Principal Component Analysis

IN5148: Statistics and Data Science with Applications in Engineering

Alan R. Vazquez
Department of Industrial Engineering

Tecnologico de Monterrey

Agenda

1. Introduction
2. Dispersion in one or more dimensions
3. Principal component analysis

Introduction

Load the libraries

Before we start, let's import the data science libraries into Python.

```
import numpy as np
import pandas as pd
import matplotlib.pyplot as plt
import seaborn as sns
from sklearn.preprocessing import StandardScaler
from sklearn.decomposition import PCA
```

Here, we use specific functions from the **pandas**, **matplotlib**, **seaborn**, and **sklearn** libraries in Python.

Types of learning

In data science, there are two main types of learning:

- Supervised learning. In which we have multiple predictors and one response. The goal is to predict the response using the predictor values.
- Unsupervised learning. In which we have only multiple predictors. The goal is to discover patterns in your data.

Unsupervised learning methods

- **Clustering Methods** aim to find subgroups with similar data in the database.
- **Principal Component Analysis** seeks an alternative representation of the data to make it easier to understand when there are many predictors in the database.

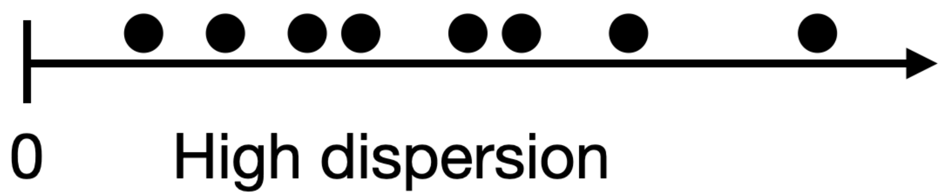
Here we will use these methods on predictors $X_1, X_2, \ldots, X_p$, which are *numerical*.

