4.1 Kernel PCA: Toy Data

Group name: DataFun

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In [1]:

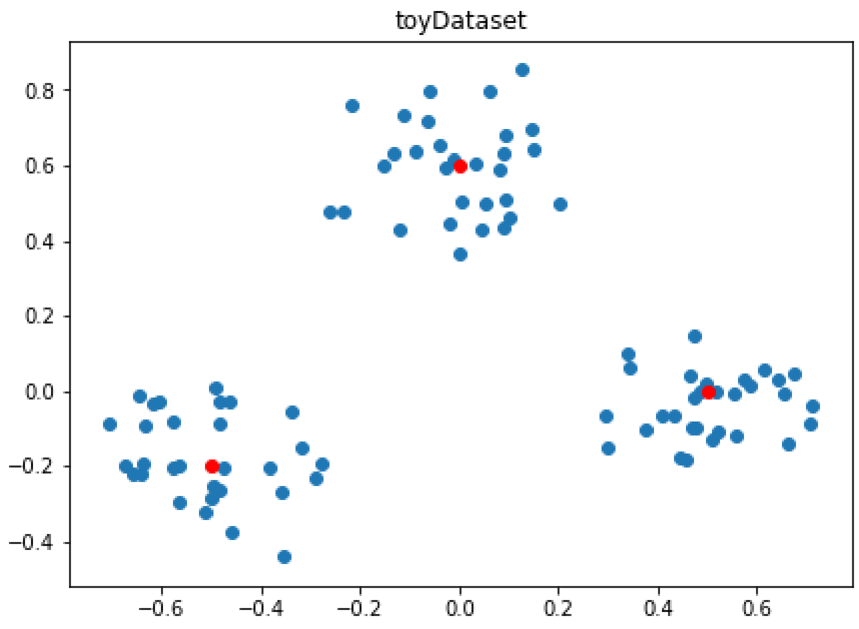
```
import numpy as np
import matplotlib.pyplot as plt
import scipy.linalg as la

from sklearn.decomposition import KernelPCA
from scipy.spatial.distance import cdist
```

(a) Create toy dataset

In [2]:

```
xMean = np.asarray([[-0.5, -0.2],[0, 0.6],[0.5, 0]])
sd = 0.1
toyDataset = np.empty([0,2])
for mean in xMean:
    toyDatasetPart = np.random.normal(mean, sd, [30,2])
    toyDataset = np.concatenate((toyDataset, toyDatasetPart), axis=0)

print("ToyDataset of shape :", toyDataset.shape)

# Plotting the results.
plt.figure(figsize=(7,5))
plt.scatter(toyDataset[:,0], toyDataset[:,1])
plt.scatter(xMean[:,0], xMean[:,1], color="r")
plt.title("toyDataset")
plt.show()
```

```
ToyDataset of shape : (90, 2)
```



(b) Apply Kernel PCA using RBF Kernel

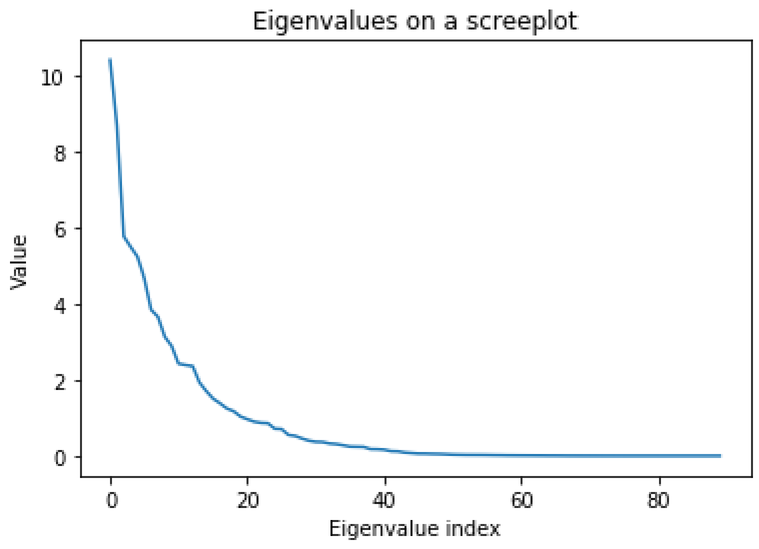
In [3]:

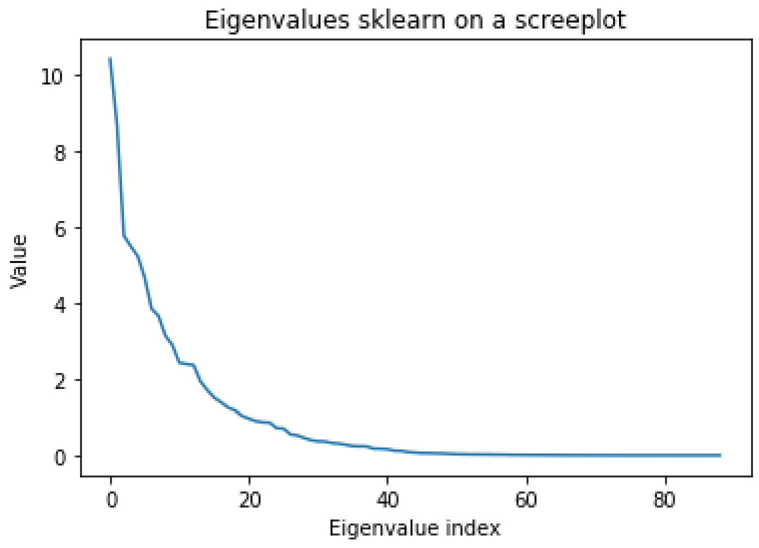
```
# Kernel function
def k(x_a, x_b, sig):
    norm = np.linalg.norm(x_a - x_b)
    return np.exp(- norm**2 / (2*sig**2))

# use kernel function to create kernel matrix K
def createKernelMatrix(x, sig):
    p = x.shape[0]
    KUnnormalized = np.empty([p,p])
    for i in range(p):
        for j in range(p):
            KUnnormalized[i,j] = k(x[i], x[j], sig)
    return KUnnormalized

def centerKernelMatrix(KUC):
    p = KUC.shape[0]
    K = np.empty([p,p])
    rowAverages = np.average(KUC, axis=0)
    lineAverages = np.average(KUC, axis=1)
    matrixAverge = np.average(KUC)
    for i in range(p):
        for j in range(p):
            K[i,j] = KUC[i,j] - rowAverages[i] - lineAverages[j] + matrixAverge
    return K

def getOrderedEig(matrix):
    eigenvals, eigenvecs = np.linalg.eig(matrix)
    orderedInd = np.argsort(eigenvals)[::-1]
    orderedEigenvals = eigenvals[orderedInd]
    orderedEigenvecs = eigenvecs[orderedInd]
    return (orderedEigenvals, orderedEigenvecs)

def normalizeEV(orderedEigenvals, orderedEigenvecs):
    p = orderedEigenvals.shape[0]
    normEV = np.empty([p,p])
    for i in range(p):
        normEV = orderedEigenvecs / np.sqrt(p*orderedEigenvals[i])
    return normEV



sig = 0.1
KernelMatrixUnnormalized = createKernelMatrix(toyDataset, sig)
#print("unnormalized KM shape: ", KernelMatrixUnnormalized.shape)
centerdKernelMatrixUnnormalized = centerKernelMatrix(KernelMatrixUnnormalized)
#print("centered KM shape:", centerdKernelMatrixUnnormalized.shape)

orderedEigenvalues, orderedEigenvectors = getOrderedEig(centerdKernelMatrixUnnor
malized)
#print("orderedEigenvectors.shape:", orderedEigenvectors.shape)
normalizedEigenvectors = normalizeEV(orderedEigenvalues, orderedEigenvectors)
#print("normalizeEigenvectors.shape:", normalizedEigenvectors.shape)

# sklearn for comparison
kpca = KernelPCA(kernel="rbf", fit_inverse_transform=True, gamma=(1/(2 * sig
**2)))
kpca.fit(toyDataset)
eigenvalues, eigenvectors = kpca.lambdas_, kpca.alphas_
```

Normalized eigenvectors:

In [4]:

```
plt.figure()
plt.plot(orderedEigenvalues)
plt.xlabel("Eigenvalue index")
plt.ylabel("Value")
plt.title("Eigenvalues on a screeplot")
plt.show()

# sklearn for comparison
plt.plot(eigenvalues)
plt.xlabel("Eigenvalue index")
plt.ylabel("Value")
plt.title("Eigenvalues sklearn on a screeplot")
plt.show()
```

