TheUnsupervised02

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1 MI2 - Exercise 02 - The Unsupervised

Group members: Niels-Ole Kühl, Philipp Marian Grulich, Johannes Giersdorf, Julius Hülsmann and Friederike Fischer

1.1 Principal Component Analysis (PCA)

1.1.1 notation and representation of data

observations: $\underline{x}^{(\alpha)} \in \mathbb{R}^N \quad \alpha = 1, \ldots, p$

centered data matrix: $X = \begin{pmatrix} \underline{x}^{(1)^T} - m^T \\ \vdots \\ \underline{x}^{(p)^T} - m^T \end{pmatrix} \in \mathbb{R}^{p \times N}$

covariance matrix: $C = \frac{1}{p} X^T X$

1.1.2 objective

Find the direction of the highest variance, which is the direction that is most informative.

$\|e_a\|_2 = 1$

Variance: $\sigma_a^2 = \underline{e}_a^T \underline{C} \underline{e}_a$

$\underline{e}_a^* = \arg\max_{e_a^*}(\sigma_a^2) \qquad \text{s.t.} \qquad \|e_a^*\|_2 = 1 \rightarrow$ maximize variance

Solution using the method of Lagrange multipliers λ returns eigenvalue problem:

$\underline{C}\underline{e}_a = \lambda \underline{e}_a$

1.1.3 Principial Components (PCs):

normalized eigenvectors $\underline{e}_a$ of $\underline{C}$, $\qquad a = 1, ..., N,$

sorted by eigenvalue $\lambda_1 > \lambda_2 > ... > \lambda_N$

feature value:

$\alpha_a = u_a(\underline{x}) = \underline{e}_1^T \underline{x}, \qquad a = 1, ..., N.$

Representation of $\underline{x}$ in the basis of PCs:

$\underline{x} = \alpha_1 \underline{e}_1 + \alpha_2 \underline{e}_2 + ... + \alpha_N \underline{e}_N$

Reconstruction using projection onto first M PCs:

$\tilde{\underline{x}} = \alpha_1 \underline{e}_1 + \alpha_2 \underline{e}_2 + ... + \alpha_M \underline{e}_M$

In [1]:
```
import os
import numpy as np
import matplotlib
import matplotlib.pyplot as plt
import matplotlib.image as img
%matplotlib inline
from mpl_toolkits.mplot3d import Axes3D
from scipy.linalg import *
```

1.2 Utilities

In [2]:
```
def plotscatter(x, title="", label="", color=""):
    if (x.shape[1]==3):
        plotscatter3d(x, title=title, label=label, color=color);
    elif (x.shape[1] ==2):
        plotscatter2d(x, title=title, label=label, color=color);
    else:
        raise ValueError("not applicable for plots \not \in \{2d, 3d\} ")


def plotscatter2d (x, title="", label="", color=""):
    if color == "":
        plt.scatter(x[:,0], x[:,1], label=label)
    else:
        plt.scatter(x[:,0], x[:,1], label=label, color=color)
    plt.title(title)
    plt.axis('equal')
    if (label != ""):
        plt.legend()


def plotscatter3d(x, title="", label="", color=""):
    fig = plt.figure()
    ax = fig.add_subplot(111, projection='3d')
    ax.scatter(x[:,0],x[:,1],x[:,2])



def arraySort (listOrder,list2):
    order    = listOrder.argsort()
    listOrder=listOrder[order[::-1]]
    list2=list2[order[::-1]]
    return (listOrder,list2)
```

1.3 logic

In [3]:
```
project     = np.dot # data, structure: np.dot(data, structur);
projectToPC = lambda point, pc: project(project(point, pc)[np.newaxis].T, \
```

```
                                    pc[np.newaxis])
```

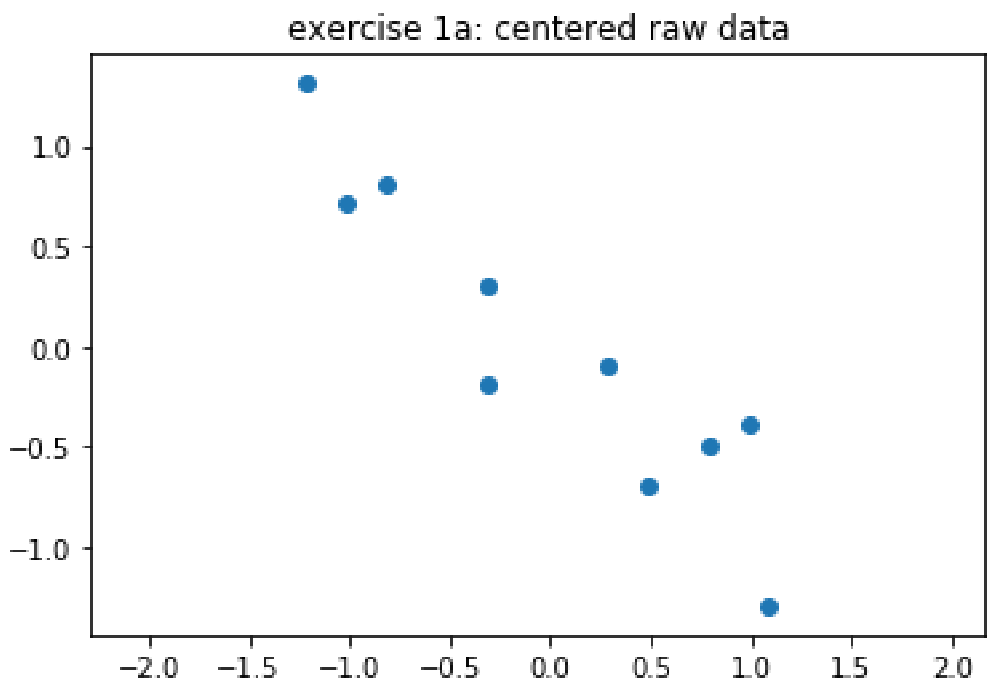
1.4 2.1 a)

- Load data, remove from mean and plot

```
In [4]: # 2.1a) logic: load data; and remove mean
        x = np.genfromtxt("pca-data-2d.dat", dtype="double", delimiter="   ")
        x = x - np.mean(x, axis=0)
        print("The shape of the data is", x.shape, ". Thus, each row consits of a tuple.")
```

```
The shape of the data is (10, 2) . Thus, each row consits of a tuple.
```

```
In [5]: # 2.1 a) plot
        plotscatter(x, title="exercise 1a: centered raw data");
```



1.5 2.1 b)

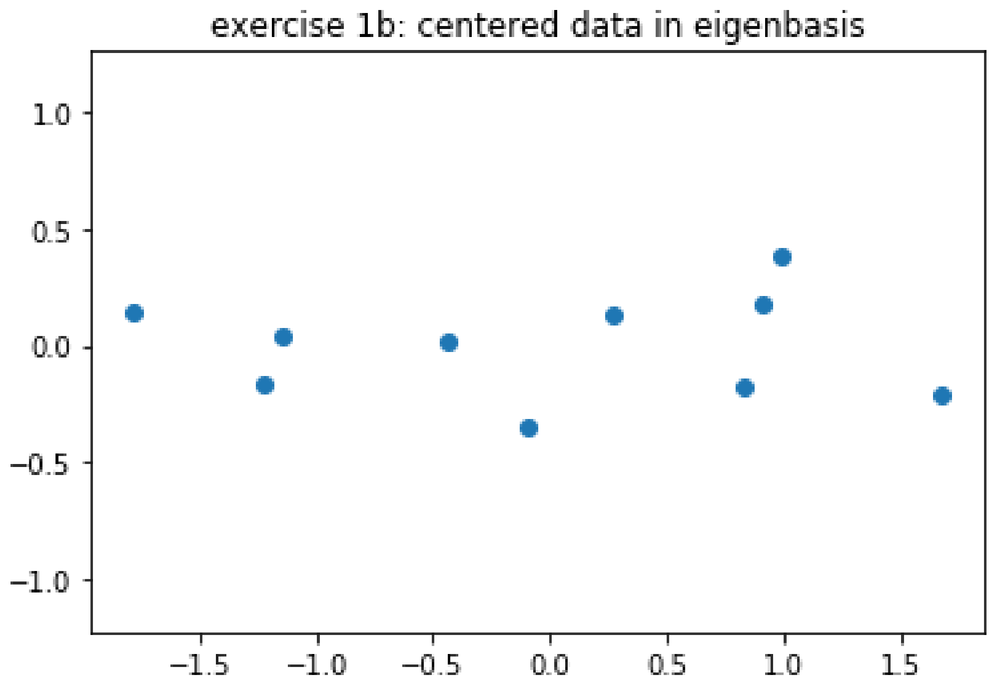
- Determine the Principal Component Directions (PCs)
- scatter plot in the coordinate system spanned by the 2 PCs.

$$x_{eig} = e_{vect}^T X$$

```
In [6]: # 2.1b) logic
        c = np.dot(x.T, x) / (x.shape[0] - 1)       # compute the covariance matrix
        evalue, evector = np.linalg.eig(c)           # eigenvalue eigenvector decomposition; evec
        evalue, evector = arraySort(evalue,evector) # sort the evector by the size of the evalue
        x_eig = project(x, evector)                  # x_eig-matrix contains data points x in eig
        print ("Each column of evector is an eigenvector: ev = (ev_1, ev_2)",
               np.dot(evector[:,0], c) - np.dot(evalue[0], evector[:,0]))
```

```
Each column of evector is an eigenvector: ev = (ev_1, ev_2) [ 0.  0.]
```

```
In [7]: # 2.1b) Plot
        plotscatter(x_eig, title="exercise 1b: centered data in eigenbasis")
```



1.6 2.1 c)

- Plot the reconstruction of the data in the original coordinate system when using
  - (i) only the first or
  - (ii) only the second PC for reconstruction. e_i

$$x_{eig} = e_{vect}^T X$$

- Reconstruction to smaller (first) evector:

