Principal Component Analysis (PCA)

This tutorial shows an example of PCA Classification.

First import required packages.

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

Write a function to plot spectral curve (reflectance v. wavelength):

In [2]:
```
def PlotSpectraAndMean(Spectra, Wv, fignum):
    ### Spectra is NBands x NSamps
    mu = np.mean(Spectra, axis=1) #calculate mean of spectra
    print(np.shape(mu)) #print shape to confirm
    plt.figure(fignum)
    plt.plot(Wv, Spectra, 'c')
    plt.plot(Wv, mu, 'r')
    plt.show()
    return mu
```

Load spectra:

In [3]:
```
filename   = '../data/PaulGader/OSBSTinyIm.mat'
ImDict     = io.loadmat(filename)
OSBSTinyIm = ImDict['OSBSTinyIm']
TinySize   = np.shape(OSBSTinyIm)
NRows      = TinySize[0]
NCols      = TinySize[1]
NBands     = TinySize[2]
print('{0:4d} {1:4d} {2:4d}'.format(NRows, NCols, NBands))
```

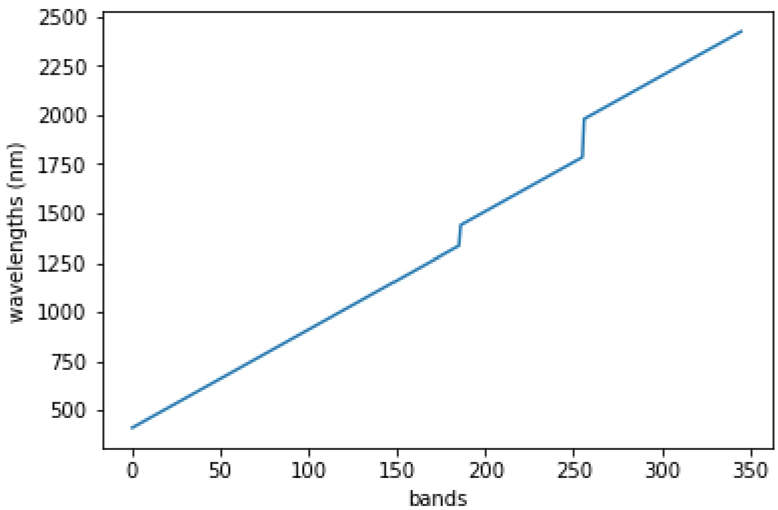
```
  62  194  346
```

Get wavelengths:

In [6]:
```
### LOAD WAVELENGTHS WITH WATER BANDS ###
### AND BAD BEGINNING AND ENDING BANDS REMOVED ###
Wv = io.loadmat('../data/PaulGader/NEONWvsNBB')
Wv = Wv['NEONWvsNBB']
print(np.shape(Wv))

plt.figure()
plt.plot(range(346), Wv)
plt.xlabel('bands'); plt.ylabel('wavelengths (nm)')
```

```
(346, 1)
```

Out[6]:
```
<matplotlib.text.Text at 0xbd47550>
```



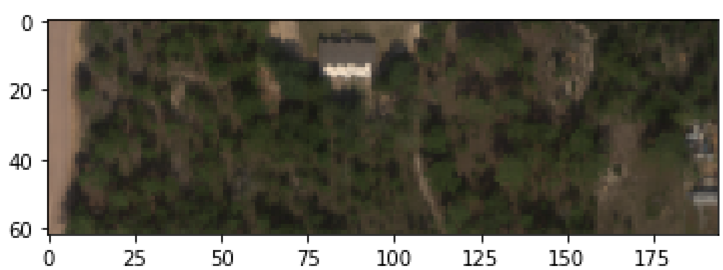
Let's load indices for Red, Green, and Blue for NEON hyperspectral data

In [7]:
```
### HAVE TO SUBTRACT AN OFFSET BECAUSE OF BAD BAND ###
### REMOVAL AND 0-BASED Python vs 1-Based MATLAB   ###
Offset     = 7

### LOAD & PRINT THE INDICES FOR THE COLORS   ###
### AND DIG THEM OUT OF MANY LAYERS OF ARRAYS ###
NEONColors = io.loadmat('../data/PaulGader/NEONColors.mat')
NEONRed    = NEONColors['NEONRed']
NEONGreen  = NEONColors['NEONGreen']
NEONBlue   = NEONColors['NEONBlue']
NEONNir    = NEONColors['NEONNir']
NEONRed    = NEONRed[0][0]-Offset
NEONGreen  = NEONGreen[0][0]-Offset
NEONBlue   = NEONBlue[0][0]-Offset
NEONNir    = NEONNir[0][0]-Offset
print('Indices:     {0:4d} {1:4d} {2:4d} {3:4d}'.format(NEONRed, NEONGreen, NE
ONBlue, NEONNir))

### CONVERT THE INDICES TO WAVELENGTHS ###
NEONRedWv    = Wv[NEONRed][0]
NEONGreenWv  = Wv[NEONGreen][0]
NEONBlueWv   = Wv[NEONBlue][0]
NEONNirWv    = Wv[NEONNir][0]
print('Wavelengths: {0:4d} {1:4d} {2:4d} {3:4d}'.format(NEONRedWv, NEONGreenWv
, NEONBlueWv, NEONNirWv))
```

```
Indices:       47   25    6  119
Wavelengths:  645  535  440 1005
```