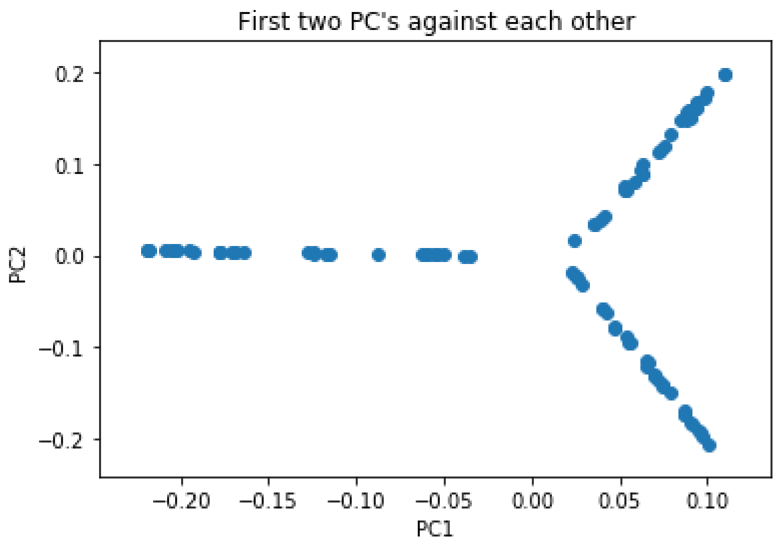


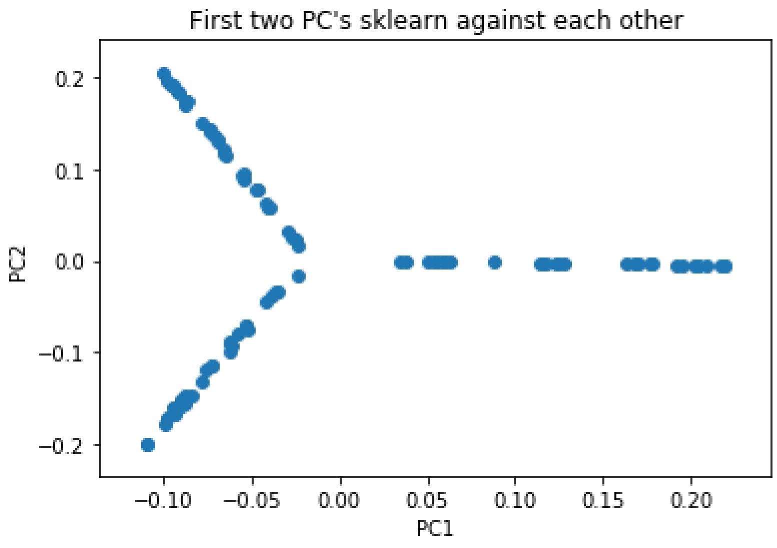


Data projected on PC1 and PC2

In [5]:

```python
plt.figure()
plt.scatter(orderedEigenvectors[:,0], orderedEigenvectors[:,1])
plt.xlabel("PC1")
plt.ylabel("PC2")
plt.title("First two PC's against each other")
plt.show()

# sklearn for comparison
plt.figure()
plt.scatter(eigenvectors[:,0], eigenvectors[:,1])
plt.xlabel("PC1")
plt.ylabel("PC2")
plt.title("First two PC's sklearn against each other")
plt.show()
```