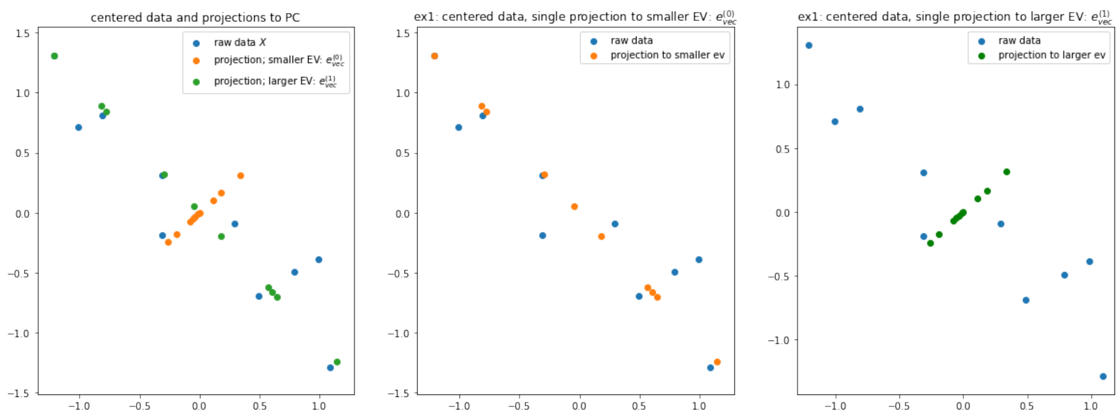
$$\left(e_{vec}^{(0)}\right)^T Ce_{vec}^{(0)} \in \mathbb{R}^2$$

- Reconstruction to larger (second) evector:

$$\left(e_{vec}^{(1)}\right)^T C e_{vec}^{(1)} \in \mathbb{R}^2$$

```
In [8]: # 2.1c) logic. Projection to principal component and reconstruction.
        # (2, 10, 2)
        x_proj = np.array([projectToPC(x, evector[i]) for i in np.arange(evector.shape[0])])
```

```
In [9]: # 2.1c) plot
        plt.figure(figsize=(20,7))
        plt.subplot(131)
        plotscatter(x, label="raw data $X$")
        plotscatter(x_proj[0,:], label="projection; smaller EV: $e_{vec}^{(0)}$")
        plotscatter(x_proj[1,:], title="centered data and projections to PC", label="projection;

        plt.subplot(132)
        plotscatter(x, label="raw data")
        plotscatter(x_proj[1], title="ex1: centered data, single projection to smaller EV: $e_{v

        plt.subplot(133)
        plotscatter(x, label="raw data")
        plotscatter(x_proj[0], title="ex1: centered data, single projection to larger EV: $e_{ve
```



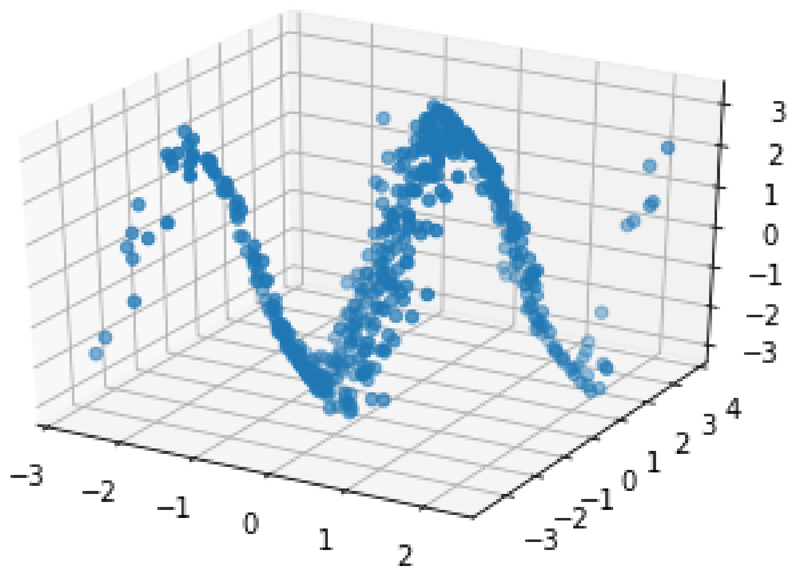
2 2.2

2.1 2.2 a)

- Load, center, plot

```
In [10]: # 2.2 a) - Logic
         x = np.genfromtxt("pca-data-3d.txt", dtype="double", delimiter=",")[1:]
         x = x - np.mean(x, axis=0)
```

```
In [11]: plotscatter3d(x)
```

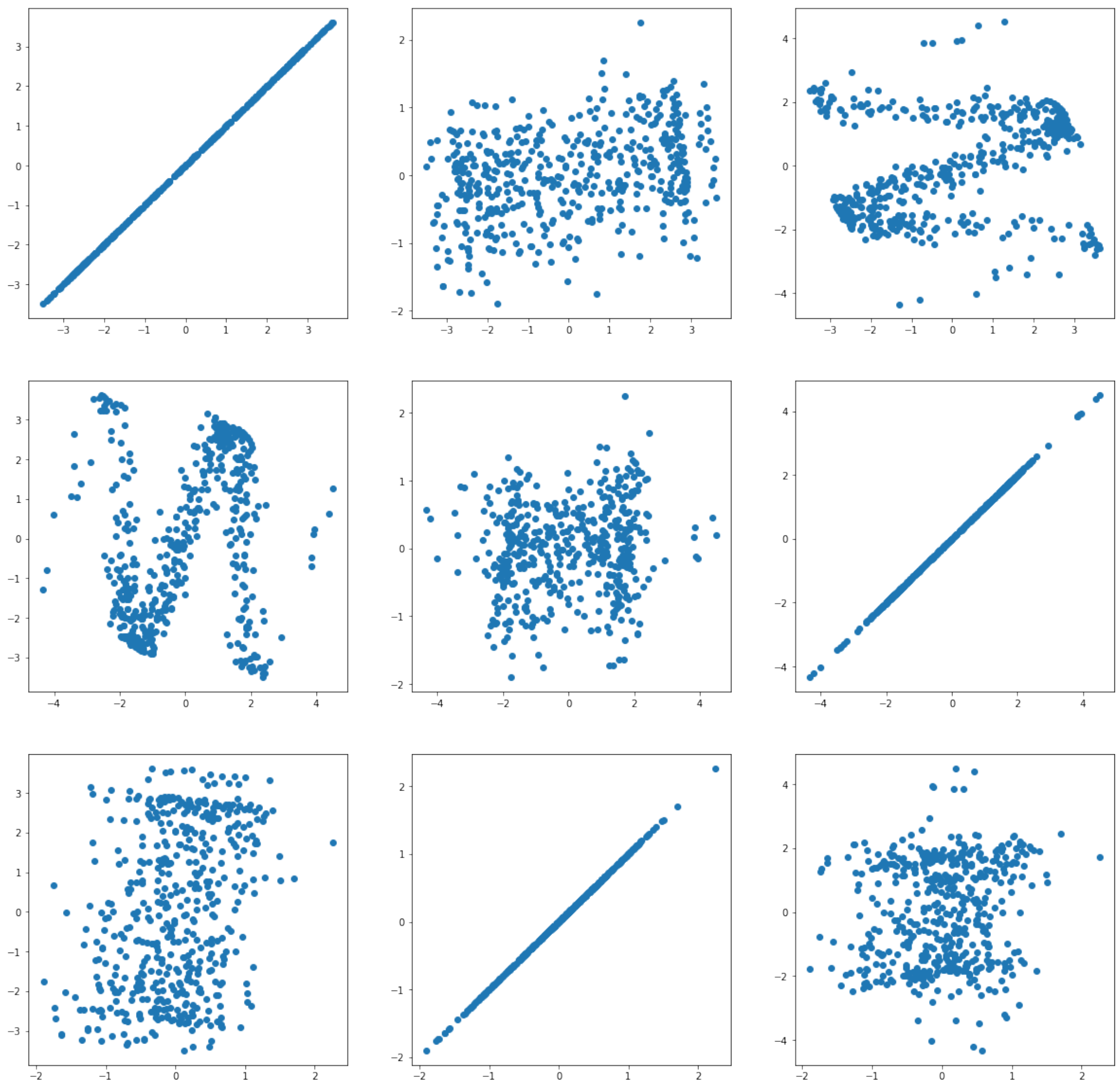


3 2.2 b)

- Determine the PCs
- Scatter plot for 2d-coordinate systems spanned by the different pairs of PCs.

```
In [12]: c = np.dot(x.T, x) / (x.shape[0]-1) # covariance matrix
         evalue, evector = np.linalg.eig(c)  # eigenvalue eigenvector decomposition; evector = P
         evalue, evector = arraySort(evalue,evector)
         x_proj = project(x, evector)         # this matrix contains the data points x in eigenb

In [13]: fig, axes = plt.subplots(nrows=3, ncols=3, figsize=(20,20))
         fig.suptitle('Scatter plots of the projection of the data according to each 2d combinat
         for i in range(0,3):
             for b in range(0,3):
                 x_proj = project(x,np.array([evector[i,:],evector[b,:]]).T)
                 axes[i,-b].scatter(x_proj[:,0], x_proj[:,1])
                 plt.plot()
```

Scatter plots of the projection of the data according to each 2d combination of PC



