Assignment 4, Exercise 7-2
Kernel PCA

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Assignment 4, Exercise 7 - 2

Consider the two-dimensional data sets pca3.csv and pca4.csv (the last data set has as a third column also a label, which should be used for coloring the plots). Perform Kernel PCA. Try at least two different kernels with at least five different kernel parameter settings to compute two principal components. Visualize the projected data.

First step is to read the data from the csv file:

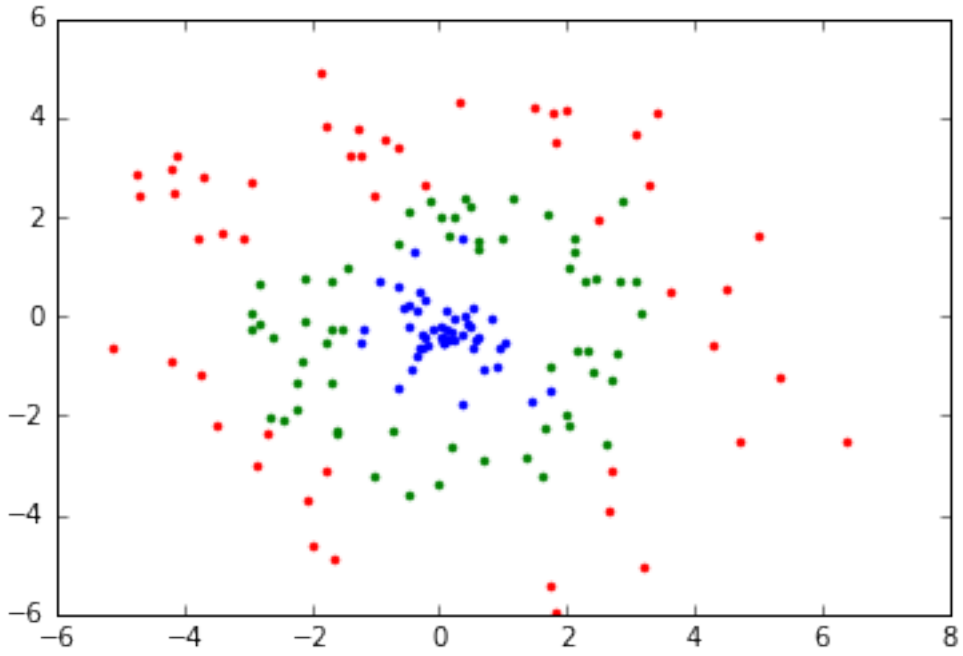
```
In [2]: import pandas as pd

        df = pd.read_csv(
            filepath_or_buffer='pca4.csv',
            header=None,
            sep=',')
```

Next, we need to center the data. For this, for each attribute, the mean of that attribute over all observations is subtracted.

```
In [3]: import numpy as np

        data = np.array(df.ix[:,:].values)  # transform to numpy array
        labels = data[:,-1]  # save the labels separately
        data = data[:,:-1]  # discard the labels
        data = data - np.mean(data, axis=0)
```

First, visualize the unprojected data. We make a 2D plot. We notice the data is shaped like 3 concentric circles.

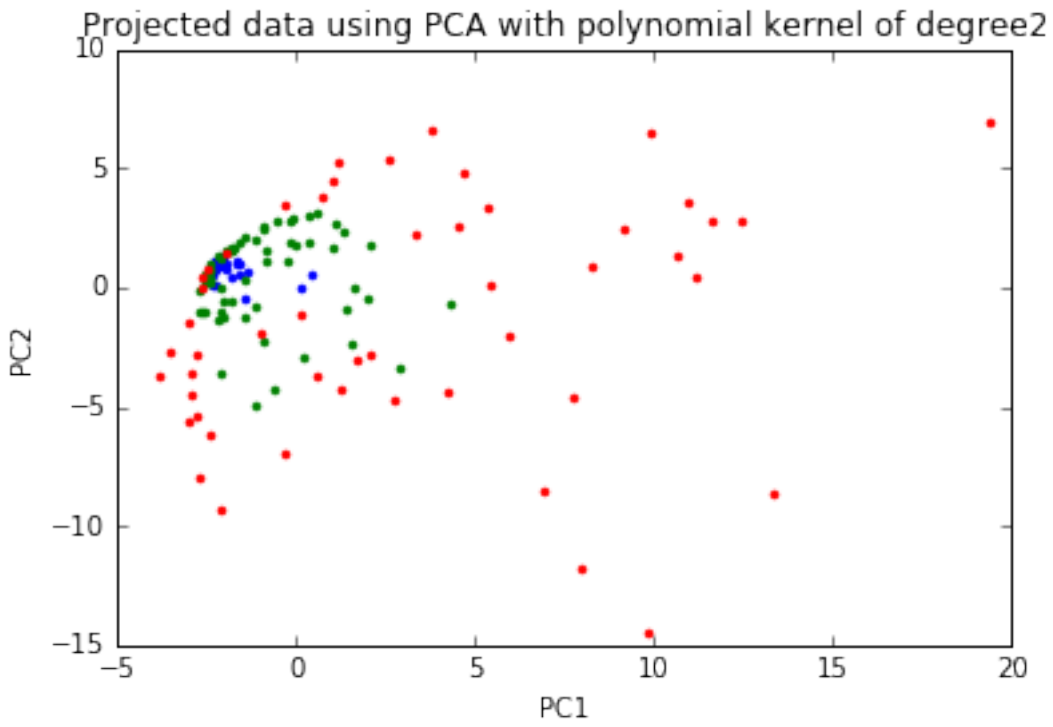
```
In [4]: %matplotlib inline
        import matplotlib.pyplot as plt
        from IPython.display import set_matplotlib_formats
        set_matplotlib_formats('png', 'pdf')

        labels_set = set(labels)

        for label in labels_set:
            # select only the observations having the current label
            # for being able to plot with different colors
            data_for_label = np.array([data[i]
                                       for i in range(len(labels))
                                       if labels[i]==label])
            plt.plot(data_for_label[:,0], data_for_label[:,1], '.')
```

