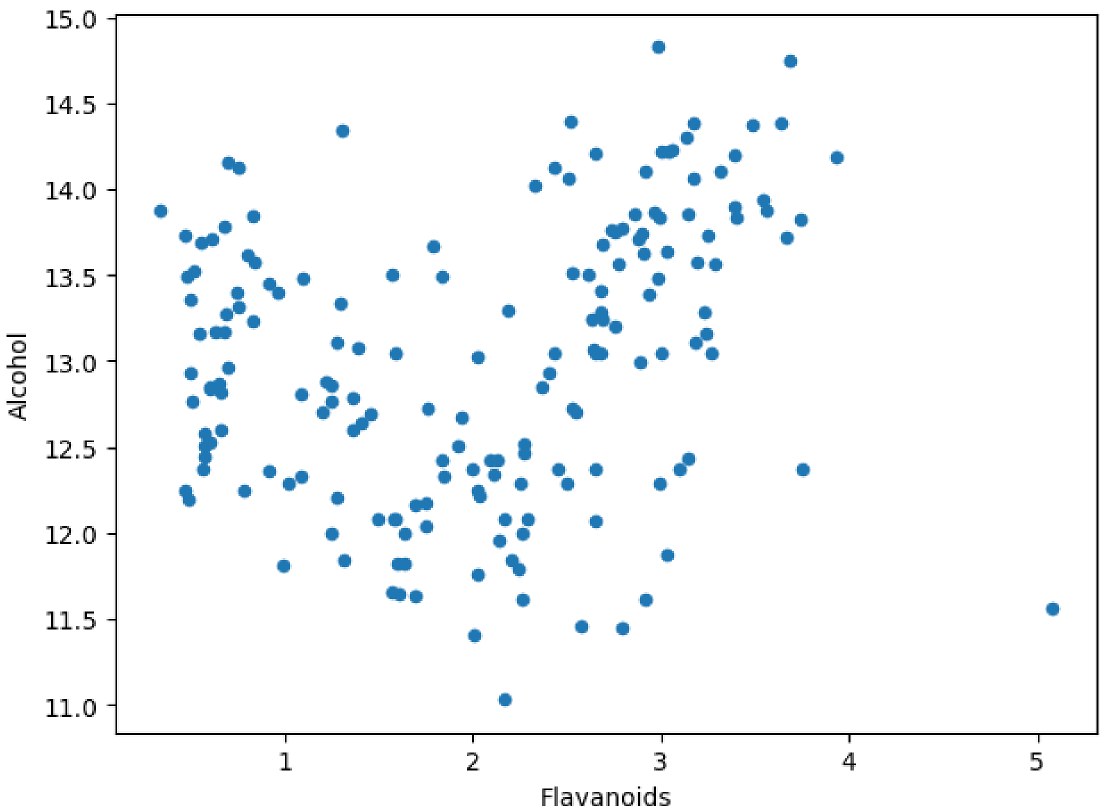


[43]:
```python
# lets examine some graphs up close
# we are looking for interesting relationships that may not be linear
# and/or may make for good engineered features.
```

```
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()
```