Now we can make a color image and display it

In [8]:
```
RGBIm = OSBSTinyIm[:, :, [NEONRed, NEONGreen, NEONBlue]]
RGBIm = np.sqrt(RGBIm)
plt.figure()
plt.imshow(RGBIm)
plt.show()
```



Now let's turn the image into a sequence of vectors so we can use matrix algebra

In [9]:
```
### HAVE TO TAKE INTO ACCOUNT DIFFERENCES BETWEEN Python AND Matlab ###
### Python USES THE    C     PROGRAMMING LANGUAGE ORDERING ###
### MATLAB USERS THE FORTRAN PROGRAMMING LANGUAGE ORDERING ###
### Python WOULD RESHAPE BY REFERENCE AND MATLAB BY VALUE  ###
### THEREFORE, WE NEED TO COPY THE VALUES EXPLICITLY       ###
TinyVecs = OSBSTinyIm.reshape(NRows*NCols, NBands, order='F').copy()

### MATLAB TREATS THE ROWS AS DATA SAMPLES ###
### np  TREATS THE COLS AS DATA SAMPLES ###
TinyVecs = np.transpose(TinyVecs)
NSamps   = np.shape(TinyVecs)[1]
np.shape(TinyVecs)
```

Out[9]:
```
(346, 12028)
```

In [12]:
```
### EXERCISE
SpecIndices = range(1000, 2000, 100)
SomeSpectra = TinyVecs[:, range(1000, 2000, 100)]
mymu        = PlotSpectraAndMean(SomeSpectra, Wv, 3)
```

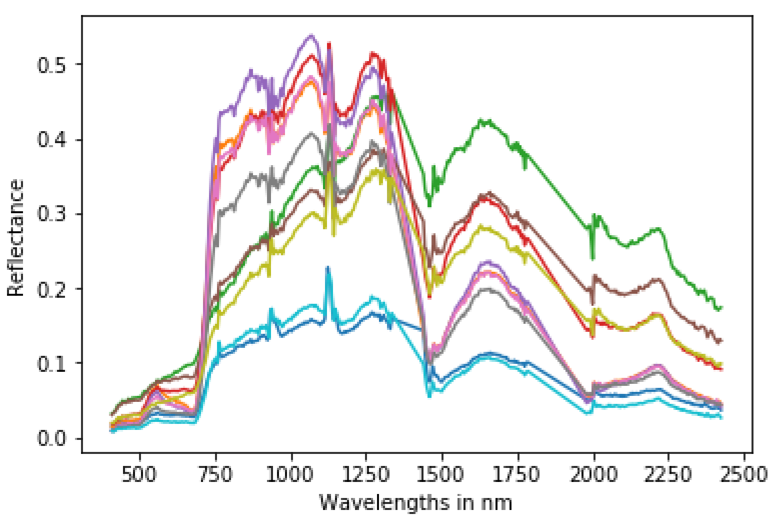
```
range(1000, 2000, 100)
```

In [13]:
```
np.shape(mymu)
```

Out[13]:
```
(346,)
```

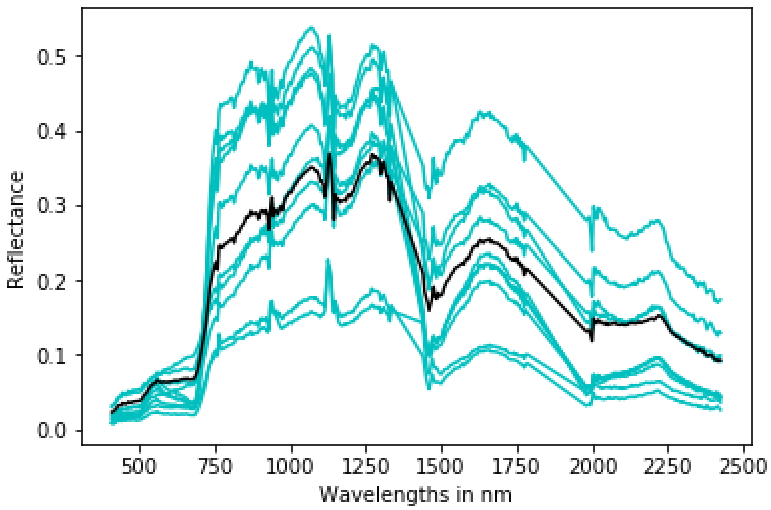
Let's plot some spectra

In [14]:
```
### Indices of Spectra to Try ###
### SpecIndices = range(0, 1000, 100) ###
SpecIndices = range(1000, 2000, 100)
SomeSpectra = TinyVecs[:, range(1000, 2000, 100)]
plt.figure(3)
plt.plot(Wv, SomeSpectra)
plt.xlabel('Wavelengths in nm')
plt.ylabel('Reflectance')
plt.show()
```



