Lab 4: Scikit Learn, Classification and Clustering

Deadline Tuesday 4/20/21 11:59 pm

scikit-learn is a popular machine learning package that contains a variety of models and tools.

All objects within scikitt-learn share a uniform common basic API consisting of 3 interfaces: an *estimator* interface for building and fitting models, a *predictor* interface for making predictions, and a *transformer* interface for converting data.

> The *estimator* interface defines object mechanism and a fit method for learning a model from training data. All supervised and unsupervised learning algorithms are offered as objects implementing this interface. Other machine learning tasks such as *feature extraction*, *feature selection*, and *dimensionality reduction* are provided as *estimators*.

For more information, check the scikit-learn API paper: [https://arxiv.org/pdf/1309.0238v1.pdf]

The general form of using models in scikit-learn:

```
clf = someModel( )
clf.fit(x_train , y_tain)
```

For Example:

```
clf = LinearSVC( )
clf.fit(x_train , y_tain)
```

> The *predictor* adds a predict method that takes an array x_test and produces predictions for x_test, based on the learned parameters of the *estimator*. In supervised learning, this method typically return predicted labels or values computed by the model. Some unsupervised learning estimators may also implement the predict interface, such as **k-means**, where the predicted values are the cluster labels.

```
clf.predict(x_test)
```

> *transform* method is used to modify or filter data before feeding it to a learning algorithm. It takes some new data as input and outputs a transformed version of that data. Preprocessing, feature selection, feature extraction and dimensionality reduction algorithms are all provided as *transformers* within the library.

This is usually done with **fit_transform** method. For example:

```
PCA = RandomizedPCA (n_components = 2)
x_train = PCA.fit_transform(x_train)
x_test = PCA.fit_transform(x_test)
```

In the example above, we first **fit** the training set to find the PC components, then they are transformed.

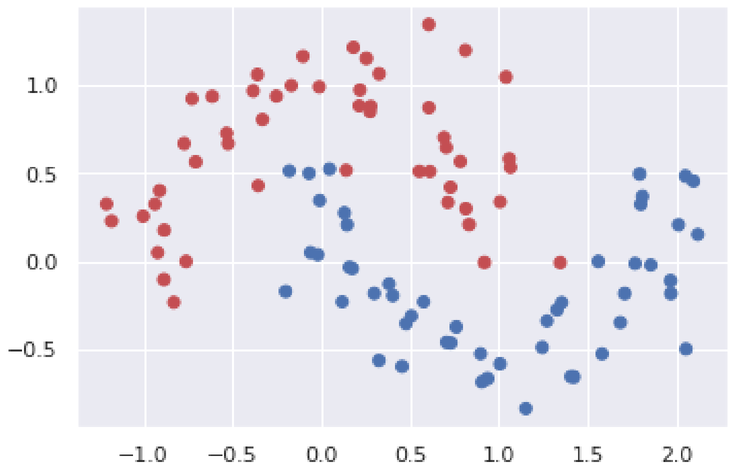
We can summarize the *estimator* as follows:

- In *all estimators*
  - `model.fit()` : fit training data. In supervised learning, fit will take two parameters: the data x and labels y. In unsupervised learning, fit will take a single parameter: the data x
- In *supervised estimators*
  - `model.predict()` : predict the label of new test data for the given model. Predict takes one parameter: the new test data and returns the learned label for each item in the test data
  - `model.score()` : Returns the score method for classification or regression methods.
- In *unsupervised estimators*
  - `model.transform()` : Tranform new data into new basis. Transform takes one parameter: new data and returns a new representation of that data based on the model

Classification: SVM

Support Vector Machines (SVM) are among the most useful and powerful supervised learning algorithm. Here we are going to look at an example of using SVM models in scikit-learn. Then, it will be your turn to try this model.

```
%matplotlib inline
import matplotlib.pyplot as plt
import seaborn as sns; sns.set()
import numpy as np


from sklearn.model_selection import train_test_split
# Import make_moons from scikit learn to generate synthetic data
from sklearn.datasets import make_moons


# 2d classification dataset
Xs , ys = make_moons( n_samples = 100,noise = 0.2 , random_state = 0)


# train-test split

Xs_train , Xs_test, ys_train, ys_test = train_test_split(Xs, ys , test_size = 0.15 )

#plot the data
colors = np.array(['r' , 'b'])
plt.scatter(Xs[:,0] , Xs[:,1]  ,c = colors[ys] )
plt.show()
```