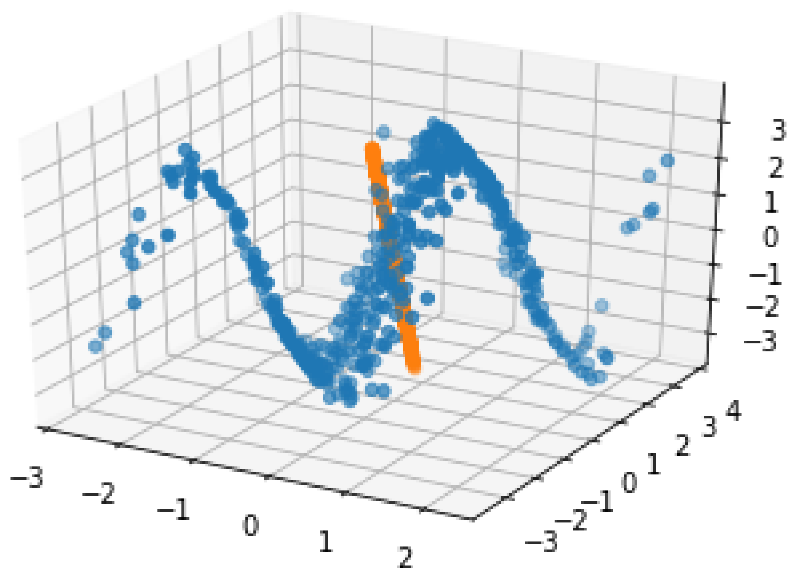
3.1 2.2 c)

- 3d-reconstruction of the data in the original coordinate systems
  - (i) the first,
  - (ii) the first two
  - (iii) all three PCs

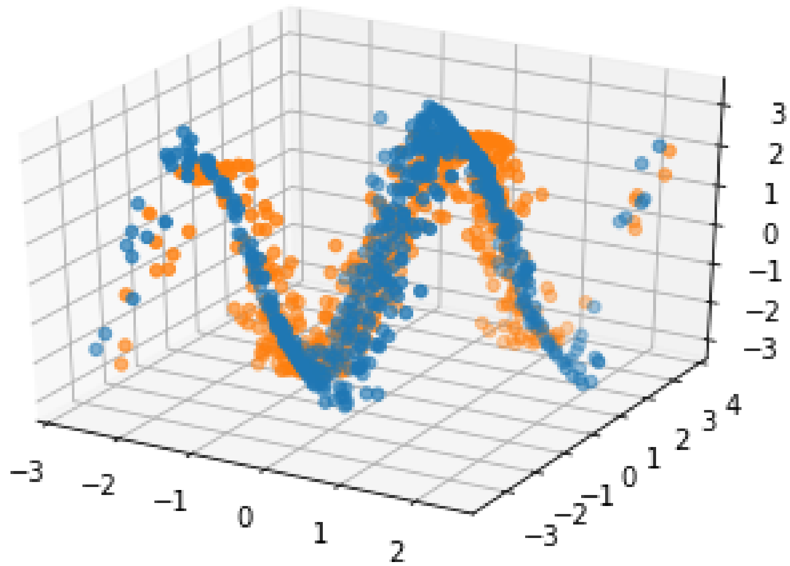
How useful are the different principal components?

```
In [14]: # 2.2 c)
         projectToPC = lambda point, pc: project(project(point, pc)[np.newaxis].T, \
                                                 pc[np.newaxis])
         x_proj = projectToPC(x, evector[0]) # (2, 10, 2)
```

```
In [15]: # 1st pc
         fig = plt.figure()
         ax = fig.add_subplot(111, projection='3d')
         ax.scatter(x[:,0],x[:,1],x[:,2])
         ax.scatter(x_proj[:,0],x_proj[:,1],x_proj[:,2])
         plt.show()
```

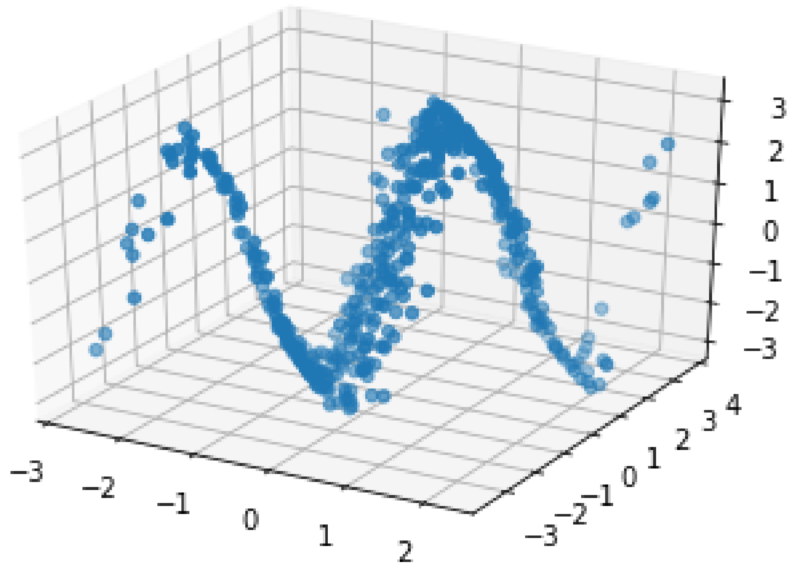



```
In [16]: # 2nd pc
         projectToPC = lambda point, pc: project(project(point, pc.T), pc)
         x_proj = projectToPC(x, evector[0:2,:]) # (2, 10, 2)

         fig = plt.figure()
         ax = fig.add_subplot(111, projection='3d')
         ax.scatter(x[:,0],x[:,1],x[:,2])
         ax.scatter(x_proj[:,0],x_proj[:,1],x_proj[:,2])
         plt.show()
```



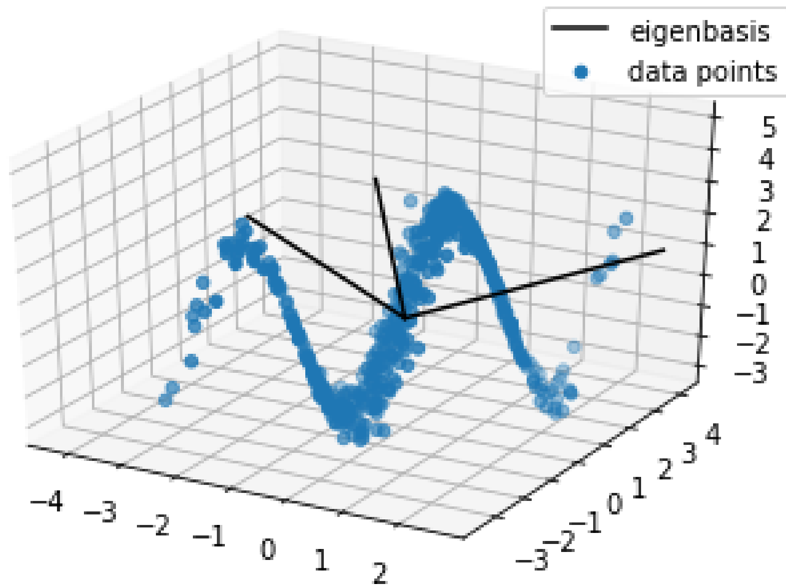

```
In [17]: print(evector[:,0:2].shape)
         projectToPC = lambda point, pc: project(project(point, pc.T), pc)
         x_proj = projectToPC(x, evector) # (2, 10, 2)

         fig = plt.figure()
         ax = fig.add_subplot(111, projection='3d')
         ax.scatter(x_proj[:,0],x_proj[:,1],x_proj[:,2]);#, color="orange")
         plt.show();
```

```
(3, 2)
```

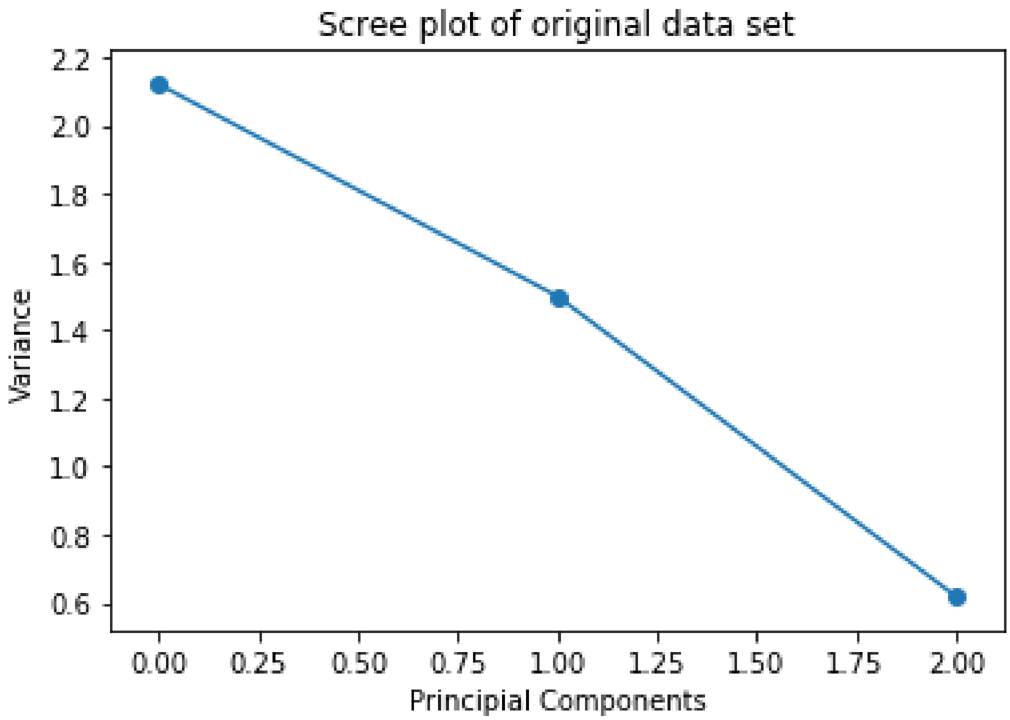


3.1.1 Discuss how useful..

```
In [18]: fig = plt.figure()
         ax = fig.add_subplot(111, projection='3d')
         ax.scatter(x[:,0],x[:,1],x[:,2], label="data points")
         ax.plot([0,5*evector[0,0]],[0,5*evector[0,1]],[0,5*evector[0,2]], color="black", label=
         ax.plot([0,5*evector[1,0]],[0,5*evector[1,1]],[0,5*evector[1,2]], color="black")
         ax.plot([0,5*evector[2,0]],[0,5*evector[2,1]],[0,5*evector[2,2]], color="black")
         plt.legend();
```




```
In [19]: plt.plot(np.arange(len(evalue)), np.sqrt(evalue))
         plt.scatter(np.arange(len(evalue)), np.sqrt(evalue))
         plt.title('Scree plot of original data set')
         plt.xlabel('Principial Components')
         plt.ylabel('Variance')
         plt.plot()

Out[19]: []
```



