```
import numpy as np
import pandas as pd
import seaborn as sb
import matplotlib.pyplot as plt

from sklearn.preprocessing import StandardScaler
```

Exercise 1

Determine PCA of a 3x2 matrix

define a matrix

```
A = np.array([[1, 2], [3, 4], [5, 6]])
print(A)
```

```
[[1 2]
 [3 4]
 [5 6]]
```

First do it manually!

1. Subtract the mean of each variable

```
col_mean = np.mean(A, axis = 0)
col_mean
```

```
array([3., 4.])
```

```
mean_centered_A = A - col_mean
mean_centered_A
```

```
array([[-2., -2.],
       [ 0.,  0.],
       [ 2.,  2.]])
```

2. Calculate the Covariance Matrix

```
covariance_matrix = np.cov(mean_centered_A, rowvar = False)
covariance_matrix
```

```
array([[4., 4.],
       [4., 4.]])
```

```
covariance_matrix.shape
```

```
(2, 2)
```

3. Compute the Eigenvalues and Eigenvectors

```
eigenvalues, eigenvectors = np.linalg.eig(covariance_matrix)
```

```
len(eigenvalues)
```

```
2
```

```
eigenvalues
```

```
array([8., 0.])
```

```
eigenvectors
```

```
array([[ 0.70710678, -0.70710678],
       [ 0.70710678,  0.70710678]])
```

```
eigenvectors.shape
```

```
(2, 2)
```

4. project data of the original matrix to the new basis

```
feature_vector = eigenvectors.T
feature_vector
```

```
array([[ 0.70710678,  0.70710678],
       [-0.70710678,  0.70710678]])
```

```
projected_data = np.dot(feature_vector, mean_centered_A.T).T
projected_data
```

```
array([[-2.82842712,  0.        ],
       [ 0.        ,  0.        ],
       [ 2.82842712,  0.        ]])
```

conclusion?

- **The column containing zeros indicate that the data has been projected alon this direction**
- **The main variation of in the original data must be along the first vector.**

Exercise 2

Ok Let's do it again but for a larger matrix 20x5

Generate a dummy dataset.

```
X = np.random.randint(10,50,100).reshape(20,5)
print(X)
```

```
[[30 16 43 20 39]
 [13 39 40 20 10]
 [18 43 22 14 12]
 [18 44 38 28 16]
 [22 10 39 44 34]
 [30 16 22 11 33]
 [22 28 26 19 41]
 [36 33 26 10 12]
 [48 28 18 47 42]
 [25 17 48 18 13]
 [31 31 44 17 40]
 [42 16 23 35 27]
 [23 39 25 47 46]
 [33 39 18 17 25]
 [11 22 25 25 18]
 [44 45 28 41 49]
 [32 43 26 40 12]
 [42 45 45 46 35]
 [43 13 26 43 18]
 [13 24 23 11 34]]
```

1. Subtract the mean of each variable

Subtract the mean of each variable from the dataset so that the dataset should be centered on the origin. Doing this proves to be very helpful when calculating the covariance matrix.

```
col_mean = np.mean(X, axis = 0)
col_mean
```

```
array([28.8 , 29.55, 30.25, 27.65, 27.8 ])
```

```
mean_centered_data = X - col_mean
mean_centered_data
```

```
array([[  1.2 , -13.55,  12.75,  -7.65,  11.2 ],
       [-15.8 ,   9.45,   9.75,  -7.65, -17.8 ],
       [-10.8 ,  13.45,  -8.25, -13.65, -15.8 ],
       [-10.8 ,  14.45,   7.75,   0.35, -11.8 ],
       [ -6.8 , -19.55,   8.75,  16.35,   6.2 ],
       [  1.2 , -13.55,  -8.25, -16.65,   5.2 ],
       [ -6.8 ,  -1.55,  -4.25,  -8.65,  13.2 ],
       [  7.2 ,   3.45,  -4.25, -17.65, -15.8 ],
       [ 19.2 ,  -1.55, -12.25,  19.35,  14.2 ],
       [ -3.8 , -12.55,  17.75,  -9.65, -14.8 ],
       [  2.2 ,   1.45,  13.75, -10.65,  12.2 ],
       [ 13.2 , -13.55,  -7.25,   7.35,  -0.8 ],
       [ -5.8 ,   9.45,  -5.25,  19.35,  18.2 ],
       [  4.2 ,   9.45, -12.25, -10.65,  -2.8 ],
       [-17.8 ,  -7.55,  -5.25,  -2.65,  -9.8 ],
       [ 15.2 ,  15.45,  -2.25,  13.35,  21.2 ],
       [  3.2 ,  13.45,  -4.25,  12.35, -15.8 ],
       [ 13.2 ,  15.45,  14.75,  18.35,   7.2 ],
       [ 14.2 , -16.55,  -4.25,  15.35,  -9.8 ],
       [-15.8 ,  -5.55,  -7.25, -16.65,   6.2 ]])
```