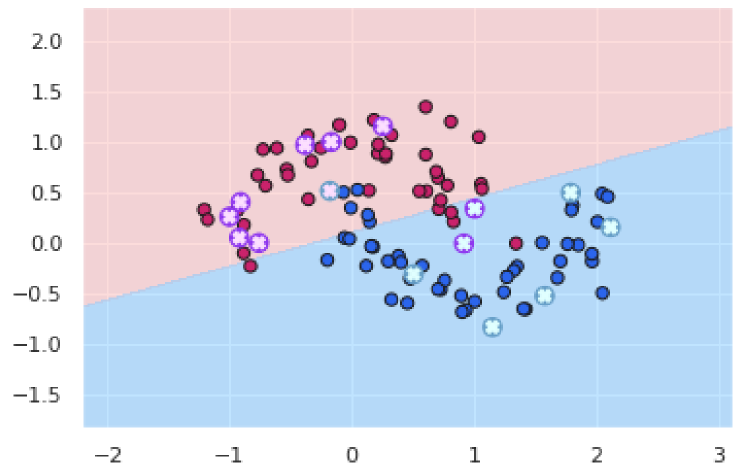


We will perform both linear and nonlinear SVM on this synthetic dataset:

```
def meshGrid (x , y , h):
    '''x is data for x-axis meshgrid
       y is data for y-axis meshgrid
       h is stepsize
    '''
    x_min, x_max = x.min() - 1 , x.max() + 1
    y_min, y_max = y.min() - 1 , y.max() + 1
    xx, yy = np.meshgrid(np.arange(x_min, x_max, h), np.arange(y_min, y_max, h))

    return xx , yy




#Import SVM
from sklearn import svm

from matplotlib.colors import ListedColormap
from sklearn import metrics


cmap_light = ListedColormap(['#FBBBB9', '#82CAFF'])
cmap_bold = ListedColormap(['#CA226B', '#2B65EC'])
cmap_test = ListedColormap(['#8E35EF', '#659EC7'])
cmap_predict = ListedColormap(['#FCDFFF', '#E0FFFF'])

# clf1 is a linear svm classifier
clf1 = svm.SVC(kernel = 'linear')

# Fit data
clf1.fit(Xs_train, ys_train)

# Predict
ys_predict = clf1.predict(Xs_test)


#Display the outcome of classification
print(metrics.classification_report(ys_test, ys_predict))
print(metrics.confusion_matrix(ys_test, ys_predict))

# Display the svm
```

```
xx , yy = meshGrid(Xs[:,0], Xs[:,1], 0.01)


Z = clf1.predict(np.c_[xx.ravel(), yy.ravel()])
Z = Z.reshape(xx.shape)

plt.figure()
plt.contourf(xx, yy, Z, cmap=cmap_light ,levels=[-1, 0, 1] ,alpha = 0.5)

# For plotting all data use the following line
#plt.scatter(Xs[:, 0], Xs[:, 1], c=ys, cmap=cmap_bold, edgecolor='k', s=50)

# For plotting train and test and prediction separatley
plt.scatter(Xs_train[:, 0], Xs_train[:, 1], c=ys_train, cmap=cmap_bold,edgecolor='k', s=40)
plt.scatter(Xs_test[:, 0], Xs_test[:, 1], alpha=1.0,c = ys_test, cmap=cmap_test,linewidth=1, marker='o'
plt.scatter(Xs_test[:, 0], Xs_test[:, 1], alpha=1.0,c = ys_predict, cmap=cmap_predict ,linewidth=1, mar
plt.xlim(xx.min(), xx.max())
plt.ylim(yy.min(), yy.max())

plt.show()
```

```
                  precision    recall  f1-score   support

               0       0.88      0.78      0.82         9
               1       0.71      0.83      0.77         6

        accuracy                           0.80        15
       macro avg       0.79      0.81      0.80        15
    weighted avg       0.81      0.80      0.80        15

    [[7 2]
     [1 5]]
```

