CSC529: Assignment #1

Matt Triano's Analysis

In [1]:
```
import pandas as pd
import matplotlib.pyplot as plt
import seaborn as sns
import numpy as np
import copy
import warnings
from scipy import stats
from IPython.display import display
from sklearn import tree
from sklearn import metrics
from sklearn.feature_selection import SelectFromModel
from sklearn.model_selection import GridSearchCV
from sklearn.model_selection import train_test_split
from sklearn import naive_bayes
from sklearn import neighbors
from sklearn import preprocessing
from sklearn.cluster import KMeans
from sklearn.metrics import accuracy_score
from sklearn.metrics import classification_report
from sklearn.model_selection import KFold, cross_val_score, cross_val_predict
from sklearn.tree import export_graphviz
import graphviz
# warnings.filterwarnings('ignore')
sns.set_style('white')
%matplotlib inline
```

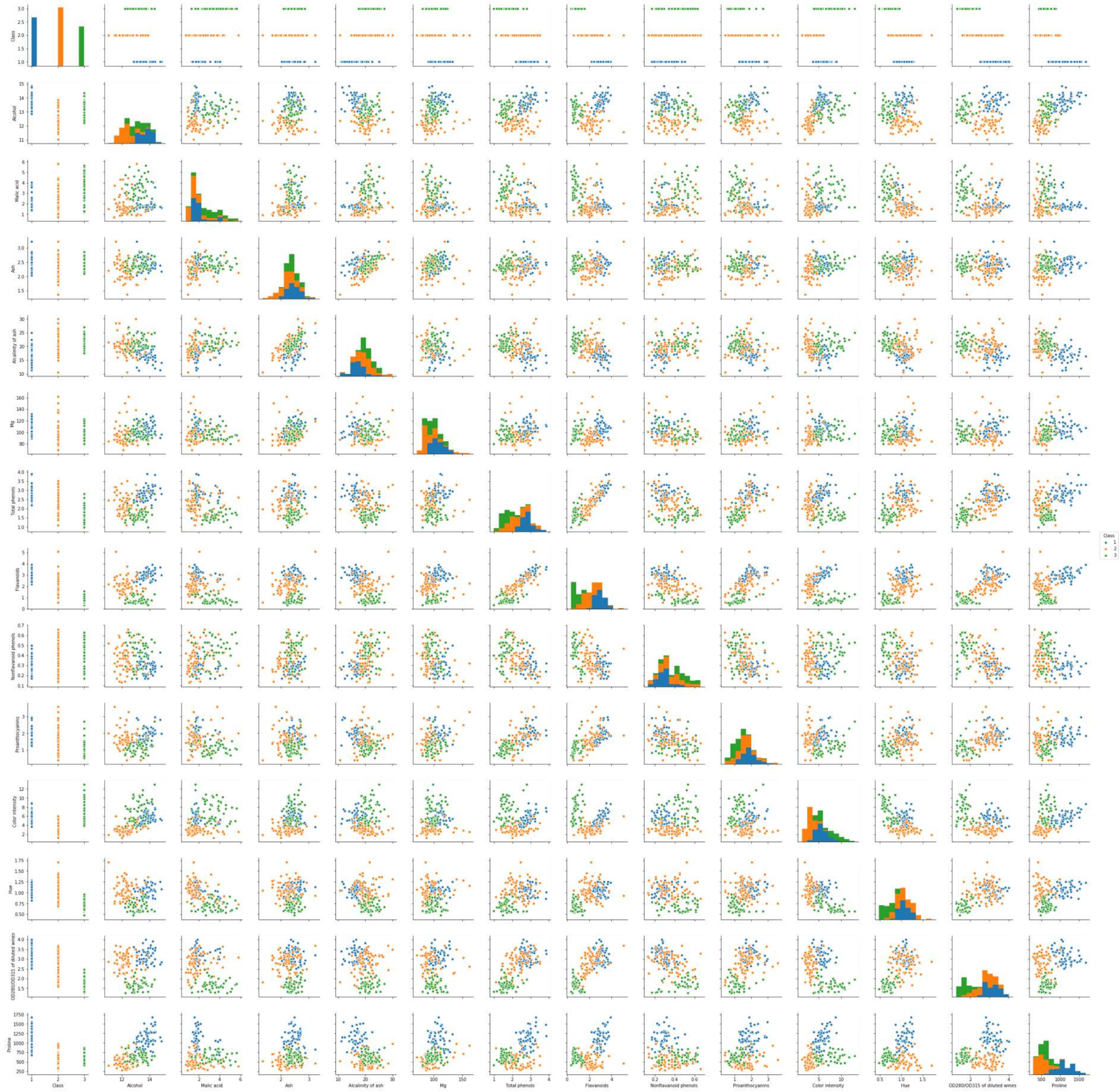
In [2]:
```
wine_df = pd.read_csv("wine.csv")
display(wine_df.columns)
wine_df.head(5)
```

```
Index(['Class', 'Alcohol', 'Malic acid', 'Ash', 'Alcalinity of ash', 'Mg',
       'Total phenols', 'Flavanoids', 'Nonflavanoid phenols',
       'Proanthocyanins', 'Color intensity', 'Hue',
       'OD280/OD315 of diluted wines', 'Proline'],
      dtype='object')
```