Compute the Average Spectrum and plot it

In [15]:
```
mu = np.mean(TinyVecs, axis=1)
plt.figure(4)
plt.plot(Wv, SomeSpectra, 'c') #plot sample of some spectra
plt.plot(Wv, mu, 'k') #plot mean spectra for the entire image in black
plt.xlabel('Wavelengths in nm')
plt.ylabel('Reflectance')
plt.show()
```

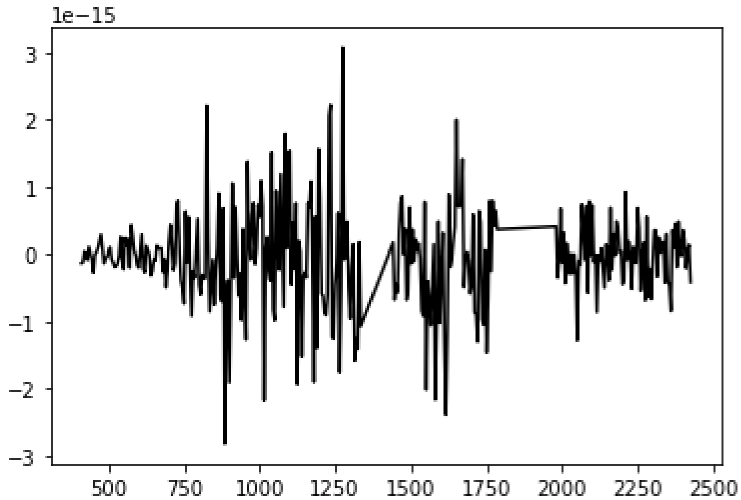


Now we want to subtract the mean from every sample

In [16]:
```
np.shape(mu)
```

Out[16]: (346,)

In [17]:
```
TinyVecsZ = np.zeros((NBands, NSamps))

#subtract mean spectra from each pixel's spectra
for n in range(NSamps):
    TinyVecsZ[range(NBands),n]= TinyVecs[(range(NBands), n)]-mu

muz = np.mean(TinyVecsZ, axis=1)
plt.figure(5)
plt.plot(Wv, muz, 'k')
#plt.ylim(-1,1)
plt.show()
```



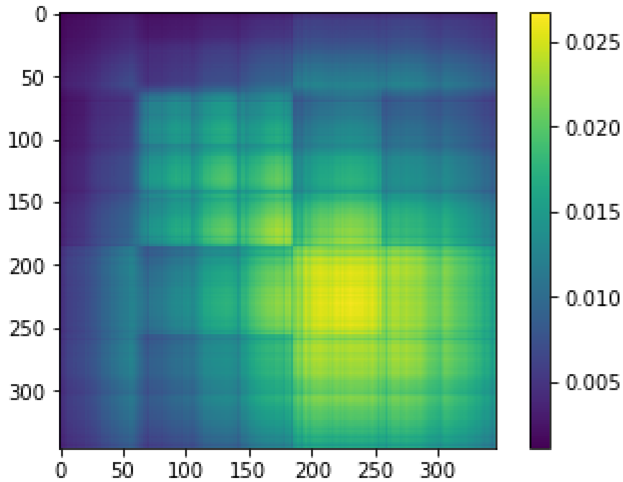
Let's make the covariance

In [20]:
```
C = np.cov(TinyVecs)
np.shape(C)
```

Out[20]: (346, 346)

We can look at some of the values but too many to look at them all. We can also view C as an image

In [22]:
```
#correlations between different bands; axes are band indices
plt.figure(6)
plt.imshow(C); plt.colorbar()
plt.show()

#this is absolute variance, not relative variance (normalized to mean)
#signal can be dominated by NIR since the reflectance values are much larger t
han in the visible portion
```



