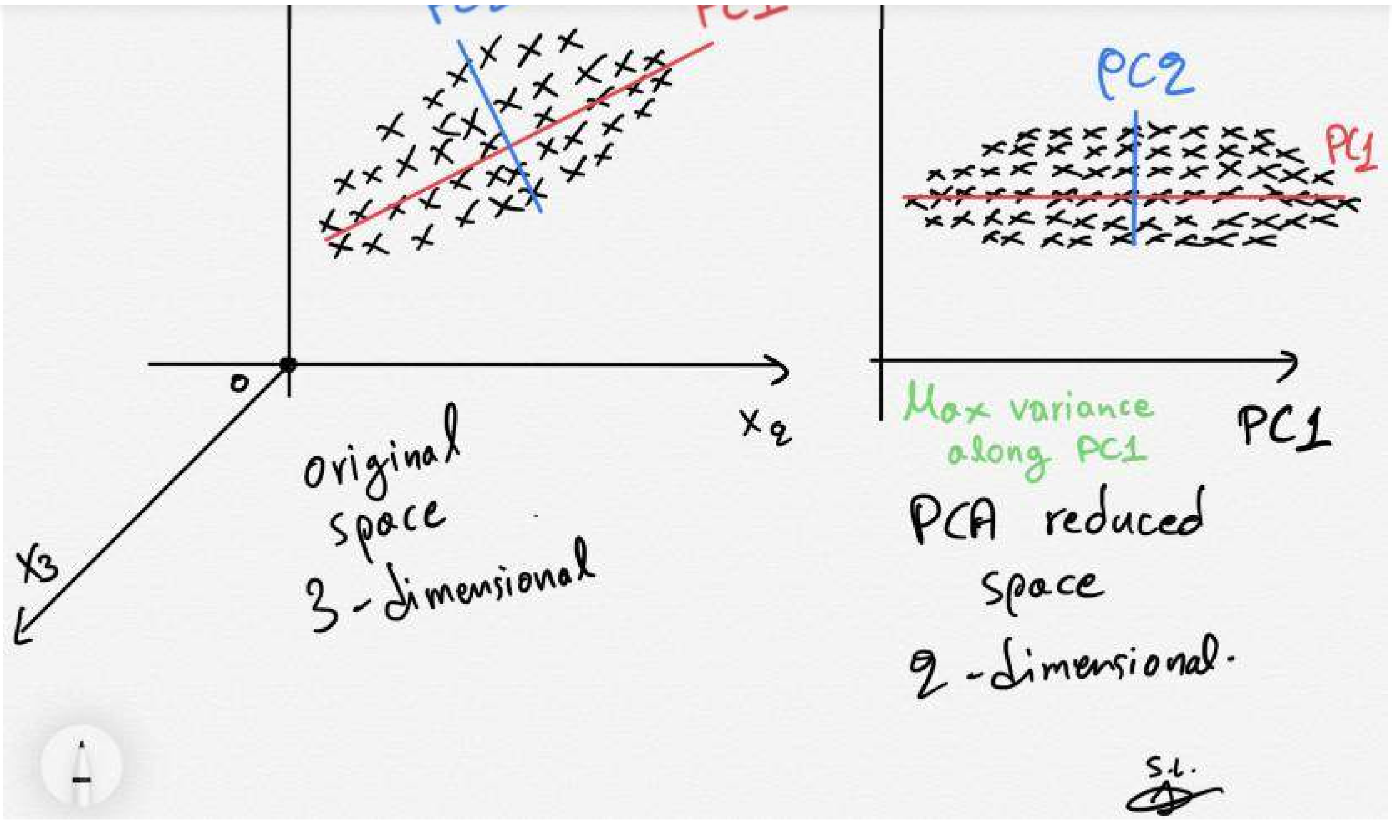
Serafeim Loukas Follow
May 30, 2020 · 7 min read · · Listen

PCA clearly explained —When, Why, How to use it and feature importance: A guide in Python

In this post I explain what PCA is, when and why to use it and how to implement it in Python using scikit-learn. Also, I explain how to get the feature importance after a PCA analysis.