Out[2]:

	Class	Alcohol	Malic acid	Ash	Alcalinity of ash	Mg	Total phenols	Flavanoids	Nonflavanoid phenols	Proant
0	1	14.23	1.71	2.43	15.6	127	2.80	3.06	0.28	2.29
1	1	13.20	1.78	2.14	11.2	100	2.65	2.76	0.26	1.28
2	1	13.16	2.36	2.67	18.6	101	2.80	3.24	0.30	2.81
3	1	14.37	1.95	2.50	16.8	113	3.85	3.49	0.24	2.18
4	1	13.24	2.59	2.87	21.0	118	2.80	2.69	0.39	1.82

In [48]:
```
g = sns.pairplot(wine_df, hue='Class')
```

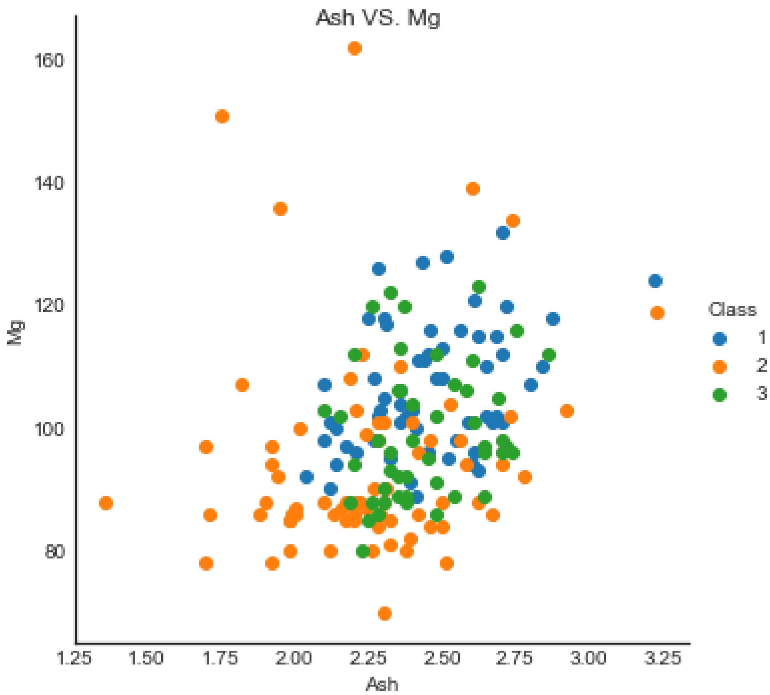


In [15]:
```
# This produces a rather attractive scatterplot
# df:         a dataframe that contains featureA, featureB, and class_variable
# featureA:   a String representation of one of the columns in DF
# featureB:   a String representation of another of the columns in DF
# class_var:  a String representation of one the class labels column in DF
def feature_compare(df, featureA, featureB, class_var):
    g = sns.FacetGrid(data=df[[class_var, featureA, featureB]],hue=class_var,
                      hue_order=[1,2,3], aspect=1, size=5)
    fig = g.fig
    g.map(plt.scatter, featureA, featureB).add_legend()
    fig.suptitle(featureA + ' VS. ' + featureB)
```