In [24]:
```
# PRINT OUT SOME "AMPLIFIED" COVARIANCE VALUES %%%
for cn in range(0, 50,5):
    w = int(Wv[cn])
    if cn==0:
        print("     ", end=" ")
    else:
        print('{0:5d}'.format(w), end=" ")
print('\n')

for rn in range(5, 50, 5):
    w = int(Wv[rn])
    print('{0:5d}'.format(w), end=" ")
    for cn in range(5,50,5):
        CovVal = int(100000*C[rn, cn])
        print('{0:5d}'.format(CovVal), end=" ")
    print('\n')

#print(round(100000*C[NEONBlue, NEONNir]))
#print(round(100000*C[NEONGreen, NEONNir]))
#print(round(100000*C[NEONRed, NEONNir]))
#print(round(100000*C[NEONGreen, NEONRed]))
```

```
      435   460   485   510   535   560   585   610   635

  435   166   181   193   201   215   238   261   275   293

  460   181   198   211   220   236   261   286   302   321

  485   193   211   226   235   252   280   306   324   344

  510   201   220   235   245   264   293   321   339   361

  535   215   236   252   264   289   322   350   369   391

  560   238   261   280   293   322   360   391   412   437

  585   261   286   306   321   350   391   428   453   481

  610   275   302   324   339   369   412   453   479   510

  635   293   321   344   361   391   437   481   510   544
```

Notice that there are no negative values. Why?

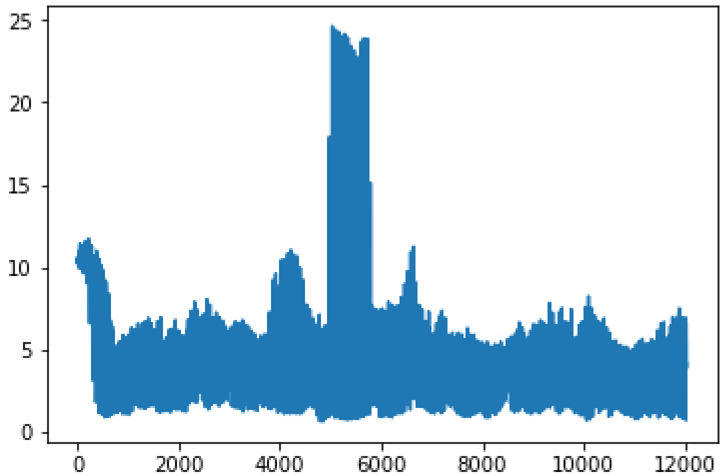
Weird covariance because they are all above their mean at the same time or below the mean at the same time -- positive correlation.

This is likely because of illumination

What if we normalize the vectors to have magnitude 1 (common strategy)

norm of a vector is the square root of the sum of the squares (pythagorean theorem)

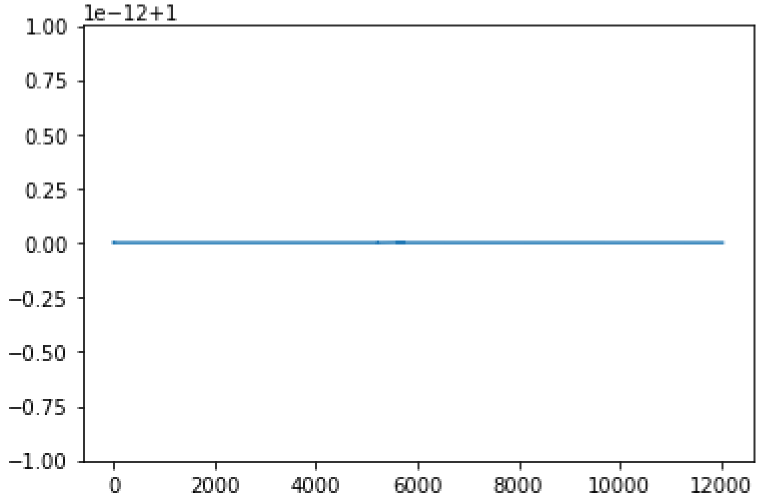
In [25]:
```
Norms = np.sqrt(np.sum(TinyVecs*TinyVecs, axis=0))
plt.figure(7)
plt.plot(Norms)
### Too many Norms.  How do we fix?
plt.show()
```



In [26]:
```
# High norms correspond to the roof on the house
print(np.shape(Norms))
print(np.shape(TinyVecs))
```

```
(12028,)
(346, 12028)
```

In [27]:
```
### Allocate Memory
TinyVecsNorm = np.zeros((NBands, NSamps))
for samp in range(NSamps):
    NormSamp = Norms[samp]
    for band in range(NBands):
        TinyVecsNorm[band, samp] = TinyVecs[band,samp]/NormSamp

#check that the norm of the norm is one
Norms1 = np.sqrt(np.sum(TinyVecsNorm*TinyVecsNorm, axis=0))
plt.figure(7)
plt.plot(Norms1)
plt.show()
BigNorm = np.max(Norms1)
LitNorm = np.min(Norms1)
print('{0:4f} {1:4f}'.format(BigNorm, LitNorm))
### Too many Norms.  How do we fix?
```