PC1
PC2
0
X2
X3
Original space 3-dimensional
PC2
PC1
Max variance along PC1
PC1
PCA reduced space 2-dimensional.
S.L.

Handmade sketch made by the **author.**

1. Introduction & Background

Principal Components Analysis (PCA) is a well-known **unsupervised dimensionality reduction** technique that constructs **relevant** features/variables through linear (linear PCA) or non-linear (kernel PCA) **combinations** of the original variables (features). In this post, we will only focus on the famous and widely used **linear PCA** method.

The construction of relevant features is achieved by **linearly transforming correlated variables** into a smaller number of **uncorrelated** variables. This is done by **projecting** (dot product) the original data into the **reduced PCA space** using the eigenvectors of the covariance/correlation matrix aka the principal components (PCs).

The **resulting projected data** are essentially **linear combinations** of the **original** data **capturing most of the variance in the data** (Jolliffe 2002).

In summary, **PCA** is an **orthogonal transformation** of the data into a series of

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2. When/Why to use PCA

- PCA technique is particularly useful in processing data where **multi-colinearity** exists between the **features/variables.**
- PCA can be used when **the dimensions of the input features are high** (e.g. a lot of variables).
- PCA can be also used for **denoising** and **data compression.**

3. Core of the PCA method

Let `X` be a matrix containing the original data with shape `[n_samples, n_features]` .

Briefly, the **PCA** analysis consists of the following **steps**:

- First, the original input variables stored in `X` are **z-scored** such each original variable (column of `X`) has zero mean and unit standard deviation.
- The next step involves the construction and **eigendecomposition** of the **covariance** matrix `Cx= (1/n)X'X` (in case of z-scored data the covariance is equal to the correlation matrix since the standard deviation of all features is 1).
- **Eigenvalues** are then **sorted** in a **decreasing** order representing decreasing variance in the data (the eigenvalues are equal to the variance — I will prove this below using Python in Paragraph 6).

normalized data by the **leading eigenvectors** of the covariance matrix **i.e.** the PCs.

- The new **reduced** PCA space **maximizes** the **variance** of the **original** data. To **visualize** the projected data as well as the contribution of the original variables, in a joint plot, we can use the **biplot**.

4. The maximum number of meaningful components

There is an **upper bound** of the **meaningful components** that can be extracted using **PCA**. This is related to the **rank** of the **covariance/correlation** matrix (`Cx`). Having a data matrix `X` with shape `[n_samples, n_features/n_variables]`, the **covariance/correlation** matrix would be `[n_features, n_features]` with **maximum rank** equal to `min(n_samples, n_features)`.