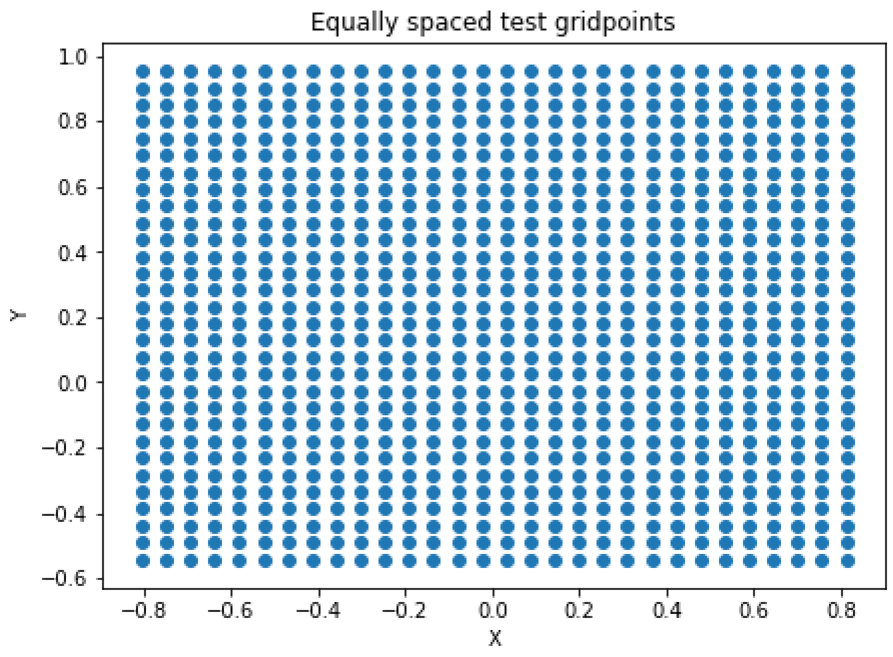




(c) Visualize first 8 PC

In [6]:

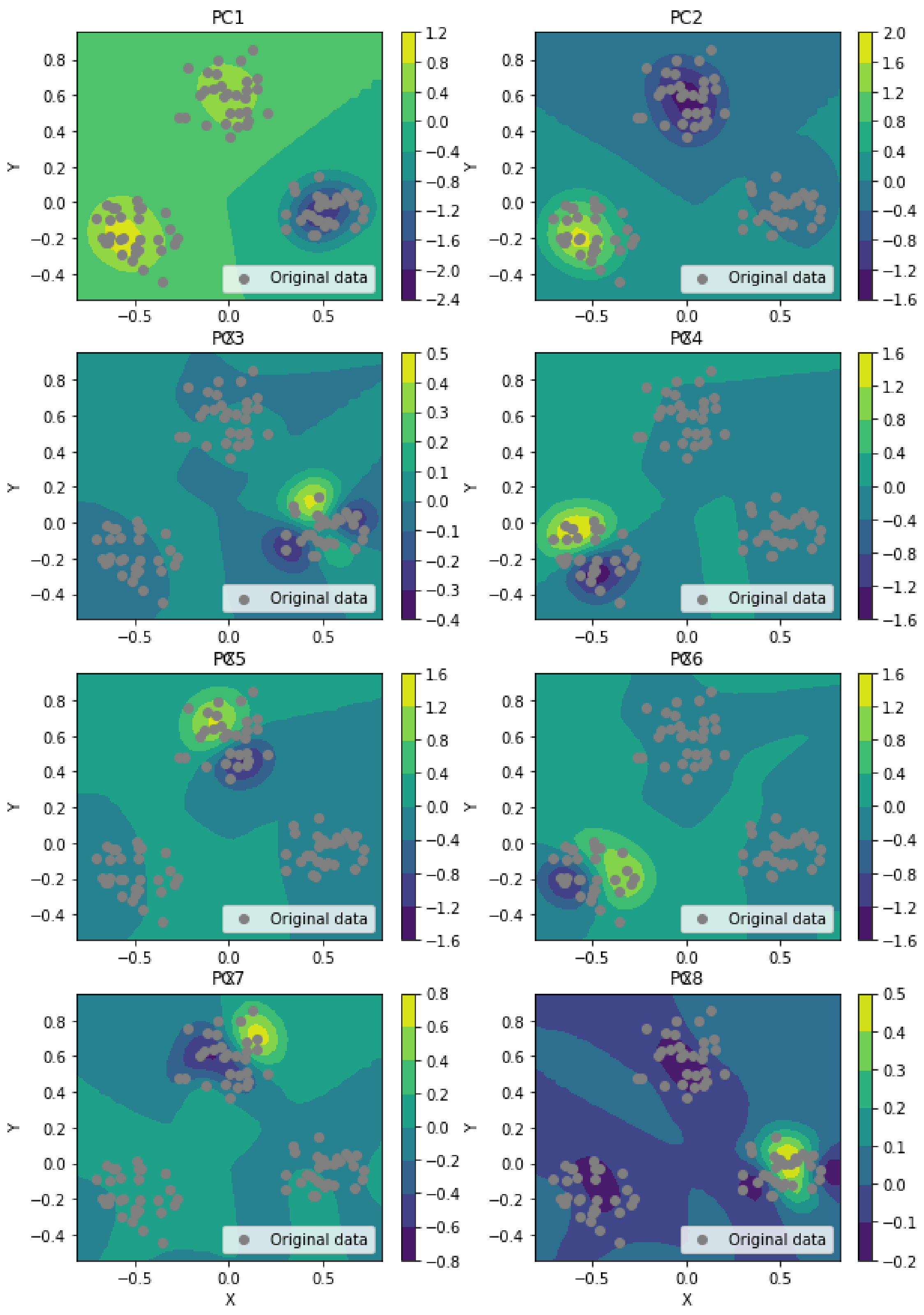
```
# Creating the test data (equally spaced gridpoints).
# Acquiring maximal and minimal values of our toy data, to be able to define
# a space.
minX, minY = np.min(toyDataset,0)
maxX, maxY = np.max(toyDataset, 0)

# Dividing the space linear. Have to add deviation.
sd=0.1
x = np.linspace(minX-sd,maxX+sd,30)
y = np.linspace(minY-sd,maxY+sd,30)

# Return coordinate matrices from coordinate vector.
xv,yv = np.meshgrid(x,y)

# Plotting the grid.
plt.figure(figsize=(7,5))
plt.scatter(xv,yv)
plt.xlabel('X')
plt.ylabel('Y')
plt.title('Equally spaced test gridpoints')
plt.show()
```