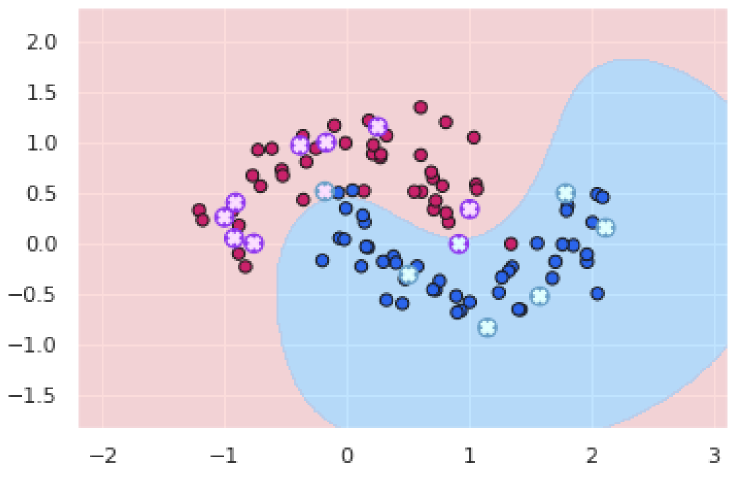


Now we apply a non-linear svm classifier

```
# clf2 is a nonlinear svm classifier

clf2 = svm.SVC(kernel = 'rbf')


# Fit data
clf2.fit(Xs_train, ys_train)

# Predict
ys_predict2 = clf2.predict(Xs_test)
```

```
#Display the outcome of classification
print(metrics.classification_report(ys_test, ys_predict2))
print(metrics.confusion_matrix(ys_test, ys_predict2))

# Display the svm
xx , yy = meshGrid(Xs[:,0], Xs[:,1], 0.01)



Z = clf2.predict(np.c_[xx.ravel(), yy.ravel()])
Z = Z.reshape(xx.shape)

plt.figure()
plt.contourf(xx, yy, Z, cmap=cmap_light ,levels=[-1, 0, 1] ,alpha = 0.5)

# For plotting all data use the following line
#plt.scatter(Xs[:, 0], Xs[:, 1], c=ys, cmap=cmap_bold, edgecolor='k', s=50)

# For plotting train and test and prediction separatley
plt.scatter(Xs_train[:, 0], Xs_train[:, 1], c=ys_train, cmap=cmap_bold,edgecolor='k', s=40)
plt.scatter(Xs_test[:, 0], Xs_test[:, 1], alpha=1.0,c = ys_test, cmap=cmap_test,linewidth=1, marker='o'
plt.scatter(Xs_test[:, 0], Xs_test[:, 1], alpha=1.0,c = ys_predict2, cmap=cmap_predict ,linewidth=1, ma
plt.xlim(xx.min(), xx.max())
plt.ylim(yy.min(), yy.max())

plt.show()
```

```
              precision    recall  f1-score   support

           0       0.89      0.89      0.89         9
           1       0.83      0.83      0.83         6

    accuracy                           0.87        15
   macro avg       0.86      0.86      0.86        15
weighted avg       0.87      0.87      0.87        15

[[8 1]
 [1 5]]
```



SVM on Wine quality dataset

Exercise 4.1 (30 pts)

Now it's your turn to work with SVM. The wine data set is loaded below. You can learn more about the dataset by using `datasett.DESCR`. Here, you need to work with the first two features to train your model.