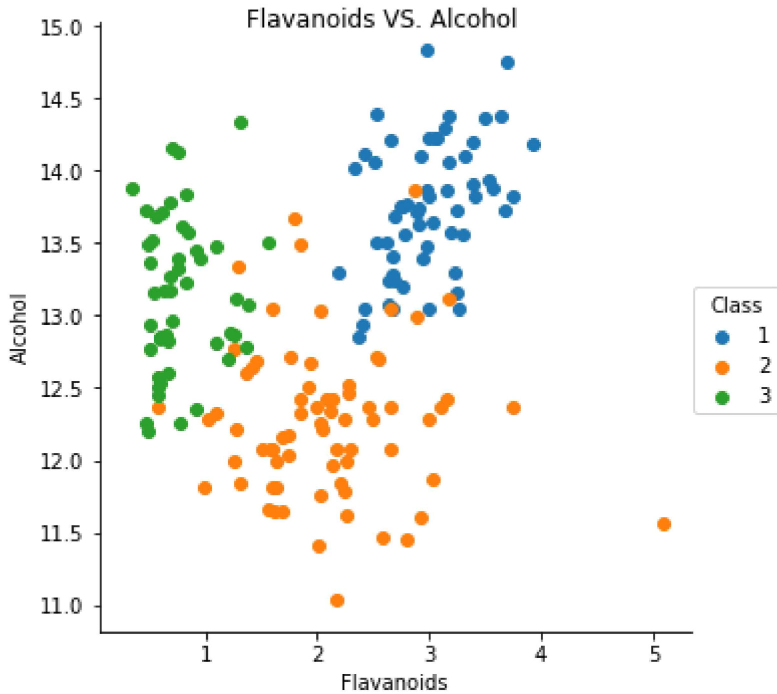
1a: Plot of 'Randomly' Selected Variables

I have to confess, I didn't pick my variables randomly. As part of my regular exploratory routine, I made a pairs plot you see above and it was pretty obvious which features were separable. Just from inspection, 'OD280/OD315 of diluted wines' vs 'Proline' looks like it generates good, distinct clusters, but 'Alcohol' and 'Flavanoids" also looks fairly well clustered. But, to highlight the fact that some of these pairings are not useful for classification, I'll show a pairing that is poorly separable, like 'Ash' and 'Mg' (I shortened magnesium because the tabular representation of the wine dataframe (above) was just a bit too wide for this notebook).

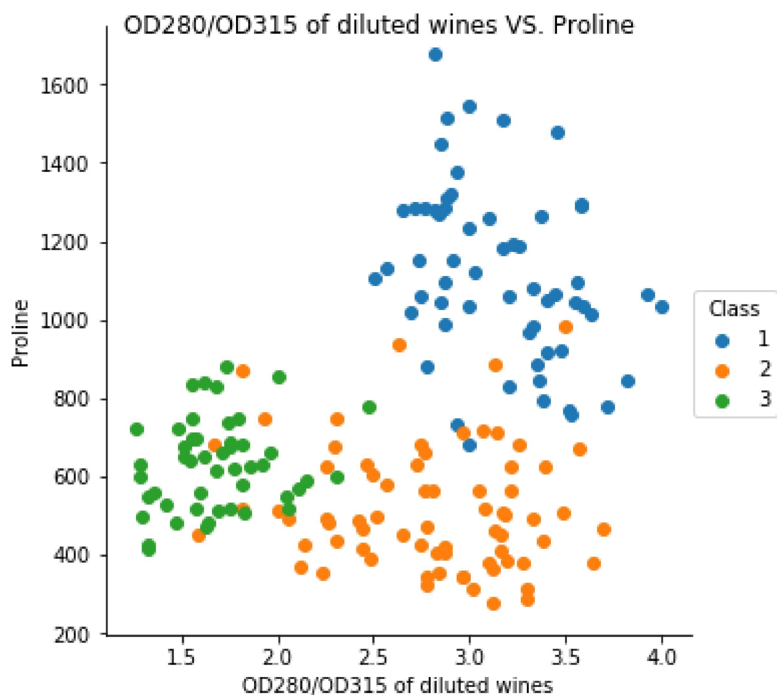
In [80]:
```
feature_compare(wine_df, 'Ash', 'Mg', 'Class')
```