2. Calculate the Covariance Matrix

Calculate the Covariance Matrix of the mean-centered data.

```
covariance_matrix = np.cov(mean_centered_data, rowvar = False)
covariance_matrix
```

```
array([[127.74736842,  -0.98947368, -15.73684211,  73.34736842,
         46.58947368],
       [ -0.98947368, 146.68157895,  -5.88157895,  14.93947368,
        -10.72631579],
       [-15.73684211,  -5.88157895,  94.19736842,   0.72368421,
         -6.31578947],
       [ 73.34736842,  14.93947368,   0.72368421, 186.55526316,
         57.76842105],
       [ 46.58947368, -10.72631579,  -6.31578947,  57.76842105,
        169.01052632]])
```

```
covariance_matrix.shape
```

```
(5, 5)
```

Note: the matrix is symmetrical

3. Compute the Eigenvalues and Eigenvectors

Now, compute the Eigenvalues and Eigenvectors for the calculated Covariance matrix.

```
eigenvalues, eigenvectors = np.linalg.eig(covariance_matrix)
```

```
eigenvalues
```

```
array([284.58791229,  68.88887528, 100.45007762, 114.80307465,
       155.46216543])
```

```
len(eigenvalues)
```

```
5
```

```
eigenvectors
```

```
array([[-0.48593246,  0.72889216,  0.43824214, -0.20113715,  0.00857548],
       [-0.03126598,  0.13053432, -0.07748173,  0.41792041,  0.8951661 ],
       [ 0.05639257,  0.48944128, -0.84450849, -0.20461209, -0.04697243],
       [-0.68529823, -0.45964887, -0.2131231 , -0.46413987,  0.24133377],
       [-0.53858917, -0.02910611, -0.20814504,  0.72635697, -0.37169305]])
```

```
eigenvectors.shape
```

```
(5, 5)
```

Note: The Eigenvectors of the Covariance matrix we get are Orthogonal to each other and each vector represents a principal axis. A Higher Eigenvalue corresponds to a higher variability. Hence the principal axis with the higher Eigenvalue will be an axis capturing higher variability in the data.

4. Sort Eigenvalues in descending order

Sort the Eigenvalues in the descending order along with their corresponding Eigenvector.

```
index_of_sorted = np.argsort(eigenvalues)[::-1]
index_of_sorted
```

```
array([0, 4, 3, 2, 1])
```

```
sorted_eigenvalues = eigenvalues[index_of_sorted]
sorted_eigenvalues
```

```
array([284.58791229, 155.46216543, 114.80307465, 100.45007762,
        68.88887528])
```

```
principal_components = eigenvectors[index_of_sorted]
principal_components
```

```
array([[-0.48593246,  0.72889216,  0.43824214, -0.20113715,  0.00857548],
       [-0.53858917, -0.02910611, -0.20814504,  0.72635697, -0.37169305],
       [-0.68529823, -0.45964887, -0.2131231 , -0.46413987,  0.24133377],
       [ 0.05639257,  0.48944128, -0.84450849, -0.20461209, -0.04697243],
       [-0.03126598,  0.13053432, -0.07748173,  0.41792041,  0.8951661 ]])
```

Note: Each column in the Eigen vector-matrix corresponds to a principal component, so arranging them in descending order of their Eigenvalue will automatically arrange the principal component in descending order of their variability. Hence the first column in our rearranged Eigen vector-matrix will be a principal component that captures the highest variability.