- Select the first two features for your X
- Split the dataset in two sets of training and testing data. Use 80% of the data for training and 20% for testing
- Perform linear and non-linear SVM on the dataset
- Display the classification report and accuracy for both models

```
from sklearn.datasets import load_wine

Xwine_full , ywine = load_wine(return_X_y = True)

#Your code here
# get two features
X_two_features = Xwine_full[:,[0,1]]

# split data
X_train , X_test, y_train, y_test = train_test_split(X_two_features, ywine, test_size = 0.2)

# linear SVM
linear_svm = svm.SVC(kernel = 'linear')

# Fit
linear_svm.fit(X_train, y_train)

# Predict
linear_predict = linear_svm.predict(X_test)

# Outcome
print(metrics.classification_report(y_test, linear_predict))

# non-linear SVM

non_linear_svm = svm.SVC(kernel = 'rbf')

# Fit
non_linear_svm.fit(X_train, y_train)

# Predict
non_linear_predict = non_linear_svm.predict(X_test)

# Outcome
print(metrics.classification_report(y_test, non_linear_predict))
```

```
              precision    recall  f1-score   support

           0       0.56      0.62      0.59         8
           1       0.81      0.94      0.87        18
           2       0.67      0.40      0.50        10

    accuracy                           0.72        36
   macro avg       0.68      0.66      0.65        36
weighted avg       0.71      0.72      0.71        36

              precision    recall  f1-score   support

           0       0.60      0.75      0.67         8
           1       0.81      0.94      0.87        18
           2       0.80      0.40      0.53        10

    accuracy                           0.75        36
   macro avg       0.74      0.70      0.69        36
weighted avg       0.76      0.75      0.73        36
```

Exercise 4.2 (10 pts)

Scaling features is another step that can affect the performance of your classifier. For the wine data, scale the features using `StandardScaler` and perform linear SVM. Display the classification report and accuracy. Did scaling data affect the classifier performance?

```
from sklearn.preprocessing import StandardScaler

scaler = StandardScaler()


#Your code here
# fit data into scaler
scaler.fit(X_train, y_train)

# transform data
tr_X_train= scaler.transform(X_train)

# same for test data
scaler.fit(X_test, y_test)
tr_X_test= scaler.transform(X_test)

# create linear svm
linear_svm_tr = svm.SVC(kernel = 'linear')

linear_svm_tr.fit(tr_X_train, y_train)

pred = linear_svm_tr.predict(tr_X_test)

print(metrics.classification_report(y_test, pred))

print('Scaled dataset has higher accuracy than non-scaled dataset.')
```

```
              precision    recall  f1-score   support

           0       0.50      0.75      0.60         8
           1       1.00      0.83      0.91        18
           2       0.78      0.70      0.74        10

    accuracy                           0.78        36
   macro avg       0.76      0.76      0.75        36
weighted avg       0.83      0.78      0.79        36

Scaled dataset has higher accuracy than non-scaled dataset.
```

Exercise 4.3 (10 pts)

scikit-learn has many other classifiers. Pick another classifier of your choice (KNN, DecisionTree, NaiveBayes, ...) and apply it to the wine dataset. Display the classification report and accuracy.

```
#Your code goes here
```

```
from sklearn.neighbors import KNeighborsClassifier

# doing a knn model

knn = KNeighborsClassifier(10)

knn.fit(X_train, y_train)

predict_knn = knn.predict(X_test)

print(metrics.classification_report(y_test, predict_knn))
```

```
              precision    recall  f1-score   support

           0       0.60      0.75      0.67         8
           1       0.94      0.94      0.94        18
           2       0.75      0.60      0.67        10

    accuracy                           0.81        36
   macro avg       0.76      0.76      0.76        36
weighted avg       0.81      0.81      0.81        36
```

Clustering

You have already seen an example of clustering using scikit-learn in lecture. In this section, you will apply `KMeans` algorithm to the wine dataset.