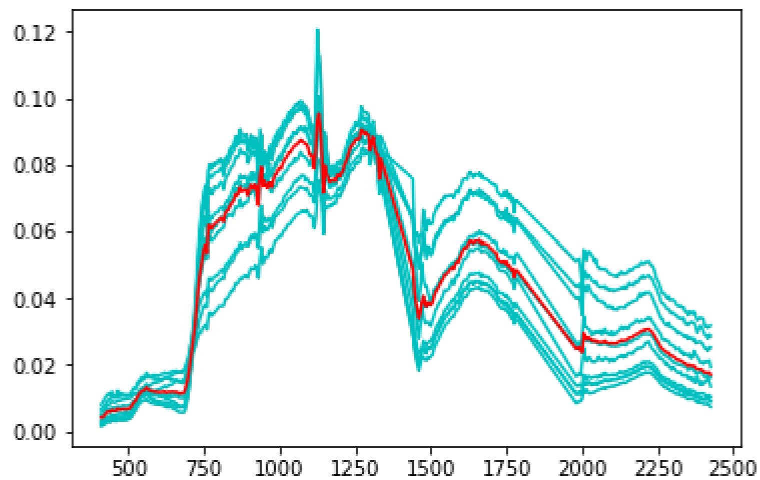



```
1.000000 1.000000
```

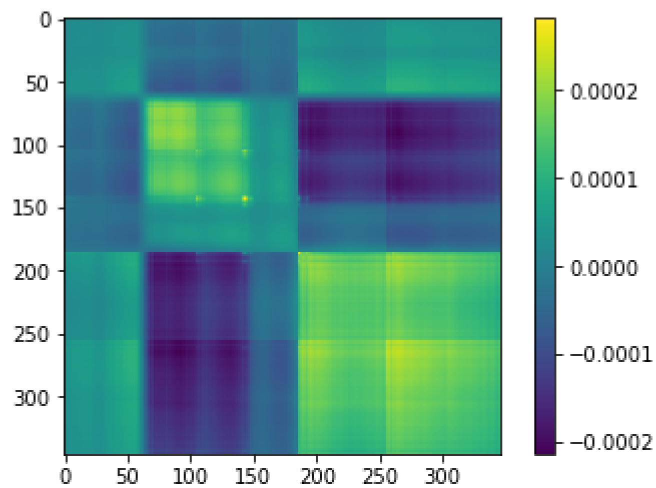
Exercise: Turn the script for plotting spectra and their mean above into a function

In [28]:
```
### Plot normalized spectra & mean in red -- this is much tighter than it used
 to be
SpecIndices      = range(1000, 2000, 100)
SomeSpectraNorm = TinyVecsNorm[:, range(1000, 2000, 100)]
MuNorm           = PlotSpectraAndMean(SomeSpectraNorm, Wv, 3)
```

```
(346,)
```



In [32]:
```
#plot covariance of normalized vectors
CNorm = np.cov(TinyVecsNorm)
plt.figure()
plt.imshow(CNorm); plt.colorbar()
plt.show()
print(np.amin(CNorm))
print(np.amax(CNorm))
```




```
-0.000213907629112
0.000281867544679
```

In [31]:
```
# PRINT OUT SOME "AMPLIFIED" COVARIANCE VALUES %%%
for cn in range(0, 50,5):
    w = int(Wv[cn])
    if cn==0:
        print("     ", end=" ")
    else:
        print('{0:5d}'.format(w), end=" ")
print('\n')


for rn in range(5, 50, 5):
    w = int(Wv[rn])
    print('{0:5d}'.format(w), end=" ")
    for cn in range(5,50,5):
        CovVal = int(10000000*CNorm[rn, cn])
        print('{0:5d}'.format(CovVal), end=" ")
    print('\n')
```

	435	460	485	510	535	560	585	610	635
435	253	259	267	263	245	258	298	317	336
460	259	269	278	275	257	271	315	335	356
485	267	278	289	286	267	282	329	351	373
510	263	275	286	284	267	283	331	353	375
535	245	257	267	267	263	281	318	334	350
560	258	271	282	283	281	303	341	358	374
585	298	315	329	331	318	341	397	423	449
610	317	335	351	353	334	358	423	455	486
635	336	356	373	375	350	374	449	486	523