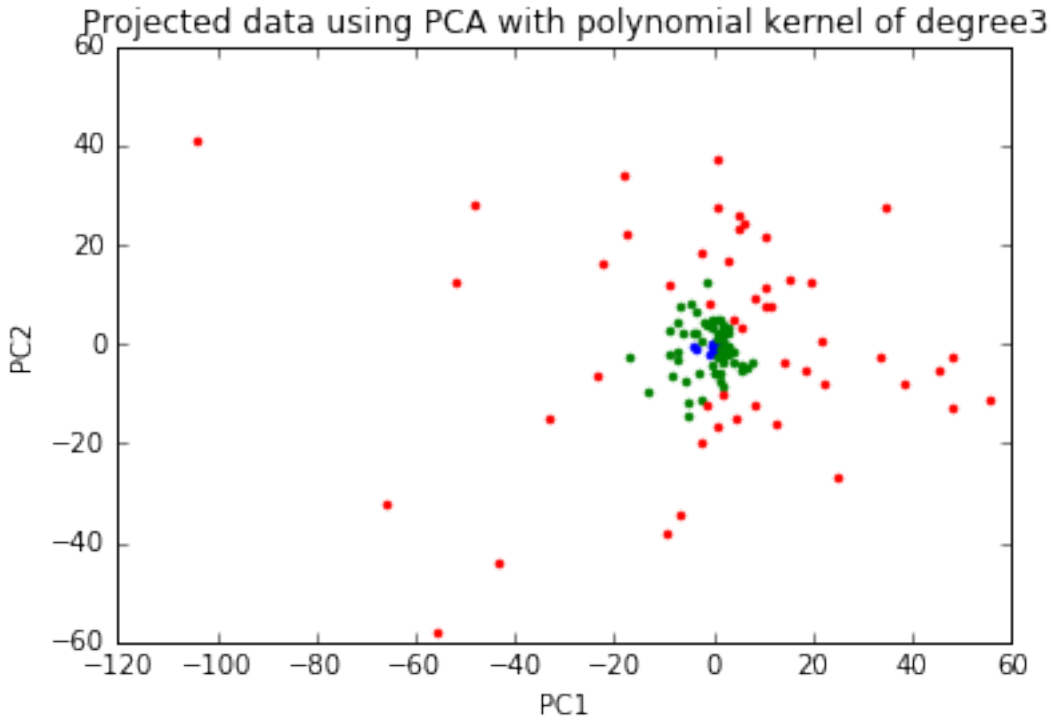


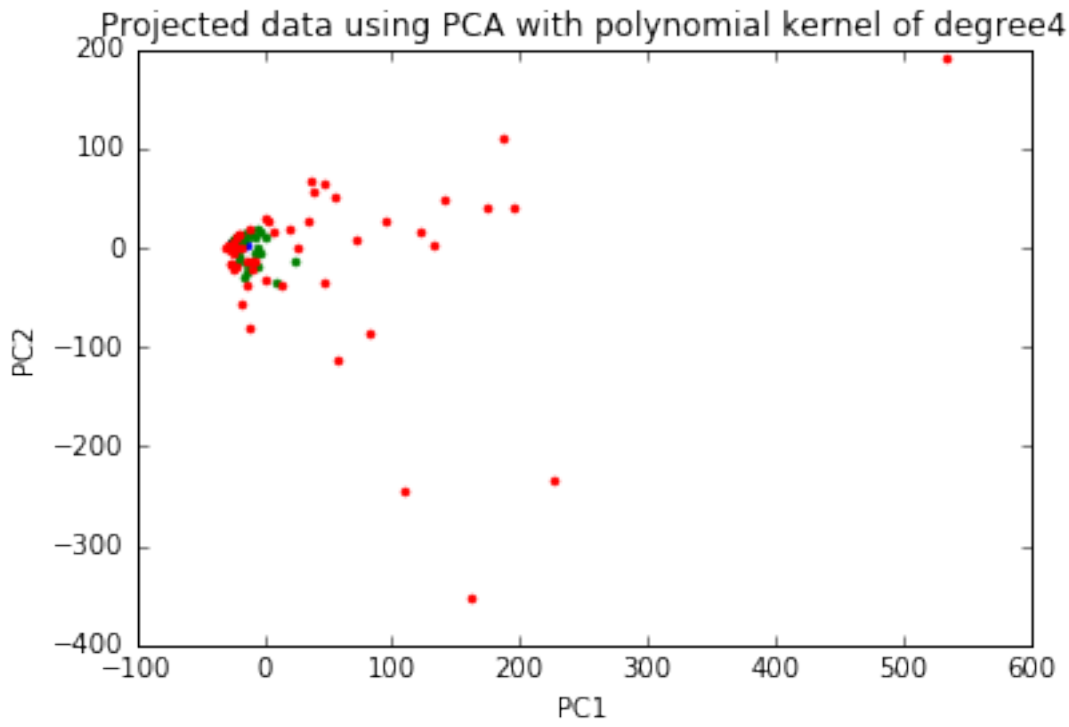
Then, apply KernelPCA with 2 different kernels: poly and rbf.