Exercise 4.4 (30 pts)

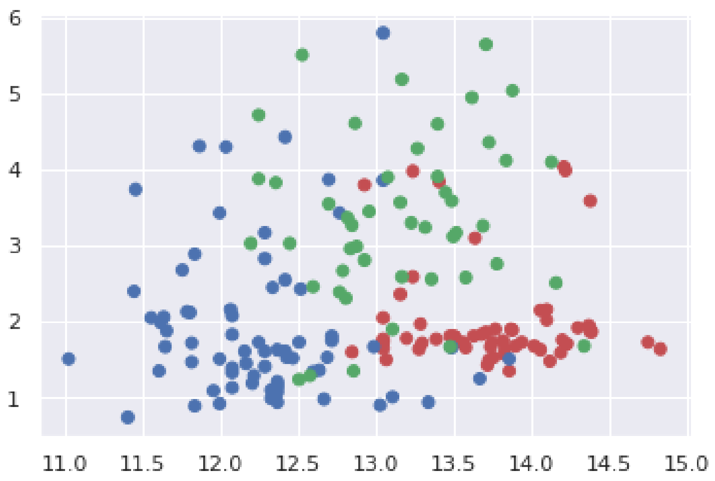
- First choose the first two features and apply kmeans clustering.
- Display cluster evaluation metrics `homogeneity_score` and `completeness_score` (both belong to sklearn.metrics)
- Plot the clusters and centroids. You have the "ground truth" or labels of your data points, your plot should create a meshgrid to display the decision boundary of your model, and add the datapoints and their true labels. (This is to observe how good your model performs on the data)

Note: For displaying decision boundaries and data points follow these steps:

1. Use meshGrid function to get the mesh for your attributes
2. Obtain labels for each point in mesh and reshape it. (Z = kmeans.predict(....))
3. Put the results into a color plot
    - Plot the colormesh --> plt.pcolormesh
    - Plot your data points --> plt.scatter
    - Plot the centroids --> plt.scatter
    - Set titles, x and y ranges
    - plt.show()

```
from sklearn.cluster import KMeans

Xwine_full , ywine = load_wine(return_X_y = True)

Xc = Xwine_full [:, :2]
```

```
colormap = np.array(['r' , 'b' , 'g'])
plt.scatter(Xc[:,0],Xc[:,1] , c = colormap[ywine])
plt.show()
```



Clustering

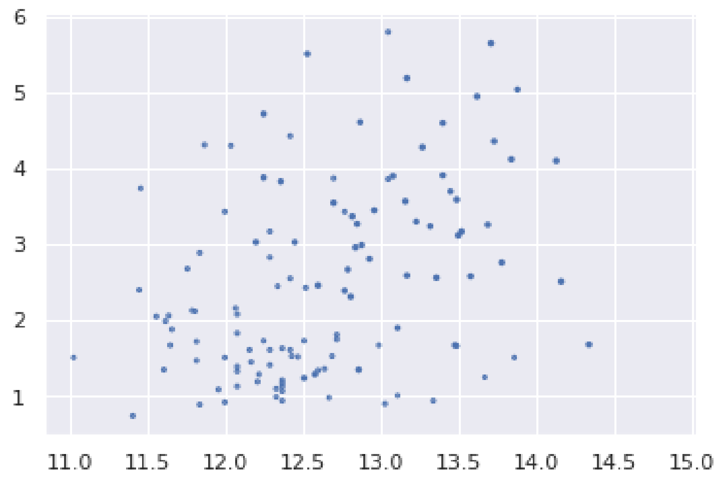
You have already seen an example of clustering using scikit-learn in lecture. In this section, you will apply `KMeans` algorithm to the wine dataset.

Exercise 4.4 (30 pts)

- First choose the first two features and apply kmeans clustering.
- Display cluster evaluation metrics `homogeneity_score` and `completeness_score` (both belong to sklearn.metrics)
- Plot the clusters and centroids. You have the "ground truth" or labels of your data points, your plot should create a meshgrid to display the decision boundary of your model, and add the datapoints and their true labels. (This is to observe how good your model performs on the data)