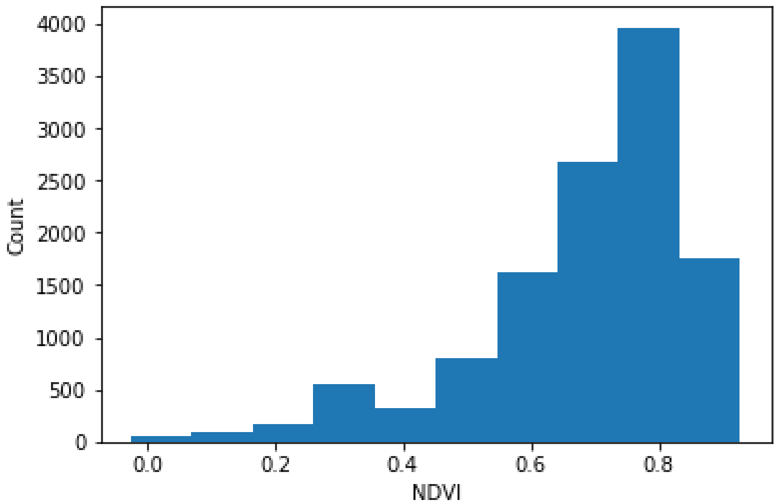
In [33]:
```
#calculate covariance of different indices by selecting bands of interest
print(np.shape(TinyVecs))
print(NEONNir)
print(NEONRed)
NIRVals  = TinyVecs[NEONNir, range(NSamps)]
RedVals  = TinyVecs[NEONRed, range(NSamps)]
NDVIVals = (NIRVals-RedVals)/(NIRVals+RedVals)
np.shape(NDVIVals)
NDVIIm   = np.reshape(NDVIVals,(NRows, NCols),order='F') #NDVI covariance
#reshape to convert from mat indices to Python; F = fortran
```

```
(346, 12028)
119
47
```

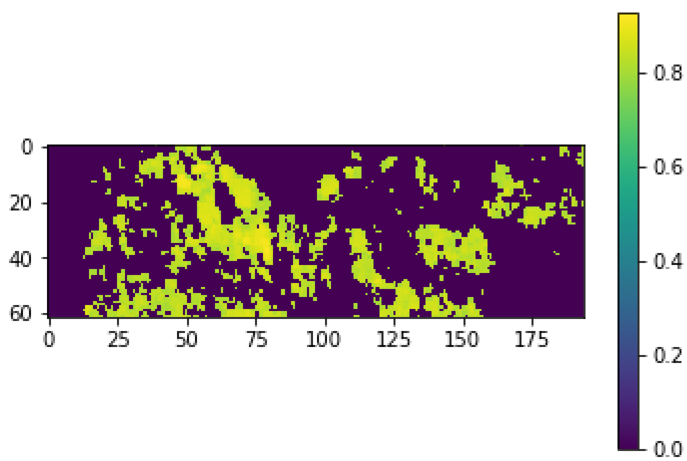
In [34]:
```
print(np.shape(NDVIIm))
```

```
(62, 194)
```

In [37]:
```
plt.figure()
plt.hist(NDVIVals); plt.xlabel('NDVI'); plt.ylabel('Count')
plt.show()
```



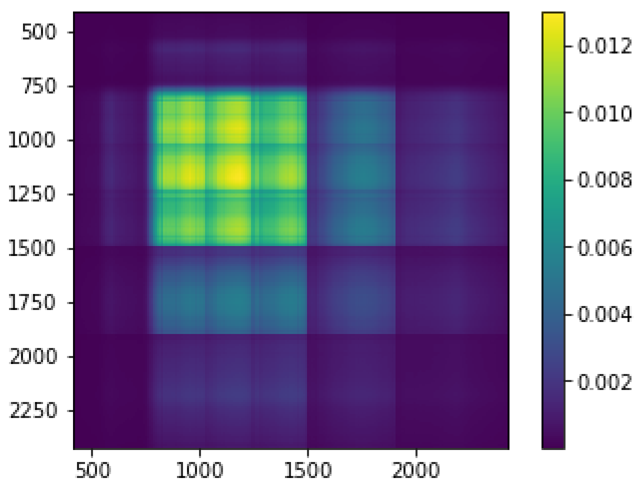
In [38]:
```
#Look only at NDVI greater than 0.8
HiNDVI = NDVIIm*(NDVIIm>0.8) #another way to mask -- multiply by boolean matri
x
plt.figure()
plt.imshow(HiNDVI); #plt.colorbar()
plt.show()
```



In [39]:
```
# plt.figure()
# plt.plot(nonzero(NDVIVals>0.8))
# plt.show()
VegIndices = np.nonzero(NDVIVals>0.8)
# print(VegIndices[0])
print(np.shape(VegIndices))
# print(np.shape(TinyVecs))
VegSpectra = TinyVecs[:, VegIndices[0]]
print(np.shape(VegSpectra))
```

```
(1, 3136)
(346, 3136)
```

In [40]:
```
#Plot covariance of vegetation (defined as NDVI > 0.8)
CVeg = np.cov(VegSpectra)
plt.figure(9)
plt.imshow?
plt.imshow(CVeg,extent=(np.amin(Wv), np.amax(Wv),np.amax(Wv), np.amin(Wv)))
plt.colorbar()
plt.show()
```



