In [1]:
```
import numpy as np
import numpy.testing as npt
from scipy.linalg import expm
import matplotlib.pyplot as plt
import scipy.spatial, scipy.linalg
import scipy.sparse.linalg
import pandas as pd
%matplotlib inline

class PCA():
    def __init__(self, X):
        # ...
        self.X = X
        self.mean = np.mean(X,axis=0)
        C = np.cov(self.X.T)
        D, U = np.linalg.eig(C)
        idx = np.argsort(-D)
        Ut = U.T
        self.U = Ut[idx]
        self.D = D[idx]


    def project(self, m):
        # ...
        U = self.U.T
        M = U[:,:m]
        Z = np.dot(M.T,self.X.T)
        Z = Z.T
        return Z

    def reconstruct(self, m):
        Z = self.project(m)
        U = self.U.T
        Y = np.dot(U[:,:m],Z.T)
        Y = Y.T
        Y = Y + self.mean
        return Y
```

3.1 Preprocessing

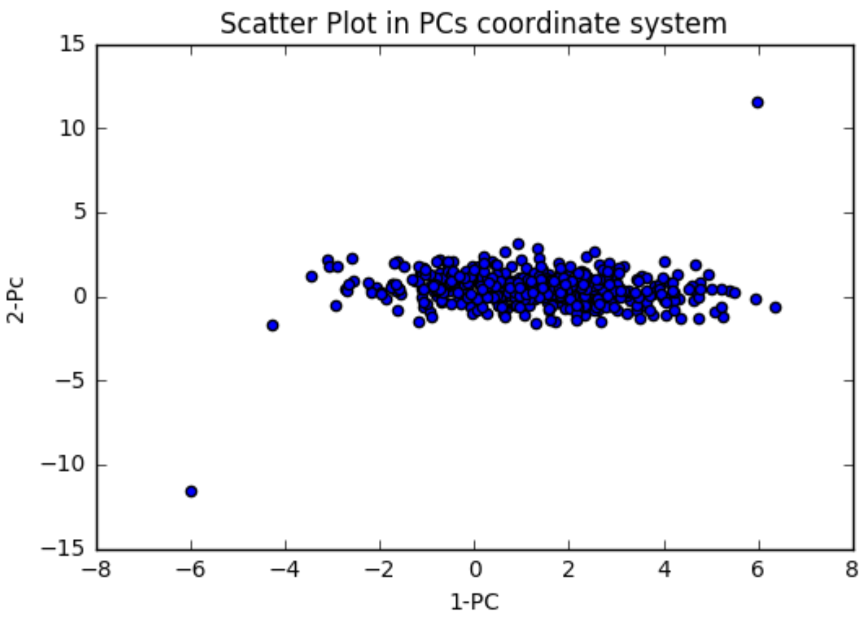
(a) Load the dataset pca2.csv. Compute the Principal Components PC1 and PC2 and plot the data in the coordinate system PC1 vs. PC2 – What do you observe?

In [2]:
```
# Load dataset
data = np.loadtxt('pca2.csv', skiprows=1, delimiter=',')
#compute PC and plot
pca2 = PCA(data)

#Do PCA and project on each PC
PC1 = pca2.U[0]
pjt1=np.dot(PC1,data.T)
PC2 = pca2.U[1]
pjt2=np.dot(PC2,data.T)

#plot
plt.scatter(pjt1, pjt2)
plt.ylim(-15,15)
plt.xlim(-8,8)
plt.xlabel('1-PC')
plt.ylabel('2-Pc')
plt.title('Scatter Plot in PCs coordinate system')
```

Out[2]: <matplotlib.text.Text at 0x7fc612c2d048>



When the dataset is projected on PC1, because of high variance the distance between outliers and inlieres are not so much different. But on PC2 because of low variance, inliers are very close to each other and outliers are separated away. With this obsevation we can use last PC to detect outliers and this is called "Novelty Filter".