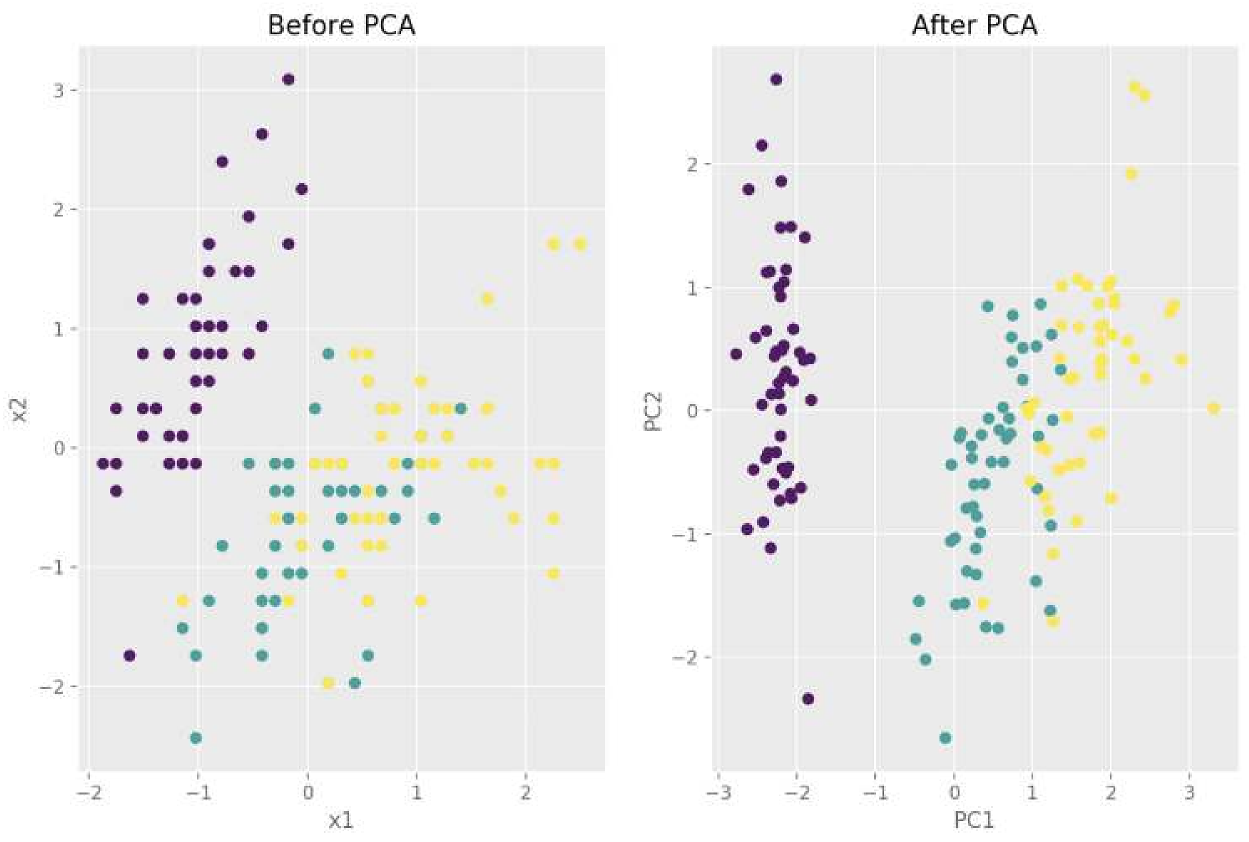
Thus, we can have at **most** `min(n_samples, n_features)` **meaningful** PC **components/dimensions** due to the **maximum** **rank** of the covariance/correlation matrix.

5. Python example using scikit-learn and the Iris dataset

```
import numpy as np
import matplotlib.pyplot as plt
from sklearn import datasets
from sklearn.decomposition import PCA
import pandas as pd
from sklearn.preprocessing import StandardScaler
plt.style.use('ggplot')

# Load the data
iris = datasets.load_iris()
X = iris.data
y = iris.target

# Z-score the features
scaler = StandardScaler()
scaler.fit(X)
X = scaler.transform(X)
```

Let’s plot the data before and **after** the **PCA** transform and also **color** code each point (sample) using the corresponding **class of the flower** `(y)` .

```
fig, axes = plt.subplots(1,2)

axes[0].scatter(X[:,0], X[:,
axes[0].set_xlabel('x1')
axes[0].set_ylabel('x2')
axes[0].set_title('Before PCA')

axes[1].scatter(X_new[:,0], X_new[:,1], c=y)
axes[1].set_xlabel('PC1')
axes[1].set_ylabel('PC2')
axes[1].set_title('After PCA')

plt.show()
```



```
print(pca.explained_variance_ratio_)
# array([0.72962445, 0.22850762])
```

6. Proof of eigenvalues of original covariance matrix being equal to the variances of the reduced space

Mathematical formulation & proof

Assuming that the original input variables stored in `X` are **z-scored** such each original variable (column of `X`) has zero mean and unit standard deviation, we have:

- The covariance of the original space is: $\mathbf{C_X} = \frac{1}{n}\mathbf{X}^T\mathbf{X}$

- PCA: Eigendecomposition of the covariance of the original space is:

$$\mathbf{C_X} = \frac{1}{n}\mathbf{X}^T\mathbf{X} = \mathbf{U}\mathbf{\Lambda}\mathbf{U}^T$$

- Let $\mathbf{Y} = \mathbf{XU}$ be the projected data (U stores the eigenvectors as columns)

