NguyenT_paper1_ipynb

July 6, 2022

1 Introduction to Machine Learning: Assignment Paper #1

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[ ]:
```
import pandas as pd
import numpy as np
from matplotlib import pyplot as plt
%matplotlib inline
import seaborn as sns
```

1.1 (1) Data Description

[ ]:
```
wines = pd.read_csv('wine.csv')
wines
```

[ ]:
```
     Wine  Alcohol  Malic.acid   Ash   Acl   Mg  Phenols  Flavanoids  \
0       1    14.23        1.71  2.43  15.6  127     2.80        3.06
1       1    13.20        1.78  2.14  11.2  100     2.65        2.76
2       1    13.16        2.36  2.67  18.6  101     2.80        3.24
3       1    14.37        1.95  2.50  16.8  113     3.85        3.49
4       1    13.24        2.59  2.87  21.0  118     2.80        2.69
..    ...      ...         ...   ...   ...  ...      ...         ...
173     3    13.71        5.65  2.45  20.5   95     1.68        0.61
174     3    13.40        3.91  2.48  23.0  102     1.80        0.75
175     3    13.27        4.28  2.26  20.0  120     1.59        0.69
176     3    13.17        2.59  2.37  20.0  120     1.65        0.68
177     3    14.13        4.10  2.74  24.5   96     2.05        0.76

     Nonflavanoid.phenols  Proanth  Color.int   Hue    OD  Proline
0                    0.28     2.29       5.64  1.04  3.92     1065
1                    0.26     1.28       4.38  1.05  3.40     1050
2                    0.30     2.81       5.68  1.03  3.17     1185
3                    0.24     2.18       7.80  0.86  3.45     1480
4                    0.39     1.82       4.32  1.04  2.93      735
..                    ...      ...        ...   ...   ...      ...
173                  0.52     1.06       7.70  0.64  1.74      740
174                  0.43     1.41       7.30  0.70  1.56      750
175                  0.43     1.35      10.20  0.59  1.56      835
```

```
176                0.53      1.46        9.30  0.60  1.62       840
177                0.56      1.35        9.20  0.61  1.60       560

[178 rows x 14 columns]
```

[ ]:
```
print('Wine columns: ', wines.columns)
print('Number of columns (features): ', len(wines.columns))
print('Number of data points (samples): ', len(wines.Wine))
```

```
Wine columns:  Index(['Wine', 'Alcohol', 'Malic.acid', 'Ash', 'Acl', 'Mg',
'Phenols',
       'Flavanoids', 'Nonflavanoid.phenols', 'Proanth', 'Color.int', 'Hue',
       'OD', 'Proline'],
      dtype='object')
Number of columns (features):  14
Number of data points (samples):  178
```

There are 14 columns (features) in this wine data set. The 14 features are: 1) Wine 2) Alcohol 3) Malic.acid 4) Ash 5) Acl 6) Mg 7) Phenols 8) Flavanoids 9) Nonflavanoid.phenols 10) Pronanth 11) Color.int 12) Hue 13) OD 14) Proline

There are 178 data points (samples).

[ ]:
```
print('Unique values for Wine column:', wines.Wine.unique())
```

```
Unique values for Wine column: [1 2 3]
```

The unique values in the Wine column are 1, 2, and 3. This means that every sample (data point) can be categorized into three categories: Wine 1, Wine 2, or Wine 3.

Summary statistics on wine data set:

[ ]:
```
wines.describe()
```

[ ]:
```
             Wine     Alcohol  Malic.acid         Ash         Acl          Mg  \
count  178.000000  178.000000  178.000000  178.000000  178.000000  178.000000
mean     1.938202   13.000618    2.336348    2.366517   19.494944   99.741573
std      0.775035    0.811827    1.117146    0.274344    3.339564   14.282484
min      1.000000   11.030000    0.740000    1.360000   10.600000   70.000000
25%      1.000000   12.362500    1.602500    2.210000   17.200000   88.000000
50%      2.000000   13.050000    1.865000    2.360000   19.500000   98.000000
75%      3.000000   13.677500    3.082500    2.557500   21.500000  107.000000
max      3.000000   14.830000    5.800000    3.230000   30.000000  162.000000

          Phenols  Flavanoids  Nonflavanoid.phenols     Proanth   Color.int  \
count  178.000000  178.000000            178.000000  178.000000  178.000000
mean     2.295112    2.029270              0.361854    1.590899    5.058090
std      0.625851    0.998859              0.124453    0.572359    2.318286
min      0.980000    0.340000              0.130000    0.410000    1.280000
25%      1.742500    1.205000              0.270000    1.250000    3.220000
```

```
50%      2.355000    2.135000              0.340000    1.555000    4.690000
75%      2.800000    2.875000              0.437500    1.950000    6.200000
max      3.880000    5.080000              0.660000    3.580000   13.000000
```

```
              Hue          OD      Proline
count  178.000000  178.000000   178.000000
mean     0.957449    2.611685   746.893258
std      0.228572    0.709990   314.907474
min      0.480000    1.270000   278.000000
25%      0.782500    1.937500   500.500000
50%      0.965000    2.780000   673.500000
75%      1.120000    3.170000   985.000000
max      1.710000    4.000000  1680.000000
```