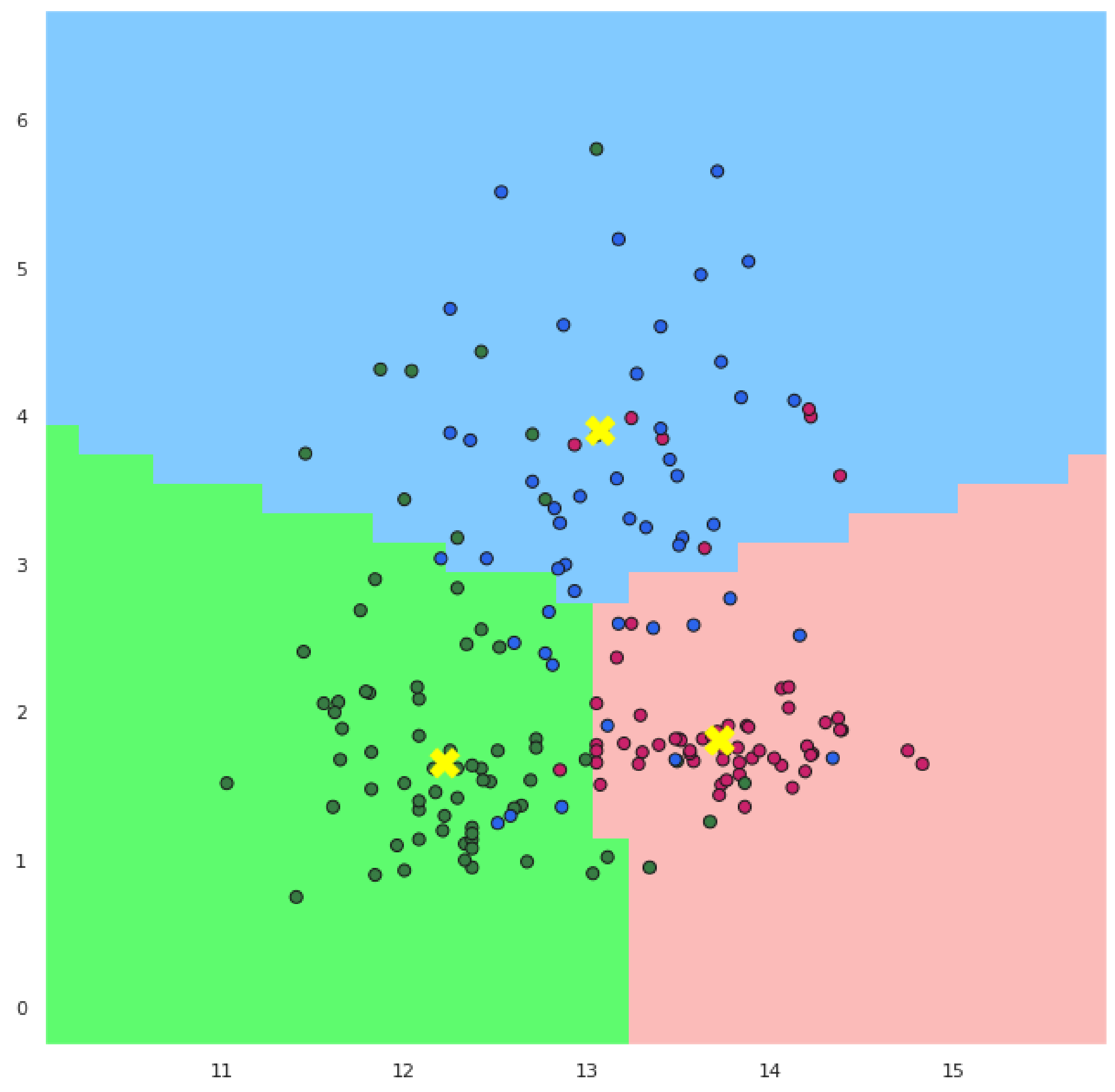
```
# Your code here

# Xc already has two features

from sklearn.metrics import homogeneity_score
from sklearn.metrics import completeness_score

# find how many labels
nlabels = len(np.unique(ywine))
print('There are',nlabels,'labels')

# apply kmeans based on labels, each cluster is a label
km = KMeans(n_clusters=nlabels)

# fit
km.fit(Xc)

# predict
pred = km.predict(Xc)

# data outcome
print('Homogeneity:',homogeneity_score(ywine, pred))
print('Completeness:',completeness_score(ywine, pred))

# plot
# colors
cmap_light = ListedColormap(['#FBBBB9', '#5EFB6E', '#82CAFF'])
cmap_bold = ListedColormap(['#CA226B', '#387C44', '#2B65EC'])

# mesh-grid
h = 0.2
x_min, x_max = Xc[:, 0].min() - 1, Xc[:, 0].max() + 1
y_min, y_max = Xc[:, 1].min() - 1, Xc[:, 1].max() + 1

xx, yy = np.meshgrid(np.arange(x_min, x_max, h),np.arange(y_min, y_max, h))

Z = km.predict(np.c_[xx.ravel(), yy.ravel()])
Z = Z.reshape(xx.shape)

# plot overall map
plt.figure()
plt.scatter(Xc[:,0], Xc[:,1] ,ywine, linewidths=2)
```

```
    There are 3 labels
    Homogeneity: 0.41035077970969713
    Completeness: 0.4080524820388843
    <matplotlib.collections.PathCollection at 0x7f28e5dd9110>
```



```
# plot predicted map
plt.figure(figsize=(11,11))
plt.pcolormesh(xx, yy, Z, cmap=cmap_light)
plt.scatter(Xc[:, 0], Xc[:, 1], c=ywine, cmap=cmap_bold, edgecolor='k', s=50)
plt.scatter(km.cluster_centers_[:,0], km.cluster_centers_[:,1], c = 'yellow', marker ='X', s=300, linew
plt.xlim(xx.min(), xx.max())
plt.ylim(yy.min(), yy.max())
```

```
(-0.26, 6.74)
```