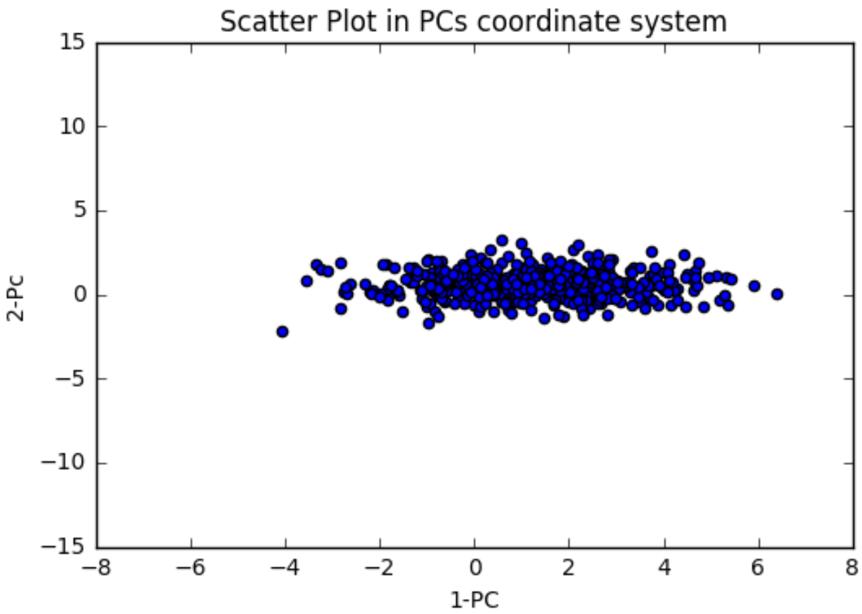
(b) Remove Observations 17 and 157 and redo the first two steps. What is the difference?

In [3]:
```
newset = np.delete(data,[16,156],0)
pca2new = PCA(newset)

#Do PCA and project on each PC
PC1new = pca2new.U[0]
pjt1new=np.dot(PC1new ,newset.T)
PC2new  = pca2new .U[1]
pjt2new =np.dot(PC2new ,newset.T)

#plot
plt.scatter(pjt1new , pjt2new )
plt.ylim(-15,15)
plt.xlim(-8,8)
plt.xlabel('1-PC')
plt.ylabel('2-Pc')
plt.title('Scatter Plot in PCs coordinate system')
```

Out[3]: <matplotlib.text.Text at 0x7fc612b7b400>



Slope became slower.

3.2 Whitening

(a) Load the dataset pca4.csv and check for outliers in the individual variables.

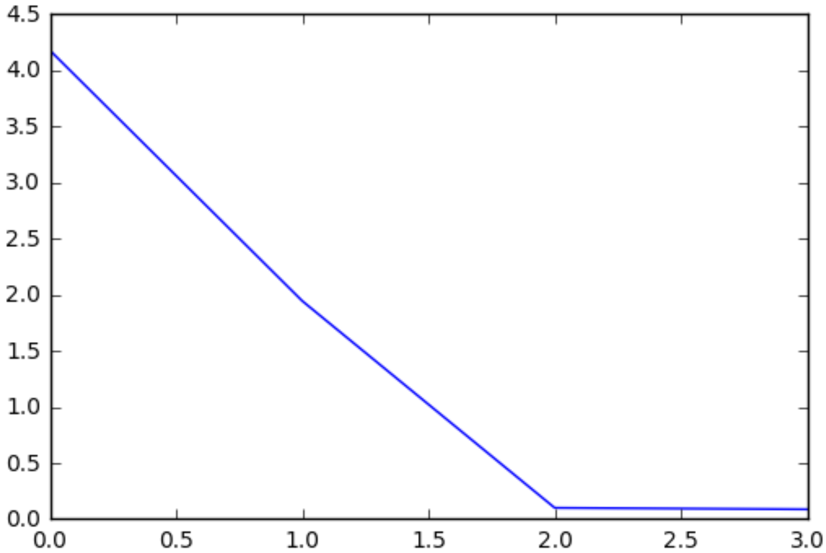
In [4]:
```
# Load dataset
data4 = np.loadtxt('pca4.csv', skiprows=1, delimiter=',')
pca4 = PCA(data4)
#Novelty Filter
nov = np.dot(pca4.U[3].reshape(1,4),data4.T)
nov = nov -np.mean(nov)
novar = np.mean(nov**2)
outidx = np.where(nov**2>novar)
print("The indecies of outliers")
print(outidx[1])
```

```
The indecies of outliers
[ 17  99 111 199 211 409 472]
```

(b) Do PCA on a reasonable subset of this data. Use a scree plot to determine how many PCs represent the data well.