In [26]:
```
feature_compare(wine_df, 'Flavanoids', 'Alcohol',  'Class')
```



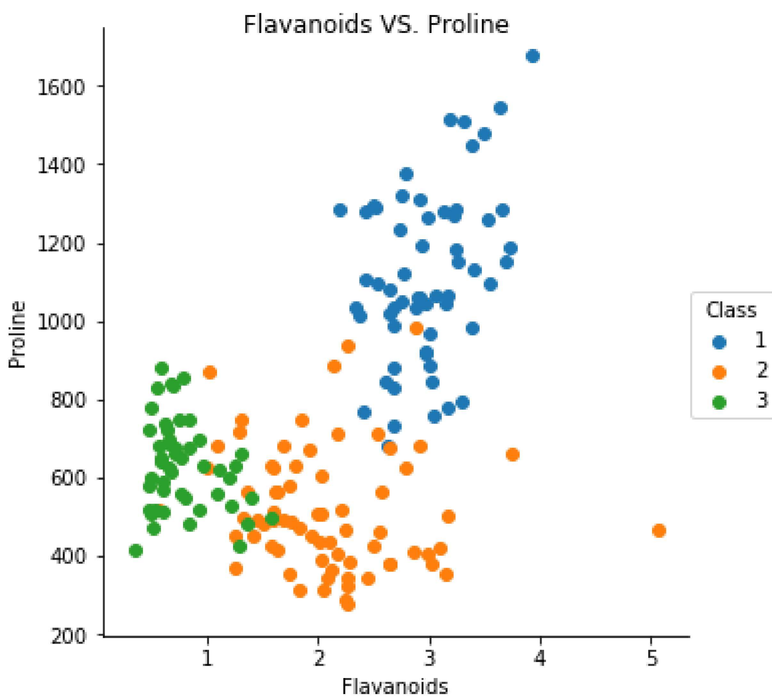
In [10]:
```
feature_compare(wine_df, 'OD280/OD315 of diluted wines', 'Proline', 'Class')
```



1b: Features Most Relevant to Classification

The decision tree classifier below indicated that largest decrease in entropy was between root node which divided data relative to a 'Proline' value of 755.0 and a node which divided data relative to a 'Flavanoids' value of 2.165. My prior guess for the clearest division was between 'Proline' and 'OD280/OD315 of diluted wines' (plotted above), but after looking at the 'Proline' vs. 'Flavanoids' plot below, it's clear that there a sharper divide between the classes, especially when projected onto the axes.

In [24]:
```
feature_compare(wine_df, 'Flavanoids', 'Proline', 'Class')
```



2: Classifiers!

2a: Decision Trees

In [4]:
```
wine_class_df = wine_df['Class']
wine_data_df = wine_df.drop('Class', axis=1)
wine_train, wine_test, class_train, class_test = train_test_split(wine_data_df
,
                                                                  wine_class_d
f,
                                                                  test_size=0.
34,
                                                                  random_state
=123)
```

In [8]:
```
from sklearn import tree
from sklearn.feature_selection import SelectFromModel
from sklearn.model_selection import GridSearchCV

parameters = {
    'criterion': ['entropy','gini'],
    'max_depth': list(range(1,10,2)),
    'min_samples_leaf': list(range(1,5,1)),
    'min_samples_split': list(range(2,10,1)),
    'random_state': [123]
}

dt_clf = tree.DecisionTreeClassifier()

dt_clf_gs = GridSearchCV(dt_clf, parameters, verbose=1, cv=10, n_jobs=4)
```

In [12]:
```
%time _ = dt_clf_gs.fit(wine_train,class_train)

dt_clf_gs.best_params_, dt_clf_gs.best_score_
```

```
Fitting 10 folds for each of 320 candidates, totalling 3200 fits
[Parallel(n_jobs=4)]: Done 222 tasks      | elapsed:    4.6s
Wall time: 7.45 s
[Parallel(n_jobs=4)]: Done 3200 out of 3200 | elapsed:    6.9s finished
```

Out[12]:
```
({'criterion': 'entropy',
  'max_depth': 3,
  'min_samples_leaf': 2,
  'min_samples_split': 2,
  'random_state': 123},
 0.90598290598290598)
```

2a.i: Decision Tree Parameters

Using scikit-learn's GridSearchCV method, I tested multiple values for the [criterion, max depth, min # of samples per leaf, and min samples for a legal split] parameters. The greatest accuracy was achieved with [criterion = entropy, max depth = 3 nodes from root, min samples per leaf = 2 samples, and min samples before a a branch can split = 2.

From the tree produced by our singular (ie non-cross-validated) holdout partitioning, we see that the **Proline** attribute provides the clearest separating line between classes, decreasing entropy from 1.5365 to 0.6891 and 1.0074 for **Proline** > 755 and **Proline** $<= 755$ respectively. As the largest descrease in entropy occurs relative to a node where **Flavanoids** provide the clearest separation, this model suggests **Proline** and **Flavanoids** are the features with the most classifying power.