Exercise 4.5 (20 pts)

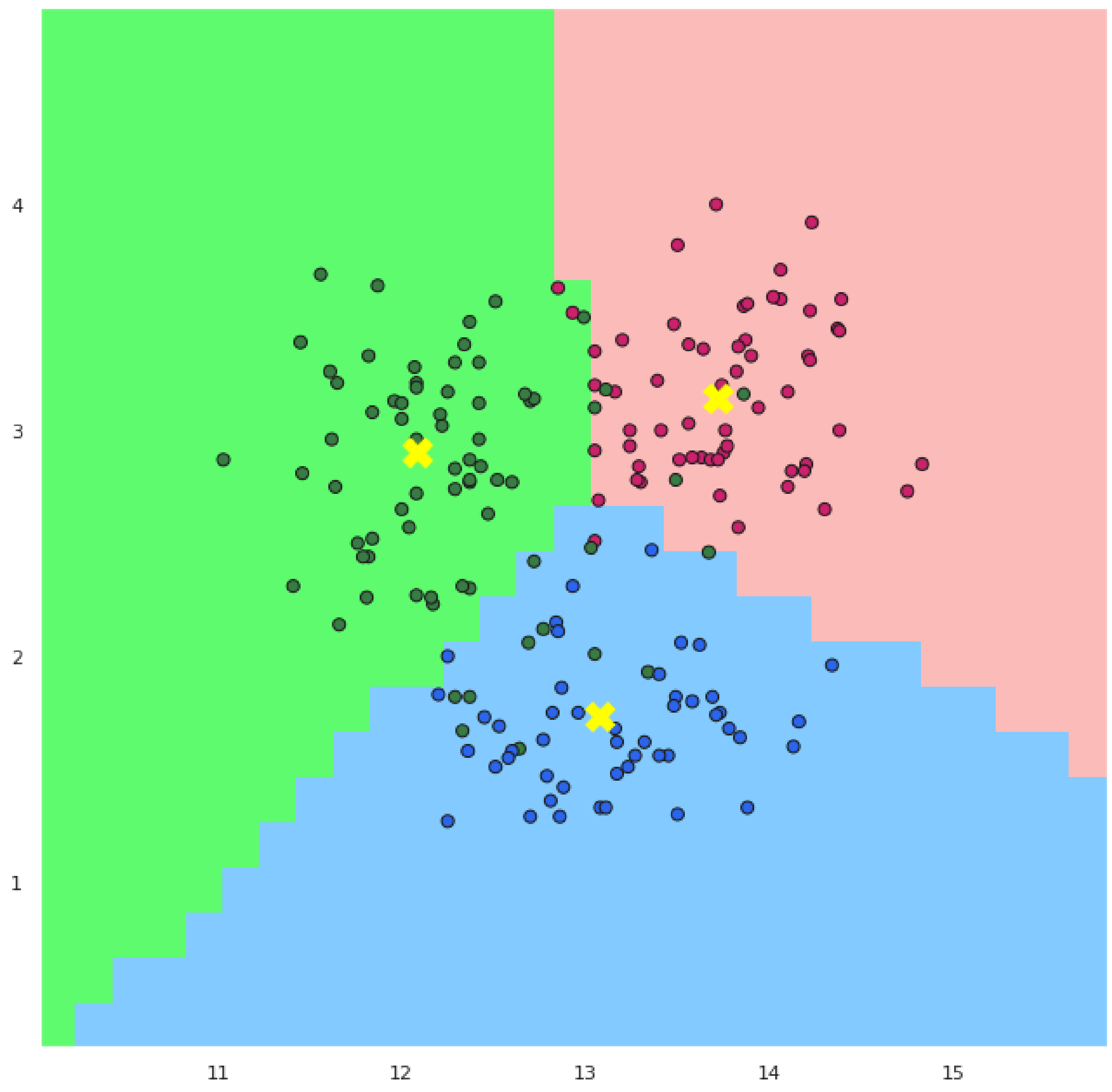
In the previous model you used the first two features: 'Alcohol' and 'Malic acid'. For this exercise, pick features 'Alcohol' and 'OD280/OD315 of diluted wines' (feature #1 and feature #12) as your two attributes and perform the tasks in Exercise 4.4. (cluster, report metrics, draw decision boundaries)