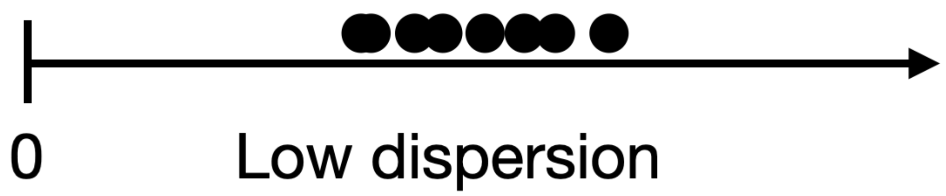
Dispersion in one or more dimensions

Dispersion in one dimension

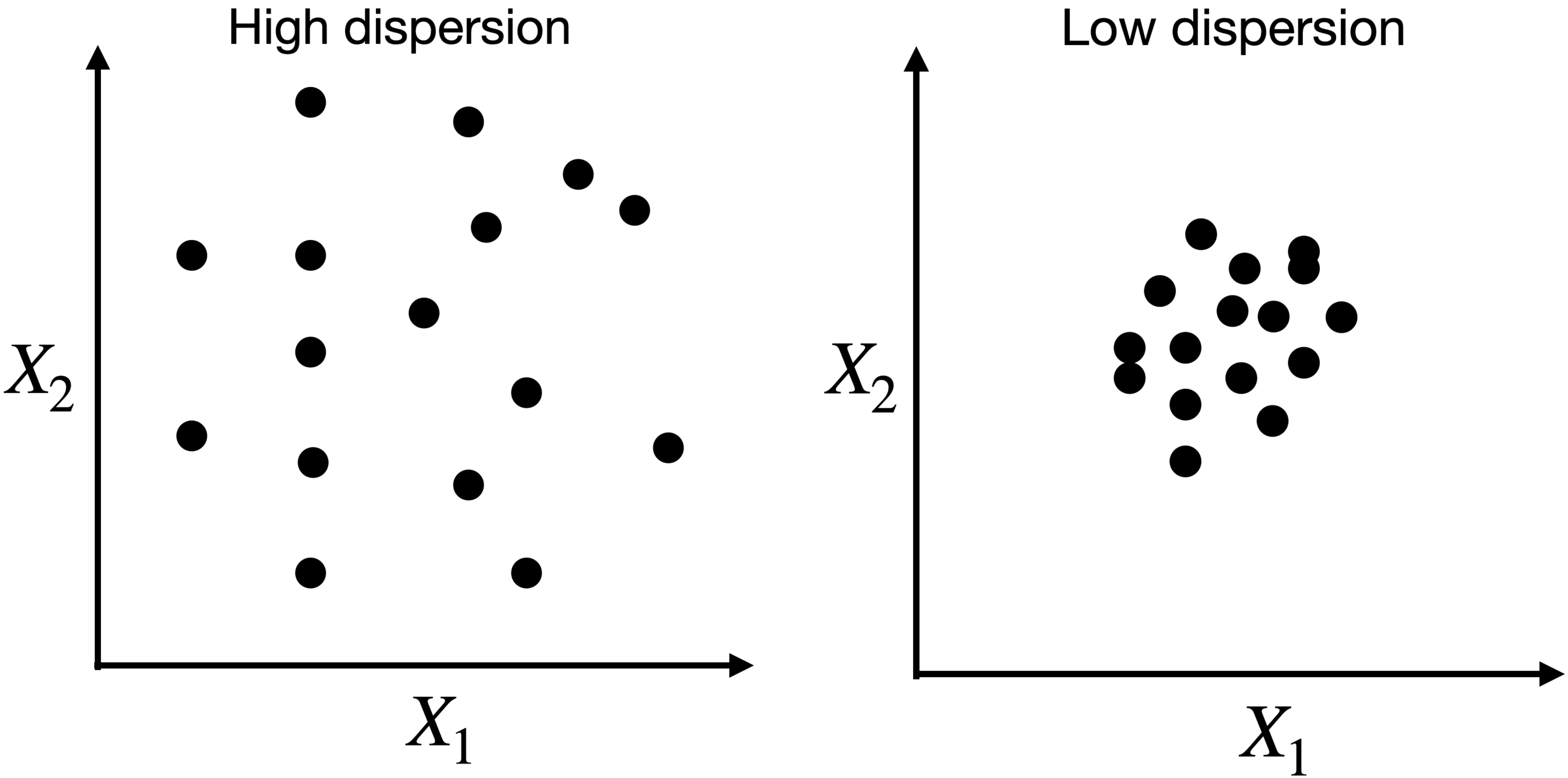
The concept of principal components requires an understanding of the dispersion or variability of the data.

Suppose we have data for a **single predictor**.