3.2 2.3 Projections of a dynamical system

3.2.1 a) Find 20 Principal Conponents

```
In [20]: # 2.3 a) PCA
         import warnings
         warnings.filterwarnings('ignore')

         # dataset: 20 processes, each measured for 100 time steps
         x = np.genfromtxt('expDat.txt', delimiter=',', dtype=int)[1:,1:]
         print(x.shape)
```

```
(100, 20)
```

```
In [21]: # covariance matrix
         c = np.dot(x.T, x) / (x.shape[0]-1)
```

```
In [22]: # eigenvalue eigenvector decomposition; evector = PCs
         evalue, evector = np.linalg.eig(c)
         evalue, evector = arraySort(evalue,evector)
         print(evector.shape)
```

```
(20, 20)
```

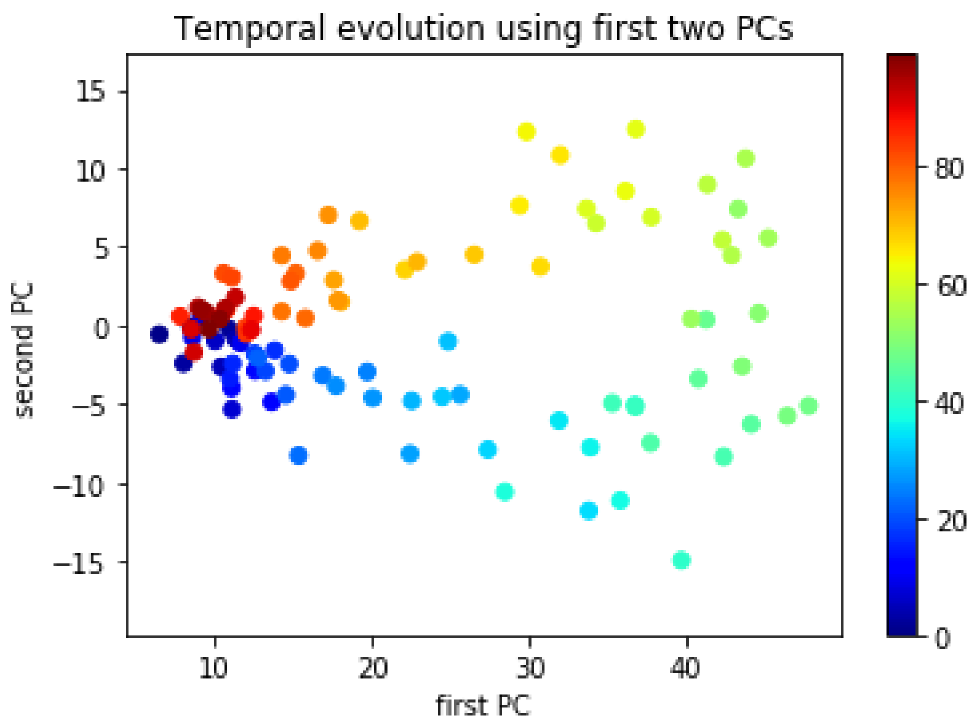
3.2.2 b) Plot temporal evolution of the system projected onto the first two PCs

```
In [23]: # 2.3 b) temporal evolution
         # x_proj contains the data points x projected onto the first two PCs
         x_proj = project(x, np.array([evector[:,0], evector[:,1]]).T)
         print(x_proj.shape)
```

```
(100, 2)
```

```
In [24]: title='Temporal evolution using first two PCs'
         plt.scatter(x_proj[:,0], x_proj[:,1], c=range(x_proj.shape[0]), cmap='jet')
         plt.title(title)
         plt.axis('equal')
         plt.xlabel('first PC')
         plt.ylabel('second PC')
         plt.legend()
         plt.colorbar()
```

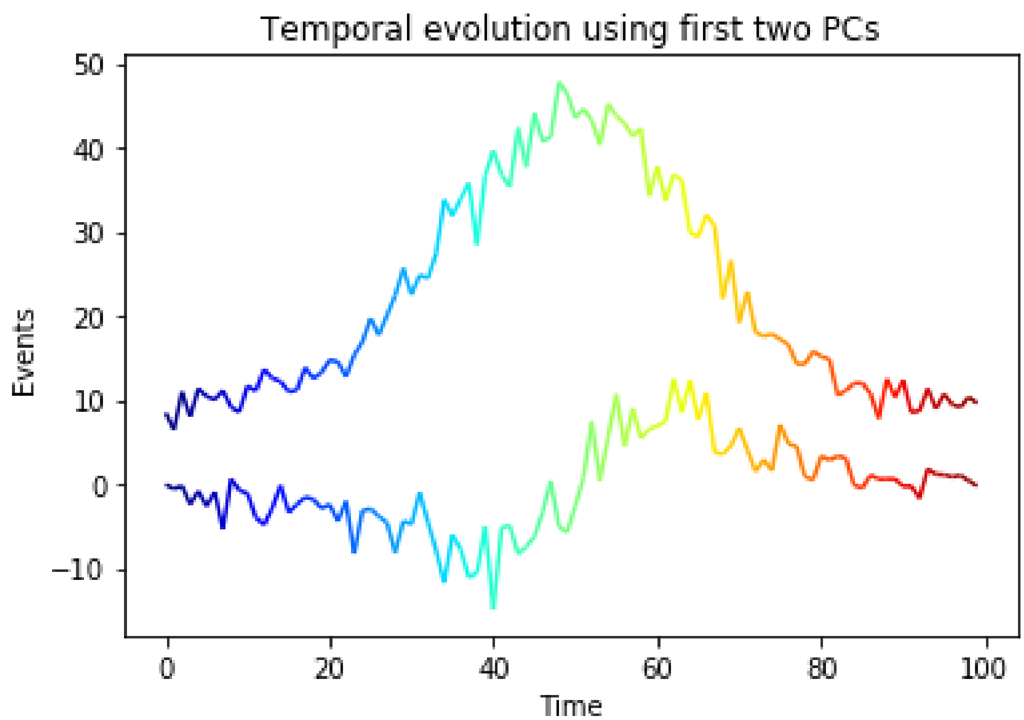
```
Out[24]: <matplotlib.colorbar.Colorbar at 0x113caca58>
```




```
In [25]: from matplotlib.collections import LineCollection
         # http://stackoverflow.com/questions/10252412/matplotlib-varying-color-of-line-to-captu

         t = np.linspace(0,1,x_proj.shape[0])
```

```
# first PC
points = np.array([np.arange(0,100),x_proj[:,0]]).transpose().reshape(-1,1,2)
segs = np.concatenate([points[:-1],points[1:]],axis=1)
lc = LineCollection(segs, cmap=plt.get_cmap('jet'))
lc.set_array(t)
plt.gca().add_collection(lc)
# second PC
points2 = np.array([np.arange(0,100),x_proj[:,1]]).transpose().reshape(-1,1,2)
segs2 = np.concatenate([points2[:-1],points2[1:]],axis=1)
lc2 = LineCollection(segs2, cmap=plt.get_cmap('jet'))
lc2.set_array(t)
plt.gca().add_collection(lc2)

plt.xlim(-5, 104)
plt.ylim(-18, 51) #plt.ylim(min(x_proj[:,0].min(), x_proj[:,1].min()), max(x_proj[:,0].
plt.title(title)
plt.xlabel('Time')
plt.ylabel('Events')
```

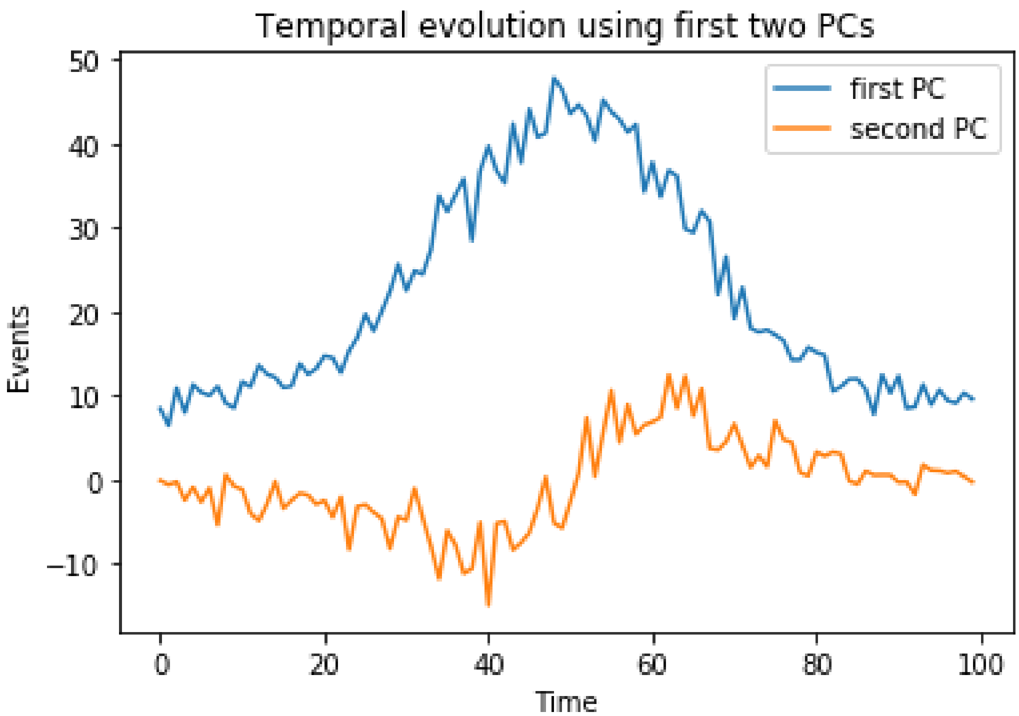
Out[25]: <matplotlib.text.Text at 0x113d69f60>



