

PCA Examples

Let's start with our implementations.

```
In [0]: import numpy as np
import pandas as pd
from sklearn.decomposition import PCA
from sklearn.preprocessing import StandardScaler
import matplotlib.pyplot as plt
```

```
In [0]: def scratch_PCA(X, k):
    demeaned_X= X - np.mean(X, axis=0)
    #we now have to caculate the covariance matrix
    cov_X= np.matmul(np.transpose(demeaned_X), demeaned_X)
    sigma,V= np.linalg.eig(cov_X)
    # you then select the k biggest eignevalues and their corresponding eigenvectors
    return sigma[:k], V[:k]
```

```
In [0]: def sklearn_PCA(X, k):
    # initialize pca with num of components (k)
    pca = PCA(n_components=k)

    # run pca on our data set
    pca.fit(X)

    # get our first k components from our solutions
    variance = pca.explained_variance_[:k]
    vectors = pca.components_[:k]
    vectors = [np.asarray(vectors[i]) for i in range(len(vectors))]

    return variance, vectors
```

We use a standard dataset (Iris) included with scikit-learn

```
In [0]: url = "https://archive.ics.uci.edu/ml/machine-learning-databases/iris/iris.data"
features = ['sepal length', 'sepal width', 'petal length', 'petal width']
iris_df = pd.read_csv(url, names=['sepal length', 'sepal width', 'petal length',
                                   'petal width', 'target'])

iris_df.head()
```

Out[0]:

	sepal length	sepal width	petal length	petal width	target
0	5.1	3.5	1.4	0.2	Iris-setosa
1	4.9	3.0	1.4	0.2	Iris-setosa
2	4.7	3.2	1.3	0.2	Iris-setosa
3	4.6	3.1	1.5	0.2	Iris-setosa
4	5.0	3.6	1.4	0.2	Iris-setosa

```
In [0]: # extract our data and labels
X = iris_df.loc[:, features].values
y = iris_df.loc[:, ['target']].values
X = StandardScaler().fit_transform(X)
```

The dataset (iris) comes with several *features* and a target, which corresponds to the classification for the row with the given values for each feature.

For PCA we just look at the features to determine the directions of maximum variance, and then we can use our principal components to map back to the targets.

Another important note: we use standard scaler on our input X as PCA is not scale invariant. In other words, by scaling all values by the same factor, our results may change. Example as follows:

Effect of Scale on PCA:

```
In [0]: scale_ex = np.array([[1, -5], [-3, -8], [7, -3]])
scale_ex
```

```
Out[0]: array([[ 1, -5],
               [-3, -8],
               [ 7, -3]])
```

```
In [0]: sklearn_PCA(scale_ex, 2)
```

```
Out[0]: (array([31.40128474,  0.26538192]),
         [array([0.89728145,  0.44145894]), array([-0.44145894,  0.89728145])])
```

```
In [0]: sklearn_PCA(2*scale_ex, 2)
```

```
Out[0]: (array([125.60513897,  1.06152769]),
         [array([0.89728145,  0.44145894]), array([-0.44145894,  0.89728145])])
```

As we see above, the amount of variance captured by the first principal component is not scaled by 2, but by the scalar squared.

Back to the Iris dataset:

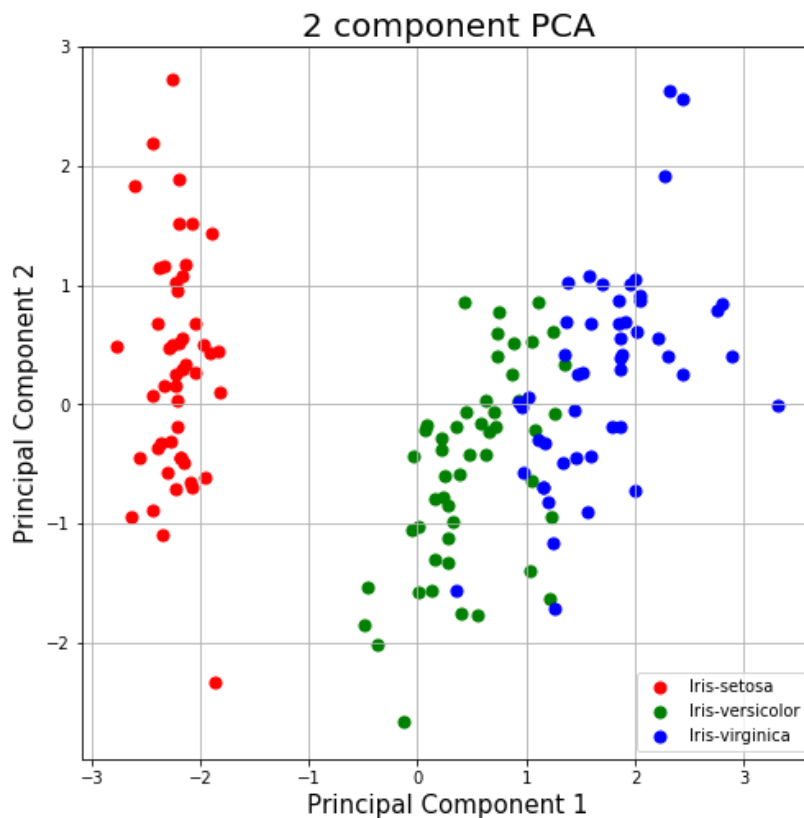
After we obtain the principal components, we project the original data using the principal component vectors.

This projection demonstrates why PCA is dimension reductionality:

```
In [0]: variance, pc = sklearn_PCA(X, 2)
projected = np.matmul(X, np.transpose(np.asarray(pc)))
principalDf = pd.DataFrame(data = projected
                           , columns = ['principal component 1', 'principal component 2'])
# add back the target
finalDf = pd.concat([principalDf, iris_df[['target']], axis = 1)
```

Visualization

```
In [0]: fig = plt.figure(figsize = (8,8))
ax = fig.add_subplot(1,1,1)
ax.set_xlabel('Principal Component 1', fontsize = 15)
ax.set_ylabel('Principal Component 2', fontsize = 15)
ax.set_title('2 component PCA', fontsize = 20)
targets = ['Iris-setosa', 'Iris-versicolor', 'Iris-virginica']
colors = ['r', 'g', 'b']
for target, color in zip(targets, colors):
    indicesToKeep = finalDf['target'] == target
    ax.scatter(finalDf.loc[indicesToKeep, 'principal component 1']
              , finalDf.loc[indicesToKeep, 'principal component 2']
              , c = color
              , s = 50)
ax.legend(targets)
ax.grid()
```



```
In [0]: print("Variance explained by Principal Component 1: " + str(variance[0]))
print("Variance explained by Principal Component 2: " + str(variance[1]))
```

Variance explained by Principal Component 1: 2.930353775589314
 Variance explained by Principal Component 2: 0.9274036215173412

As we see above, by using the first 2 principal components, we were able to compress our dataset with 4 initial variables/features, into 2 features and visualize it on a simple plot. We also see how variance factors into the split of the principal components. The first principal component shows the best split between the data, and very clearly sets apart the two plant species, despite the PCA being carried out on data without any labels (knowledge of which species a row belongs to). Accordingly, the first principal component also captures the most variance of the original dataset.

Credit:

Visualization: <https://towardsdatascience.com/pca-using-python-scikit-learn-e653f8989e60> (<https://towardsdatascience.com/pca-using-python-scikit-learn-e653f8989e60>)