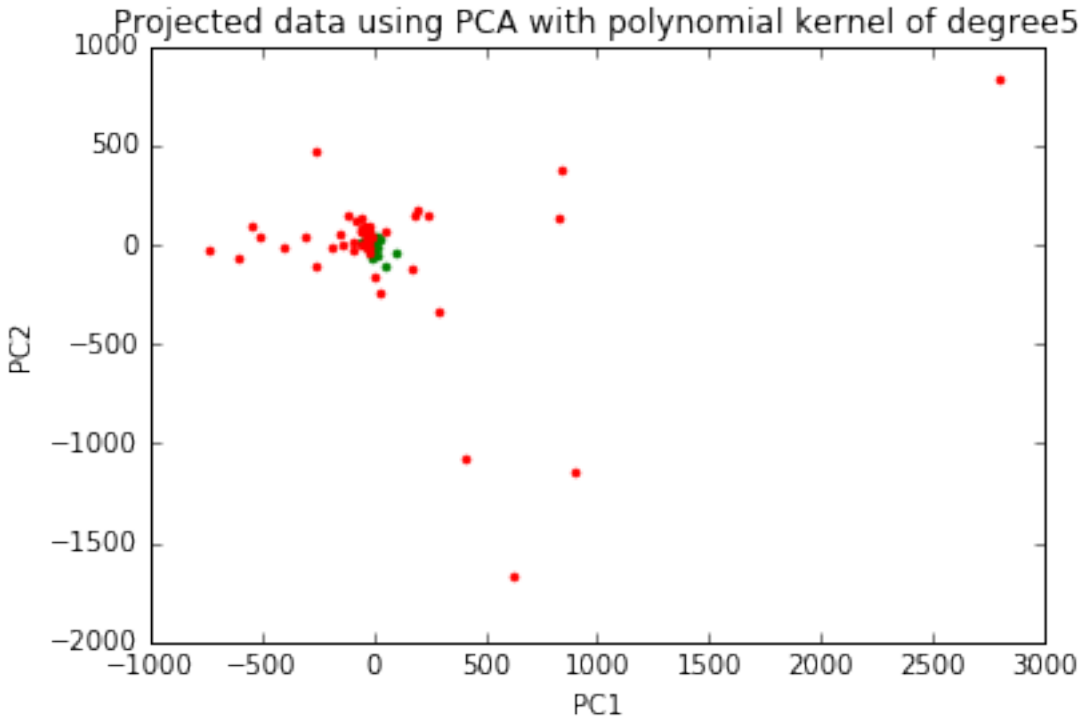
1. The polynomial kernel with various degrees:

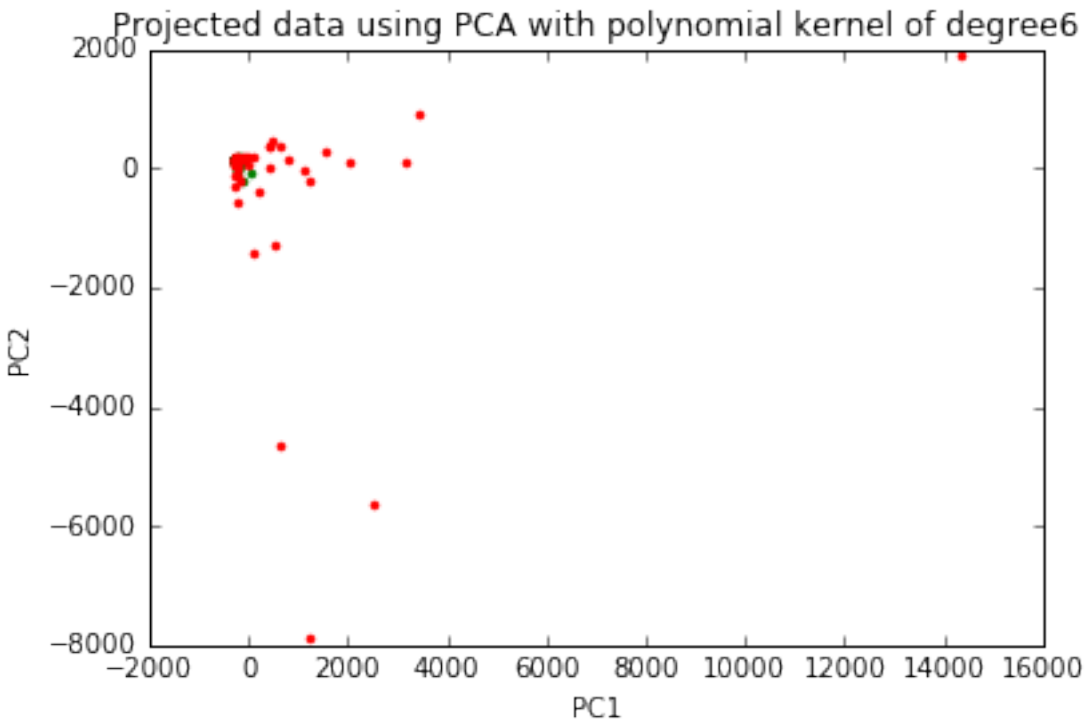
In [5]:
```
from sklearn.decomposition import KernelPCA


figure_index = 0
# define some degrees for the polynomial kernel
poly_kernel_degrees = [2,3,4,5,6]
for poly_kernel_degree in poly_kernel_degrees:

    kpca = KernelPCA(n_components=2, kernel='poly', degree=poly_kernel_degree)
    transformed_data = kpca.fit_transform(data)
    # make a plot using the labels for coloring

    for label in labels_set:
        # select only the observations having the current label
        data_for_label = np.array([transformed_data[i]
                                   for i in range(len(labels))
                                   if labels[i]==label])
        plt.figure(figure_index)
        plt.plot(data_for_label[:,0], data_for_label[:,1],'.')
        plt.xlabel("PC1")
        plt.ylabel("PC2")
        plt.title("Projected data using PCA with polynomial kernel of degree"
                  + str(poly_kernel_degree))

    figure_index+=1
```


Projected data using PCA with polynomial kernel of degree2
PC2
PC1
10
5
0
−5
−10
−15
−5
0
5
10
15
20