In [26]:
```
first_pc = plt.plot(x_proj[:,0], label='first PC')
second_pc = plt.plot(x_proj[:,1], label='second PC')
plt.legend()
```

```
plt.title(title)
plt.xlabel('Time')
plt.ylabel('Events')
```

Out[26]: <matplotlib.text.Text at 0x113dd6438>



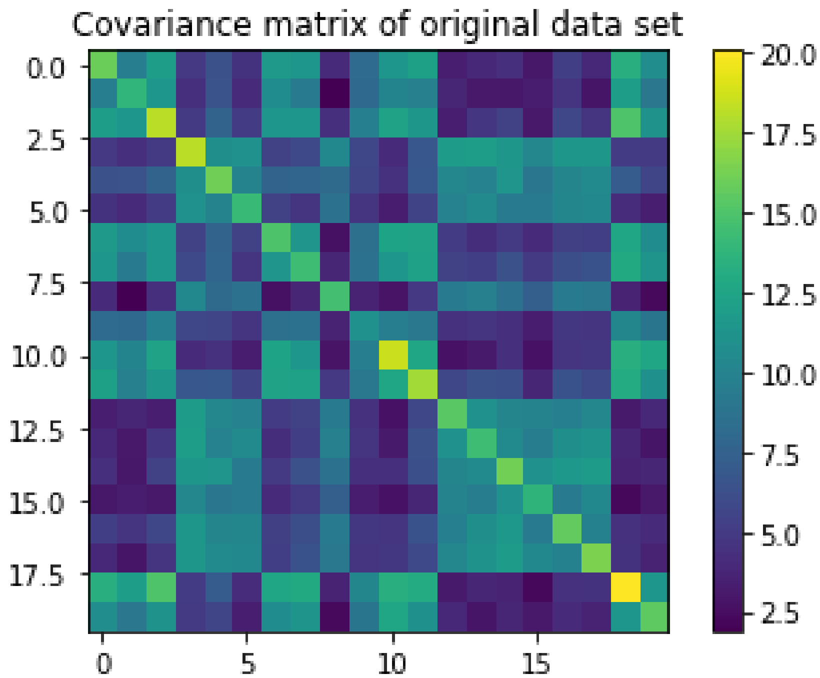
3.2.3 c) New shuffled data set

In [27]:
```
# 2.3 c) shuffle values within event column
x_per = np.array([np.random.permutation(i) for i in x.T]).T
```

3.2.4 d) Plot covariance matrices and scree plots for original and shuffled data

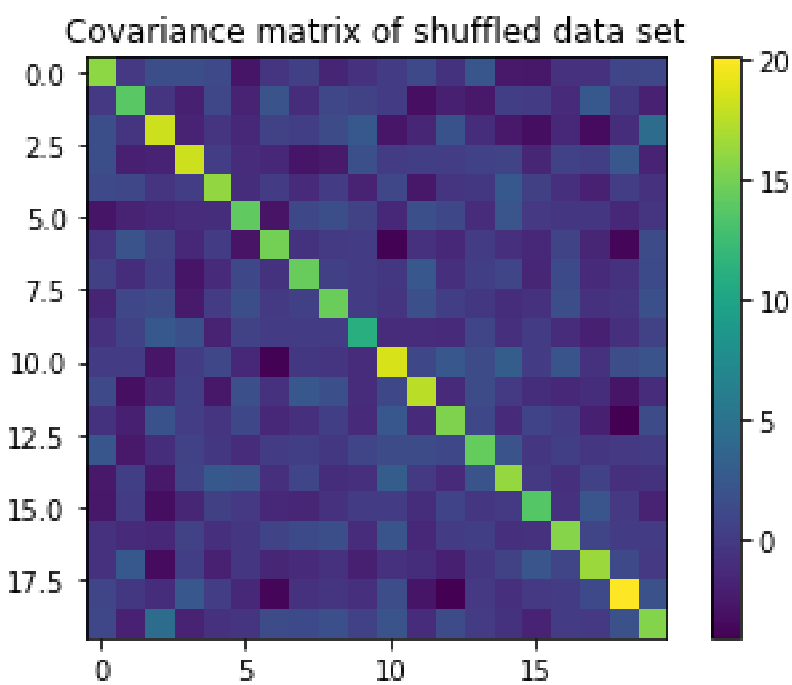
In [28]:
```
# 2.3 d) comparison covariance and scree plots
C_x = np.cov(x,rowvar=False)
C_per = np.cov(x_per,rowvar=False)

plt.imshow(C_x)
plt.title('Covariance matrix of original data set')
plt.colorbar()
```

Out[28]: <matplotlib.colorbar.Colorbar at 0x11403c9e8>



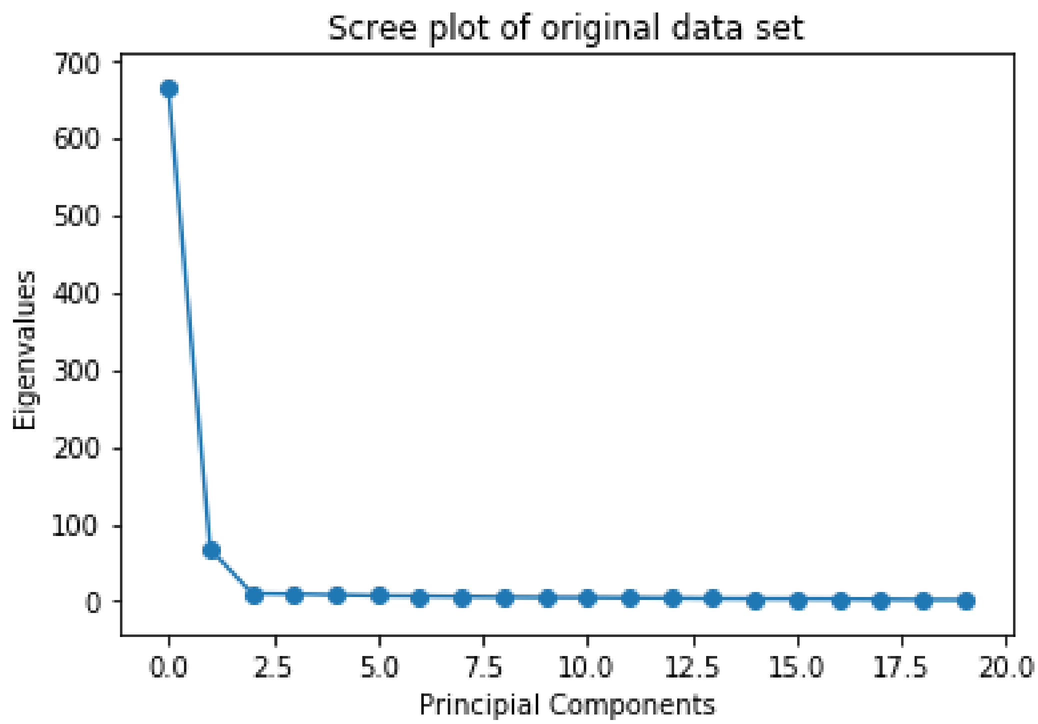

```
In [29]: plt.imshow(C_per)
         plt.title('Covariance matrix of shuffled data set')
         plt.colorbar()
```

```
Out[29]: <matplotlib.colorbar.Colorbar at 0x1142c6a20>
```



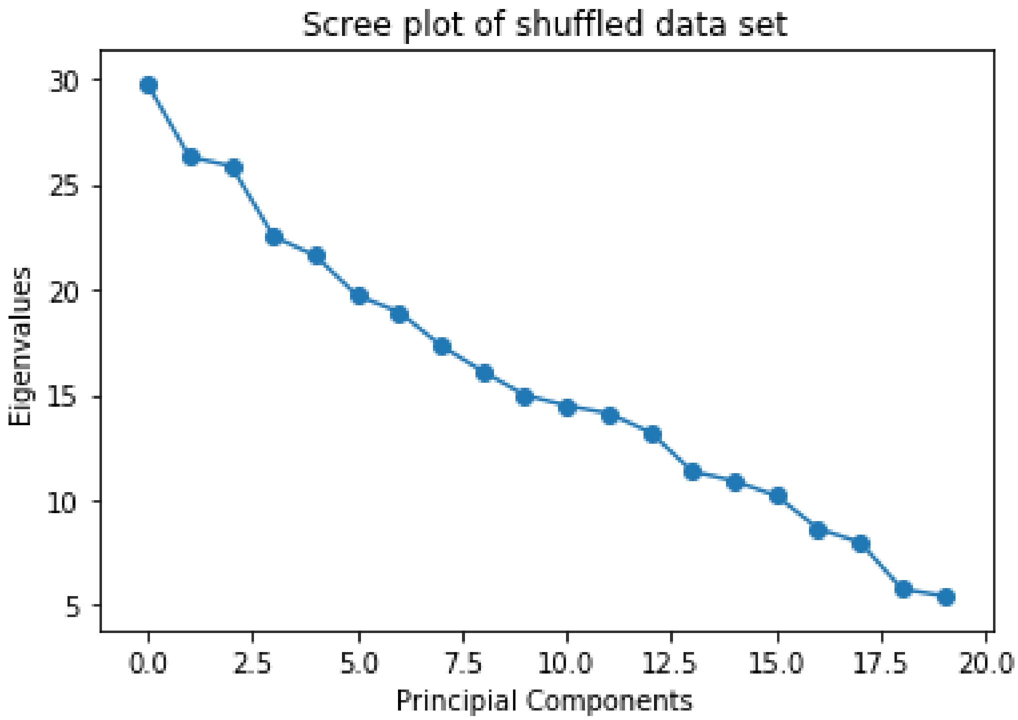
In [30]:
```
plt.plot(np.arange(len(evalue)), evalue)
plt.scatter(np.arange(len(evalue)), evalue)
plt.title('Scree plot of original data set')
plt.xlabel('Principial Components')
plt.ylabel('Eigenvalues')
```

Out[30]: <matplotlib.text.Text at 0x113aa37b8>



In [31]:
```
evalue_per, evector_per = np.linalg.eig(C_per)  # eigenvalue eigenvector decomposition;
evalue_per, evector_per = arraySort(evalue_per, evector_per)

plt.plot(np.arange(len(evalue_per)), evalue_per)
plt.scatter(np.arange(len(evalue_per)), evalue_per)
plt.title('Scree plot of shuffled data set')
plt.xlabel('Principial Components')
plt.ylabel('Eigenvalues')
```

Out[31]: <matplotlib.text.Text at 0x111e95940>



3.2.5 Interpretation

Covariance matrices The corellation in the original data set is visible in the plot of the covariance matrix. There is no visible correlation in the shuffeld data set, because all values other than the diagonal are equally low. #### Scree plots Original data set: the first two PCs are relevant for data variance, the rest of the PCs are irrelevant and can be interpreted as noise. Shuffled data set: the line form follows from ordering the eigenvalues from largest to smallest, there is no possiblity to distinguish between relevant and irrelevant PCs.