5. Select a subset from the rearranged Eigenvalue matrix

Select a subset of n first eigenvectors from the rearranged Eigenvector matrix as per our need, n is desired dimension of your final reduced data. i.e. "n_components=2" means you selected the first two principal components.

```
n_components=2

top_n_principal_components = principal_components[:n_components]
top_n_principal_components
```

```
array([[-0.48593246,  0.72889216,  0.43824214, -0.20113715,  0.00857548],
       [-0.53858917, -0.02910611, -0.20814504,  0.72635697, -0.37169305]])
```

```
feature_vector = top_n_principal_components.T
feature_vector
```

```
array([[-0.48593246, -0.53858917],
       [ 0.72889216, -0.02910611],
       [ 0.43824214, -0.20814504],
       [-0.20113715,  0.72635697],
       [ 0.00857548, -0.37169305]])
```

Note: The final dimensions of X_reduced will be (20, 2) and originally the data was of higher dimensions (20, 5).

6. Transform the data

Finally, transform the data by having a dot product between the Transpose of the Eigenvector subset and the Transpose of the mean-centered data. By transposing the outcome of the dot product, the result we get is the data reduced to lower dimensions from higher dimensions.

```
row_feature_vector_transpose = np.transpose(feature_vector)
row_feature_vector_transpose
```

```
array([[-0.48593246,  0.72889216,  0.43824214, -0.20113715,  0.00857548],
       [-0.53858917, -0.02910611, -0.20814504,  0.72635697, -0.37169305]])
```

```
row_mean_centered_data = np.transpose(mean_centered_data)
row_mean_centered_data
```

```
array([[  1.2 , -15.8 , -10.8 , -10.8 ,  -6.8 ,   1.2 ,  -6.8 ,   7.2 ,
         19.2 ,  -3.8 ,   2.2 ,  13.2 ,  -5.8 ,   4.2 , -17.8 ,  15.2 ,
          3.2 ,  13.2 ,  14.2 , -15.8 ],
       [-13.55,   9.45,  13.45,  14.45, -19.55, -13.55,  -1.55,   3.45,
         -1.55, -12.55,   1.45, -13.55,   9.45,   9.45,  -7.55,  15.45,
         13.45,  15.45, -16.55,  -5.55],
       [ 12.75,   9.75,  -8.25,   7.75,   8.75,  -8.25,  -4.25,  -4.25,
        -12.25,  17.75,  13.75,  -7.25,  -5.25, -12.25,  -5.25,  -2.25,
         -4.25,  14.75,  -4.25,  -7.25],
       [ -7.65,  -7.65, -13.65,   0.35,  16.35, -16.65,  -8.65, -17.65,
         19.35,  -9.65, -10.65,   7.35,  19.35, -10.65,  -2.65,  13.35,
         12.35,  18.35,  15.35, -16.65],
       [ 11.2 , -17.8 , -15.8 , -11.8 ,   6.2 ,   5.2 ,  13.2 , -15.8 ,
         14.2 , -14.8 ,  12.2 ,  -0.8 ,  18.2 ,  -2.8 ,  -9.8 ,  21.2 ,
        -15.8 ,   7.2 ,  -9.8 ,   6.2 ]])
```

```
eigen_dot = np.dot(feature_vector_transpose, row_mean_centered_data)
eigen_dot
```

```
array([[ 12.96490482, -19.18008846, -23.36997019, -17.20701989,
         15.55924032,   5.83724346,  -3.77568923,  -5.0347186 ,
         17.23717899,   5.42702442,   2.87986656,  17.78454148,
         -4.21834464,  -9.11003579,  -9.2586001 ,   4.74157704,
         -8.14273835,   5.67307626,  21.34552149, -10.15296961],
       [-15.52040507, -13.35707662,   3.45613385,  -7.34335236,
        -11.40924928,   0.92525087,  -2.63812307,   5.15718898,
         21.27229899, -19.89695028, -13.67264537,  10.84960573,
          6.19934858,  12.12264648,  -4.54971291,  12.55068131,
         11.6078114 ,  -0.46781325,  10.600405  ,  -5.88604298]])
```

```
X_reduced = eigen_dot.T
X_reduced
```

```
array([[ 12.96490482, -15.52040507],
       [-19.18008846, -13.35707662],
       [-23.36997019,   3.45613385],
       [-17.20701989,  -7.34335236],
       [ 15.55924032, -11.40924928],
       [  5.83724346,   0.92525087],
       [ -3.77568923,  -2.63812307],
       [ -5.0347186 ,   5.15718898],
       [ 17.23717899,  21.27229899],
       [  5.42702442, -19.89695028],
       [  2.87986656, -13.67264537],
       [ 17.78454148,  10.84960573],
       [ -4.21834464,   6.19934858],
       [ -9.11003579,  12.12264648],
       [ -9.2586001 ,  -4.54971291],
       [  4.74157704,  12.55068131],
       [ -8.14273835,  11.6078114 ],
       [  5.67307626,  -0.46781325],
       [ 21.34552149,  10.600405  ],
       [-10.15296961,  -5.88604298]])
```

```
X_reduced.shape
```

```
(20, 2)
```

Exercise 3

Now, let’s just combine everything above by making a function and try our Principal Component analysis from scratch on an example.