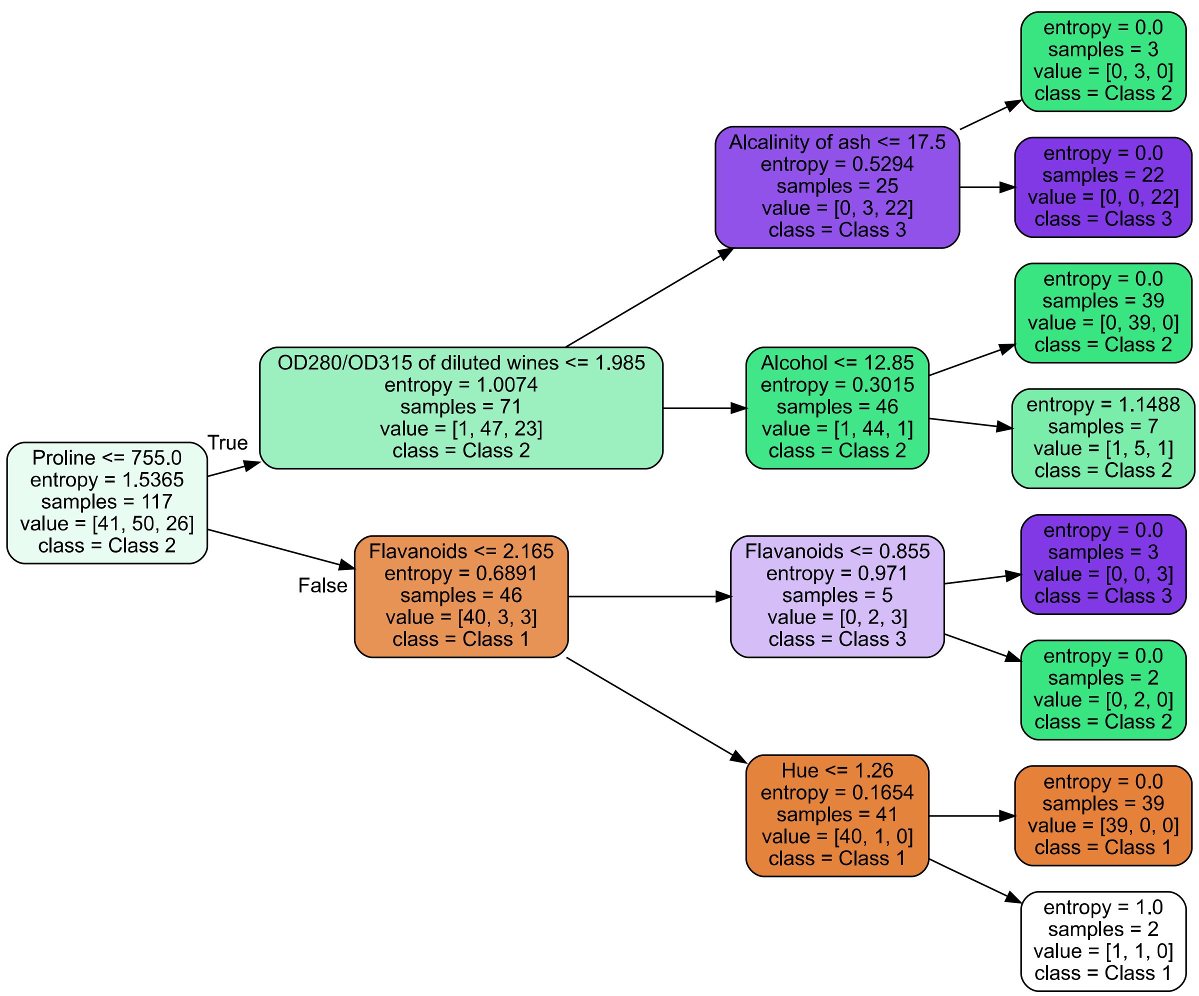
In [84]:
```
wine_tree_clf = tree.DecisionTreeClassifier(criterion='entropy',
                                            max_depth=3,
                                            min_samples_leaf=2,
                                            min_samples_split=2,
                                            random_state=123)
wine_tree_clf.fit(wine_train, class_train)
```

Out[84]:
```
DecisionTreeClassifier(class_weight=None, criterion='entropy', max_depth=3,
            max_features=None, max_leaf_nodes=None,
            min_impurity_split=1e-07, min_samples_leaf=2,
            min_samples_split=2, min_weight_fraction_leaf=0.0,
            presort=False, random_state=123, splitter='best')
```