Projected data using PCA with polynomial kernel of degree3
PC2
PC1
60
40
20
0
−20
−40
−60
−120
−100
−80
−60
−40
−20
0
20
40
60

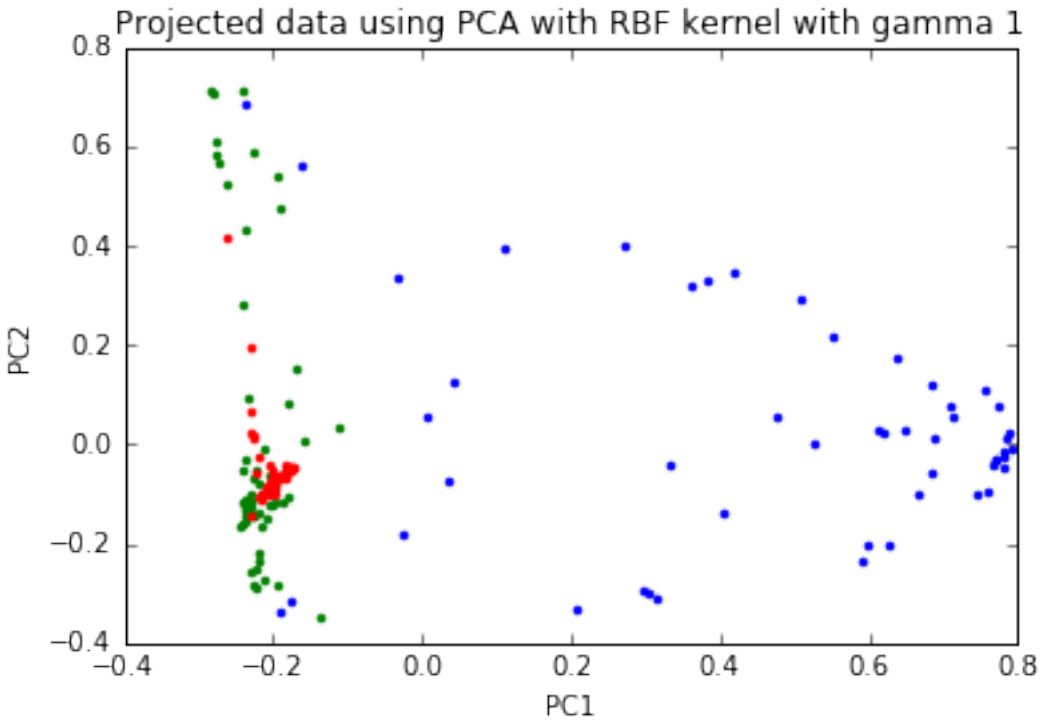

Projected data using PCA with polynomial kernel of degree4
PC2
PC1
200
100
0
−100
−200
−300
−400
−100
0
100
200
300
400
500
600

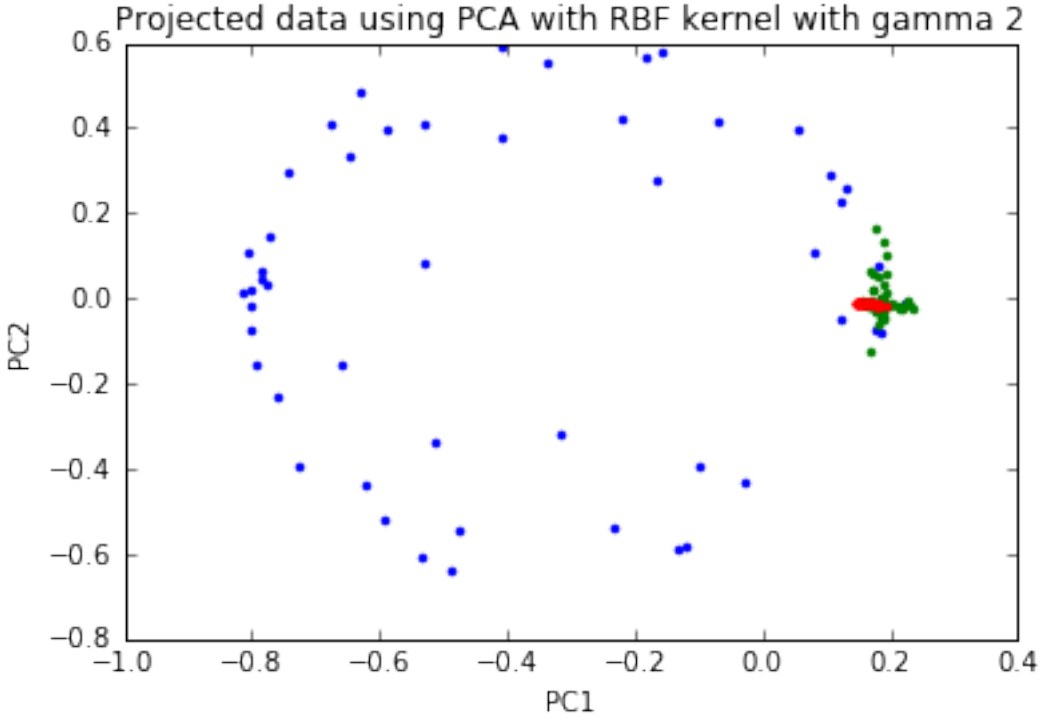

Projected data using PCA with polynomial kernel of degree5
PC2
PC1
1000
500
0
−500
−1000
−1500
−2000
−1000
−500
0
500
1000
1500
2000
2500
3000