In [5]:
```
subset = np.delete(data4,outidx[1],0)
newpca4 = PCA(subset)
plt.plot(newpca4.D)
```

Out[5]:
```
[<matplotlib.lines.Line2D at 0x7fc612b14978>]
```



We choose first 2 PCs to represent.

In [6]:
```
Error = np.linalg.norm(subset -newpca4.reconstruct(2))
print("Error ||subset-represented subset||: ",Error)
```

```
Error ||subset-represented subset||:  9.95655530615
```

(c) “Whiten” the data, i.e. create a set of 4 uncorrelated variables with mean 0 and standard deviation equal to 1. This can be done e.g. using the transformation

$$Z = \tilde{X}E\Lambda^{-1/2}$$

The new variables z_i form the columns of Z, E is a matrix containing in its columns the normalized eigenvectors of the covariance matrix C of the centered data $\tilde{X}$ (variables columnwise) and Λ is a diagonal matrix containing the corresponding eigenvalues.

In [7]:
```
cenX = subset - np.mean(subset,axis=0)
C = np.cov(cenX.T)
D,E = np.linalg.eig(C)
nomE = np.empty((4,4))
nomE = E/np.linalg.norm(E,axis=0)
Lambda12 = np.diag(D**(-1/2))
Z = np.dot(np.dot(cenX,nomE),Lambda12)
```

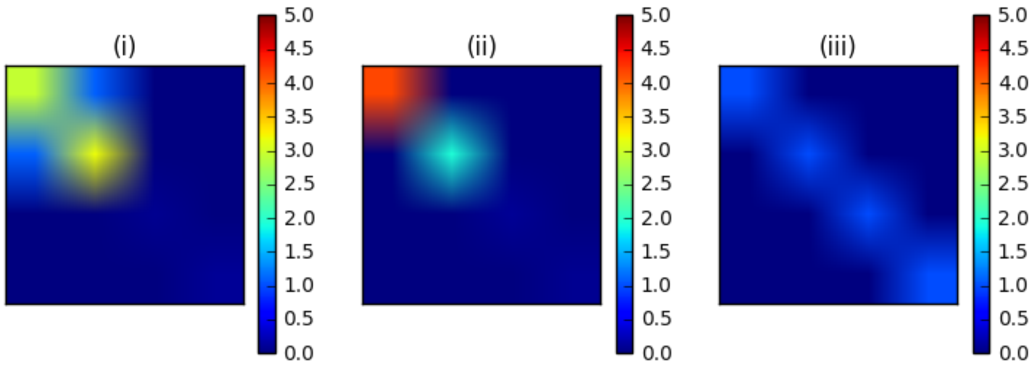
(d) Make 3 heat plots of the (i) 4x4 covariance matrix C, (ii) the covariance matrix of the data projected onto PC1-PC4, and (iii) of the whitened variables.

In [8]:
```
plt.figure(figsize=(9,3))
# 4x4 covariance matrix C
plt.subplot(131)
plt.title("(i)")
plt.imshow(C,vmin=0, vmax=5)
plt.colorbar()
plt.xticks([])
plt.yticks([])

plt.subplot(132)
covpro=np.cov(newpca4.project(4).T)
plt.title("(ii)")
plt.imshow(covpro,vmin=0, vmax=5)
plt.colorbar()
plt.xticks([])
plt.yticks([])

plt.subplot(133)
plt.title("(iii)")
plt.imshow(np.cov(Z.T),vmin=0, vmax=5)
plt.colorbar()
plt.xticks([])
plt.yticks([])
```

