Performing Kernel Principal Components Analysis

PCA is good at reducing the number of dimensions, but it works in a linear manner. If the data is not organized in a linear fashion, PCA fails to do the required job. This is where Kernel PCA comes into the picture. You can learn more about it at http://www.ics.uci.edu/~welling/classnotes/papers_class/Kernel-PCA.pdf. Let's see how to perform Kernel PCA on the input data and compare it to how PCA performs on the same data.

How to do it...

1. Create a new Python file, and import the following packages:

```
import numpy as np
import matplotlib.pyplot as plt

from sklearn.decomposition import PCA, KernelPCA
from sklearn.datasets import make_circles
```

2. Define the seed value for the random number generator. This is needed to generate the data samples for analysis:

```
# Set the seed for random number generator
np.random.seed(7)
```

3. Generate data that is distributed in concentric circles to demonstrate how PCA doesn't work in this case:

```
# Generate samples
X, y = make_circles(n_samples=500, factor=0.2, noise=0.04)
```

4. Perform PCA on this data:

```
# Perform PCA
pca = PCA()
```

```
X_pca = pca.fit_transform(X)
```

5. Perform Kernel PCA on this data:

```
# Perform Kernel PCA
kernel_pca = KernelPCA(kernel="rbf", fit_inverse_transform=True, gamma=10)
X_kernel_pca = kernel_pca.fit_transform(X)
X_inverse = kernel_pca.inverse_transform(X_kernel_pca)
```

6. Plot the original input data:

```
# Plot original data
class_0 = np.where(y == 0)
class_1 = np.where(y == 1)
plt.figure()
plt.title("Original data")
plt.plot(X[class_0, 0], X[class_0, 1], "ko", mfc='none')
plt.plot(X[class_1, 0], X[class_1, 1], "kx")
plt.xlabel("1st dimension")
plt.ylabel("2nd dimension")
```

7. Plot the PCA-transformed data:

```
# Plot PCA projection of the data
plt.figure()
plt.plot(X_pca[class_0, 0], X_pca[class_0, 1], "ko", mfc='none')
plt.plot(X_pca[class_1, 0], X_pca[class_1, 1], "kx")
plt.title("Data transformed using PCA")
plt.xlabel("1st principal component")
plt.ylabel("2nd principal component")
```

8. Plot Kernel PCA-transformed data:

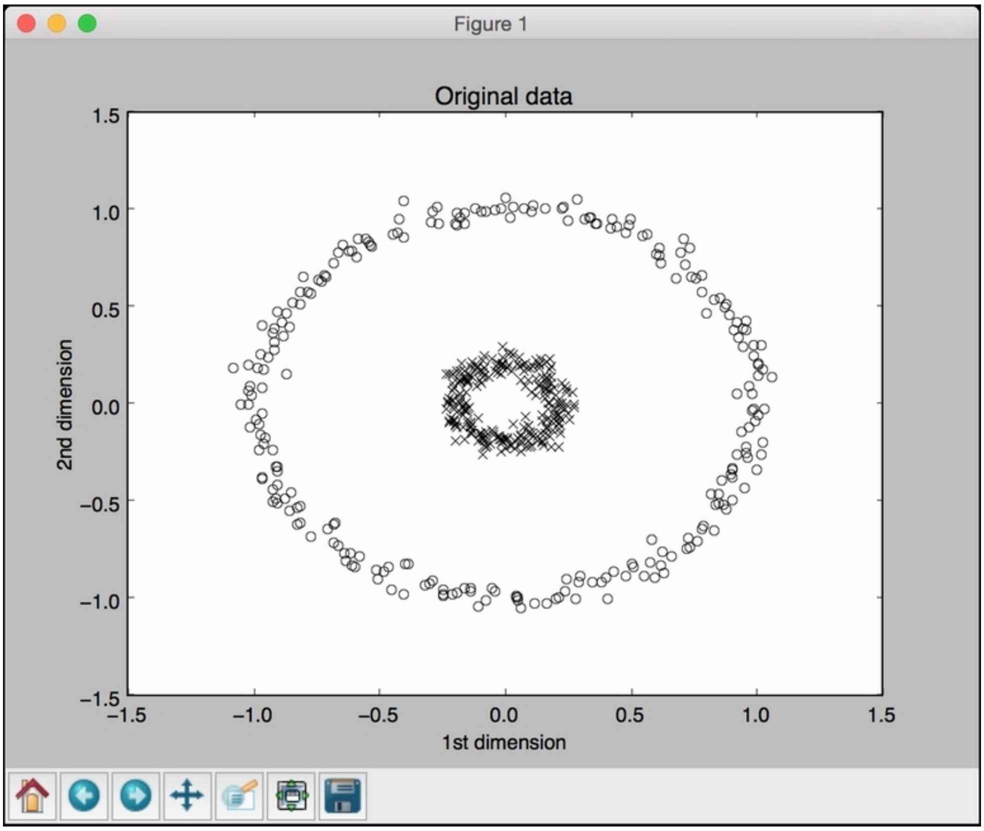
```
# Plot Kernel PCA projection of the data
plt.figure()
plt.plot(X_kernel_pca[class_0, 0], X_kernel_pca[class_0, 1], "ko", mfc='no
plt.plot(X_kernel_pca[class_1, 0], X_kernel_pca[class_1, 1], "kx")
plt.title("Data transformed using Kernel PCA")
plt.xlabel("1st principal component")
plt.ylabel("2nd principal component")
```