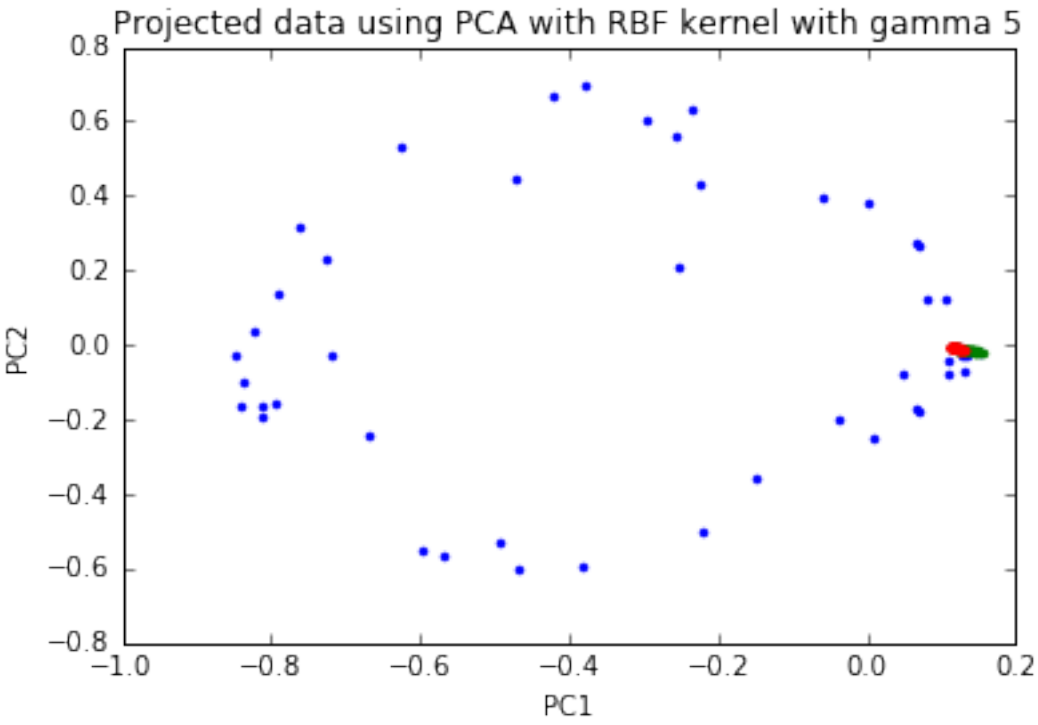


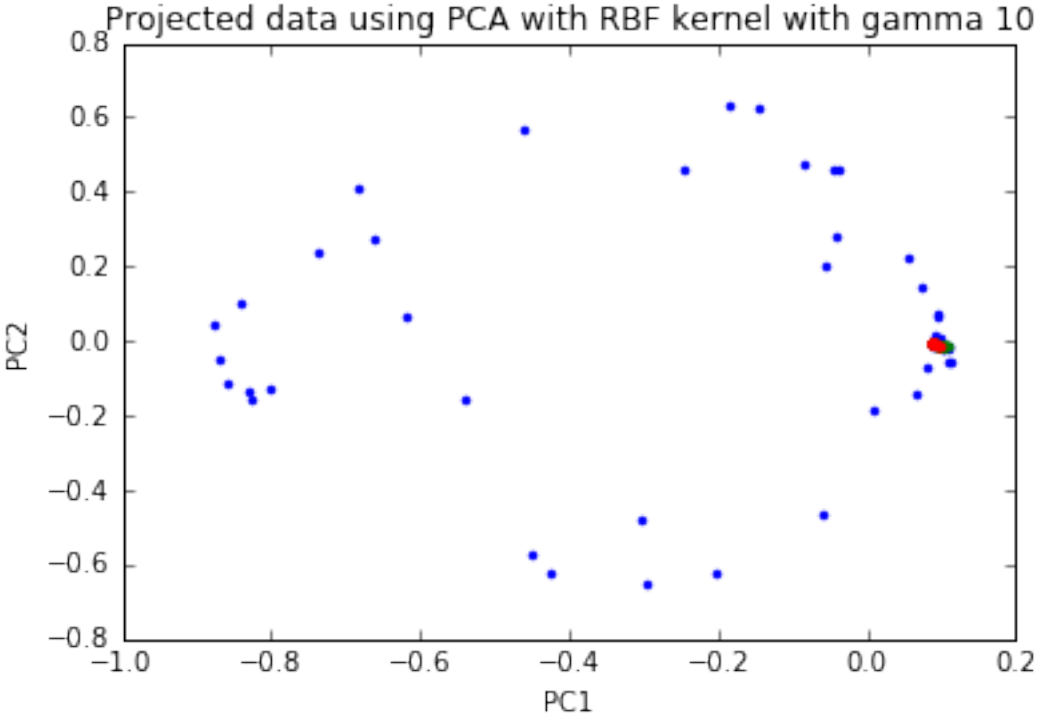
1. The RBF kernel with various values for gamma:

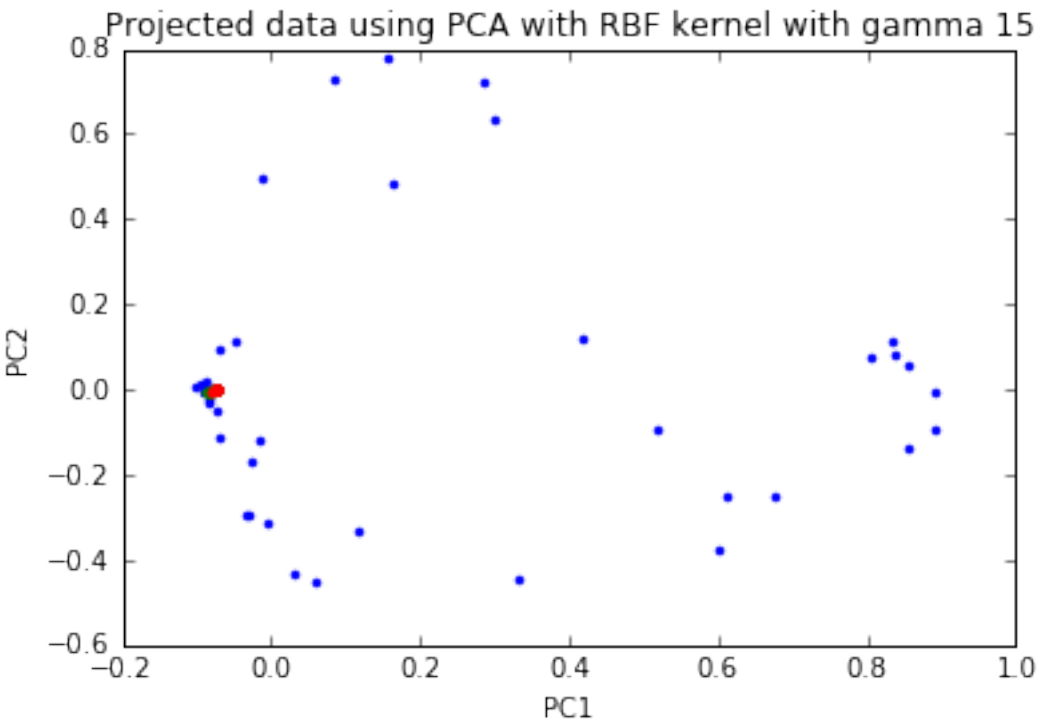
```
In [6]: figure_index = 0
        # define some values for gamma for the polynomial kernel
        rbf_kernel_gammas = [1,2,5,10,15]

        for rbf_kernel_gamma in rbf_kernel_gammas:

            kpca = KernelPCA(n_components=2, kernel='rbf', gamma=rbf_kernel_gamma)
            transformed_data = kpca.fit_transform(data)
            # make a plot using the labels for coloring

            for label in labels_set:
                # select only the observations having the current label
                data_for_label = np.array([transformed_data[i]
                                           for i in range(len(labels))
                                           if labels[i]==label])
                plt.figure(figure_index)
                plt.plot(data_for_label[:,0], data_for_label[:,1],'.')
                plt.xlabel("PC1")
                plt.ylabel("PC2")
                plt.title("Projected data using PCA with RBF kernel with gamma "
                          + str(rbf_kernel_gamma))

            figure_index+=1
```


Projected data using PCA with RBF kernel with gamma 1
PC2
PC1
0.8
0.6
0.4
0.2
0.0
−0.2
−0.4
−0.4
−0.2
0.0
0.2
0.4
0.6
0.8


Projected data using PCA with RBF kernel with gamma 2
PC2
PC1
0.6
0.4
0.2
0.0
−0.2
−0.4
−0.6
−0.8
−1.0
−0.8
−0.6
−0.4
−0.2
0.0
0.2
0.4

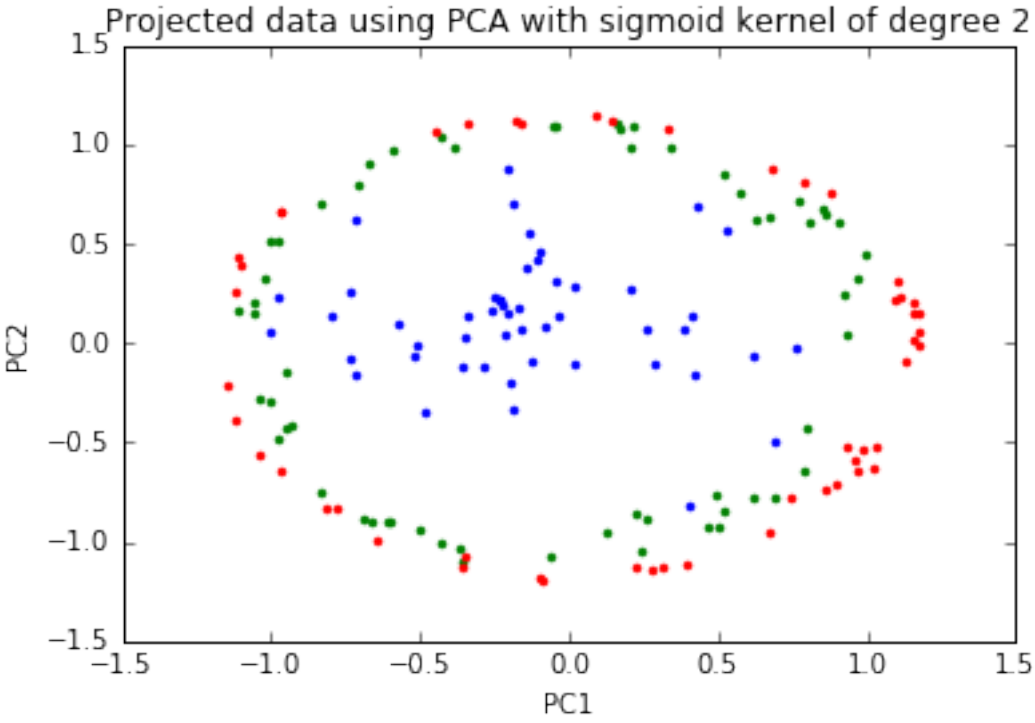

Projected data using PCA with RBF kernel with gamma 5
PC2
PC1
0.8
0.6
0.4
0.2
0.0
−0.2
−0.4
−0.6
−0.8
−1.0
−0.8
−0.6
−0.4
−0.2
0.0
0.2