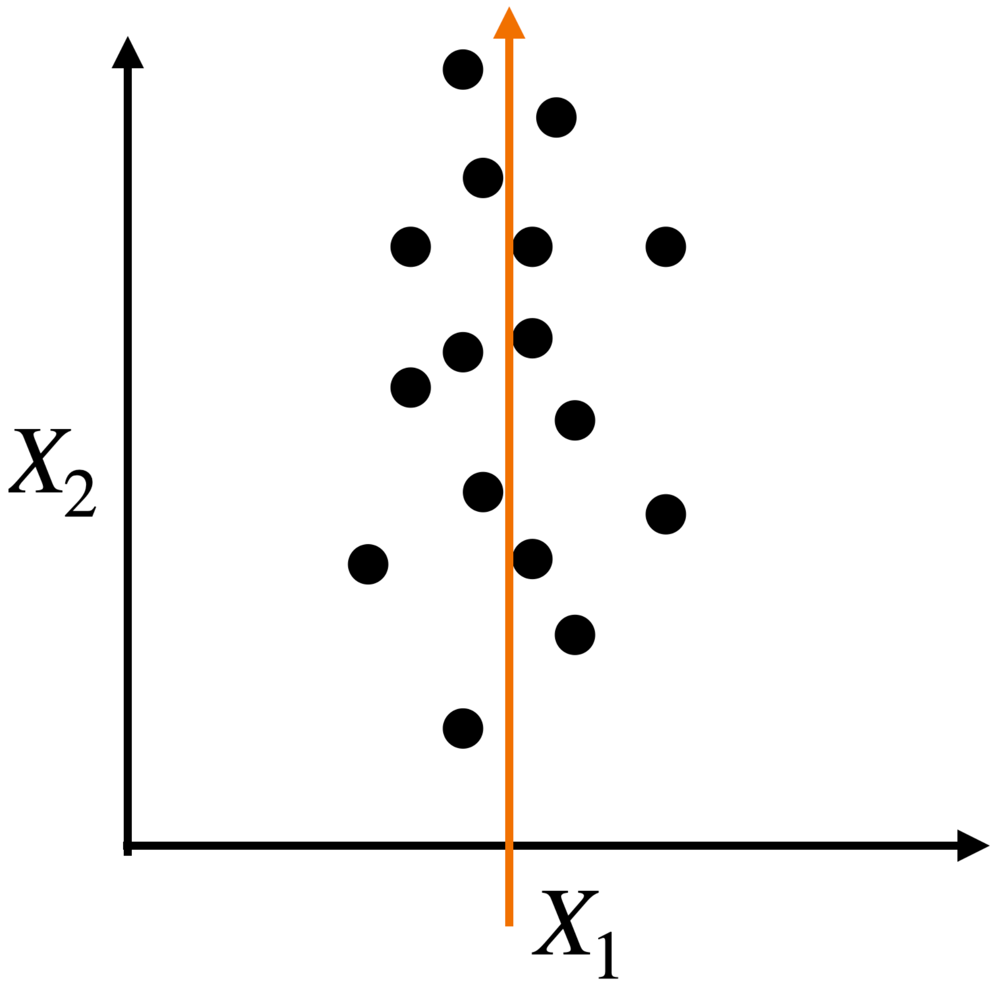


Dispersion in two dimensions


High dispersion
Low dispersion
X_1
X_2
X_1
X_2

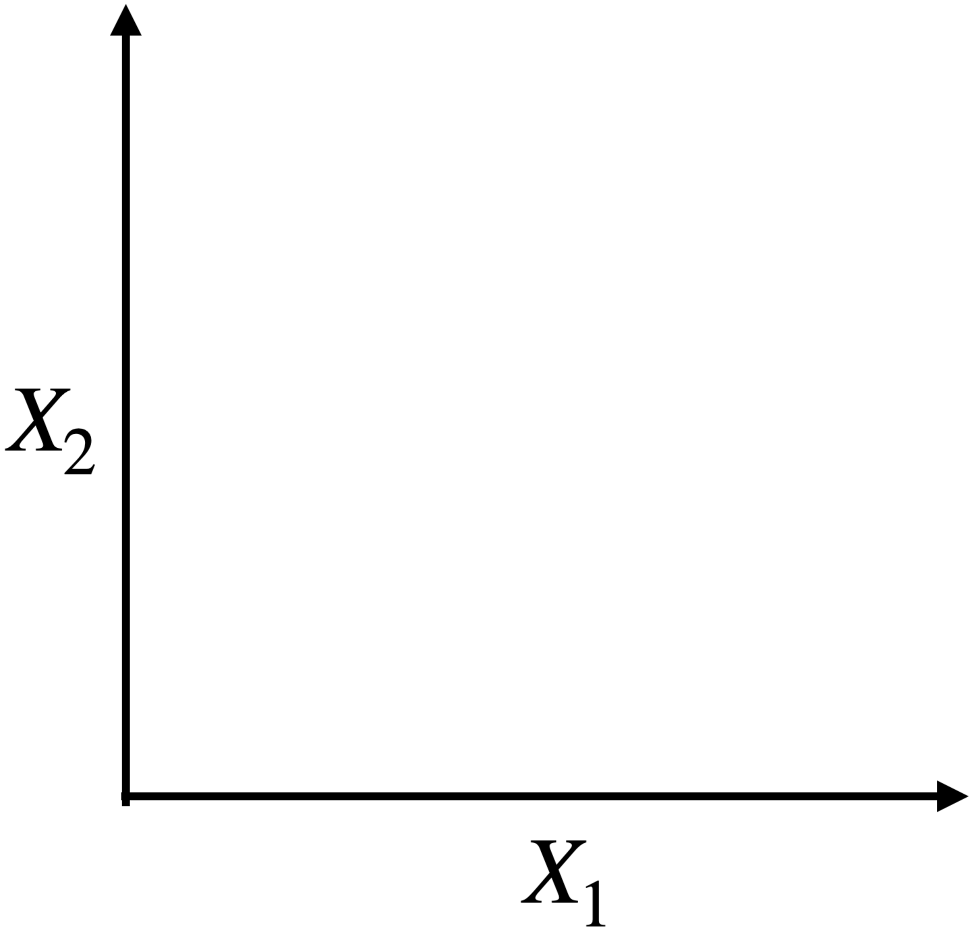
Capturing dispersion

In some cases, we can capture the spread of data in two dimensions (predictors) using a single dimension.