In [85]:
```
export_graphviz(wine_tree_clf,out_file='wine_tree.dot', feature_names=wine_dat
a_df.columns,
                rounded=True, rotate=True, filled=True,
                class_names=['Class 1', 'Class 2', 'Class 3'])
```

In [16]:
```
with open('wine_tree.dot') as f:
    dot_graph = f.read()
graphviz.Source(dot_graph)
```

Out[16]:



In [82]:
```
dt_cv = cross_val_score(wine_tree_clf, wine_data_df, wine_class_df, cv=30)
dt_cv
```

Out[82]:
```
array([ 0.85714286,  1.        ,  0.71428571,  0.85714286,  0.57142857,
        0.57142857,  1.        ,  1.        ,  1.        ,  1.        ,
        0.85714286,  1.        ,  0.83333333,  0.83333333,  1.        ,
        1.        ,  1.        ,  1.        ,  1.        ,  1.        ,
        1.        ,  0.8       ,  1.        ,  1.        ,  1.        ,
        1.        ,  1.        ,  1.        ,  1.        ,  1.        ])
```

In [83]:
```
print("Decision Tree Classifier accuracy on Training Set: {:0.3f}"
      .format(wine_tree_clf.score(wine_train, class_train)))
print("Decision Tree Classifier accuracy on Testing Set: {:0.3f}"
      .format(wine_tree_clf.score(wine_test, class_test)))
print("CV Classification Accuracy: {:0.3f} +/- {:0.3f})".format(dt_cv.mean(),
dt_cv.std()))
```

```
Decision Tree Classifier accuracy on Training Set: 0.974
Decision Tree Classifier accuracy on Testing Set: 0.885
CV Classification Accuracy: 0.930 +/- 0.124)
```

2a.ii.1&2: Decision Tree Accuracy

- **Training Data:** 0.974
- **Testing Data:** 0.885

There was a possibly significant difference between the accuracy of the model with the training and testing data, but that was just based off of 1 partitioning of the data. Decision trees are predisposed to overfitting, so we have to apply cross-validation to get a better estimate of accuracy. Using 30 folds, I obseved an accuracy of 0.930 ± 0.124 for this decision tree classifier.

2a.iii: Distributional Assumptions for Decision Trees

Decision tree modeling makes no assumptions about the distribution. Independence between variables isn't necessary, variables can be categorical or continuous.

2b: Naive Bayes

In [6]:
```
nb_gauss_clf = naive_bayes.GaussianNB()
nb_gauss_clf = nb_gauss_clf.fit(wine_train, class_train)
nb_gauss_preds = nb_gauss_clf.predict(wine_test)
accuracy_score(class_test, nb_gauss_preds)

nb_cv = cross_val_score(nb_gauss_clf, wine_data_df, wine_class_df, cv=30)
```

In [7]:
```
print("Naive Bayes Classifier accuracy on Training Set: {:0.3f}"
      .format(nb_gauss_clf.score(wine_train, class_train)))
print("Naive Bayes Classifier accuracy on Testing Set:  {:0.3f}"
      .format(nb_gauss_clf.score(wine_test, class_test)))
print("CrossValidated Naive Bayes Classifier Accuracy:  {:0.3f} +/- {:0.3f})"
      .format(nb_cv.mean(), nb_cv.std()))
```

```
Naive Bayes Classifier accuracy on Training Set: 0.983
Naive Bayes Classifier accuracy on Testing Set:  1.000
CrossValidated Naive Bayes Classifier Accuracy:  0.973 +/- 0.060)
```

In [8]:
```
nb_cv = cross_val_score(nb_gauss_clf, wine_data_df, wine_class_df, cv=30)
nb_cv
```

Out[8]:
```
array([ 0.85714286,  1.        ,  1.        ,  0.85714286,  1.        ,
        1.        ,  1.        ,  1.        ,  0.85714286,  1.        ,
        1.        ,  1.        ,  0.83333333,  1.        ,  1.        ,
        1.        ,  1.        ,  1.        ,  1.        ,  1.        ,
        1.        ,  0.8       ,  1.        ,  1.        ,  1.        ,
        1.        ,  1.        ,  1.        ,  1.        ,  1.        ])
```

2b.ii: Naive Bayes Model Assumptions

Naive Bayes classifiers make the assumption that dataset features are weakly correlated and can be treated as independent, because Bayes' theorem (which is the engine of naive Bayes classifiers) applies to independent variables. From the accuracy results above, where we achieved a 0.973 accuracy using a 30-fold cross validated classifier, it's pretty safe to make the assumption of independence.