1.2 (2) Feature Selection

Chosen features: Alcohol, Flavanoids, Proline, Color.int

1) Wines often vary in their alcohol content, so choosing the Alcohol feature could be useful.
2) Flavanoids affect many aspects of wine including its color, taste, and texture, so Flavanoids can be another useful feature.
3) Proline is an amino acid that is prevalent in wine, so this feature can also be useful in helping us categorize various wines.
4) Different wines often have different and distinct colors, so Color.int can be a useful feature.

All possible pairs of the four features:

[ ]:
```
from itertools import combinations

features = ['Alcohol', 'Flavanoids', 'Proline', 'Color.int']

pairs = list(combinations(features, 2))

print('All possible pairs from the four features')
pairs
```

```
All possible pairs from the four features
```

[ ]:
```
[('Alcohol', 'Flavanoids'),
 ('Alcohol', 'Proline'),
 ('Alcohol', 'Color.int'),
 ('Flavanoids', 'Proline'),
 ('Flavanoids', 'Color.int'),
 ('Proline', 'Color.int')]
```

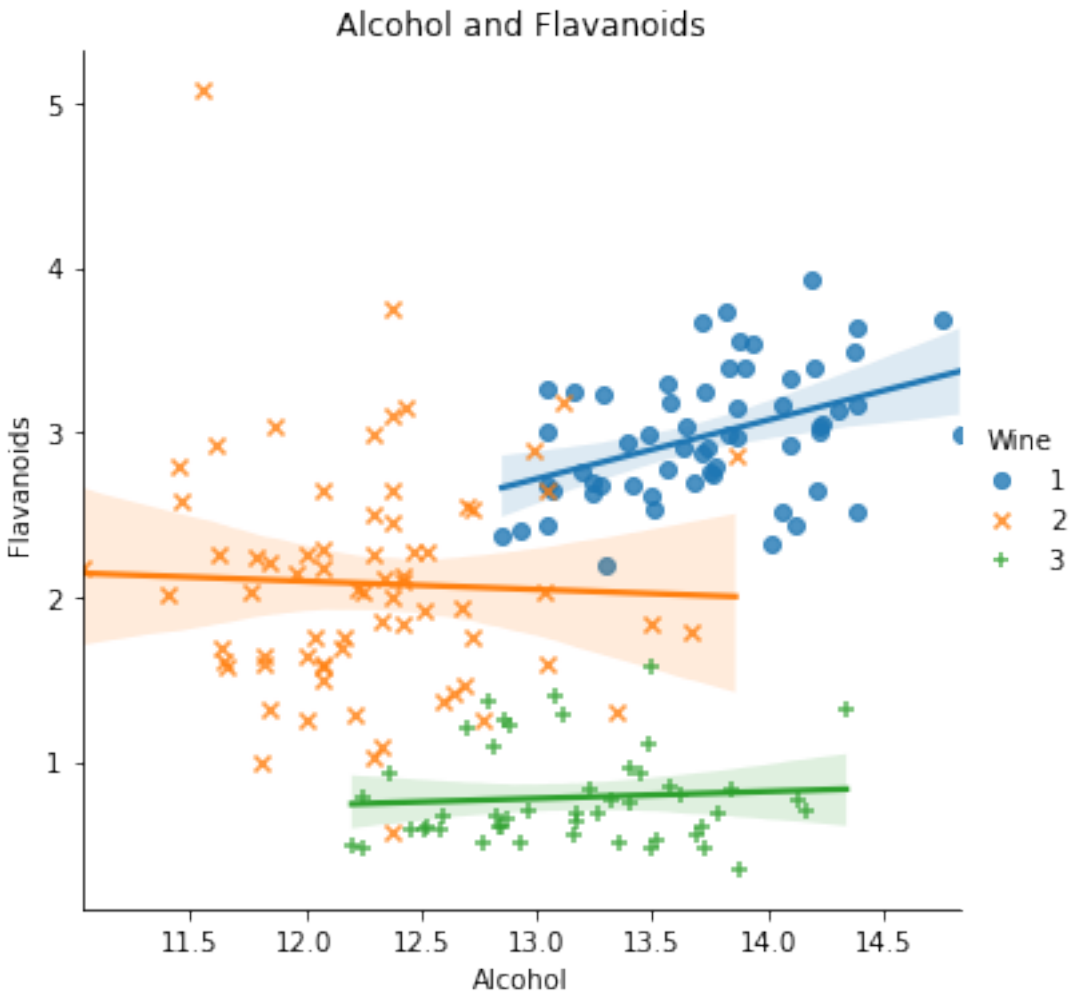
Line plots of the 6 pairs:

[ ]:
```
sns.lmplot('Alcohol', 'Flavanoids',
    data = wines, fit_reg = True,
    markers = ["o", "x", "+"],
```

```
    hue = "Wine")
plt.title('Alcohol and Flavanoids')
```

```
/Users/theodorenguyen/opt/anaconda3/lib/python3.8/site-
packages/seaborn/_decorators.py:36: FutureWarning: Pass the following variables
as keyword args: x, y. From version 0.12, the only valid positional argument
will be `data`, and passing other arguments without an explicit keyword will
result in an error or misinterpretation.
  warnings.warn(
```

[ ]: `Text(0.5, 1.0, 'Alcohol and Flavanoids')`

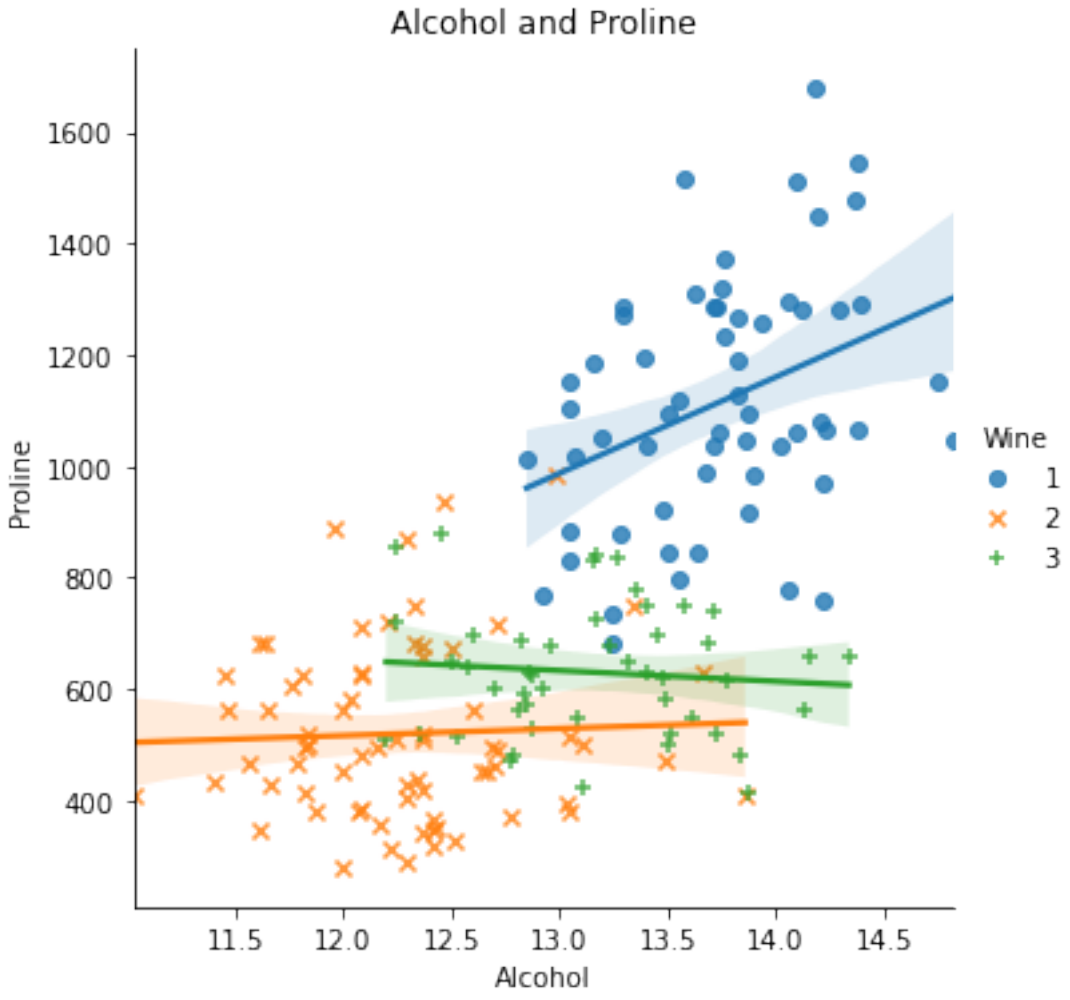


[ ]:
```
sns.lmplot('Alcohol', 'Proline',
    data = wines, fit_reg = True,
    markers = ["o", "x", "+"],
    hue = "Wine")
```

```
plt.title('Alcohol and Proline')
```

```
/Users/theodorenguyen/opt/anaconda3/lib/python3.8/site-
packages/seaborn/_decorators.py:36: FutureWarning: Pass the following variables
as keyword args: x, y. From version 0.12, the only valid positional argument
will be `data`, and passing other arguments without an explicit keyword will
result in an error or misinterpretation.
  warnings.warn(
```