Out[8]:
```
([], <a list of 0 Text yticklabel objects>)
```



3.3 Oja's Rule: Derivation

Consider a linear connectionist neuron whose output $y = y(t)$ at time t is an inner product of the N-dim input vector $x = x(t)$ with the N-dim weight vector w:

$$y = w^T x$$

The Hebbian update rule for learning the weights can be written as

$$w_i(t+1) = w_i(t) + \epsilon y(t) x_i(t), \quad i = 1, 2, , , , N$$

where ϵ is the learning-rate parameter and t the iteration step. As was shown in the lecture, the Hebbian learning rule leads to a divergence of the length of the weight vector. Therefore, the following normalization was introduced by Oja:

$$w_i(t+1) = \frac{w_i(t) + \epsilon y(t) x_i(t)}{\left(\sum_{j=1}^{N} [w_j(t) + \epsilon y(t) x_j(t)]^2\right)^{\frac{1}{2}}}$$

Task: Derive an approximation to this update rule for a small value of the learning-rate parameter ϵ by Taylor expanding the right hand side of this equation with respect to ϵ around ϵ = 0. Show that neglecting terms of second or higher order in ϵ gives Oja's rule:

$$w_i(t+1) = w_i(t) + \epsilon y(t)[x_i(t) - y(t) w_i(t)]$$

Anser: The formula of Taylor expanding is

$$\sum_{n=0}^{\infty} \frac{f^{(n)}}{n!}(x-a)^n$$

And

$$w(t+1) = f(\epsilon) = \frac{w_i(t) + \epsilon y(t) x_i(t)}{(\sum_{j=1}^N [w_j(t) + \epsilon y(t) x_j(t)]^2)^{\frac{1}{2}}}$$

$$|w| = \sum_{j=1}^N [w_j(t)]^2 = 1, \quad \sum_{j=0}^N [x_j(t) w_j(t)] = y(t)$$

Neglecting terms of second or higher order in ϵ so we have to expand only until 1st order

$$\begin{aligned}
f^{(0)}(0) + f^{(1)}(0)\epsilon &= \frac{w_i(t)}{(\sum_j^N w_j^2(t))^{\frac{1}{2}}} + \epsilon \left(\frac{y(t)x_i(t)}{(\sum_{j=1}^N [w_j(t) + 0y(t)x_j(t)]^2)^{\frac{1}{2}}} - \frac{1}{2} \frac{w_i(t) + 0y(t)x_i(t)}{(\sum_{j=1}^N [w_j(t) + 0y(t)x_j(t)]^2)^{\frac{3}{2}}} 2 \right. \\
&= \frac{w_i(t)}{(\sum_j^N w_j^2(t))^{\frac{1}{2}}} + \epsilon \left(\frac{y(t)x_i(t)}{(\sum_{j=1}^N [w_j(t)]^2)^{\frac{1}{2}}} - \frac{w_i(t)}{(\sum_{j=1}^N [w_j(t)]^2)^{\frac{3}{2}}} y(t) \sum_{j=0}^N [x_j(t) w_j(t)] \right) \\
&= w_i(t) + \epsilon \left(y(t)x_i(t) - y(t)^2 w_i(t) \right) \\
&= w_i(t) + \epsilon y(t)[(x_i(t) - y(t) w_i(t)]
\end{aligned}$$

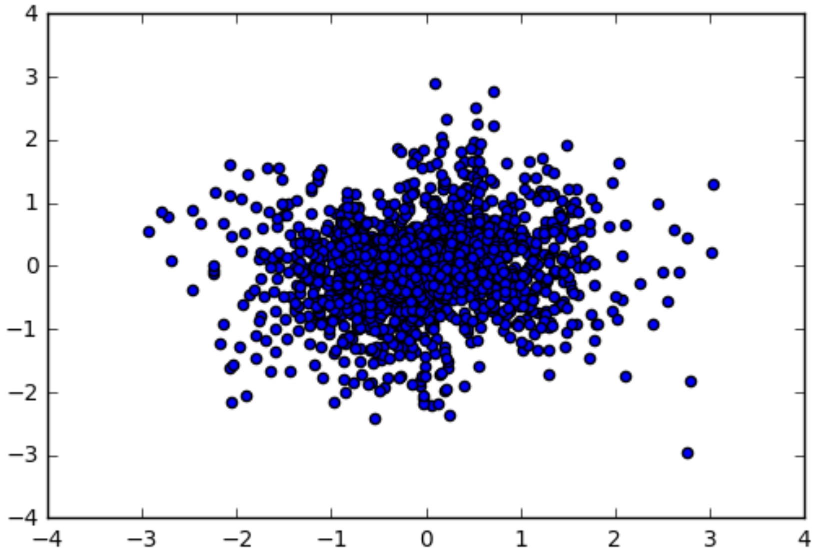
3.4 Oja's Rule: Application

The file data-onlinePCA.txt contains observations from an artificial experiment run over an interval of time (i.e. the first datapoint was observed at $t_0 = 0$ and the last at $t_N = 10s$).

