

PCA

November 6, 2018

1 Principal Component Analysis

The goal of this question is to build a conceptual understanding of dimensionality reduction using PCA and implement it on a toy dataset. Only have to use numpy and matplotlib for this question.

```
In [1]: import numpy as np
import matplotlib
import matplotlib.pyplot as plt

In [2]: # (a) Load data (features)
def load_data():
    data = np.load('q3-data/features.npy')
    labels = np.load('q3-data/labels.npy')

    mean = np.mean(data, axis=0)
    mean = np.array(mean, ndmin=2)
    data = np.subtract(data, mean)

    mean2 = np.mean(data, axis=0)
    stdvn = np.std(data, axis=0)
    stdvn = np.array(stdvn, ndmin=2)
    print(stdvn.shape, stdvn)

    data = data/stdvn
    print(np.std(data, axis=0))

    return data, labels

datafile, labels = load_data()

(1, 8) [[0.82530129 0.43214658 1.75852918 0.76061262 1.29681839 1.18787014
1.93816328 1.22044697]]
[1. 1. 1. 1. 1. 1. 1. 1.]

In [3]: labels = labels.astype(int)
print(labels.shape, labels.dtype)
```

(150,) int64

```
In [4]: # (b) Perform eigen decomposition and return eigen pairs in descending order of eigen
def eigendecomp(X):

    # covariance matrix:

    # cov_mat = (X - np.mean(X, axis=0)).T.dot((X - np.mean(X, axis=0))) / (X.shape[0])
    cov_mat = np.cov(X.T)
    print(cov_mat.shape, type(cov_mat), cov_mat)

    # Eigendecomposition on covariance matrix, cov_mat:

    eig_vals, eig_vecs = np.linalg.eig(cov_mat)

    print('Eigenvectors \n%s' %eig_vecs)
    print('\nEigenvalues \n%s' %eig_vals)

    # sorting eigenvalues in decreasing order and corresponding eigenvectors:

    idx = eig_vals.argsort()[::-1]
    sorted_eig_vals = eig_vals[idx]
    sorted_eig_vecs = eig_vecs[:,idx]

    return (sorted_eig_vals, sorted_eig_vecs)

sorted_evalues, sorted_evecs = eigendecomp(datafile)

print(sorted_evalues)
print(sorted_evecs)

(8, 8) <class 'numpy.ndarray'> [[ 1.00671141 -0.11010327  0.87760486  0.82344326  0.61123001 -0.
 0.776564  0.48190166]
 [-0.11010327  1.00671141 -0.42333835 -0.358937  0.07459068  0.52416995
 -0.28731011 -0.06998508]
 [ 0.87760486 -0.42333835  1.00671141  0.96921855  0.4704054 -0.25019762
 0.85445501  0.51042104]
 [ 0.82344326 -0.358937  0.96921855  1.00671141  0.44634059 -0.21541033
 0.8273983  0.54484244]
 [ 0.61123001  0.07459068  0.4704054  0.44634059  1.00671141  0.70151359
 0.84012249  0.93454714]
 [-0.07220205  0.52416995 -0.25019762 -0.21541033  0.70151359  1.00671141
 0.2731165  0.659988 ]
 [ 0.776564 -0.28731011  0.85445501  0.8273983  0.84012249  0.2731165
 1.00671141  0.88321462]
```

```

[ 0.48190166 -0.06998508  0.51042104  0.54484244  0.93454714  0.659988
 0.88321462  1.00671141]]
Eigenvectors
[[-0.39124937  0.13884872 -0.46160937  0.58034539  0.24934936  0.21747713
 -0.38816186  0.1118572 ]
 [ 0.11687696 -0.4391715  -0.78711289 -0.2905579  -0.12725786  0.02806659
 0.21689908  0.15922802]
 [-0.40655289  0.29080021 -0.13961871 -0.12636707 -0.54994554 -0.61159334
 -0.17223991  0.13591601]
 [-0.39944906  0.26454833 -0.16206048 -0.54404218  0.49904279  0.01470075
 0.05047577 -0.44213114]
 [-0.3778555  -0.35426671  0.07790627  0.42060984  0.12822569 -0.34172774
 0.6099293  -0.17576426]
 [-0.09816172 -0.64299795  0.11941452 -0.04972667 -0.0795516  -0.07714852
 -0.59620498 -0.43768069]
 [-0.45509399 -0.03231459  0.12200908 -0.08034689 -0.51935676  0.67406772
 0.18983425 -0.14979985]
 [-0.38587285 -0.30545597  0.29393481 -0.28457653  0.27864817 -0.02358821
 -0.08099129  0.70942501]]