Create a PCA function accepting data matrix and the number of components as input arguments.

```
def pca(X, n_components):
  col_mean = np.mean(X, axis = 0)
  mean_centered_data = X - col_mean
  covariance_matrix = np.cov(mean_centered_data, rowvar = False)

  eigenvalues, eigenvectors = np.linalg.eig(covariance_matrix)

  index_of_sorted = np.argsort(eigenvalues)[::-1]
  sorted_eigenvalues = eigenvalues[index_of_sorted]
```

```
principal_components = eigenvectors[index_of_sorted]

eigen_sum = np.sum(sorted_eigenvalues)
#explainability = np.empty(len(sorted_eigenvalues))
explainability = {}


#for idx, eigen_val in enumerate(sorted_eigenvalues):
for eigen_val in sorted_eigenvalues:
  #explainability[idx] = np.sum(sorted_eigenvalues[:idx + 1]) / eigen_sum
  #explainability[eigen_val] = np.sum(sorted_eigenvalues[:idx + 1]) / eigen_sum
  explainability[eigen_val] = str((eigen_val / eigen_sum) * 100) + ' %'


top_n_principal_components = principal_components[:n_components]
feature_vector = top_n_principal_components.T

row_feature_vector = np.transpose(feature_vector)
row_mean_centered_data = np.transpose(mean_centered_data)

eigen_dot = np.dot(row_feature_vector, row_mean_centered_data)
X_reduced = eigen_dot.T

return X_reduced, explainability
```

Let's use the IRIS dataset to test our PCA function, and by the same way see if we can classify the dataset in the projected space

```
#Get the IRIS dataset
url = "https://archive.ics.uci.edu/ml/machine-learning-databases/iris/iris.data"
data = pd.read_csv(url, names=['sepal length','sepal width','petal length','petal width','target'])
data.head()
```

	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

1. prepare the dataset & target set for classification

```
Y = data['target']
Y.head()
```

```
0    Iris-setosa
1    Iris-setosa
2    Iris-setosa
3    Iris-setosa
4    Iris-setosa
Name: target, dtype: object
```

```
len(Y)
```

```
150
```

```
X_var = data.iloc[:, :-1]
X_var.head()
```

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

```
X_var.shape
```

```
(150, 4)
```

```
scaler = StandardScaler().set_output(transform="pandas")
X_new = scaler.fit_transform(X_var)
X_new.head()
```

	sepal length	sepal width	petal length	petal width
0	-0.900681	1.032057	-1.341272	-1.312977
1	-1.143017	-0.124958	-1.341272	-1.312977
2	-1.385353	0.337848	-1.398138	-1.312977
3	-1.506521	0.106445	-1.284407	-1.312977
4	-1.021849	1.263460	-1.341272	-1.312977