1. Make a scatter plot of the data and indicate the time index by the color of the datapoints you can e.g. break the full dataset into 10 blocks corresponding to 1 second length each and therefore use 10 different colors).
2. Determine the principal components (using batch PCA) and plot the first PC (e.g. as an arrow or the endpoint of it) for each of the 10 blocks in the same plot as the original data.
3. Implement Oja's rule and apply it with a learning-rate parameter $\epsilon \in [0:002, 0:04, 0:45]$ to the dataset. In each iteration randomly sample one data point and apply the learning step. Plot the weights at each timestep (as points whose x vs. y coordinates are given by the weight for x and y) in the same plot as the original data (use the colors from 1. to indicate the time index for each plotted weight). Interpret your results.

In [9]:
```
dtonln = np.loadtxt('data-onlinePCA.txt', skiprows=1, delimiter=',',usec
ols=np.arange(1,3))
plt.scatter(dtonln[:,0],dtonln[:,1])
```

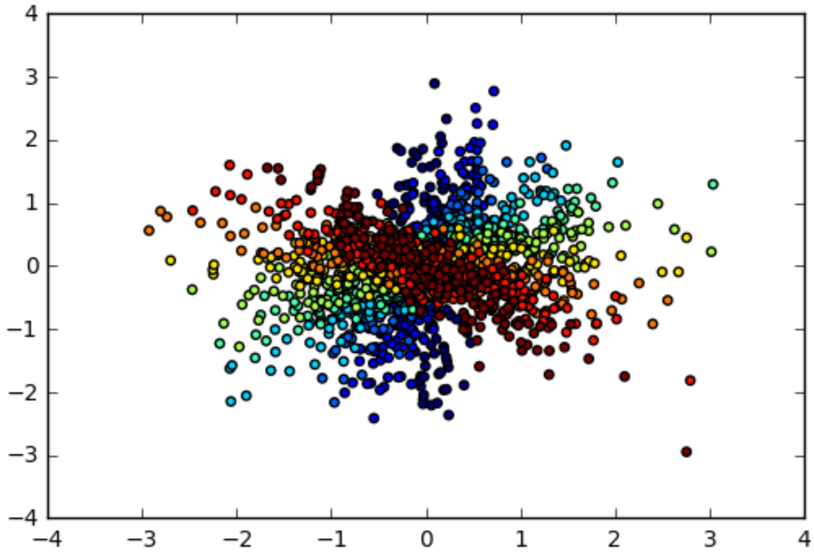
Out[9]: <matplotlib.collections.PathCollection at 0x7fc612834c88>



In [10]:
```
# Divided by time steps
label = np.empty((10,200))
for i in range(10):
    label[i] =np.ones(200)*i
label = label.reshape(1,2000)
```

In [11]:
```
# Make a scatter plot
plt.scatter(dtonln[:,0],dtonln[:,1],15,label[0])
```

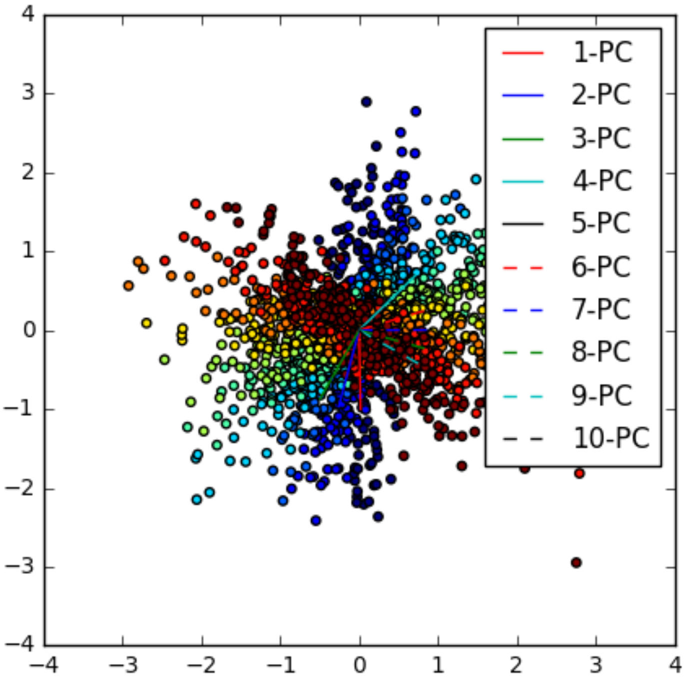
Out[11]: <matplotlib.collections.PathCollection at 0x7fc61281f080>