In [7]:

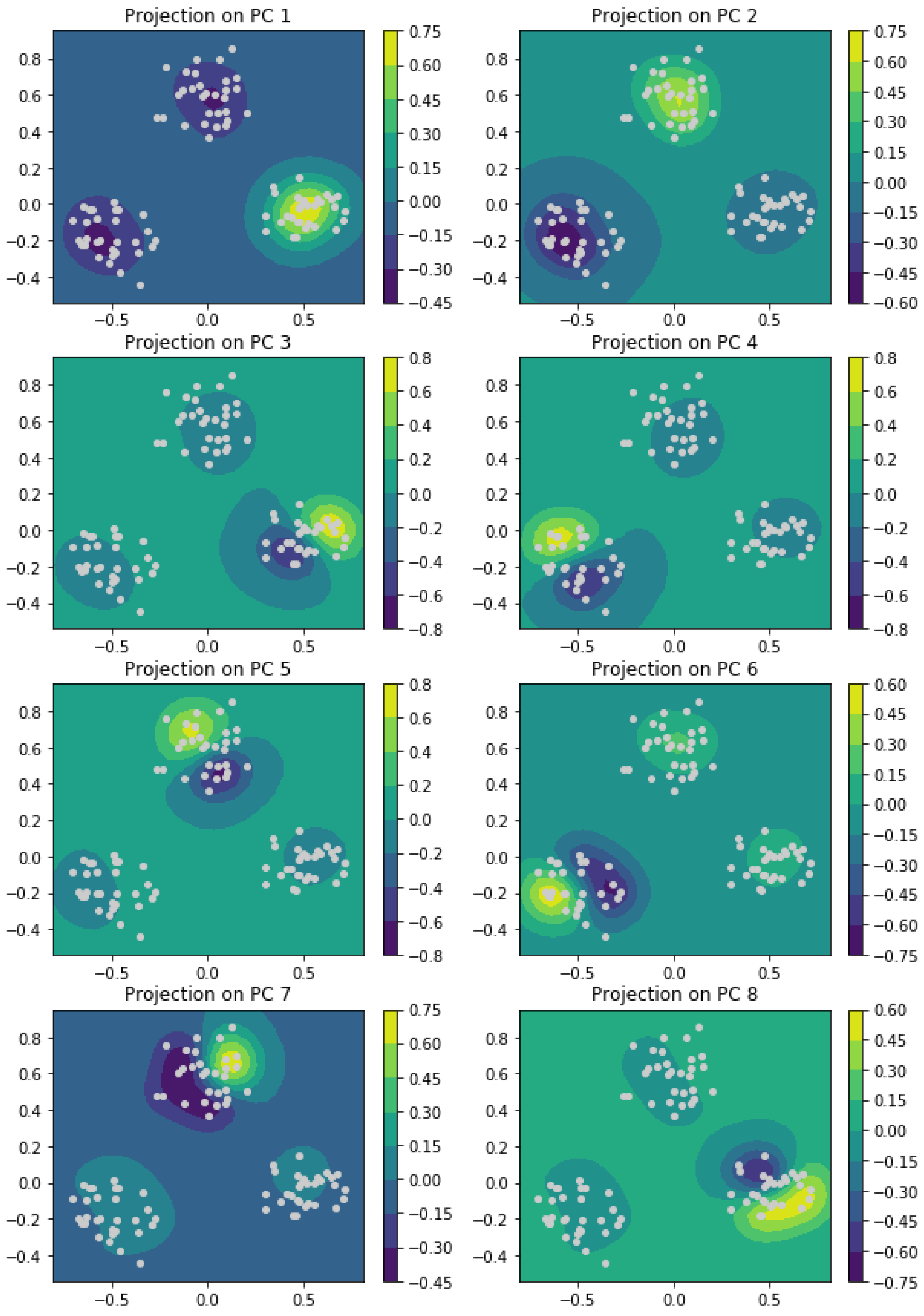
```
# Goal: Reshaping 30x30 matrixes into 900x2 vectors.
# Reshaping to one dimensional vectors.
xVec = np.reshape(xv,(30*30,1))
yVec = np.reshape(yv,(30*30,1))
# Concatanating the previous vectors.
meshgrid = np.concatenate((xVec,yVec),1)

# Calculating difference between test data and sample data.
# Third parameter means that we count the squared euclidean distance
# (what we need for RBF kernel) --> it is squared already!
newKernelMatrix = np.exp(-(cdist(meshgrid,toyDataset,'sqeuclidean'))/(2*sig**2))
print(newKernelMatrix.shape)
# The new kernel matrix is 900x90 (#TData X #SampleData).
centeredNewKernelMatrix = newKernelMatrix

# Project onto the first 8 PCs using matrix multiplication operator.
# 900x90 @ 90x8 = 90x8
requiredPCs = orderedEigenvectors[:,0:8]
projection = newKernelMatrix @ requiredPCs

plt.figure(figsize=(10,15))
for i in range(0,8):
    plt.subplot(4, 2, i+1)
    plt.contourf(xv, yv, np.reshape(projection[:,i],((30,30))))
    plt.colorbar()
    plt.scatter(toyDataset[:,0],toyDataset[:,1],c='grey',label='Original data')
    plt.xlabel('X')
    plt.ylabel('Y')
    plt.title('PC'+str(i+1))
    plt.legend()
plt.show()
```

```
(900, 90)
```



In [8]:

```
#projet to pc1-8
projectedMesh = kpca.transform(meshgrid).reshape(30, 30, -1)

#plot
num = 8
plt.figure(figsize=(10,15))

for i in range(num):
    plt.subplot(4, 2, i+1)
    plt.title('Projection on PC {:d}'.format(i+1))
    plt.contourf(x, y, projectedMesh[:,:,i])
    plt.colorbar
    plt.plot(toyDataset[:,0], toyDataset[:,1], 'o', color='#CCCCCC',
markersize=4)
    plt.colorbar()
plt.show()
```



(d) Discuss suitable applications for KPCA

PCA:

- detect linear features in data
- reduce data to linear subspaces
- to cluster data linearly.

If features do not follow linear but NON-LINEAR features, the PCA by itself cannot be used.

KERNEL-PCA:

- can be applied do detect even highly non-linear features in a given dataset.
- can be used to find a lower-dimensional non-linear subspace that the data is confined to.
- allows to cluster data according to non-linear patterns, by mapping them to a N-dimensional space and separating them there with a hyperplane

Limitations/Challenges:

1. For large datasets storing K (of size NxN) can become expensive. It can be adressed by clustering data in smaller subsets and/or by only calculating some of the eigenvalues and eigenvectors
2. When the Kernel scale is chosen poorly the eigenvalues (data variations) can be of about the same value. This might not allow for an efficient dimensionality reduction