3.2.6 e) New shuffled data set: randomized row order

The timesteps will be in a different order, but the correlation between the different timesteps will be preserved. We expect the plot of the temporal evolution using the first two PCs to be similar to the one with the original data, only the color code showing the circle evolution over time will change, because the order of the timesteps changed.

3.3 2.4

```
In [32]: # load directory which contains unzipped images
         from os import listdir
         from os.path import isfile, join
         mypath = "imgpca"
         onlyfiles = [f for f in listdir(mypath) if (isfile(join(mypath, f)) and ("_" not in str
         images_by_category = dict()
```

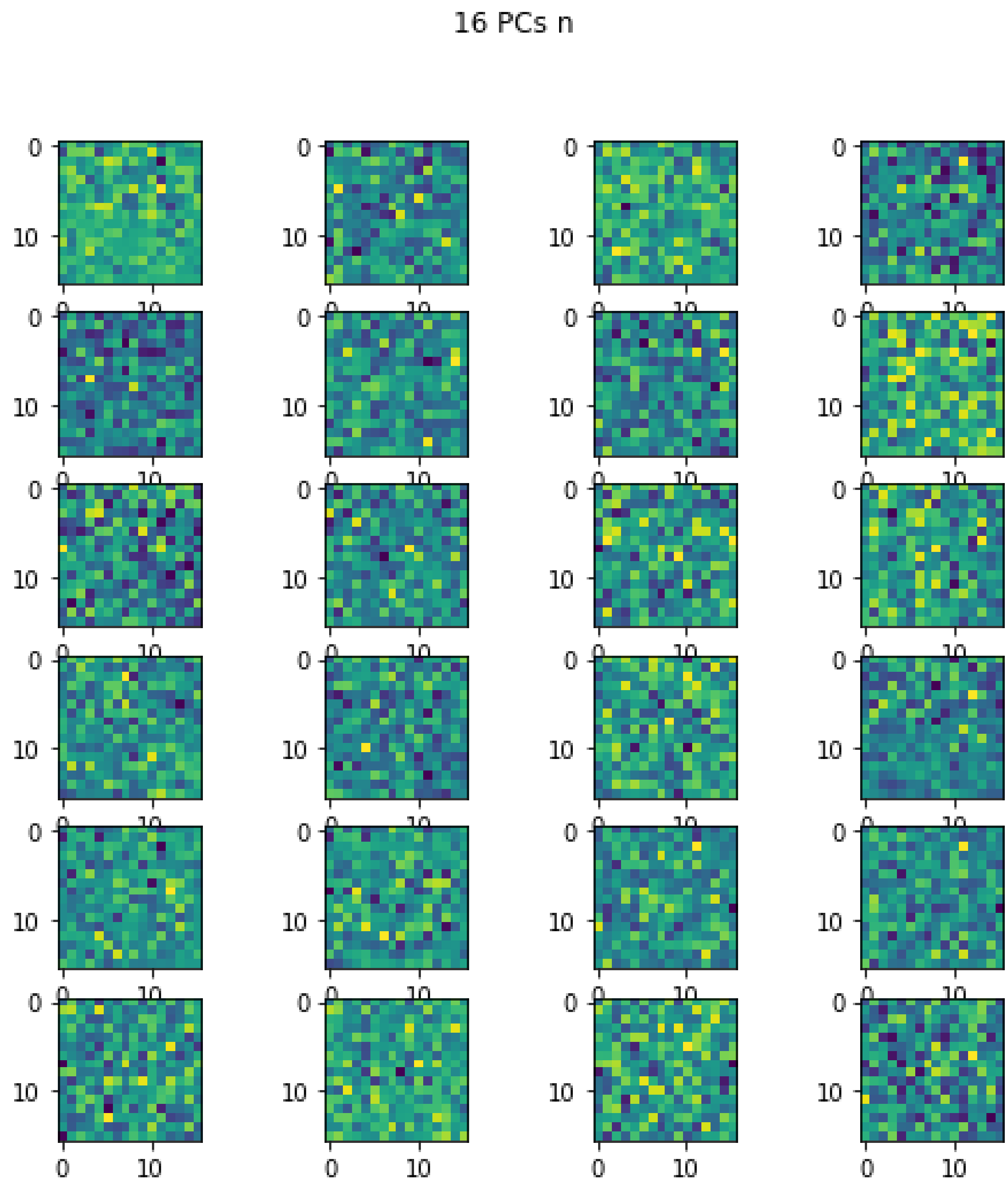
```
        for file in onlyfiles:
            try:
                images_by_category[file[0]].append(file)
            except KeyError:
                images_by_category[file[0]] = [file,]
        print(images_by_category)
```

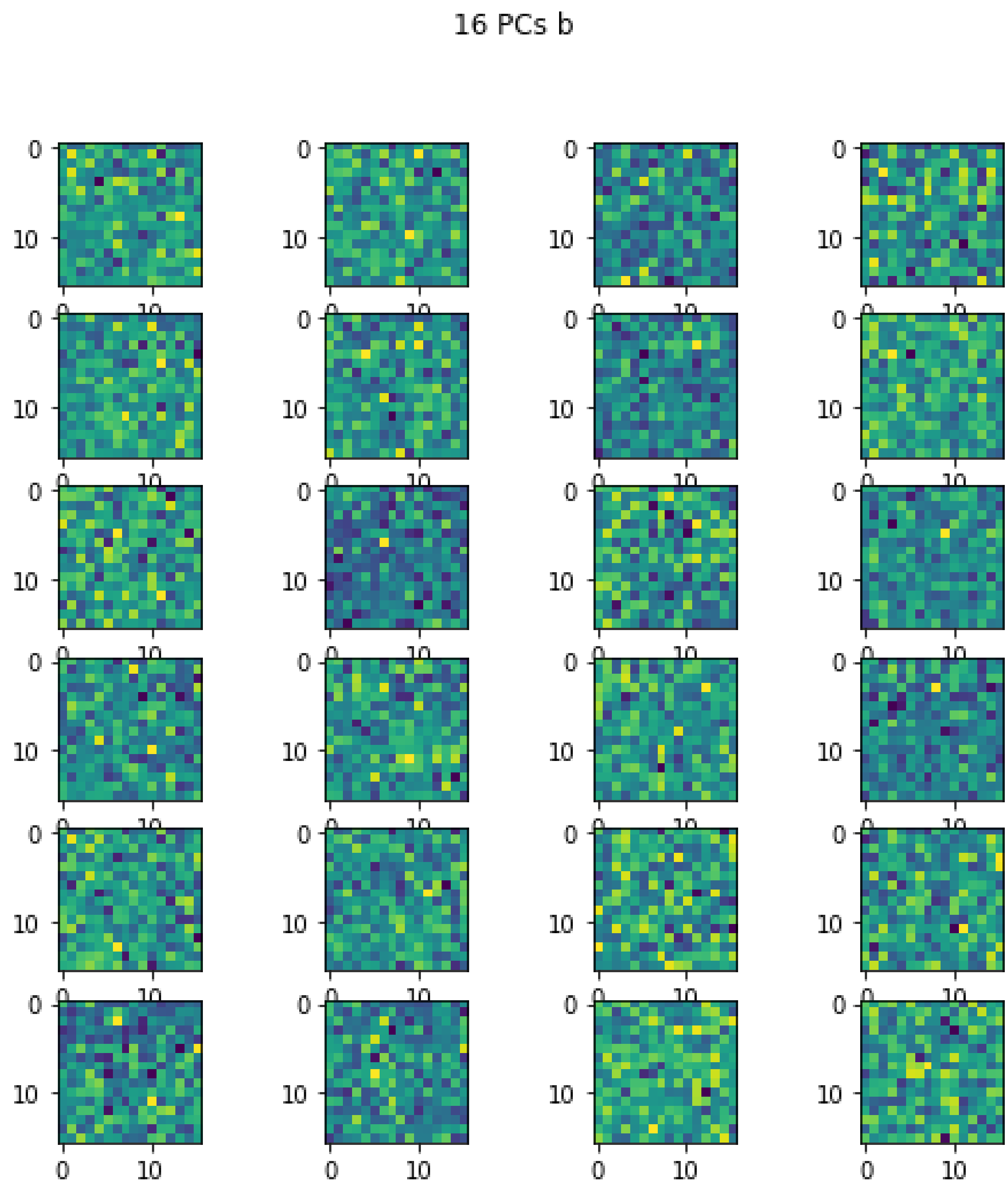
```
{'b': ['b1.jpg', 'b10.jpg', 'b2.jpg', 'b3.jpg', 'b4.jpg', 'b5.jpg', 'b6.jpg', 'b7.jpg', 'b8.jpg'
```

```
In [33]: # Sample subset
         width = 16
         patches_per_image = 500
         #exercise a: Create Nx256 matrix
         eigenwerte = dict()
         eigenvectors = dict()
         for prefix in ["n","b"]:
             patches = np.zeros(shape=(len(images_by_category[prefix])*patches_per_image,256))
             for idx, f in enumerate(images_by_category[prefix]):
                 image = img.imread(join(mypath,f))
                 # Sample 500 16*16 patches per image
                 for i in range(0,patches_per_image-1):
                     column = np.random.randint(0,image.shape[0]-width)
                     row = np.random.randint(0,image.shape[1]-width)
                     patch = image[column:column+width,row:row+width].flatten()
                     patches[idx*patches_per_image + i] = patch

             #Exercise b: Calculate PCs and show them as images
             m_patches = patches - np.mean(patches, axis=0)
             print(patches.argmax())
             print(m_patches.max())
             c = np.dot(m_patches.T, m_patches) / (m_patches.shape[0]-1)
             evalue, evector = np.linalg.eig(c)

             # Plot the PCs
             fig, axes = plt.subplots(nrows=6, ncols=4, figsize=(8,8))
             fig.suptitle("16 PCs {}".format(prefix))
             print(evector.shape)
             for c in range(0,4):
                 for r in range(0,6):
                     axes[r,c].imshow(evector[c+(r*4)].reshape(16,16))

             # Save copy for scree plot
             eigenwerte[prefix] = evalue[:]
             eigenvectors[prefix] = evector[:]
```