- The covariance of the reduced PCA space is:

$$\begin{aligned}\mathbf{C_Y} &= \frac{1}{n}\mathbf{Y}^T\mathbf{Y}\\ &= \frac{1}{n}(\mathbf{XU})(\mathbf{XU})^T\\ &= \frac{1}{n}\mathbf{U}^T\mathbf{X}^T\mathbf{XU}\\ &= \mathbf{U}^T\left(\frac{1}{n}\mathbf{X}^T\mathbf{X}\right)\mathbf{U}\end{aligned}$$

$$\mathbf{C_Y} = \mathbf{U}^T\mathbf{C_X}\mathbf{U}$$

Verify using Python

The **maximum variance proof** can be also seen by estimating the **covariance** matrix of the **reduced space:**

```
np.cov(X_new.T)

array([[2.93808505e+00, 4.83198016e-16],
       [4.83198016e-16, 9.20164904e-01]])
```

We observe that these values (on the diagonal we have the variances) are **equal** to the **actual eigenvalues** of the covariance stored in `pca.explained_variance_`:

```
pca.explained_variance_
array([2.93808505, 0.9201649 ])
```

7. Feature importance

The **importance** of each **feature** is reflected by the **magnitude** of the **corresponding values in the eigenvectors** (higher magnitude — higher importance).

Let’s find the **most important features:**

```
print(abs( pca.components_ ))

[[0.52106591 0.26934744 0.5804131 0.56485654]
 [0.37741762 0.92329566 0.02449161 0.06694199]]
```

Here, `pca.components_` has shape `[n_components, n_features]` Thus, by looking at the **PC1** (first Principal Component) which is the **first row** can state that **feature 2** and then **1** are the **most important** for **PC2.**

*To sum up, we look at the absolute values of the eigenvectors' components corresponding to the **k** largest eigenvalues. In sklearn the components are sorted by explained variance.* ***The larger they are these absolute values, the more a specific feature contributes to that principal component.***

8. The biplot

The **biplot** is the best way to visualize **all-in-one** following a **PCA** analysis.