2. Apply the PCA function

```
reduced_X, explainability = pca(X_new.to_numpy(), 3)
reduced_X
```

```
array([[-0.2316583 , -0.87967436,  0.31762646],
       [ 0.07253025,  0.25502854,  0.20117481],
       [-0.18536908, -0.12326756,  0.04254146],
       [-0.24451042,  0.15034585, -0.00698258],
       [-0.38110853, -1.06194072,  0.24231575],
       [-0.44050933, -1.82346152,  0.32276436],
       [-0.42753067, -0.52226744, -0.13496883],
       [-0.24979851, -0.61982431,  0.26009048],
       [-0.15778746,  0.62875583, -0.14609035],
       [-0.08907179,  0.07093576,  0.30963548],
       [-0.2550866 , -1.38999448,  0.52716354],
       [-0.41738895, -0.54224064,  0.1272438 ],
       [-0.02520974,  0.30325906,  0.23607563],
       [-0.21867964,  0.42151973, -0.14010673],
       [-0.13737131, -2.20145476,  0.77020078],
       [-0.59940097, -3.01760131,  0.49362145],
       [-0.27650482, -1.878515  ,  0.29071661],
       [-0.19721296, -0.89599473,  0.21229633],
       [-0.19891512, -1.6886951 ,  0.64426382],
       [-0.49668081, -1.52476091,  0.20566408],
       [-0.07862214, -0.71993819,  0.55783159],
       [-0.3760799 , -1.32690476,  0.10521534],
       [-0.47028264, -0.98935358, -0.07144924],
       [-0.07901452, -0.45899233,  0.03543466],
       [-0.54039234, -0.50095053,  0.15127961],
       [ 0.05382265,  0.25064512,  0.28762799],
       [-0.22190896, -0.63870169,  0.05744215],
       [-0.20936477, -0.89782114,  0.3960677 ],
       [-0.08220807, -0.69740799,  0.39293716],
       [-0.30837246, -0.08197745,  0.06657727],
       [-0.15892223,  0.10028892,  0.14188798],
       [ 0.07227079, -0.78010568,  0.33114746],
       [-0.76074355, -2.16655987,  0.47210947],
       [-0.58156868, -2.50655059,  0.56517394],
       [-0.08907179,  0.07093576,  0.30963548],
       [ 0.04551602, -0.23276139,  0.24581745],
       [ 0.06252146, -1.02107834,  0.59133176],
       [-0.08907179,  0.07093576,  0.30963548],
       [-0.2029419 ,  0.40081594, -0.15898368],
       [-0.18650385, -0.65173447,  0.33051979],
       [-0.21950649, -0.87784794,  0.13385508],
       [ 0.49788711,  1.85182103, -0.15971474],
       [-0.37525305, -0.02753709, -0.16874647],
       [-0.23917386, -0.88551895, -0.1580995 ],
       [-0.62623998, -1.4860278 ,  0.1323817 ],
       [ 0.04368094,  0.27061832,  0.02541537],
       [-0.57212727, -1.49467717,  0.31900615],
       [-0.28966486, -0.07759403, -0.01987591],
       [-0.31838126, -1.35808433,  0.45673423],
       [-0.12264181, -0.41941117,  0.25695993],
       [ 0.28971372, -0.58509099,  0.67085989],
       [ 0.02639337, -0.43747718,  0.12693003],
       [ 0.26501772, -0.32779795,  0.51600572],
       [ 0.36825659,  1.74112676, -0.29240064],
       [ 0.39330919,  0.4010821 ,  0.22489685],
       [-0.14093761,  0.67524071, -0.13588931],
       [-0.17061378, -0.60853717, -0.03768694],
       [ 0.08600496,  1.67102869, -0.45995107],
```

```
reduced_X.shape
```

```
(150, 3)
```

```
explainability
```

```
{2.930353775589317: '72.77045209380135 %',
 0.9274036215173419: '23.03052326768065 %',
 0.14834222648163944: '3.683831957627379 %',
 0.02074601399559593: '0.5151926808906321 %'}
```

3. Create a Pandas Dataframe of reduced Dataset with target data

```
reduced_dataset = pd.DataFrame(reduced_X)
reduced_dataset['Target'] = Y
reduced_dataset.head()
```

	0	1	2	Target
0	-0.231658	-0.879674	0.317626	Iris-setosa
1	0.072530	0.255029	0.201175	Iris-setosa
2	-0.185369	-0.123268	0.042541	Iris-setosa
3	-0.244510	0.150346	-0.006983	Iris-setosa
4	-0.381109	-1.061941	0.242316	Iris-setosa

```
reduced_dataset.shape
```

```
(150, 4)
```

4. Vizualize the data with one and two principal components

```
def plot_iris_pca(df, n_components):

  # Settin different colours for various categories in the Target column
  target_colors = {
      'Iris-setosa': 'red',
      'Iris-versicolor': 'green',
      'Iris-virginica': 'blue'}

  # Scatter plot
  plt.figure(figsize=(10, 8))

  for target, color in target_colors.items():
    subset = df[df['Target'] == target]
    if n_components == 1:
      plt.scatter(subset[[0]], subset[[0]]*0, label=target, c=color)
    if n_components == 2:
      plt.scatter(subset[[0]], subset[[1]], label=target, c=color)

  # Axis labels and legend
  if n_components == 1:
    plt.xlabel('Component 0')
    plt.ylabel('Component 0')

  if n_components == 2:
    plt.xlabel('Component 0')
    plt.ylabel('Component 1')

  plt.legend()

  # Show the plot
  plt.show()
```