9. Transform the data back to the original space using the Kernel method to show that the inverse is maintained:

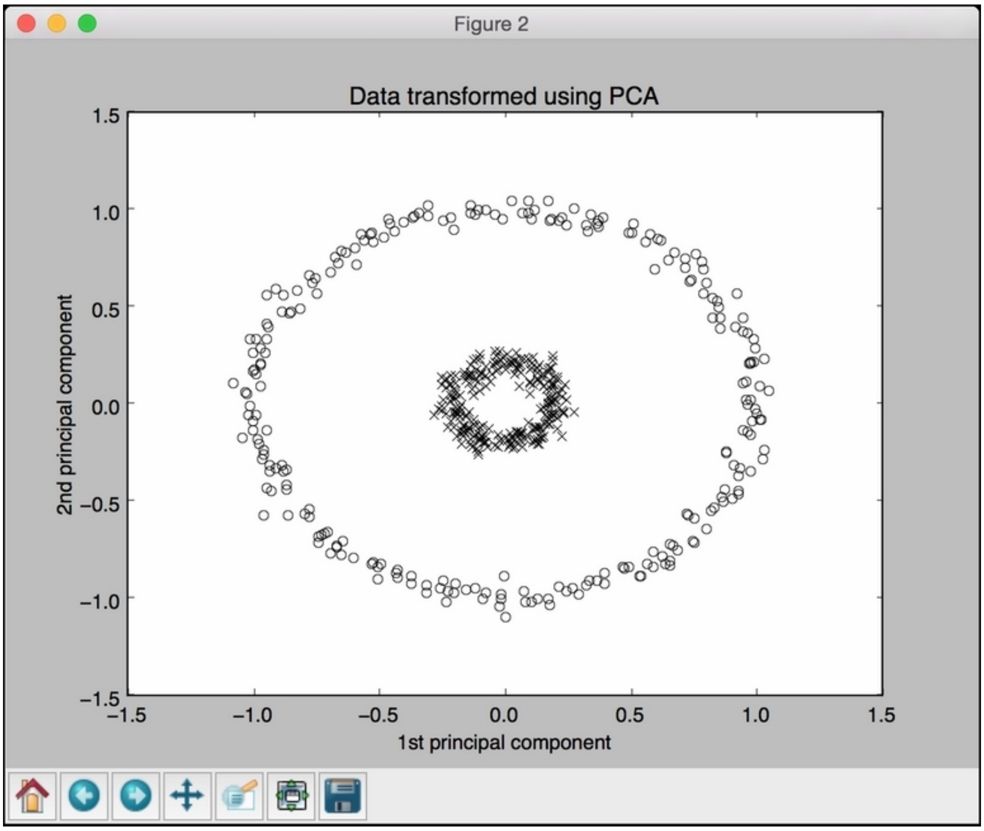
```
# Transform the data back to original space
plt.figure()
plt.plot(X_inverse[class_0, 0], X_inverse[class_0, 1], "ko", mfc='none')
plt.plot(X_inverse[class_1, 0], X_inverse[class_1, 1], "kx")
plt.title("Inverse transform")
plt.xlabel("1st dimension")
plt.ylabel("2nd dimension")

plt.show()
```