Which model performs better?

```
# your code here

# get features #1, #12 -> column 0, 11
special_X = Xwine_full [:,[0,11]]

# find how many labels
nlabels = len(np.unique(ywine))
print('There are',nlabels,'labels')

# apply kmeans based on labels, each cluster is a label
km2 = KMeans(n_clusters=nlabels)
```

```
# fit
km2.fit(special_X)

# predict
pred2 = km2.predict(special_X)

# data outcome
print('Homogeneity:',homogeneity_score(ywine, pred2))
print('Completeness:',completeness_score(ywine, pred2))

# plot
# colors
cmap_light = ListedColormap(['#FBBBB9', '#5EFB6E', '#82CAFF'])
cmap_bold = ListedColormap(['#CA226B', '#387C44', '#2B65EC'])

# mesh-grid
h = 0.2
x_min, x_max = special_X[:, 0].min() - 1, special_X[:, 0].max() + 1
y_min, y_max = special_X[:, 1].min() - 1, special_X[:, 1].max() + 1

xx, yy = np.meshgrid(np.arange(x_min, x_max, h),np.arange(y_min, y_max, h))

Z = km2.predict(np.c_[xx.ravel(), yy.ravel()])
Z = Z.reshape(xx.shape)

# plot overall map
plt.figure(figsize=(11,11))
plt.pcolormesh(xx, yy, Z, cmap=cmap_light)
plt.scatter(special_X[:, 0], special_X[:, 1], c=ywine, cmap=cmap_bold, edgecolor='k', s=50)
plt.scatter(km2.cluster_centers_[:,0], km2.cluster_centers_[:,1], c = 'yellow', marker ='X', s=300, lin
plt.xlim(xx.min(), xx.max())
plt.ylim(yy.min(), yy.max())
```

```
There are 3 labels
Homogeneity: 0.7072039236692641
Completeness: 0.7006853440435565
(0.27, 4.870000000000001)
```



```
print('The model with features #1 and #12 has Homogeneity: {}, Completeness:{}'.format(homogeneity_scor
print('Overall performing a lot better than the model with features #1, #2.')
```

```
The model with features #1 and #12 has Homogeneity: 0.7072039236692641, Completeness:0.700685344043
Overall performing a lot better than the model with features #1, #2.
```

✓ 0s completed at 6:47 PM