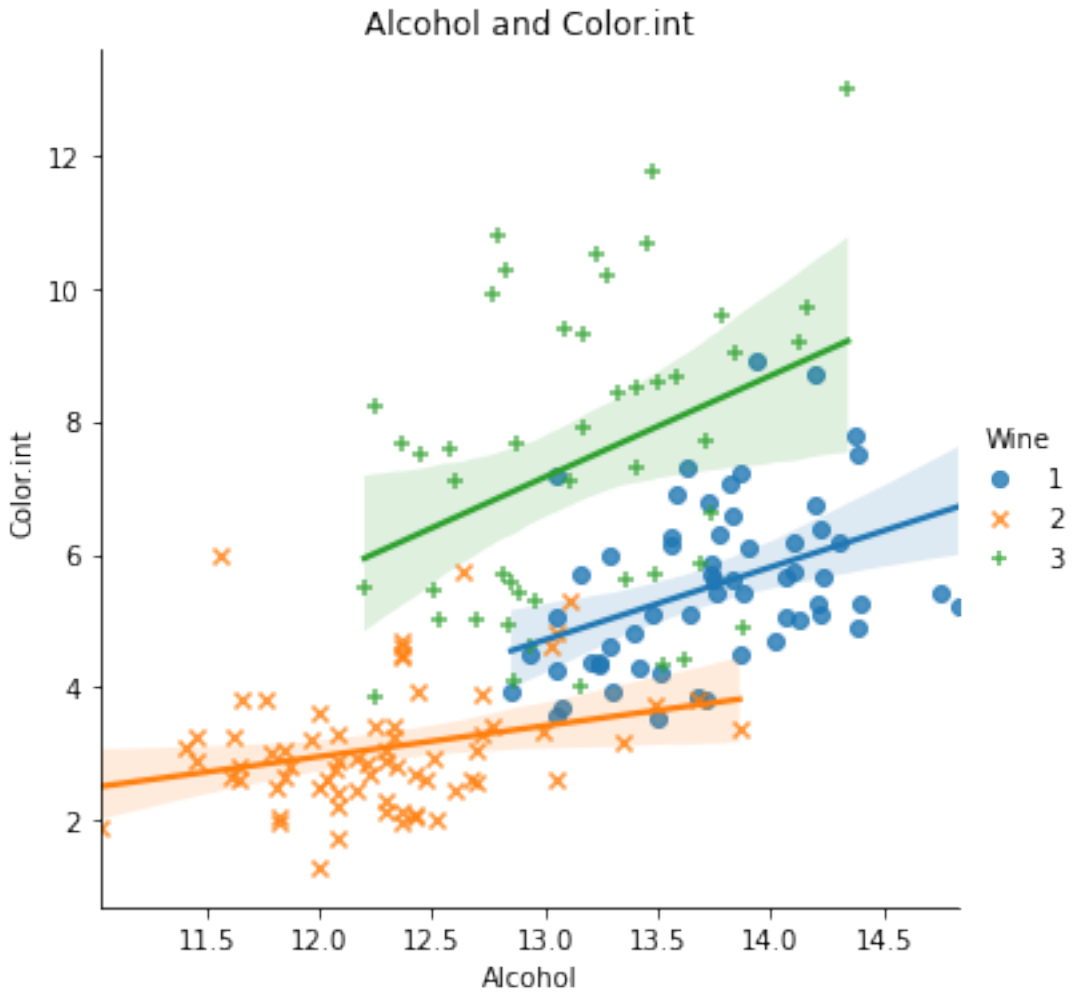
[ ]: Text(0.5, 1.0, 'Alcohol and Proline')



[ ]:
```
sns.lmplot('Alcohol', 'Color.int',
    data = wines, fit_reg = True,
    markers = ["o", "x", "+"],
    hue = "Wine")
plt.title('Alcohol and Color.int')
```

```
/Users/theodorenguyen/opt/anaconda3/lib/python3.8/site-
packages/seaborn/_decorators.py:36: FutureWarning: Pass the following variables
as keyword args: x, y. From version 0.12, the only valid positional argument
will be `data`, and passing other arguments without an explicit keyword will
result in an error or misinterpretation.
  warnings.warn(
```