In [12]:
```
# Determine the principal components
PCs=np.empty((10,2,2))
X = np.empty((10,200,2))
for i in range(10):
    idx = np.where(label==i)[1]
    X[i] = dtonln[idx]
    opca = PCA(dtonln[idx])
    PCs[i] = opca.U
firstPCs = PCs[:,0,:]
```

In [13]:
```
# Plot the first PC (e.g. as an arrow or the endpoint of it) for each of
the 10 blocks
plt.figure(figsize=(5,5))
colors = ['r','b','g','c','k','r--','b--','g--','c--','k--',]
for i in range(len(firstPCs)):
    vector = firstPCs[i];
    plt.plot((0,vector[0]),(0,vector[1]), colors[i], label='%d-PC' % (i+
1) )
    plt.legend()
plt.scatter(dtonln[:,0],dtonln[:,1],15,label[0])
```

Out[13]: <matplotlib.collections.PathCollection at 0x7fc610ec75c0>



Oja's rule:

$$w_i(t+1) = w_i(t) + \epsilon y(t)[x_i(t) - y(t)w_i(t)]$$

where:

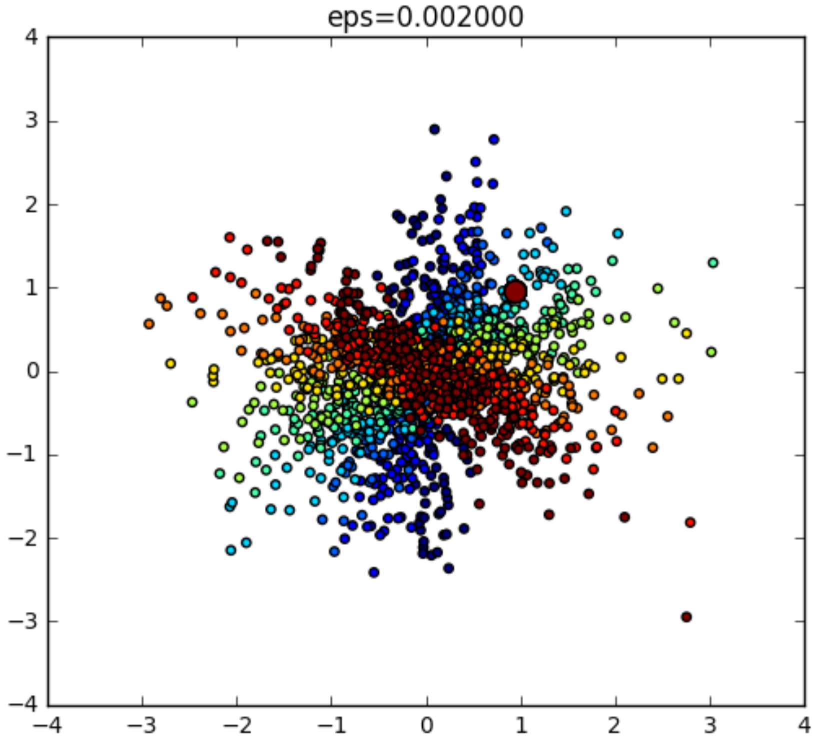
$$y = w^T x$$

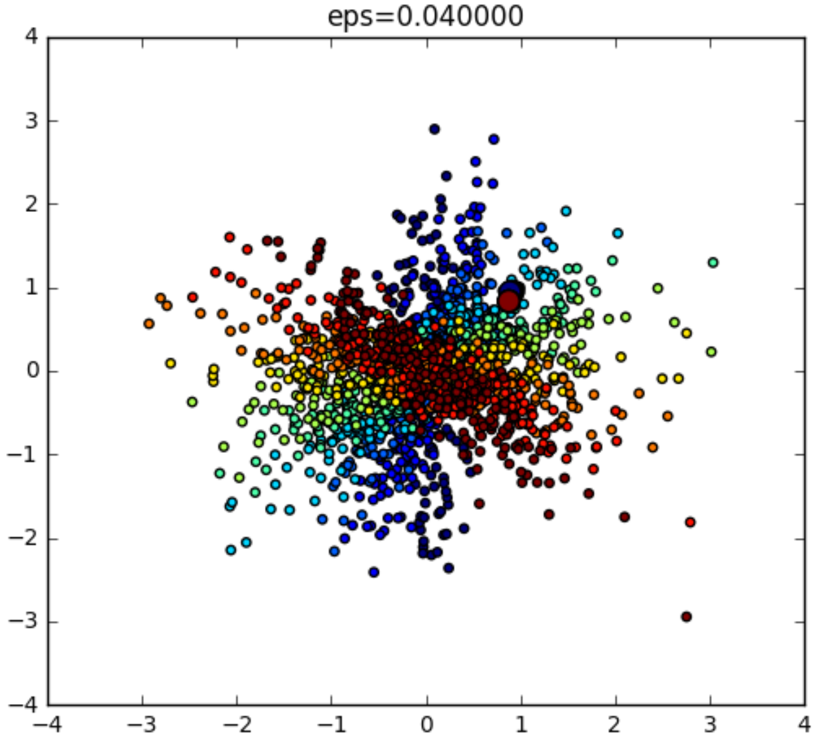
In [44]:
```
# Oja
ite = 10
W = np.empty((3,ite,2))
eps = [0.002, 0.04, 0.45]
```

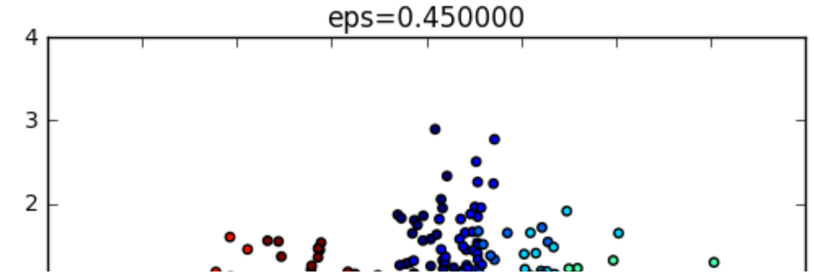
In [45]:
```
w = np.random.randn(1,2)
```

In [46]:
```
k = 0