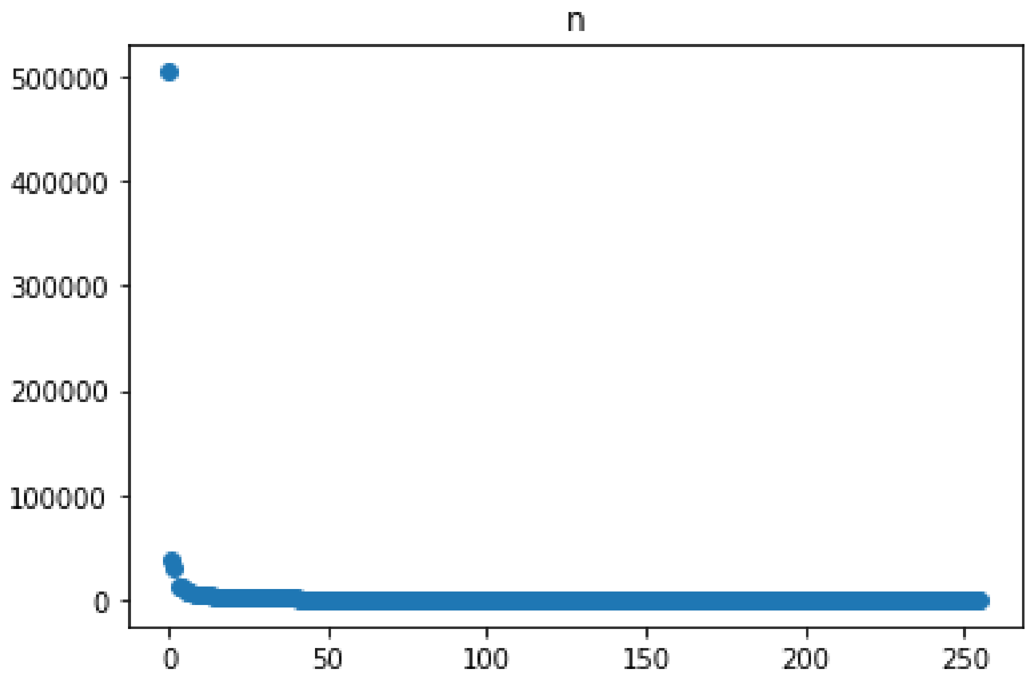
```
18476
152.896923077
```

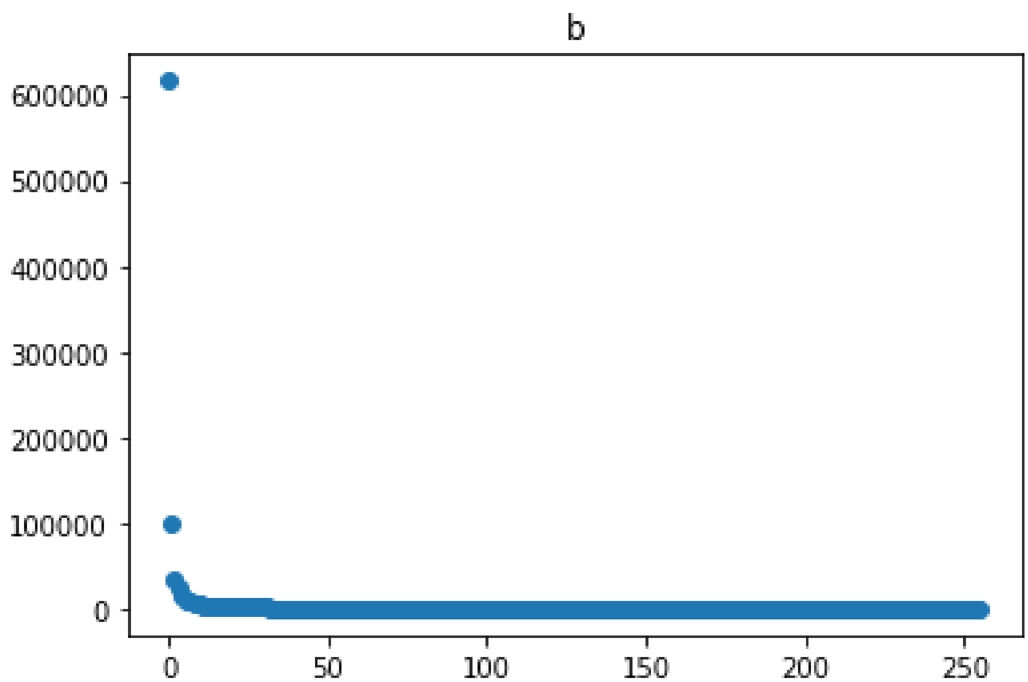
```
(256, 256)
8
139.734
(256, 256)
```





```
In [34]: # Scree plot of Eigenwerte
         for prefix in ["n","b"]:
             eigenwerte[prefix].sort()
             y = eigenwerte[prefix][::-1]
             x = np.asarray(range(0,len(y)))
             plt.figure()
             plt.title(prefix)
             plt.scatter(x,y)
```





As can be seen in the scree-plot, only the first few PCs make sense to use. For category **n** this is **3** and for **b** it is 2-3 (we will go with **3**).

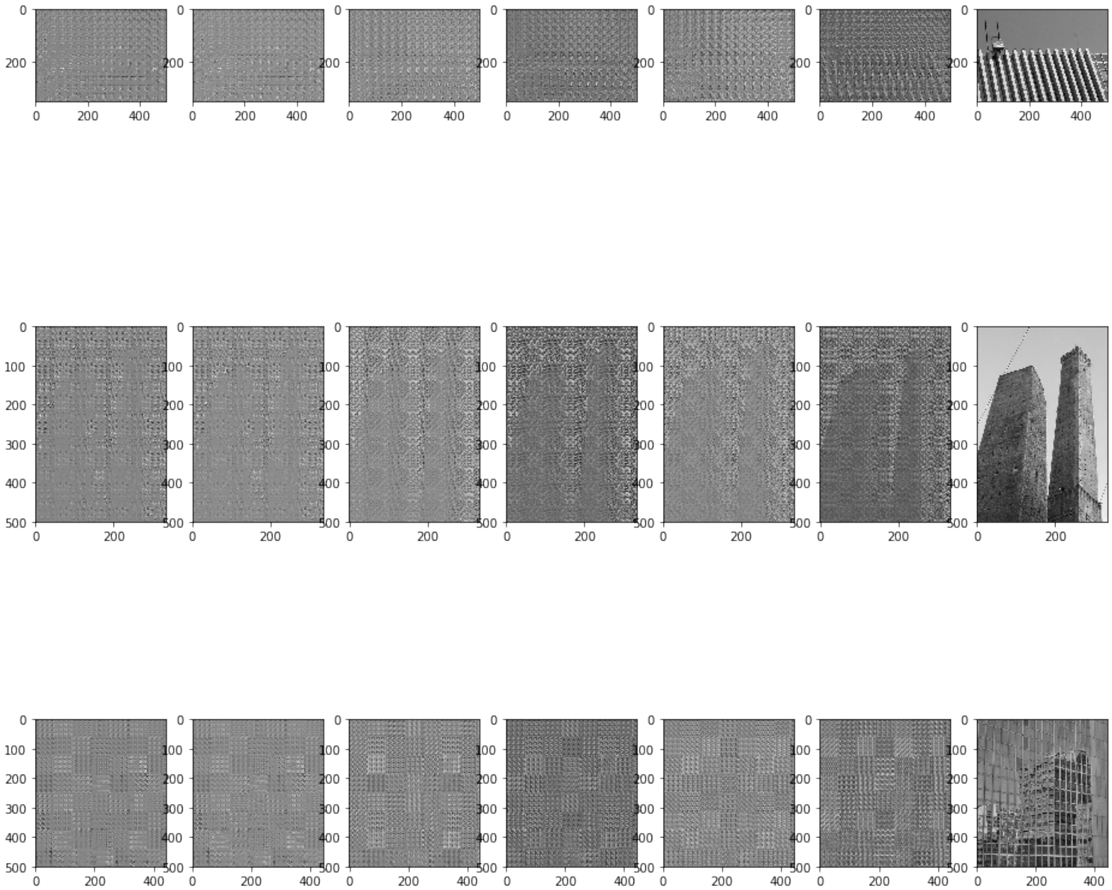
3.4 TODO: What is the respective compression ratio? (is it 3 / 256 + the overhead of storing the vectors?)