[ ]:
```
Text(0.5, 1.0, 'Alcohol and Color.int')
```

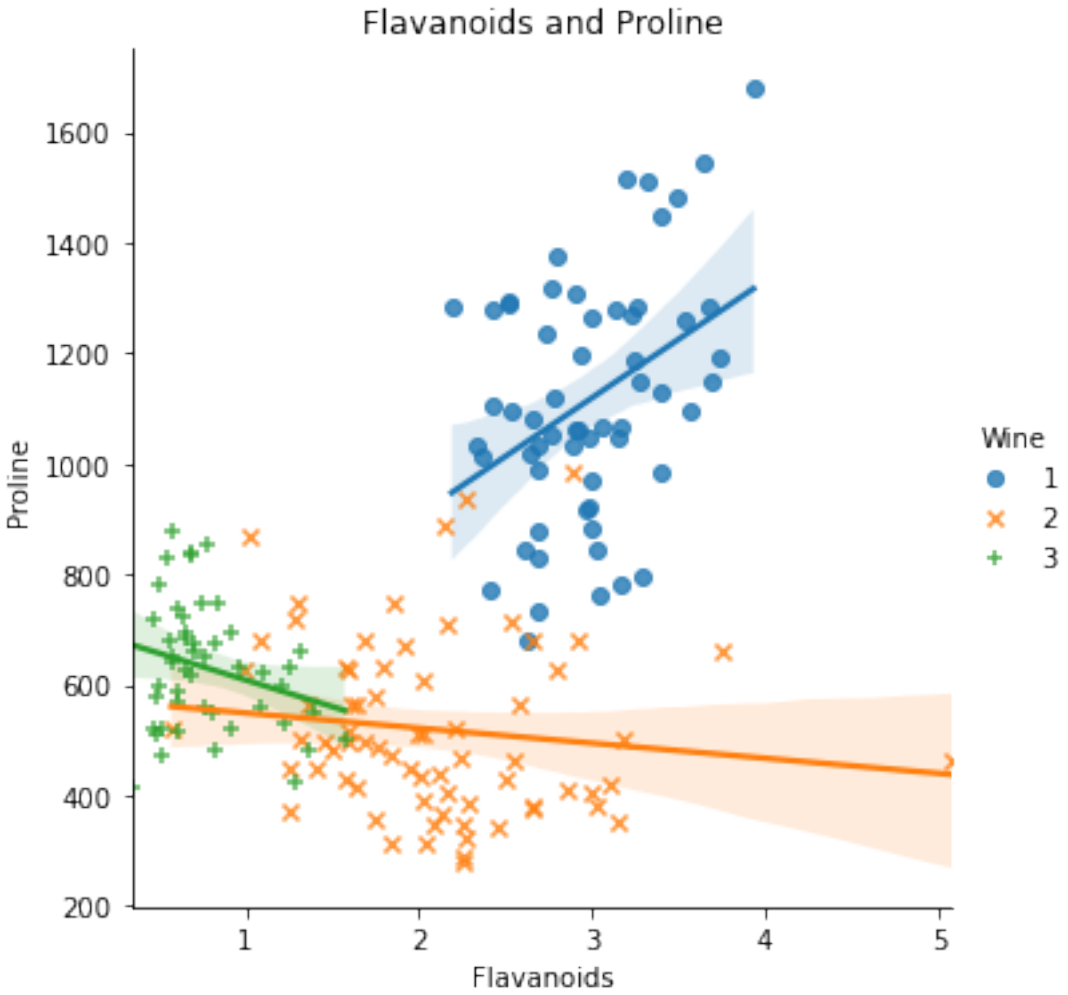


[ ]:
```
sns.lmplot('Flavanoids', 'Proline',
    data = wines, fit_reg = True,
    markers = ["o", "x", "+"],
    hue = "Wine")
plt.title('Flavanoids and Proline')
```

```
/Users/theodorenguyen/opt/anaconda3/lib/python3.8/site-
packages/seaborn/_decorators.py:36: FutureWarning: Pass the following variables
```

```
as keyword args: x, y. From version 0.12, the only valid positional argument
will be `data`, and passing other arguments without an explicit keyword will
result in an error or misinterpretation.
  warnings.warn(
```