For PCA with 1 pricipal component

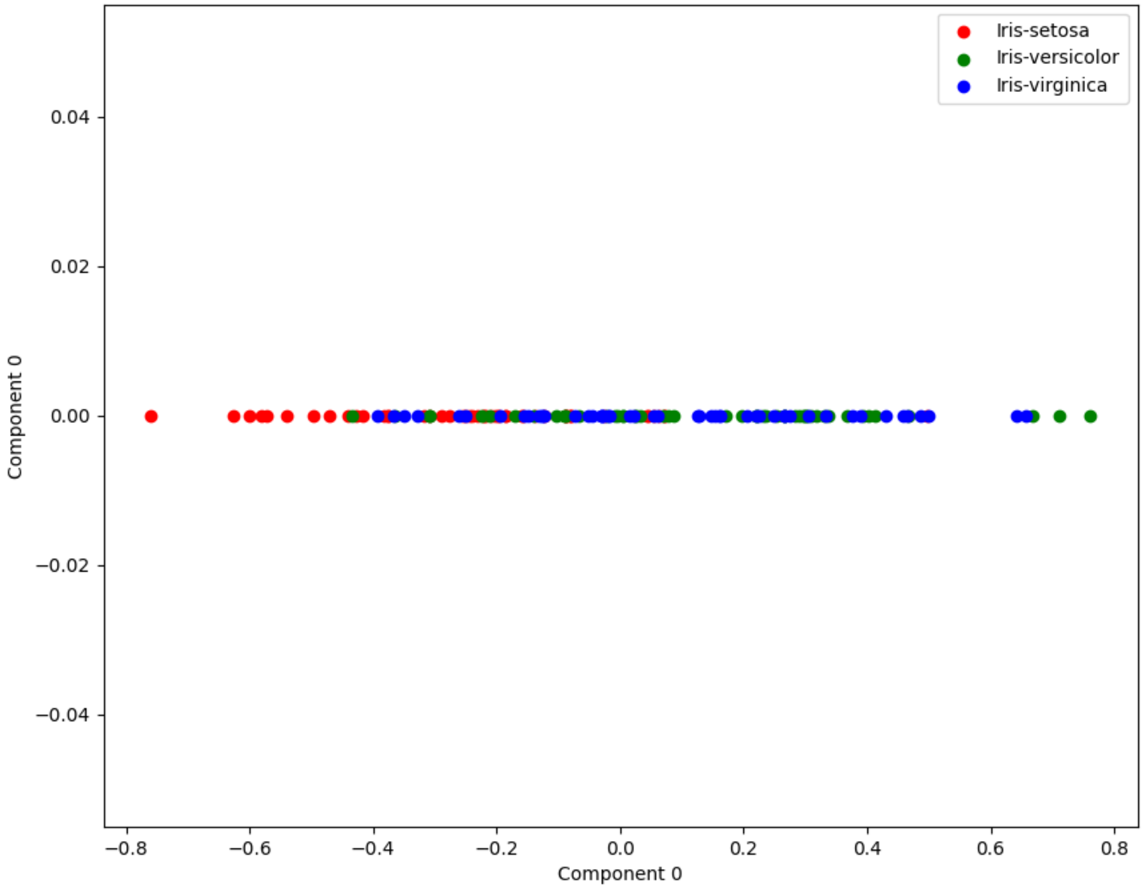
```
reduced_X, explainability = pca(X_new.to_numpy(), 1)
reduced_dataset = pd.DataFrame(reduced_X)
reduced_dataset['Target'] = Y

print(reduced_dataset.shape)
reduced_dataset.head()
```

```
(150, 2)
```

	0	Target
0	-0.231658	Iris-setosa
1	0.072530	Iris-setosa
2	-0.185369	Iris-setosa
3	-0.244510	Iris-setosa
4	-0.381109	Iris-setosa

```
plot_iris_pca(reduced_dataset, 1)
```




```
explainability
```

```
{2.930353775589317: '72.77045209380135 %',
 0.9274036215173419: '23.03052326768065 %',
 0.14834222648163944: '3.683831957627379 %',
 0.020746013995559593: '0.5151926808906321 %'}
```