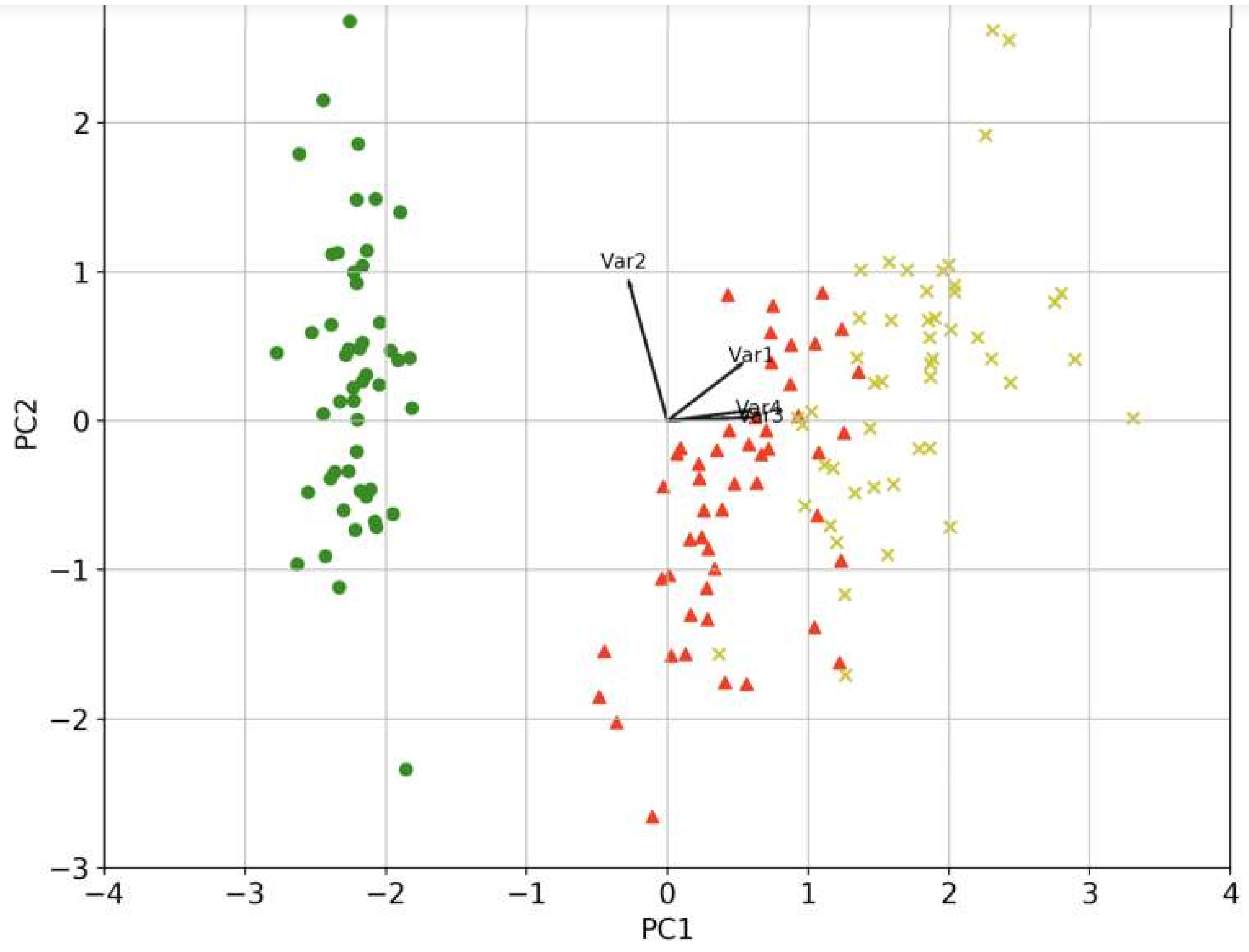
There is an implementation in **R** but there is no standard implementation in **python** so I decided to write my **own function** for that:

```
def biplot(score, coeff , y):
    '''
    Author: Serafeim Loukas, serafeim.loukas@epfl.ch
    Inputs:
       score: the projected data
       coeff: the eigenvectors (PCs)
       y: the class labels
   '''

    xs = score[:,0] # projection on PC1
    ys = score[:,1] # projection on PC2
    n = coeff.shape[0] # number of variables
    plt.figure(figsize=(10,8), dpi=100)
    classes = np.unique(y)
    colors = ['g','r','y']
    markers=['o','^','x']
    for s,l in enumerate(classes):
        plt.scatter(xs[y==l],ys[y==l], c = colors[s],
marker=markers[s]) # color based on group
    for i in range(n):
        #plot as arrows the variable scores (each variable has a score
for PC1 and one for PC2)
        plt.arrow(0, 0, coeff[i,0], coeff[i,1], color = 'k', alpha =
0.9,linestyle = '-',linewidth = 1.5, overhang=0.2)
        plt.text(coeff[i,0]* 1.15, coeff[i,1] * 1.15, "Var"+str(i+1),
color = 'k', ha = 'center', va = 'center',fontsize=10)
```

```
    plt.ylim([-limy,limy])
    plt.grid()
    plt.tick_params(axis='both', which='both', labelsize=14)
```

Call the function (make sure to run first the initial blocks of code where we load the iris data and perform the PCA analysis):

```
import matplotlib as mpl
mpl.rcParams.update(mpl.rcParamsDefault) # reset ggplot style

# Call the biplot function for only the first 2 PCs
biplot(X_new[:,0:2], np.transpose(pca.components_[0:2, :]), y)
plt.show()
```



The PCA biplot using my custom function.

We can again verify **visually** that **a)** the variance is maximized and **b)** that **feature 1, 3 and 4** are the **most important** for **PC1.** Similarly, **feature 2** and then **1** are the **most important** for **PC2.**

Furthermore, **arrows** (variables/features) that point into the **same direction** indicate **correlation** between the variables that they represent whereas, the arrows heading in **opposite directions** indicate a **contrast** between the variables they represent.

Verify the above using **code:**

```
# Var 3 and Var 4 are extremely positively correlated
np.corrcoef(X[:, 2], X[:, 3])[1,0]
```

That's all folks! Hope you liked this article!

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References

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