[ ]:
```
Text(0.5, 1.0, 'Flavanoids and Proline')
```

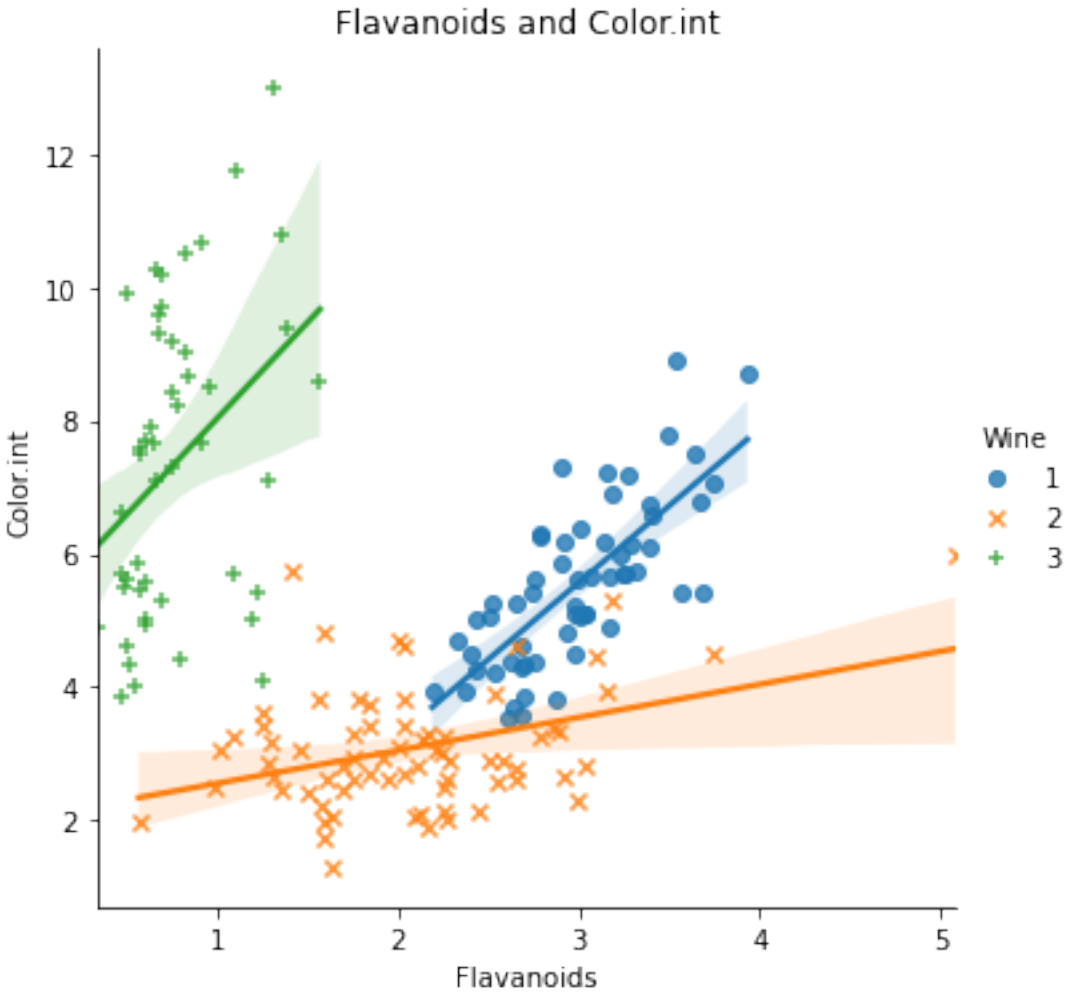


[ ]:
```
sns.lmplot('Flavanoids', 'Color.int',
    data = wines, fit_reg = True,
    markers = ["o", "x", "+"],
    hue = "Wine")
plt.title('Flavanoids and Color.int')
```

```
/Users/theodorenguyen/opt/anaconda3/lib/python3.8/site-
packages/seaborn/_decorators.py:36: FutureWarning: Pass the following variables
as keyword args: x, y. From version 0.12, the only valid positional argument
will be `data`, and passing other arguments without an explicit keyword will
```

```
result in an error or misinterpretation.
  warnings.warn(
```

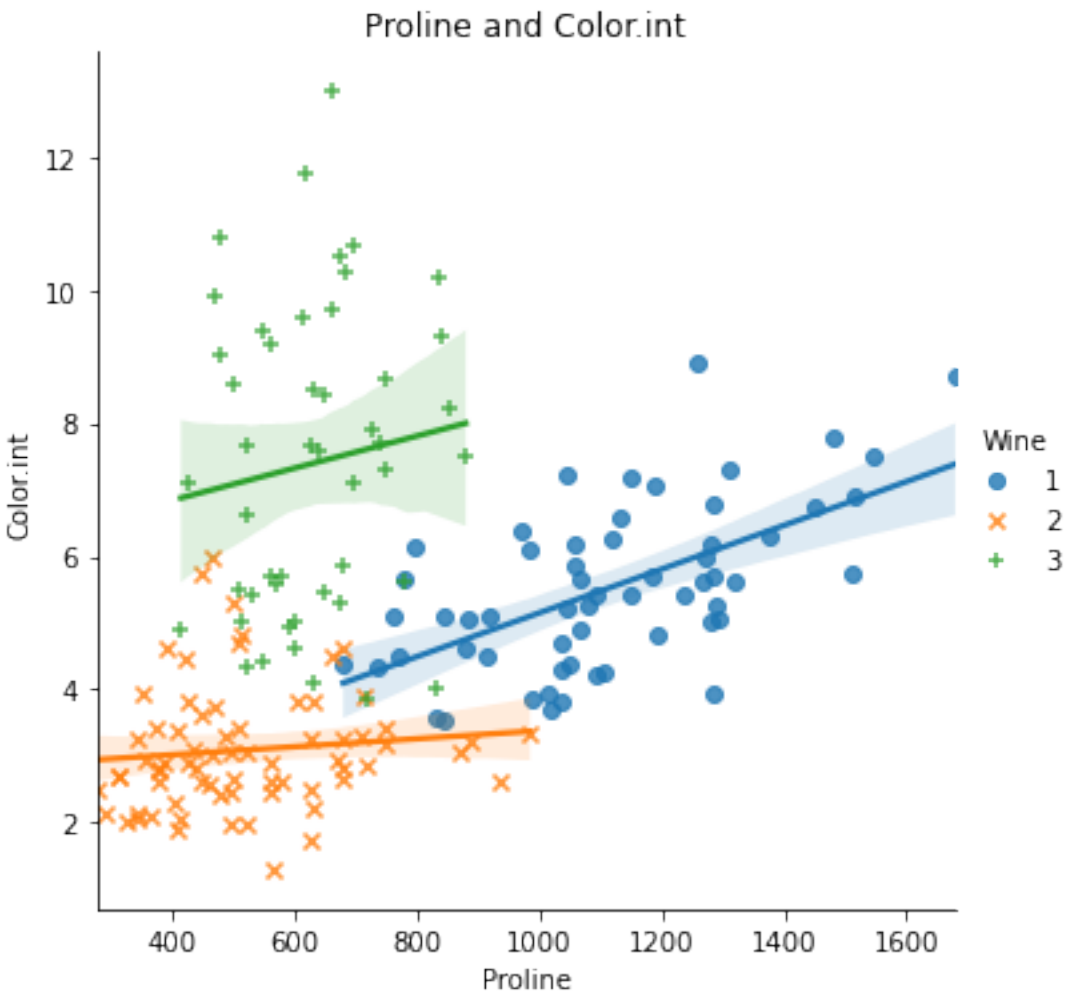
[ ]:
```
Text(0.5, 1.0, 'Flavanoids and Color.int')
```