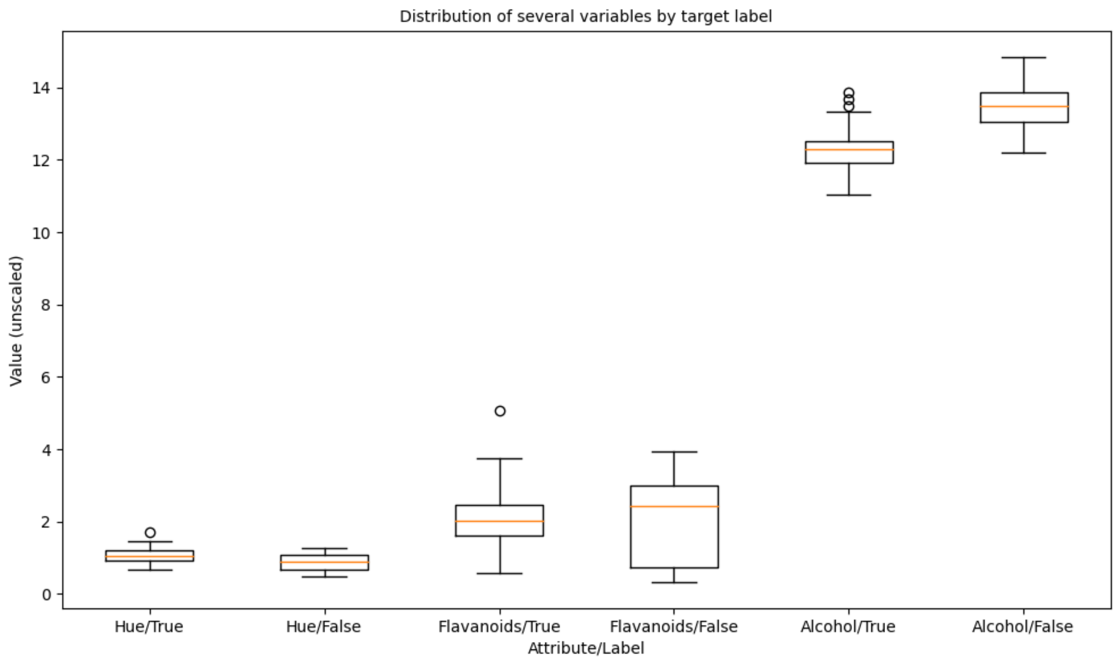



15.0
14.5
14.0
13.5
13.0
12.5
12.0
11.5
11.0
Alcohol
2
4
6
8
10
12
Color_intensity



[69]:
```
# 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',
```

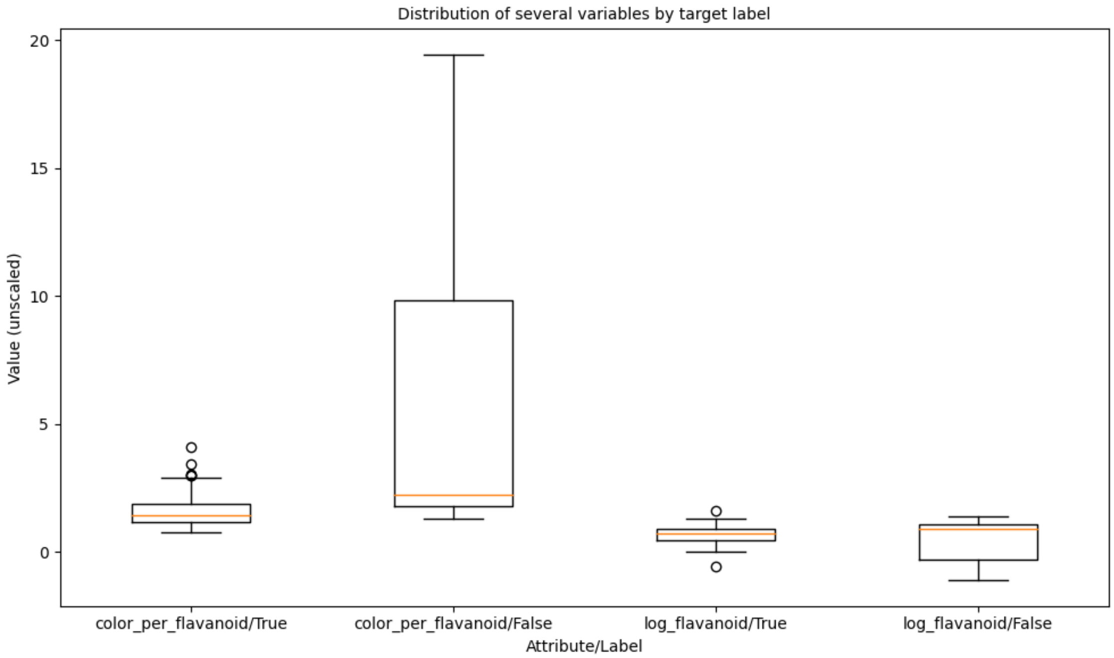
```
    xlabel='Attribute/Label',
    ylabel='Value (unscaled)',
    xticklabels=[
        'Hue/True',
        'Hue/False',
        'Flavanoids/True',
        'Flavanoids/False',
        'Alcohol/True',
        'Alcohol/False',
    ]
)
utils.save_fig('box_plots')
```



EDA: Engineering features

[75]:
```
# 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
```

```python
# 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

[50]:
```
# 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)
```

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


x_training
```

[50]:

```
     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
29                           3.59   1035.0
16                           2.65   1280.0
147                          1.86    625.0
97                           2.74    428.0
159                          1.78    620.0
..                            ...      ...
133                          1.29    600.0
137                          1.69    515.0
72                           2.78    472.0
140                          2.31    600.0
37                           2.51   1105.0

[151 rows x 13 columns]
```

[58]:
```python
# 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,)
```

[61]:
```python
# 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()),
])
```

[62]:
```python
# 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")),
])
```

[63]:
```python
# 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
```

[63]:
```
ColumnTransformer(transformers=[('pipeline-1',
                                 Pipeline(steps=[('impute',
SimpleImputer(strategy='median')),
                                                 ('standardize',
                                                  StandardScaler())]),
<sklearn.compose._column_transformer.make_column_selector object at
0x7ff32accb450>),
                                ('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
0x7ff32accb210>)])
```

[64]:
```
# 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()
```

[64]:
```
     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
```

Deployment: Model selection (without data transformations)

[ ]:
```python
# This is where next work will resume...
```