2c: KNN Classifier

2c.i: KNN Classifier Accuracy

for k=1

- **Training Data:** 1.000
- **Testing Data:** 0.984
- **30 fold, CV KNN:** 0.951 ± 0.085

for k=3

- **Training Data:** 1.000
- **Testing Data:** 0.967
- **30 fold, CV KNN:** 0.957 ± 0.081

for k=5

- **Training Data:** 1.000
- **Testing Data:** 1.000
- **30 fold, CV KNN:** 0.954 ± 0.080

for k=25

- **Training Data:** 1.000
- **Testing Data:** 0.967
- **30 fold, CV KNN:** 0.978 ± 0.056

2c.ii: Model Notes

For this KNN classifier, I used the euclidean distance as the similarity measure, and I used MinMax scaling on the data to account for the differences in unit sizes between variables. Without normalizing the data, the features represented with very small or very large units (relative to other features) will distort the distance between data, leading to less accurate classification.

In [9]:
```
def knn_classifier(k, data_df, class_df, weight='distance', print_acc=True):
    knn_clf = neighbors.KNeighborsClassifier(k, weights=weight)
    data_train, data_test, class_train, class_test = train_test_split(data_df,
                                                                    class_df,
                                                                    test_size=0.
34,
                                                                    random_state
=123)
    min_max_scaler = preprocessing.MinMaxScaler().fit(data_train)
    data_norm_train = min_max_scaler.transform(data_train)
    data_norm_test = min_max_scaler.transform(data_test)
    knn_clf.fit(data_norm_train, class_train)
    knn_pred = knn_clf.predict(data_norm_test)
    if print_acc:
        print("KNN Classifier accuracy (for k = {:0.0f}) on Training Set: {:0.
3f}"
              .format(k, knn_clf.score(data_norm_train, class_train)))
        print("KNN Classifier accuracy (for k = {:0.0f}) on Testing Set: {:0.3
f}"
              .format(k, knn_clf.score(data_norm_test, class_test)))

def knn_classifier_cv(k, data_df, class_df, print_acc=True, weight='distance'
):
    knn_clf = neighbors.KNeighborsClassifier(k, weights=weight)
    min_max_scaler = preprocessing.MinMaxScaler().fit(data_df)
    data_norm = min_max_scaler.transform(data_df)
    knn_cv = cross_val_score(knn_clf, data_norm, class_df, cv=30)
    if print_acc:
        print("CrossValidated KNN Classifier Accuracy (k = {:0.0f}): {:0.3f}
 +/- {:0.3f})"
              .format(k, knn_cv.mean(), knn_cv.std()))
    return knn_cv.mean(), knn_cv.std()

def knn_clf_k_finder(ks, data_df, class_df, print_acc=True, weight='distance'
):
    results = []
    stdevs = []
    for k in ks:
        k_mean, k_stdevs = knn_classifier_cv(k, data_df, class_df, print_acc)
        results.append(k_mean)
        stdevs.append(k_stdevs)
    return results, stdevs
```

In [10]:
```
knn_classifier(1, wine_data_df, wine_class_df, weight='distance')
knn_classifier_cv(1, wine_data_df, wine_class_df)
```

```
KNN Classifier accuracy (for k = 1) on Training Set: 1.000
KNN Classifier accuracy (for k = 1) on Testing Set: 0.984
CrossValidated KNN Classifier Accuracy (k = 1): 0.951 +/- 0.085)
```

Out[10]:
```
(0.95063492063492072, 0.085152331894729136)
```

In [8]:
```
knn_classifier(3, wine_data_df, wine_class_df, weight='distance')
knn_classifier_cv(3, wine_data_df, wine_class_df)
```

```
KNN Classifier accuracy (for k = 3) on Training Set: 1.000
KNN Classifier accuracy (for k = 3) on Testing Set: 0.967
CrossValidated KNN Classifier Accuracy (k = 3): 0.957 +/- 0.081)
```

Out[8]: `(0.9573015873015873, 0.080816724182147984)`

In [9]:
```
knn_classifier(5, wine_data_df, wine_class_df, weight='distance')
knn_classifier_cv(5, wine_data_df, wine_class_df)
```