[ ]:
```
sns.lmplot('Proline', 'Color.int',
    data = wines, fit_reg = True,
    markers = ["o", "x", "+"],
    hue = "Wine")
plt.title('Proline and Color.int')
```

```
/Users/theodorenguyen/opt/anaconda3/lib/python3.8/site-
packages/seaborn/_decorators.py:36: FutureWarning: Pass the following variables
as keyword args: x, y. From version 0.12, the only valid positional argument
will be `data`, and passing other arguments without an explicit keyword will
result in an error or misinterpretation.
  warnings.warn(
```

[ ]: Text(0.5, 1.0, 'Proline and Color.int')



1.3 (3) Train/Test Split

Data trimming:

[ ]:
```
wines.drop(['Malic.acid', 'Ash', 'Acl', 'Mg', 'Phenols', 'Nonflavanoid.
↪phenols', 'Proanth', 'Hue', 'OD'], axis = 1, inplace = True)
```

[ ]:
```
wines.head()
```

[ ]:

	Wine	Alcohol	Flavanoids	Color.int	Proline
0	1	14.23	3.06	5.64	1065
1	1	13.20	2.76	4.38	1050
2	1	13.16	3.24	5.68	1185
3	1	14.37	3.49	7.80	1480

```
4     1    13.24         2.69        4.32       735
```

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

train, test = train_test_split(wines, test_size = 0.2)

print('train size: ', len(train))
print('test size: ', len(test))
```

```
train size:  142
test size:  36
```

1.4 (4) Pickle

[ ]:
```
# Produce two .pkl files: wines_train.pkl and wines_test.pkl
import pickle

with open('wines_train.pkl', 'wb') as train_data:
    pickle.dump(train, train_data)

with open('wines_test.pkl', 'wb') as test_data:
    pickle.dump(test, test_data)
```

File names: * wines_train.pkl * wines_test.pkl

1.5 (5) Number of k's

[ ]:
```
# Open two .pkl files
with open ('wines_train.pkl', 'rb') as train_data:
    train = pickle.load(train_data)

with open('wines_test.pkl', 'rb') as test_data:
    test = pickle.load(test_data)
```

[ ]:
```
print('train size: ', len(train))
print('test size: ', len(test))
```

```
train size:  142
test size:  36
```

[ ]:
```
from sklearn.neighbors import KNeighborsClassifier

# find best k, range from 3 to half of the number of data
max_k = len(train) // 2
k_list = []
for i in range(3, max_k, 1):
    k_list.append(i)
```

```
print('max_k: ', max_k)
print('Generated ', len(k_list), ' k\'s')
```

```
max_k:  71
Generated  68  k's
```

1.6 (6) Number of Cross Validation Scores

[ ]:
```
from sklearn.model_selection import cross_val_score

# Use the four features we selected in (2) (Alcohol, Flavanoids, Proline, Color.
 ↪int).
# These are the predictor variables.
x_train = train[['Alcohol', 'Flavanoids', 'Proline', 'Color.int']]

# Our target variable is Wine (1, 2, or 3)
y_train = train['Wine']
```

[ ]:
```
# 10-fold cross validation

# Create list to store cv scores
cv_scores = []

# Set the best cross validation score to be negative infinity
best_score = -np.inf

for k in k_list:
    # k-Nearest Neighbor algorithm
    knn = KNeighborsClassifier(n_neighbors = k)
    # Store the average of 10 cross validation scores in cv_scores
    cv_scores.append(cross_val_score(knn, x_train, y_train, cv = 10, scoring =␣
 ↪'accuracy').mean())