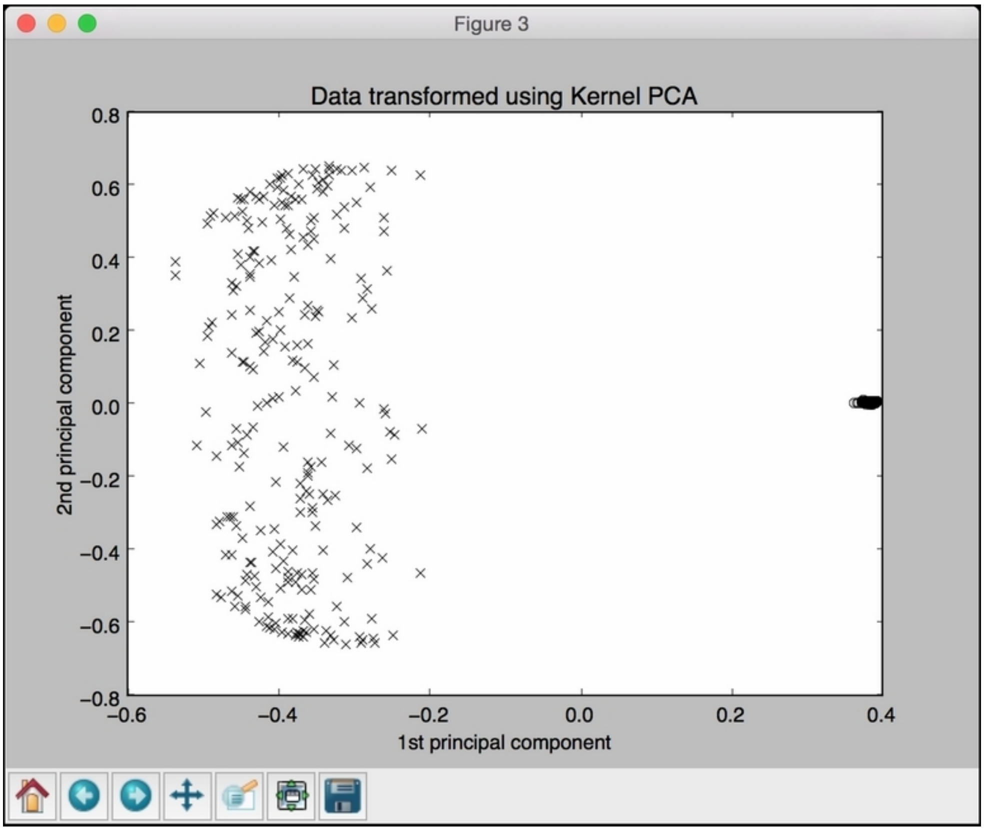
10. The full code is given in the `kpca.py` file that's already provided to you for reference. If you run this code, you will see four figures. The first figure is the original data:



The second figure depicts the data transformed using PCA:



The third figure depicts the data transformed using Kernel PCA. Note how the points are clustered in the right part of the figure:



The fourth figure depicts the inverse transform of the data back to the original space:

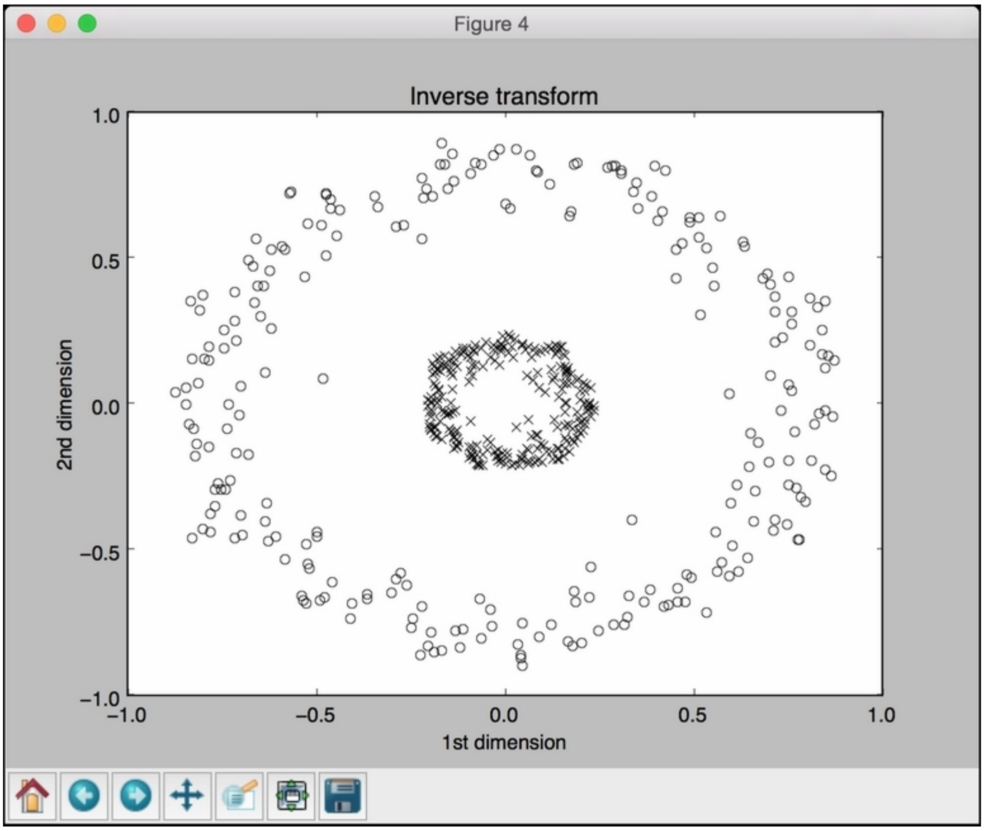


Figure 4
Inverse transform
1.0
0.5
0.0
−0.5
−1.0
2nd dimension
−1.0
−0.5
0.0
0.5
1.0
1st dimension