In [ ]:
```
#positive covariance in NIR bands (750-1500nm?) --> vegetation
```

OK, Let's do PCA

Recall that TinyVecsZ is the mean-subtracted version of the original spectra

In [41]:
```
C   = np.cov(TinyVecs)
D,V = linalg.eig(C) #calculates eigenvalues
D   = D.real #Python gives you eigenvalues as complex numbers ;
             #covariance will never have complex numbers, so extract only the
 real portion
print(np.shape(D)) #
print(np.shape(V))
print(TinyVecs.shape)
print(V[0,0])
```

```
(346,)
(346, 346)
(346, 12028)
-0.0124822914573
```

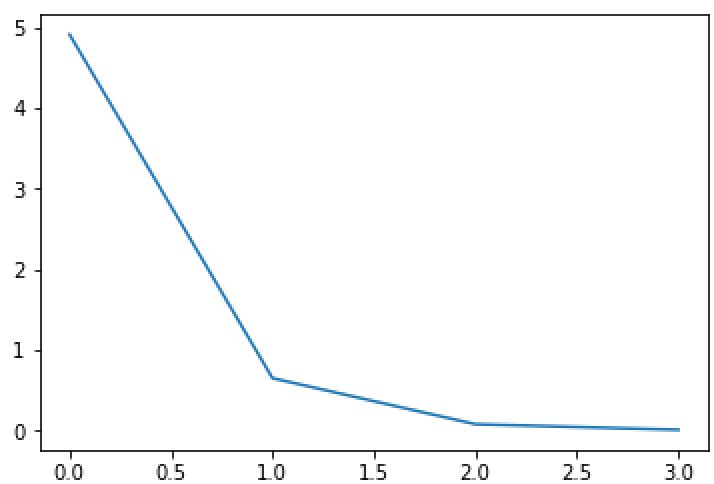
$$S = V^T D V$$

In [60]:
```
# plt.figure(10)
print(D.shape)
DiagD = np.diag(D)
print('Diagonal Shape:',DiagD.shape)
```

```
(346,)
Diagonal Shape: (346, 346)
```

In [53]:
```
print(D.shape) #Diagonal matrix is an array with 346 elements - this differs f
rom Matlab
plt.plot(D[0:4]) # plot only first 5 eigenvalues
#Exercise
#plt.plot(D[range(10)])
#plt.plot(D[range(10, 30, 10)])
plt.show()
```

```
(346,)
```



There are 346 eigenvalues, but only the first few contain information. By the second coordinate, the eigenvalue drops below 1. According to PCA, this data does not have many dimensions (~3).

In [57]:
```
TinyVecsPCA = np.dot(V.T, TinyVecsZ) #V transpose times x - mean
PCACovar    = np.cov(TinyVecsPCA)
D,V         = linalg.eig(C)
D           = D.real
print(D.shape)
print(PCACovar.shape)
for r in range(10):
    print('{0:5f} {1:5f}'.format(D[r], PCACovar[r,r]))
print()
for r in range(10):
    for c in range(10):
        NextVal = int(10000*PCACovar[r,c])
        print('{0:5d}'.format(NextVal), end=" ")
    print('\n')
# #Delta       = np.sum(np.sum((PCACovar-D), axis=0), axis=0)
# print(Delta)
# plt.figure(11)
# plt.plot(np.diag(PCACovar))
# plt.show()
```

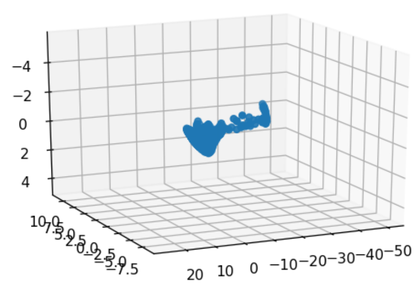
```
(346,)
(346, 346)
4.911250 4.911250
0.653442 0.653442
0.083168 0.083168
0.013260 0.013260
0.004038 0.004038
0.003201 0.003201
0.001390 0.001390
0.000931 0.000931
0.000705 0.000705
0.000561 0.000561

49112     0     0     0     0     0     0     0     0     0

    0  6534     0     0     0     0     0     0     0     0

    0     0   831     0     0     0     0     0     0     0

    0     0     0   132     0     0     0     0     0     0

    0     0     0     0    40     0     0     0     0     0

    0     0     0     0     0    32     0     0     0     0

    0     0     0     0     0     0    13     0     0     0

    0     0     0     0     0     0     0     9     0     0

    0     0     0     0     0     0     0     0     7     0

    0     0     0     0     0     0     0     0     0     5
```

Notice that the values on the diagonal are the variances of each coordinate in the PCA transformed data. They drop off rapidly which is why one can reduce dimensionality by discarding components that have low variance. Also, notice that the diagonal matrix D produce by diagonalizing the covariance of x is the covariance of y = PCA(x).

If the data are Gaussian, then the coordinates of y are uncorrelated and independent. If not, then only uncorrelated.

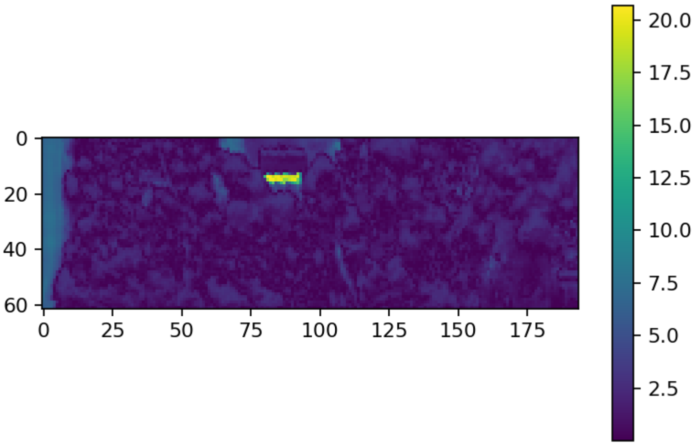
Let's pull out the first 3 dimensions and plot them'

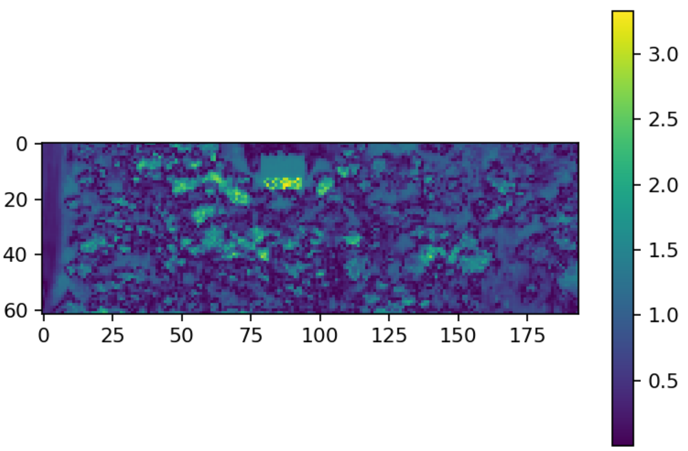
In [56]:
```
%matplotlib notebook #interactive mode so you can rotate
fig = plt.figure(13)
ax = fig.add_subplot(111, projection='3d') #make 3D plot
#plot only 0th,1st, & 2nd elements
ax.scatter(TinyVecsPCA[0,range(NSamps)],TinyVecsPCA[1,range(NSamps)],TinyVecsP
CA[2,range(NSamps)], marker='o')
plt.show()
```

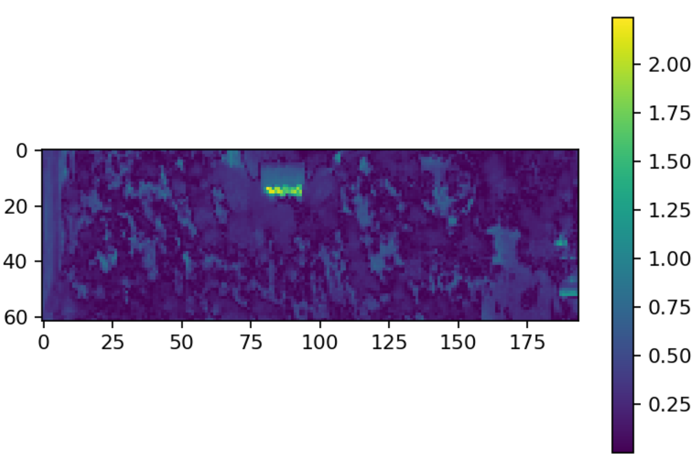


We can also display principal components as images

In [58]:
```
for coord in range(3):
    P1 = TinyVecsPCA[coord, :]
    PCAIm      = np.reshape(P1, (NRows, NCols), order='F')
    plt.figure(14+coord)
    plt.imshow(np.abs(PCAIm))
    plt.colorbar()
    plt.show()
```


0
20
40
60
0 25 50 75 100 125 150 175
20.0
17.5
15.0
12.5
10.0
7.5
5.0
2.5


0
20
40
60
0 25 50 75 100 125 150 175
3.0
2.5
2.0
1.5
1.0
0.5


0
20
40
60
0 25 50 75 100 125 150 175
2.00
1.75
1.50
1.25
1.00
0.75
0.50
0.25

EXERCISE:

Write a function that calculates PCA of spectra and plots the first 3 components.