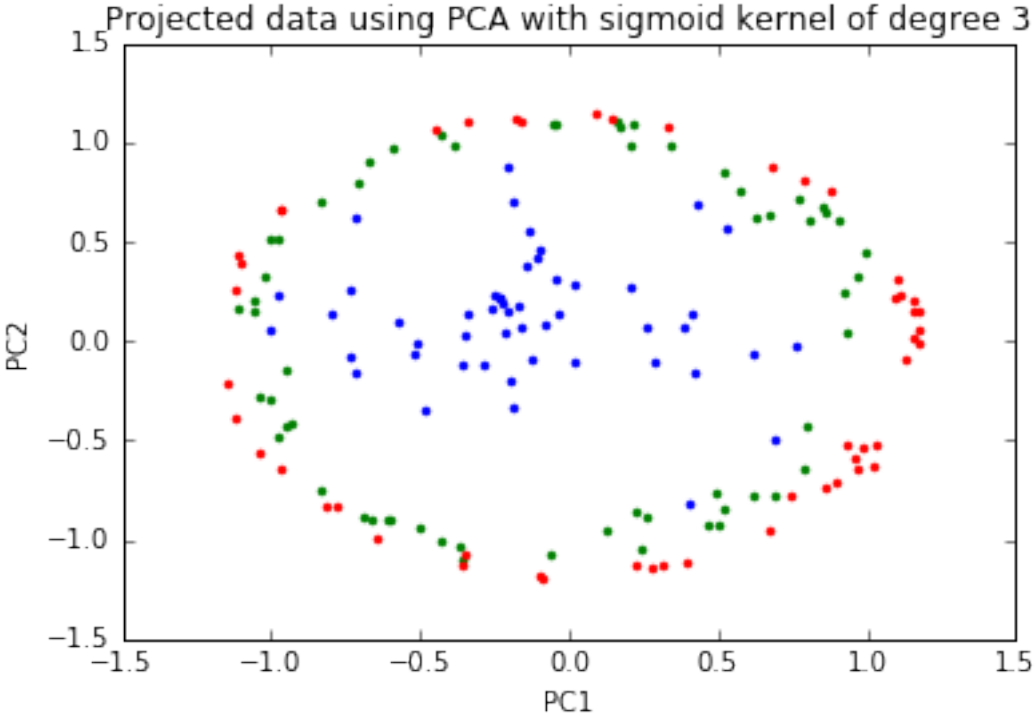

Projected data using PCA with RBF kernel with gamma 10
PC2
PC1
0.8
0.6
0.4
0.2
0.0
−0.2
−0.4
−0.6
−0.8
−1.0
−0.8
−0.6
−0.4
−0.2
0.0
0.2

