

Sheet 1: Principal Components Analysis

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1 Sheet 1: Principal Component Analysis

In [1]: `%matplotlib inline`

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

In [2]: `from sklearn import datasets`
`from sklearn.decomposition import PCA`
`from sklearn.metrics.pairwise import cosine_similarity`
`from sklearn.metrics.pairwise import euclidean_distances`
`from mpl_toolkits.mplot3d import Axes3D`

In [3]: `# set printing of matrices to 3 decimal places for clarity`
`# this doesn't change the values stored inside the matrices`
`np.set_printoptions(formatter={'float': lambda x: "{0:0.3f}".format(x)})`

1.1 Question 2

In [4]: `data_matrix = np.array([[10, 60, 10, 90],`
 `[20, 50, 40, 70],`
 `[30, 50, 30, 40],`
 `[20, 50, 20, 60],`
 `[10, 60, 30, 10]])`

In [5]: `norm = linalg.norm(data_matrix, axis=1)`
`print norm`

[109.087 96.954 76.811 83.066 68.557]

In [6]: `cosine_sim = cosine_similarity(data_matrix)`
`print cosine_sim`

```
[[1.000 0.936 0.859 0.971 0.655]
 [0.936 1.000 0.953 0.981 0.767]
 [0.859 0.953 1.000 0.956 0.874]
 [0.971 0.981 0.956 1.000 0.773]
 [0.655 0.767 0.874 0.773 1.000]]
```

In [7]: `euclidean_distances(data_matrix)`

Out[7]: `array([[0.000, 38.730, 58.310, 34.641, 82.462],`
 `[38.730, 0.000, 33.166, 22.361, 62.450],`
 `[58.310, 33.166, 0.000, 24.495, 37.417],`
 `[34.641, 22.361, 24.495, 0.000, 52.915],`
 `[82.462, 62.450, 37.417, 52.915, 0.000]])`

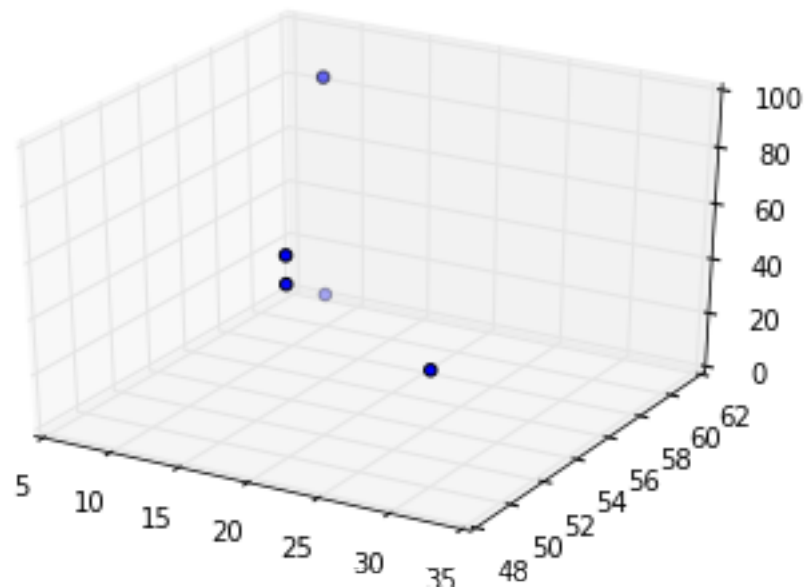
1.2 Question 3

```
In [8]: data_matrix = np.array([[10, 60, 90],
                                [20, 50, 70],
                                [30, 50, 40],
                                [20, 50, 60],
                                [10, 60, 10]])
```

1.2.1 Scatter Plot

```
In [9]: fig = plt.figure()
        ax = fig.add_subplot(111, projection='3d')
        ax.scatter(data_matrix[:,0], data_matrix[:,1], data_matrix[:,2], marker='o')
```

```
Out[9]: <mpl_toolkits.mplot3d.art3d.Path3DCollection at 0xa3231d0>
```



1.2.2 Mean Vector and data centering

```
In [10]: mean = np.mean(data_matrix, axis=0)
         print mean
```

```
[18.000 54.000 54.000]
```

```
In [11]: centered_data = np.empty([5,3])
         for i in range(0,3):
             centered_data[:,i] = data_matrix[:,i] - mean[i]
         print data_matrix
```

```
[[10 60 90]
 [20 50 70]
 [30 50 40]
 [20 50 60]
 [10 60 10]]
```

1.2.3 covariance matrix

```
In [12]: # rowvar=False means that columns are variables (and rows are instances)
         covariance = np.cov(centered_data, rowvar=False)
         print covariance

[[70.000 -40.000 -15.000]
 [-40.000 30.000 -20.000]
 [-15.000 -20.000 930.000]]
```

1.2.4 eigen values and eigen vectors

```
In [13]: eigenvalues, eigenvectors = linalg.eigh(covariance)

In [14]: for i in range(0,3):
         print "{}, {}".format(eigenvalues[i], eigenvectors[i])

4.60865706553, [0.526 0.850 -0.016]
94.7153745646, [0.850 -0.526 -0.021]
930.67596837, [0.027 0.003 1.000]

In [15]: # verify that (eigenvec * (eigenvals * eigenvec.transpose)) = Covariance
         np.matmul(eigenvectors, np.matmul(np.diag(eigenvalues), eigenvectors.transpose()))
         print eigenvectors.transpose()

[[0.526 0.850 0.027]
 [0.850 -0.526 0.003]
 [-0.016 -0.021 1.000]]
```

1.2.5 variance and projection to lower dimensions

The variance by the eigenvector of the largest eigenvalue corresponds to $\frac{930.7}{930.7+94.7+4.6} = 0.903$ of the total variance which is good enough to represent the original dataset.

```
In [16]: # compute the projection matrix
         # (column vectors corresponding to the eigenvectors of the highest eigenvalues)
         proj_matrix = np.column_stack((eigenvectors[1], eigenvectors[2]))
```

The projection matrix P corresponding to the top two eigen vectors of the matrix U is

$$P = \begin{bmatrix} 0.850 & 0.027 \\ -0.526 & 0.003 \\ -0.021 & 1.000 \end{bmatrix}$$

The projected data is just transforming the original dataset to the new subspace by applying the projection matrix on the dataset.

```
In [17]: # computing the projected data
         proj_data = np.matmul(data_matrix, proj_matrix)
```

$$ProjData = \begin{bmatrix} -25.014 & 90.396 \\ -10.821 & 70.646 \\ -1.677 & 40.926 \\ -10.606 & 60.649 \\ -23.296 & 10.425 \end{bmatrix}$$

1.2.6 Plotting the new projected data

```
In [18]: fig = plt.figure()
         ax = fig.add_subplot(111)
         ax.scatter(proj_data[:,0], proj_data[:,1], marker='o')
```

```
Out[18]: <matplotlib.collections.PathCollection at 0xa5a3710>
```