```

Eigenvalues

```

[ 4.74298961e+00  2.29585309e+00  7.76910512e-01  2.04172901e-01
 3.37651661e-02 -8.56766184e-16 -1.16776912e-16  5.26888208e-16]
[ 4.74298961e+00  2.29585309e+00  7.76910512e-01  2.04172901e-01
 3.37651661e-02  5.26888208e-16 -1.16776912e-16 -8.56766184e-16]
[[-0.39124937  0.13884872 -0.46160937  0.58034539  0.24934936  0.1118572
 -0.38816186  0.21747713]
 [ 0.11687696 -0.4391715  -0.78711289 -0.2905579  -0.12725786  0.15922802
 0.21689908  0.02806659]
 [-0.40655289  0.29080021 -0.13961871 -0.12636707 -0.54994554  0.13591601
 -0.17223991 -0.61159334]
 [-0.39944906  0.26454833 -0.16206048 -0.54404218  0.49904279 -0.44213114
 0.05047577  0.01470075]
 [-0.3778555  -0.35426671  0.07790627  0.42060984  0.12822569 -0.17576426
 0.6099293  -0.34172774]
 [-0.09816172 -0.64299795  0.11941452 -0.04972667 -0.0795516  -0.43768069
 -0.59620498 -0.07714852]
 [-0.45509399 -0.03231459  0.12200908 -0.08034689 -0.51935676 -0.14979985
 0.18983425  0.67406772]
 [-0.38587285 -0.30545597  0.29393481 -0.28457653  0.27864817  0.70942501
 -0.08099129 -0.02358821]]

```

After sorting the eigenpairs, the next question is “how many principal components are we going to choose for our new feature subspace?” A useful measure is the so-called “explained variance,” which can be calculated from the eigenvalues.

- The explained variance tells us how much information (variance) can be attributed to each of the principal components.

```

In [5]: # (c) Evaluate using variance_explained as the metric
def eval(sorted_evalues, sorted_evectors):

    tot = sum(sorted_evalues)
    var_exp = [(i / tot)*100 for i in sorted(sorted_evalues, reverse=True)]
    cum_var_exp = np.cumsum(var_exp)

    var_exp = np.array(var_exp, ndmin=2)
    cum_var_exp = np.array(cum_var_exp, ndmin=2)

    sorted_evalues = np.array(sorted_evalues, ndmin=2)
    np.set_printoptions(suppress=True)
    eval_var = np.concatenate((np.array(sorted_evalues.T, ndmin=2), np.array(var_exp.T, ndmin=2)), axis=1)
    cum_eval_var = np.concatenate((np.array(eval_var, ndmin=2), np.array(cum_var_exp.T, ndmin=2)), axis=1)
    print("[EigenValue      Variance      Cumulative_Variance]")
    print(cum_eval_var)

    return var_exp, cum_var_exp

var, cum_var = eval(sorted_evalues, sorted_evectors)

[EigenValue      Variance      Cumulative_Variance]
[[ 4.74298961  58.89212098  58.89212098]
 [ 2.29585309  28.50684249  87.39896347]
 [ 0.77691051   9.64663886  97.04560233]
 [ 0.2041729    2.53514686  99.58074919]
 [ 0.03376517   0.41925081 100.         ]
 [ 0.          0.         100.         ]
 [-0.         -0.         100.         ]
 [-0.         -0.         100.         ]]

```

I would pick $k = 3$ for this problem, as it covers 97% of the variance. Remaining of the values are quite insignificant and thus can be left out without much loss of information.

In []:

The construction of the projection matrix that will be used to transform the Iris data onto the new feature subspace. Although, the name “projection matrix” has a nice ring to it, it is basically just a matrix of our concatenated top k eigenvectors.

- Here, we are reducing the 8-dimensional feature space to a 2-dimensional feature subspace, by choosing the “top 2” eigenvectors with the highest eigenvalues to construct our 2-dimensional eigenvector matrix.

```

In [6]: matrix_w = np.hstack((sorted_evectors[:, 0].reshape(8,1), sorted_evectors[:, 1].reshape(8,1)))
print('Matrix W:\n', matrix_w)

```

```
Y = datafile.dot(matrix_w)
```

Matrix W:

```
[[-0.39124937  0.13884872]
 [ 0.11687696 -0.4391715 ]
 [-0.40655289  0.29080021]
 [-0.39944906  0.26454833]
 [-0.3778555   -0.35426671]
 [-0.09816172 -0.64299795]
 [-0.45509399 -0.03231459]
 [-0.38587285 -0.30545597]]
```

In this last step we will use the 8CE2-dimensional projection matrix W to transform our samples onto the new subspace via the equation $Y=XCEW$, where Y is a 150CE2 matrix of our transformed samples.

In [7]: # (d) Visualize after projecting to 2-D space

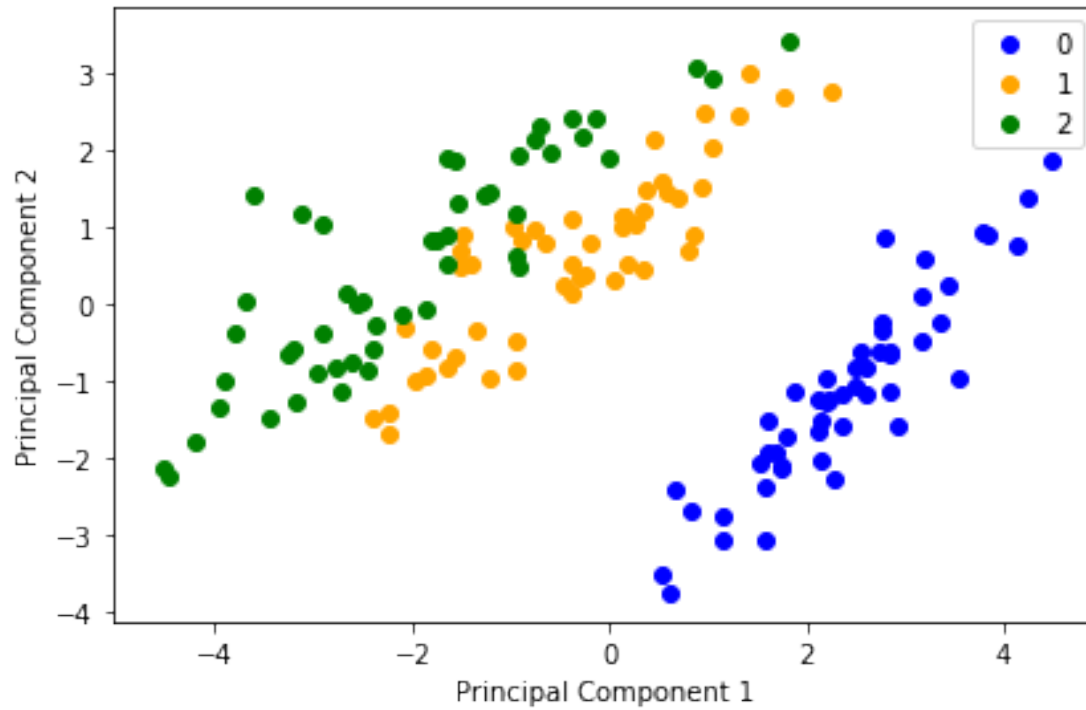
```
def viz(Y, y, x):

    plt.figure(figsize=(6, 4))

    for lab, col in zip((0, 1, 2), ('blue', 'orange', 'green')):
        plt.scatter(Y[y==lab, 0],
                    Y[y==lab, 1],
                    label=lab,
                    c=col)

    plt.xlabel('Principal Component 1')
    plt.ylabel('Principal Component 2')
    plt.legend(loc='upper right')
    plt.tight_layout()
    plt.show()

viz(Y, labels, datafile)
```



```
In [8]: def main():

        eval(sorted_evalues, sorted_evecs)
        viz(Y, labels, datafile)

    if __name__ == "__main__":
        main()
```

[EigenValue	Variance	Cumulative_Variance]
[[4.74298961	58.89212098	58.89212098]
[2.29585309	28.50684249	87.39896347]
[0.77691051	9.64663886	97.04560233]
[0.2041729	2.53514686	99.58074919]
[0.03376517	0.41925081	100.]
[0.	0.	100.]
[-0.	-0.	100.]
[-0.	-0.	100.]]