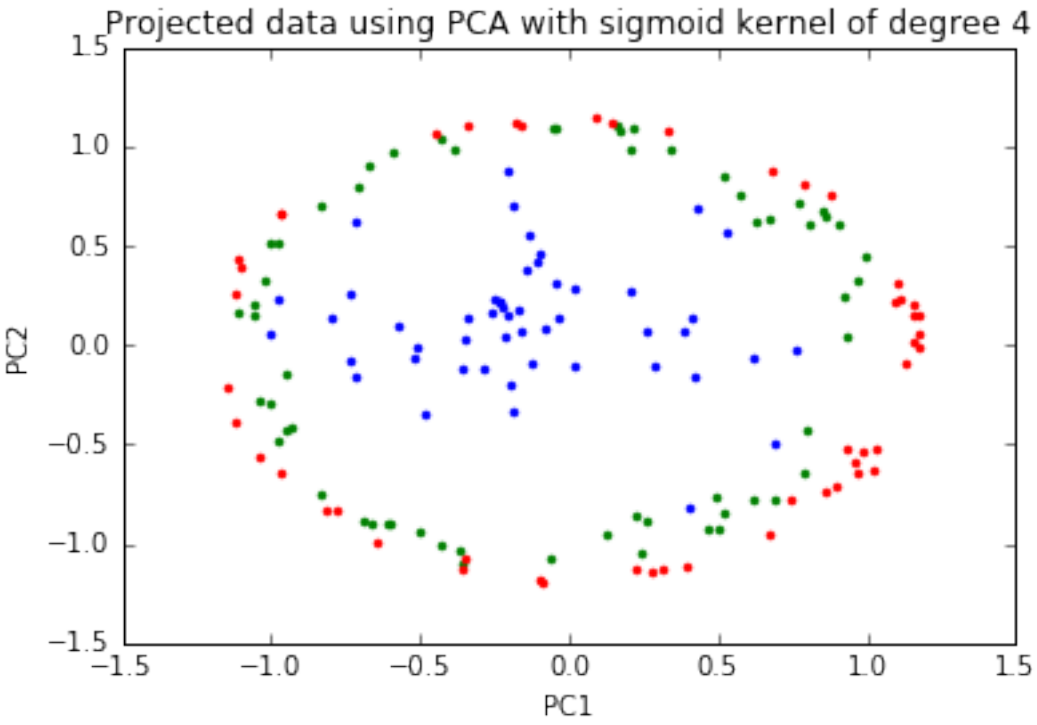


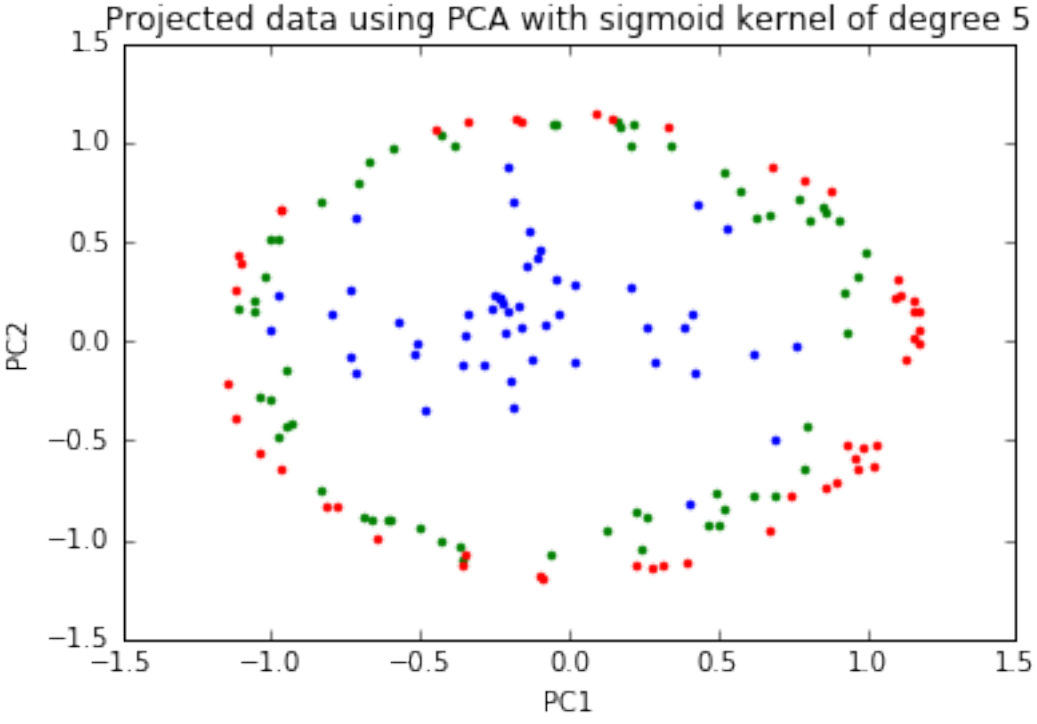
3. The Sigmoid kernel with various degrees:

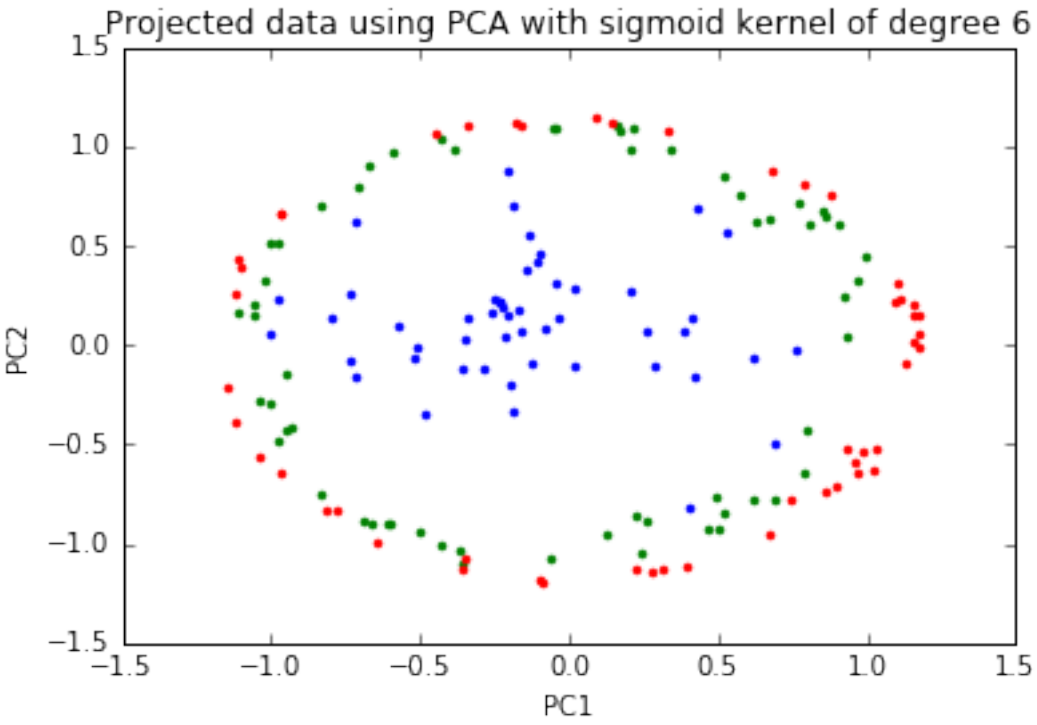
```
In [7]: figure_index = 0

        for kernel_degree in poly_kernel_degrees:

            kpca = KernelPCA(n_components=2, kernel='sigmoid', degree=kernel_degree)
            transformed_data = kpca.fit_transform(data)
            # make a plot using the labels for coloring

            for label in labels_set:
                # select only the observations having the current label
                data_for_label = np.array([transformed_data[i] for i in range(len(labels)) if labels[i]=
                plt.figure(figure_index)
                plt.plot(data_for_label[:,0], data_for_label[:,1],'.')
                plt.xlabel("PC1")
                plt.ylabel("PC2")
                plt.title("Projected data using PCA with sigmoid kernel of degree "+str(kernel_degree))

            figure_index+=1
```


Projected data using PCA with sigmoid kernel of degree 2
PC2
PC1
1.5
1.0
0.5
0.0
−0.5
−1.0
−1.5
−1.5
−1.0
−0.5
0.0
0.5
1.0
1.5


Projected data using PCA with sigmoid kernel of degree 3
PC2
PC1
1.5
1.0
0.5
0.0
−0.5
−1.0
−1.5
−1.5
−1.0
−0.5
0.0
0.5
1.0
1.5


Projected data using PCA with sigmoid kernel of degree 4
PC2
PC1
1.5
1.0
0.5
0.0
−0.5
−1.0
−1.5
−1.5
−1.0
−0.5
0.0
0.5
1.0
1.5


Projected data using PCA with sigmoid kernel of degree 5
PC2
PC1
1.5
1.0
0.5
0.0
−0.5
−1.0
−1.5
−1.5
−1.0
−0.5
0.0
0.5
1.0
1.5


Projected data using PCA with sigmoid kernel of degree 6
PC2
PC1
1.5
1.0
0.5
0.0
−0.5
−1.0
−1.5
−1.5
−1.0
−0.5
0.0
0.5
1.0
1.5