for e in eps:
    for i in range(ite):
        x = X[i][np.random.choice(200,1)]
        y = np.dot(w.reshape(1,2),x.reshape(2,1))
        w= w + e*y*(x-y*w)
        W[k][i]= w
    k = k+1
```

In [47]:
```
plt.figure(figsize=(6,18))
wlabel = np.arange(0,10)*0
wlabel[9] =1
j=0
for e in eps:
    plt.subplot(3,1,j+1)
    plt.title("eps=%f" % e )
    plt.scatter(dtonln[:,0],dtonln[:,1],15,label[0])
    plt.scatter(W[j][:,0],W[j][:,1],90,wlabel)
    j=j+1
```


eps=0.002000
4
3
2
1
0
−1
−2
−3
−4
−4 −3 −2 −1 0 1 2 3 4


eps=0.040000
4
3
2
1
0
−1
−2
−3
−4
−4 −3 −2 −1 0 1 2 3 4


eps=0.450000
4
3
2

In upper plots big blue circle means in the convergence step and red one means final position of the weight. If we choose too small epsilon=0.002, the weight moves so small that it seems stoped. With epsilon= 0,04 the weight moves but too slow to be converged in this iteration step. If we more iterate it can be converged but also take time. With eps=0.45 the weight converged very well but if we choose higher eps, it might be not converged.

In [ ]:

```

```

In [ ]:

```

```