    # If the most recent cv score is better than best_score,
    # reassign best_score and assign k to best_k
    if cv_scores[-1] > best_score:
        best_score = cv_scores[-1]
        best_k = k

print('Generated ', len(cv_scores), ' cross validation scores')
```

```
Generated  68  cross validation scores
```

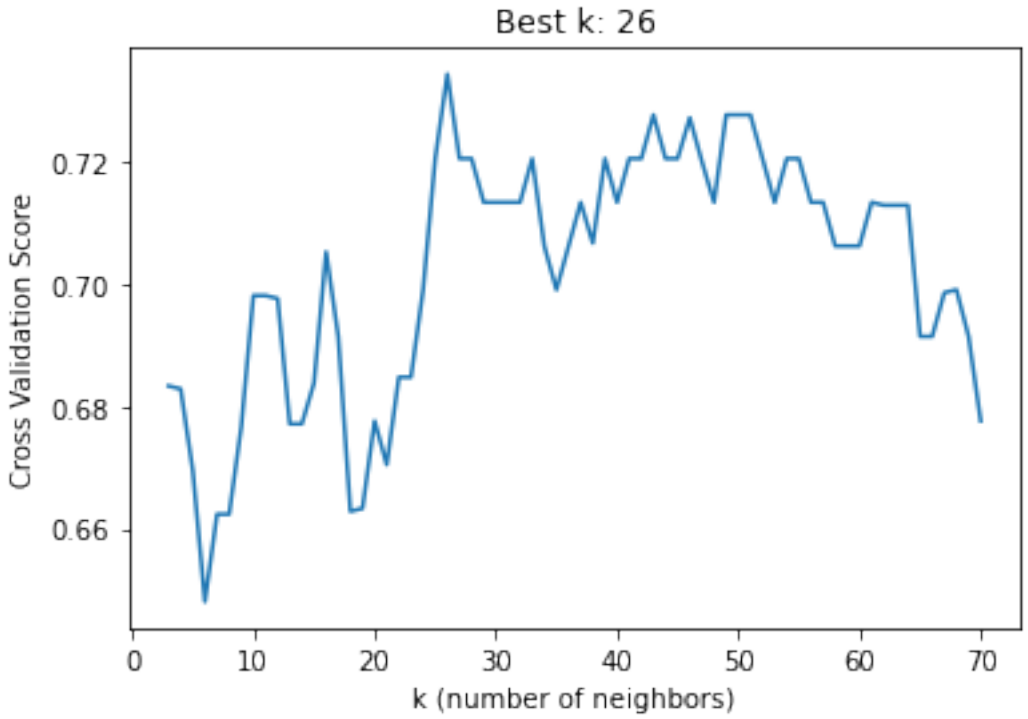
1.7 (7) Optimal Value of k

[ ]:
```
print('Best cross validation score: ', best_score)
print('Best k: ', best_k)
```

```
Best cross validation score:  0.7342857142857143
Best k:  26
```

[ ]:
```
fig, ax = plt.subplots(1)
ax.plot(k_list, cv_scores)
ax.set(title = 'Best k: ' + str(best_k),
    xlabel = 'k (number of neighbors)',
    ylabel = 'Cross Validation Score')
```

[ ]:
```
[Text(0.5, 1.0, 'Best k: 26'),
 Text(0.5, 0, 'k (number of neighbors)'),
 Text(0, 0.5, 'Cross Validation Score')]
```



1.8 (8) Accuracy Score

[ ]:
```
from sklearn.metrics import accuracy_score

# knn with n_neighbors = best_k chosen from cross validation above
knn = KNeighborsClassifier(n_neighbors = best_k)
```

```
# set up knn using train data
knn.fit(x_train, y_train)

# select data features to be used for prediction on test data
x_test = test[['Alcohol', 'Flavanoids', 'Proline', 'Color.int']]
# select target value for test data
y_test = test['Wine']

# test
predictions = knn.predict(x_test)

# check ground truth with knn prediction
comparison = pd.DataFrame(
    {'prediction' : predictions,
     'ground truth' : y_test}
)

comparison
```

[ ]:

	prediction	ground truth
110	3	2
137	2	3
131	2	3
17	1	1
109	3	2
162	3	3
89	3	2
117	2	2
104	3	2
39	3	1
62	3	2
168	3	3
19	1	1
91	2	2
108	2	2
12	1	1
166	3	3
5	1	1
125	2	2
85	2	2
140	3	3
175	1	3
32	1	1
34	1	1
71	2	2
38	1	1

```
124          2            2
155          3            3
14           1            1
107          2            2
105          2            2
116          2            2
167          3            3
20           3            1
92           2            2
55           1            1
```

[ ]:
```
# check accuracy
print('Accuracy is ' + str(accuracy_score(y_test, predictions)))
```

```
Accuracy is 0.7222222222222222
```