In [35]:
```
# Reconstruct 3 arbitrary images by projecting all of its constituent (non-overlapping1
# patches onto the first n PCs of that image category

patch_width = 16
N = [1,2,4,8,16,100,256]
def projecting_haze(eigenwerte, eigenvectors,file_names,prefix):
    fig, axes = plt.subplots(nrows=3, ncols=len(N), figsize=(16,16))
    fig.suptitle(prefix)
    # Choose 3 images
    for image_number, f in [(i,image) for (i,image) in enumerate(file_names) if i < 3]:
        print(f)
        image = img.imread(join(mypath,f))
        print(image.shape)

        # Iterate over the image and fill patches into array. At boundaries we need to
        for i,n in enumerate(N):
            flat_image = image[:].flatten()
            proj_image = np.zeros(flat_image.shape)
            reconstructed_image = np.zeros(image.shape)
            # Take the first n vectors
            _, pcs = arraySort(eigenwerte,eigenvectors)
            pcs = pcs[:n].T
            # Project the patches using the PCs

            # +1 offset to make sure, we always have a patch for the end (range ends ex
            for column_pixel in range(0,image.shape[1]+1,patch_width):
                # overlap at  boundary
                if column_pixel + patch_width >= image.shape[1]:
                    column_pixel = image.shape[1] - patch_width
                for row_pixel in range(0,image.shape[0]+1,patch_width):
                    if row_pixel + patch_width >= image.shape[0]:
                        row_pixel = image.shape[0] - patch_width
                    # Extract the patch by taking a square from (0,0) to (15,15) with a
                    patch = image[row_pixel:row_pixel + patch_width,column_pixel:column
                    #
                    projected_patch = np.dot(patch.flatten(),pcs)
                    reconstructed_patch = np.dot(projected_patch,pcs.T)
                    #print(reconstructed_patch)
                    reconstructed_image[row_pixel:row_pixel + patch_width,column_pixel:
                        reconstructed_patch.reshape((patch_width,patch_width))

            # Plot the picture with n used PCs
            axes[image_number,i].imshow(reconstructed_image,cmap='gray')

for prefix in ["n","b"]:
```

```
projecting_haze(eigenwerte[prefix],eigenvectors[prefix],images_by_category[prefix],
```

```
n1.jpg
(256, 512)
n10.jpg
(256, 512)
n11.jpg
(256, 512)
b1.jpg
(353, 500)
b10.jpg
(500, 334)
b2.jpg
(500, 443)
```

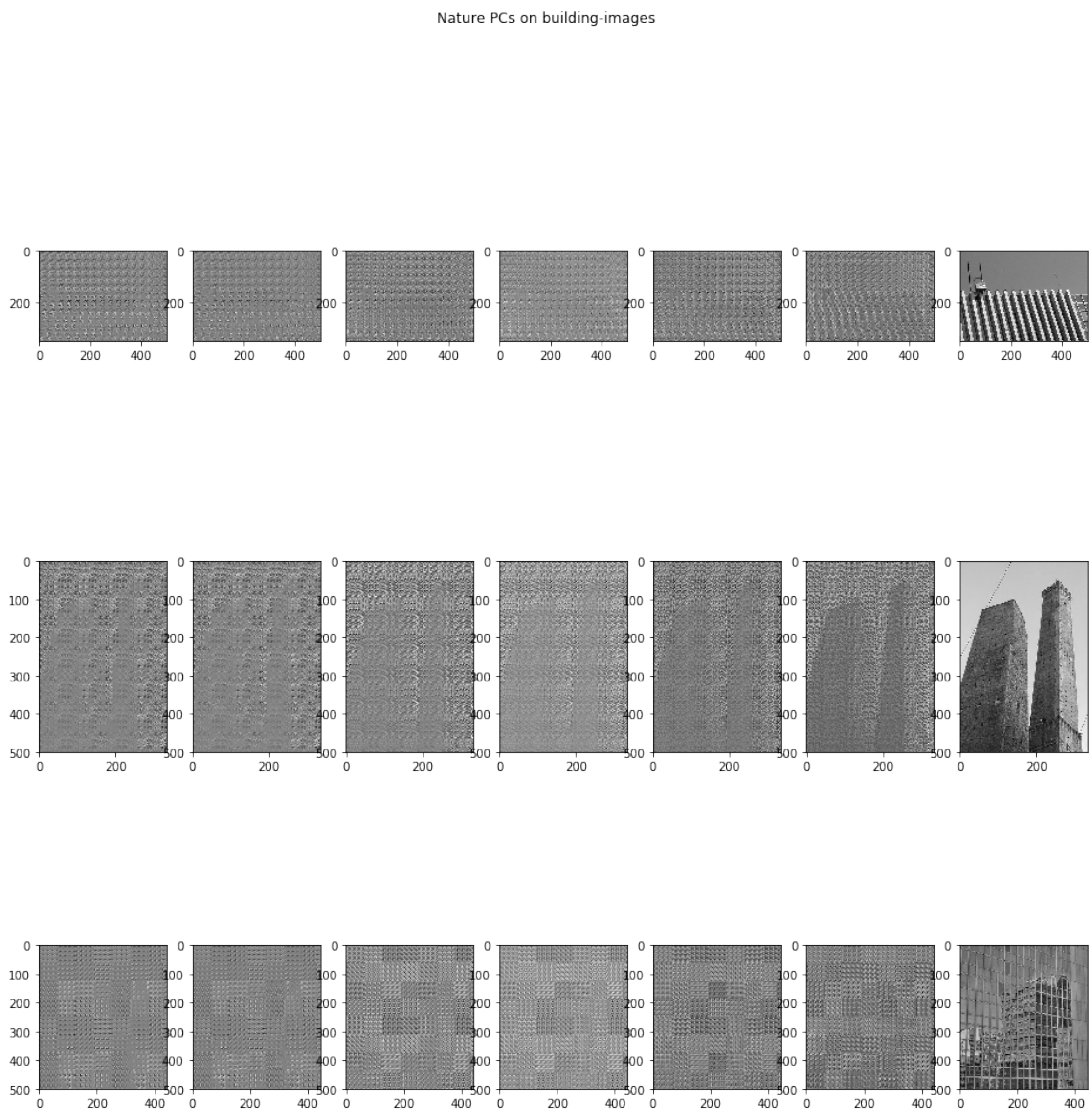
The Building PCs for building. Nature PCs for nature



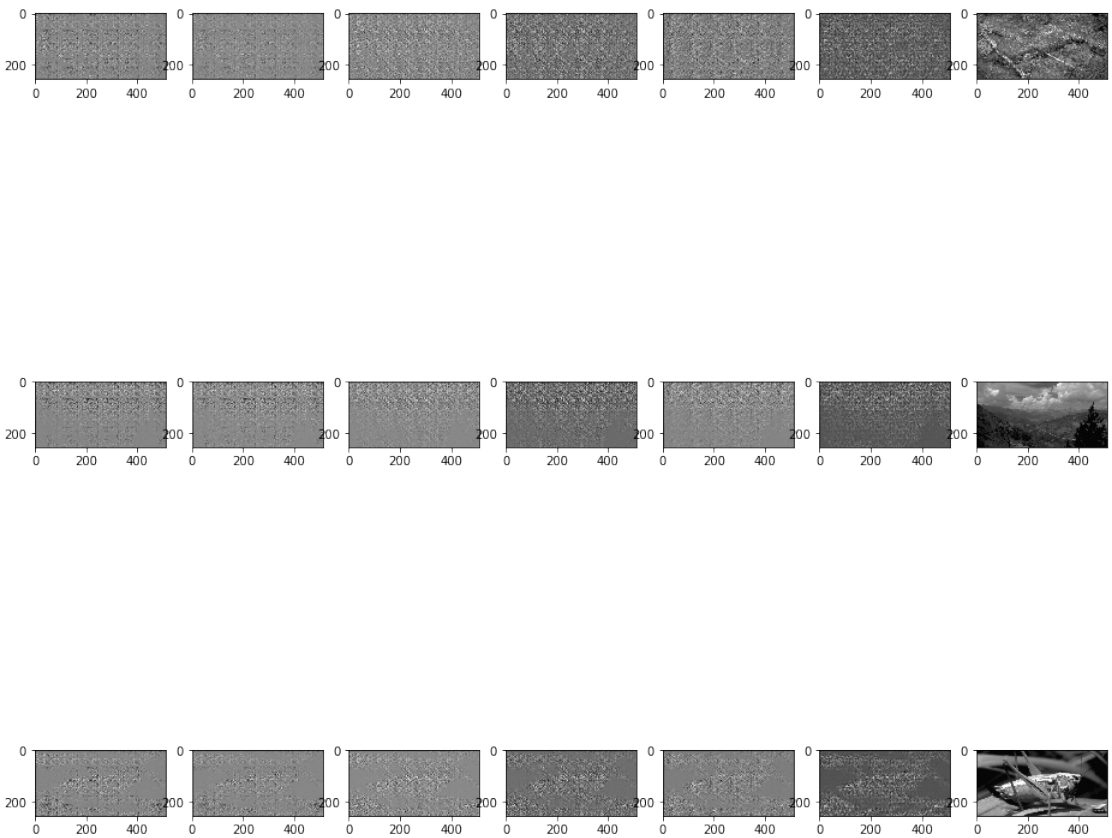
In [36]:
```
print("Nature PCs on building-images")
projecting_haze(eigenwerte["n"],eigenvectors["n"],images_by_category["b"],"Nature PCs o
print("Building PCs on nature-images")
projecting_haze(eigenwerte["b"],eigenvectors["b"],images_by_category["n"],"Building PCs
```

```
Nature PCs on building-images
b1.jpg
(353, 500)
b10.jpg
(500, 334)
b2.jpg
(500, 443)
Building PCs on nature-images
```

```
n1.jpg
(256, 512)
n10.jpg
(256, 512)
n11.jpg
(256, 512)
```



Building PCs on nature-images



In [ ]: