PCA_example

February 12, 2018

This notebook presents an example of using Principle Component Analysis.

Date Created: 12 Feb 2018 Last Modified: 12 Feb 2018 Humans Responsible: The Prickly Pythons Kernel used: Python 2 Most material below is from http://sebastianraschka.com/Articles/2014_pca_step_by_step.html Very nice slide presentation including Principle Component Regression: http://www.stats.uwo.ca/faculty/braun/ss3850/notes/sas10.pdf

```
In [1]: from IPython.display import Image
        Image(filename='illustration.png',width=700)
```

Out[1]:

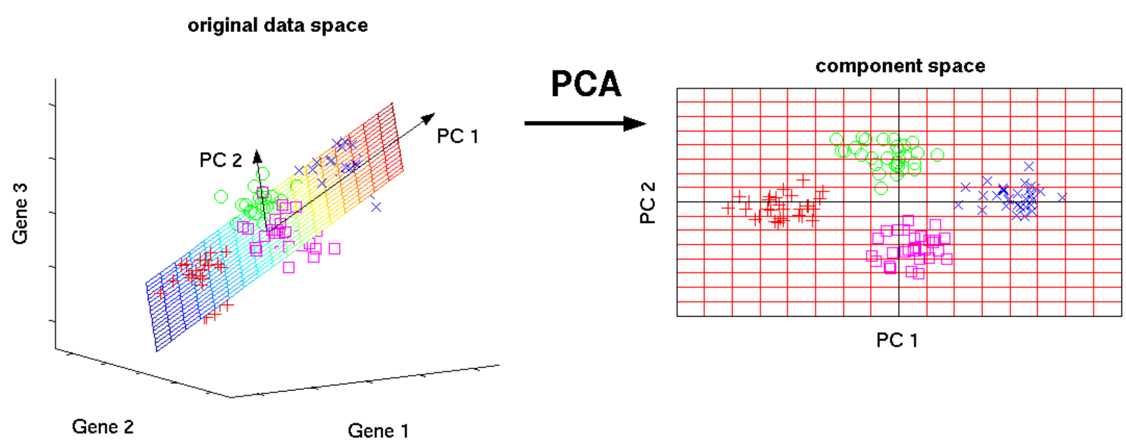


Illustration (and nice explanation) here: https://www.analyticsvidhya.com/blog/2016/03/practical-guide-principal-component-analysis-python/

0.1 Setup

```
In [2]: import numpy as np
        from matplotlib import pyplot as plt
        from mpl_toolkits.mplot3d import Axes3D
        from mpl_toolkits.mplot3d import proj3d
        np.random.seed(2342347) # random seed for consistency
```

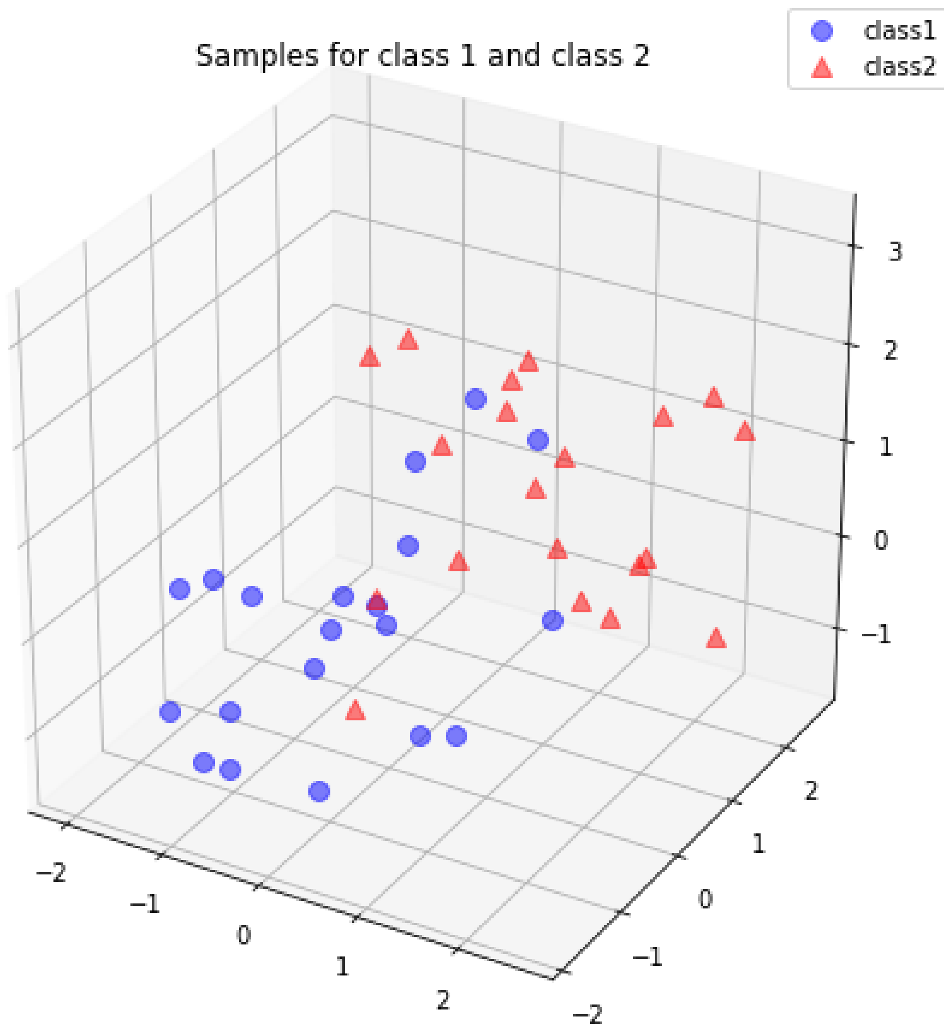
1 Reducing a 3D dataset to a 2D dataset by dropping 1 dimension.

Start by creating some vectors of data:

```
In [3]: mu_vec1 = np.array([0,0,0])
        cov_mat1 = np.array([[1,0,0],[0,1,0],[0,0,1]])
        class1_sample = np.random.multivariate_normal(mu_vec1, cov_mat1, 20).T
        assert class1_sample.shape == (3,20), "The matrix has not the dimensions 3x20"

        mu_vec2 = np.array([1,1,1])
        cov_mat2 = np.array([[1,0,0],[0,1,0],[0,0,1]])
        class2_sample = np.random.multivariate_normal(mu_vec2, cov_mat2, 20).T
        assert class2_sample.shape == (3,20), "The matrix has not the dimensions 3x20"
```

```
In [4]: %pylab inline

        fig = plt.figure(figsize=(8,8))
        ax = fig.add_subplot(111, projection='3d')
        plt.rcParams['legend.fontsize'] = 10
        ax.plot(class1_sample[0,:], class1_sample[1,:], class1_sample[2,:], 'o', markersize=8, c
        ax.plot(class2_sample[0,:], class2_sample[1,:], class2_sample[2,:], '^', markersize=8, a

        plt.title('Samples for class 1 and class 2')
        ax.legend(loc='upper right')

        plt.show()
```

```
Populating the interactive namespace from numpy and matplotlib
```



Because we don't need class labels for the PCA analysis, let us merge the samples for our 2 classes into one 3Œ403Œ40-dimensional array.

```
In [5]: all_samples = np.concatenate((class1_sample, class2_sample), axis=1)
        assert all_samples.shape == (3,40), "The matrix has not the dimensions 3x40"
```

1.1 1. The mean vector

```
In [6]: mean_x = np.mean(all_samples[0,:])
        mean_y = np.mean(all_samples[1,:])
        mean_z = np.mean(all_samples[2,:])

        mean_vector = np.array([[mean_x],[mean_y],[mean_z]])

        print('Mean Vector:\n', mean_vector)
```

```
('Mean Vector:\n', array([[ 0.32576538],
       [ 0.37601327],
       [ 0.33054809]]))
```

1.2 2. The Scatter Matrix

```
In [7]: scatter_matrix = np.zeros((3,3))
        for i in range(all_samples.shape[1]):
            scatter_matrix += (all_samples[:,i].reshape(3,1) - mean_vector).dot((all_samples[:,i
        print('Scatter Matrix:\n', scatter_matrix)
```

```
('Scatter Matrix:\n', array([[ 53.3484232 ,  23.19069091,  21.46467362],
       [ 23.19069091,  52.8014702 ,  17.55487511],
       [ 21.46467362,  17.55487511,  51.1236242 ]]))
```

1.3 3. The Covariance Matrix

```
In [8]: cov_mat = np.cov([all_samples[0,:],all_samples[1,:],all_samples[2,:]])
        print('Covariance Matrix:\n', cov_mat)
```

```
('Covariance Matrix:\n', array([[ 1.36790829,  0.5946331 ,  0.55037625],
       [ 0.5946331 ,  1.35388385,  0.450125  ],
       [ 0.55037625,  0.450125  ,  1.31086216]]))
```

1.4 4. Computing eigenvectors and values

```
In [9]: # eigenvectors and eigenvalues for the from the scatter matrix
        eig_val_sc, eig_vec_sc = np.linalg.eig(scatter_matrix)

        # eigenvectors and eigenvalues for the from the covariance matrix
        eig_val_cov, eig_vec_cov = np.linalg.eig(cov_mat)

        for i in range(len(eig_val_sc)):
            eigvec_sc = eig_vec_sc[:,i].reshape(1,3).T
            eigvec_cov = eig_vec_cov[:,i].reshape(1,3).T
            assert eigvec_sc.all() == eigvec_cov.all(), 'Eigenvectors are not identical'

            print('Eigenvector {}: \n{}'.format(i+1, eigvec_sc))
            print('Eigenvalue {} from scatter matrix: {}'.format(i+1, eig_val_sc[i]))
            print('Eigenvalue {} from covariance matrix: {}'.format(i+1, eig_val_cov[i]))
            print('Scaling factor: ', eig_val_sc[i]/eig_val_cov[i])
            print(40 * '-')
```

```
Eigenvector 1:
[[ 0.6131328 ]
 [ 0.57507225]
```

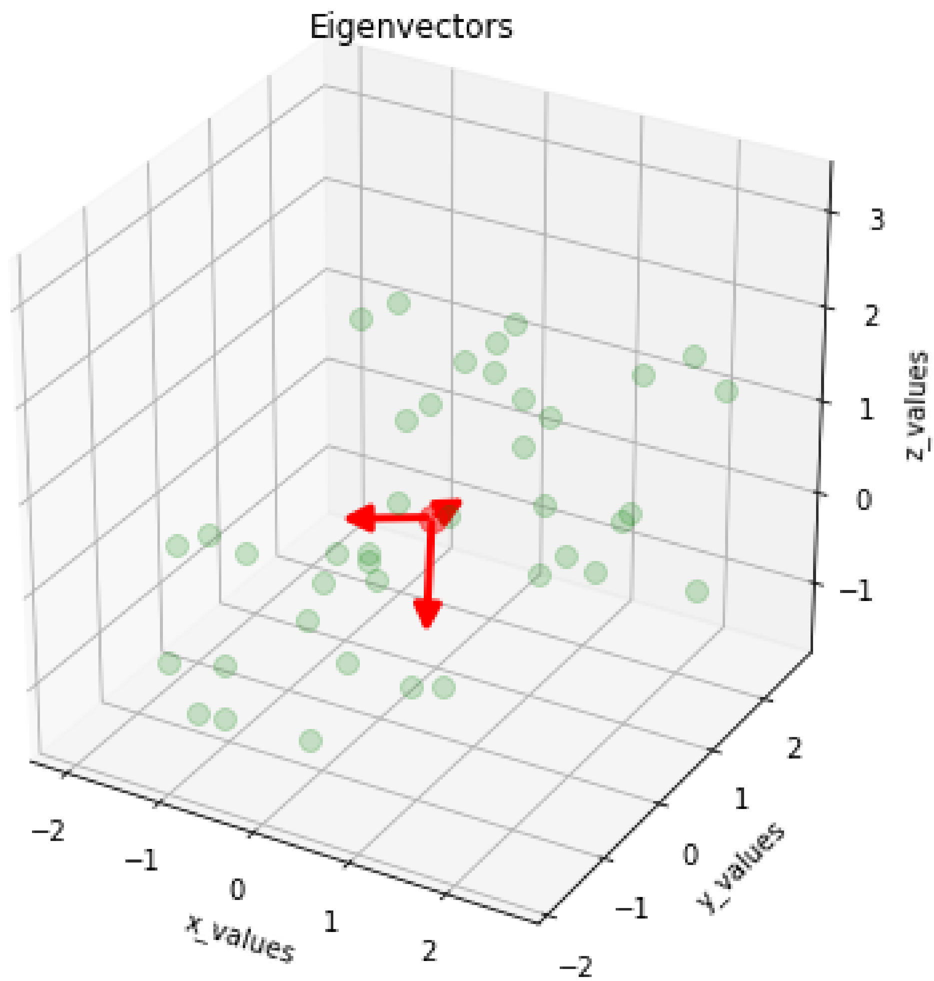
```
 [ 0.54162726]]
Eigenvalue 1 from scatter matrix: 94.060933071
Eigenvalue 1 from covariance matrix: 2.41181879669
('Scaling factor: ', 38.999999999999972)
----------------------------------------
Eigenvector 2:
[[ 0.78845466]
 [-0.48805716]
 [-0.37435206]]
Eigenvalue 2 from scatter matrix: 28.8020178753
Eigenvalue 2 from covariance matrix: 0.738513278854
('Scaling factor: ', 38.999999999999979)
----------------------------------------
Eigenvector 3:
[[-0.04906558]
 [-0.65657606]
 [ 0.75266224]]
Eigenvalue 3 from scatter matrix: 34.4105666541
Eigenvalue 3 from covariance matrix: 0.882322221899
('Scaling factor: ', 38.999999999999993)
----------------------------------------
```

1.4.1 4.1 Visualize the eigenvectors

In [10]:
```
%pylab inline

from matplotlib import pyplot as plt
from mpl_toolkits.mplot3d import Axes3D
from mpl_toolkits.mplot3d import proj3d
from matplotlib.patches import FancyArrowPatch


class Arrow3D(FancyArrowPatch):
    def __init__(self, xs, ys, zs, *args, **kwargs):
        FancyArrowPatch.__init__(self, (0,0), (0,0), *args, **kwargs)
        self._verts3d = xs, ys, zs

    def draw(self, renderer):
        xs3d, ys3d, zs3d = self._verts3d
        xs, ys, zs = proj3d.proj_transform(xs3d, ys3d, zs3d, renderer.M)
        self.set_positions((xs[0],ys[0]),(xs[1],ys[1]))
        FancyArrowPatch.draw(self, renderer)

fig = plt.figure(figsize=(7,7))
ax = fig.add_subplot(111, projection='3d')

ax.plot(all_samples[0,:], all_samples[1,:], all_samples[2,:], 'o', markersize=8, color=
```

```
ax.plot([mean_x], [mean_y], [mean_z], 'o', markersize=10, color='red', alpha=0.5)
for v in eig_vec_sc.T:
    a = Arrow3D([mean_x, v[0]], [mean_y, v[1]], [mean_z, v[2]], mutation_scale=20, lw=3
    ax.add_artist(a)
ax.set_xlabel('x_values')
ax.set_ylabel('y_values')
ax.set_zlabel('z_values')

plt.title('Eigenvectors')

plt.show()
```

```
Populating the interactive namespace from numpy and matplotlib
```



1.5 5. Sorting the eigenvectors by decreasing eigenvalues

```
In [11]: for ev in eig_vec_sc:
             numpy.testing.assert_array_almost_equal(1.0, np.linalg.norm(ev))

         # Make a list of (eigenvalue, eigenvector) tuples
         eig_pairs = [(np.abs(eig_val_sc[i]), eig_vec_sc[:,i]) for i in range(len(eig_val_sc))]

         # Sort the (eigenvalue, eigenvector) tuples from high to low
         eig_pairs.sort(key=lambda x: x[0], reverse=True)

         # Visually confirm that the list is correctly sorted by decreasing eigenvalues
         for i in eig_pairs:
             print(i[0])
```

```
94.060933071
34.4105666541
28.8020178753
```

1.6 6. Choose k eigenvectors with the largest eigenvalues

```
In [12]: matrix_w = np.hstack((eig_pairs[0][1].reshape(3,1), eig_pairs[1][1].reshape(3,1)))
         print('Matrix W:\n', matrix_w)
```

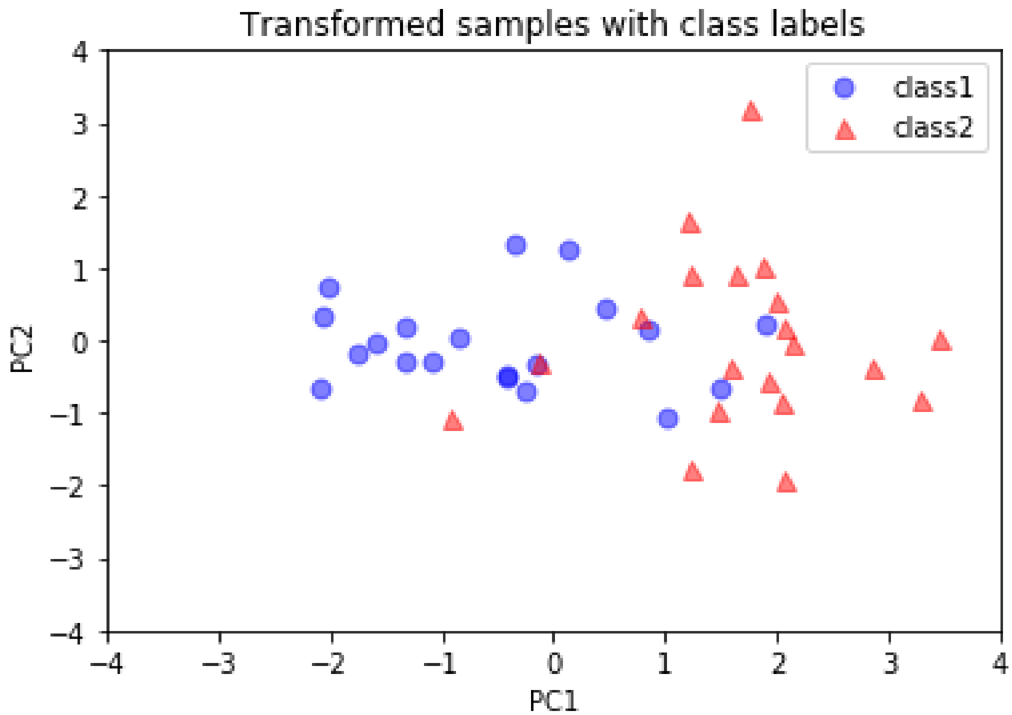
```
('Matrix W:\n', array([[ 0.6131328 , -0.04906558],
       [ 0.57507225, -0.65657606],
       [ 0.54162726,  0.75266224]]))
```

1.7 7. Transform the samples onto the new subspace

```
In [13]: transformed = matrix_w.T.dot(all_samples)
         assert transformed.shape == (2,40), "The matrix is not 2x40 dimensional."
```

1.7.1 7.1 Visualize result

```
In [14]: plt.plot(transformed[0,0:20], transformed[1,0:20], 'o', markersize=7, color='blue', alp
         plt.plot(transformed[0,20:40], transformed[1,20:40], '^', markersize=7, color='red', al
         plt.xlim([-4,4])
         plt.ylim([-4,4])
         plt.xlabel('PC1')
         plt.ylabel('PC2')
         plt.legend()
         plt.title('Transformed samples with class labels')

         plt.show()
```



Principle Component Regression will use the components with the most variance to do regression on a selected variable, see these slides (from slide number 11): http://www.stats.uwo.ca/faculty/braun/ss3850/notes/sas10.pdf