For PCA with 2 pricipal components

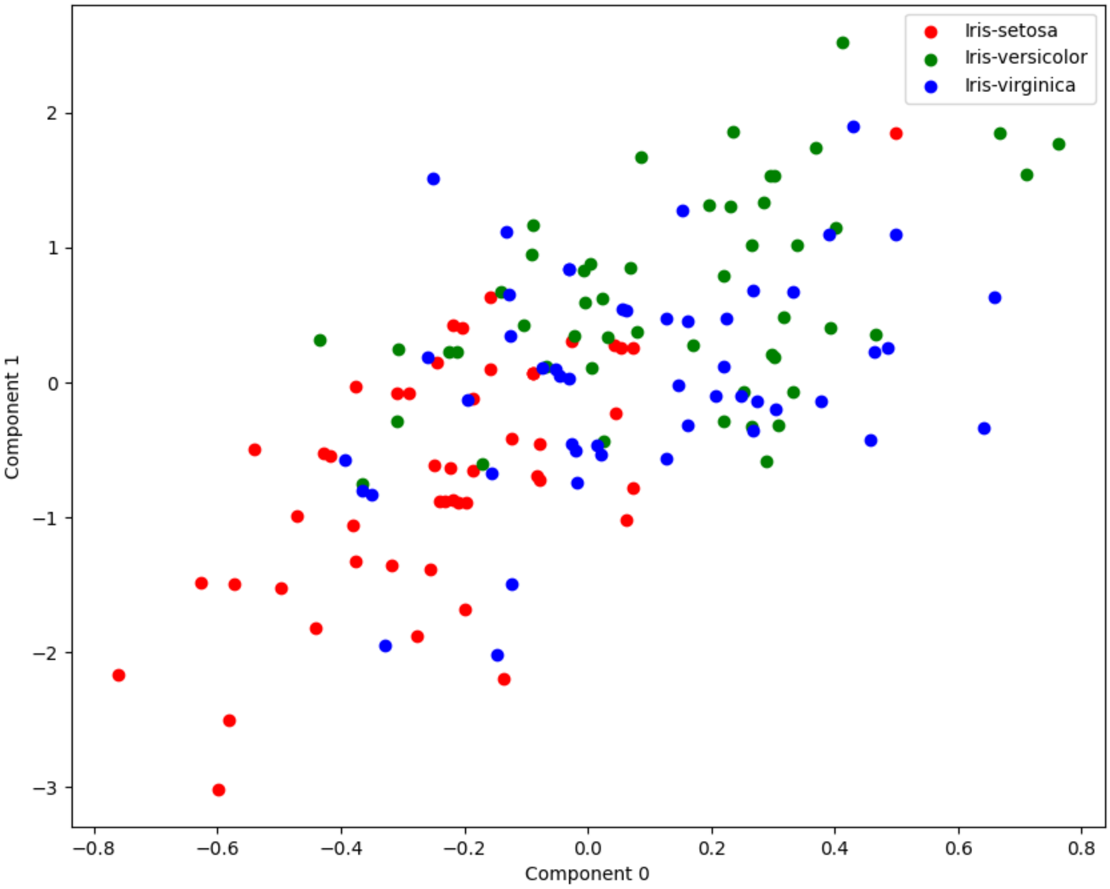
```
reduced_X, explainability = pca(X_new.to_numpy(), 2)
reduced_dataset = pd.DataFrame(reduced_X)
reduced_dataset['Target'] = Y

print(reduced_dataset.shape)
reduced_dataset.head()
```

```
(150, 3)
```

	0	1	Target
0	-0.231658	-0.879674	Iris-setosa
1	0.072530	0.255029	Iris-setosa
2	-0.185369	-0.123268	Iris-setosa
3	-0.244510	0.150346	Iris-setosa
4	-0.381109	-1.061941	Iris-setosa

```
plot_iris_pca(reduced_dataset, 2)
```




```
explainability
```

```
{2.930353775589317: '72.77045209380135 %',
 0.9274036215173419: '23.03052326768065 %',
 0.14834222648163944: '3.683831957627379 %',
 0.02074601399559593: '0.5151926808906321 %'}
```

conclusions?

- **The pricipal components corresponding to eigen values 2.930353775589317 and 0.9274036215173419 is able to explain 72.77% and 23.03% of the data respectively.**
- **Therfore, PCA with one principal component alone is able to account for 72.77% of the data.**
- **Similarly, PCA with two principal components able to account for 95.8% of the data.**

More?

Go to: https://jakevdp.github.io/PythonDataScienceHandbook/05.09-principal-component-analysis.html

+ Code + Text