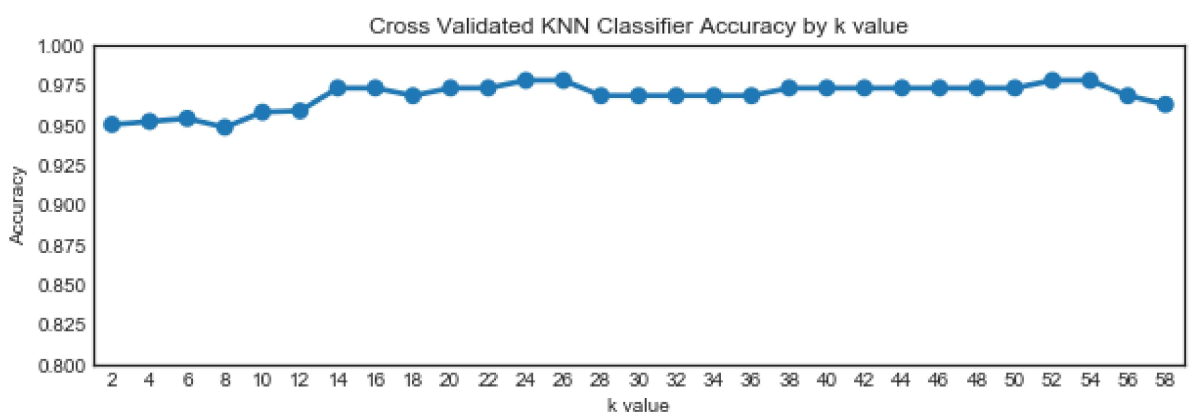
```
KNN Classifier accuracy (for k = 5) on Training Set: 1.000
KNN Classifier accuracy (for k = 5) on Testing Set: 1.000
CrossValidated KNN Classifier Accuracy (k = 5): 0.954 +/- 0.080)
```

Out[9]: `(0.95365079365079375, 0.080492938365624184)`

In [102]:
```
k_list = list(range(2,60,2))
res, stds = knn_clf_k_finder(k_list, wine_data_df, wine_class_df, print_acc=False)
```

In [137]:
```
fig, ax = plt.subplots(figsize=(10,3))
sns.pointplot(x=k_list, y=res, ax=ax)
ax.set_title('Cross Validated KNN Classifier Accuracy by k value')
ax.set_xlabel('k value')
ax.set_ylabel('Accuracy')
ax.set_ylim(.8,1)
```

Out[137]: `(0.8, 1)`



In [138]:
```
knn_classifier(25, wine_data_df, wine_class_df, weight='distance')
knn_classifier_cv(25, wine_data_df, wine_class_df)
```

```
KNN Classifier accuracy (for k = 25) on Training Set: 1.000
KNN Classifier accuracy (for k = 25) on Testing Set: 0.984
CrossValidated KNN Classifier Accuracy (k = 25): 0.978 +/- 0.056)
```

Out[138]: `(0.97825396825396826, 0.05609735805050816)`

3: Basic Concepts

3.1: Training Error

When making a classifier, we are trying to make a model that we can apply to data that wasn't used in building the model. We can add parameters to our classifier so that we correctly classify every data point (ie we can overfit the model), but if that doesn't improve our ability to classify new data, then it's not valuable. We want to build a classifier that performs best (ie has the lowest prediction error) with data that wasn't used to build the classifier.

3.2: Collective Relevance

As the picture showing the chessboard problem demonstrates, the data's projection onto either axes, x_1 or x_2, appears to show the data points are randomly distributed and well mixed, but from visual inspection, there are obvious well-defined clusters separated by class. If the classes weren't recognized, features x_1 or x_2 would appear to be uncorrelated and independent, and that's clearly not correct.

3.3: Irrelevant features

As picture 5 shows, the green triangles and red circles are similarly distributed along the horizontal axis (on the right side of the picture) and this would lead to a KNN classifier incorrectly classifying many of the data points. Performing LDA on this data clearly reveals the optimal axes orientation for this data (shown on the left side) which eliminates the unnecessary axis. This is also an example of the "Curse of Dimensionality".

3.4: Occam's Razor

The picture with the Occam's razor caption doesn't quite fit with the understanding of Occam's razor I gained in my physics education. The forumlation I learned basically says that, when comparing multiple possible explanations for some observed phenomena (after eliminating the theories that are contradicted by the observed data), prefer the simplest theory until new data forces you to add complexity.

I guess I could relate it to the image by saying that the simplest model (which would survive Occam's razor) will only try to explain the data that has been seen and won't include features that expand the domain to unseen data.