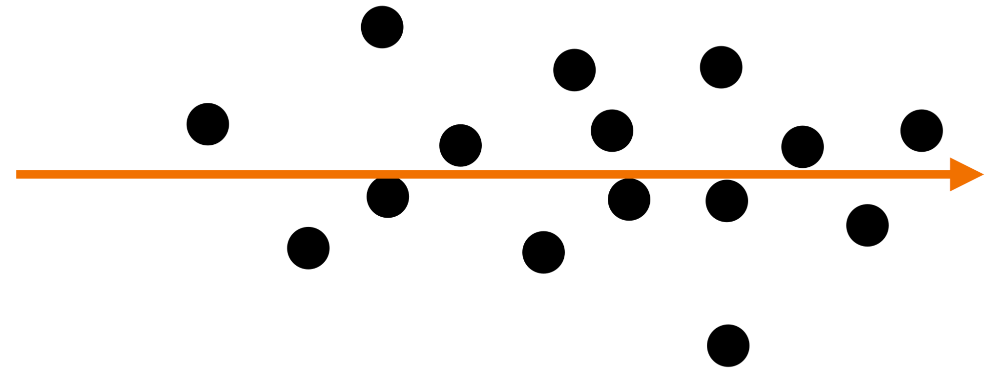

X_2
X_1

Capturing dispersion

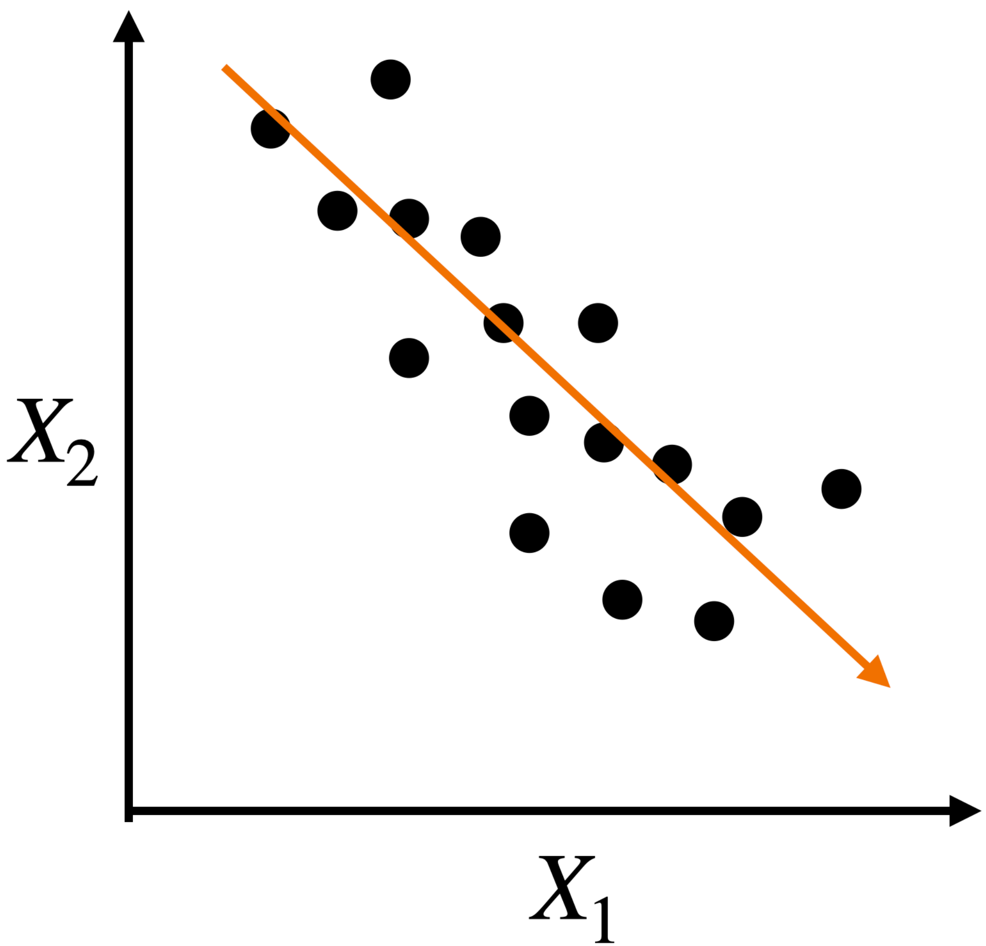
In some cases, we can capture the spread of data in two dimensions (predictors) using a single dimension.



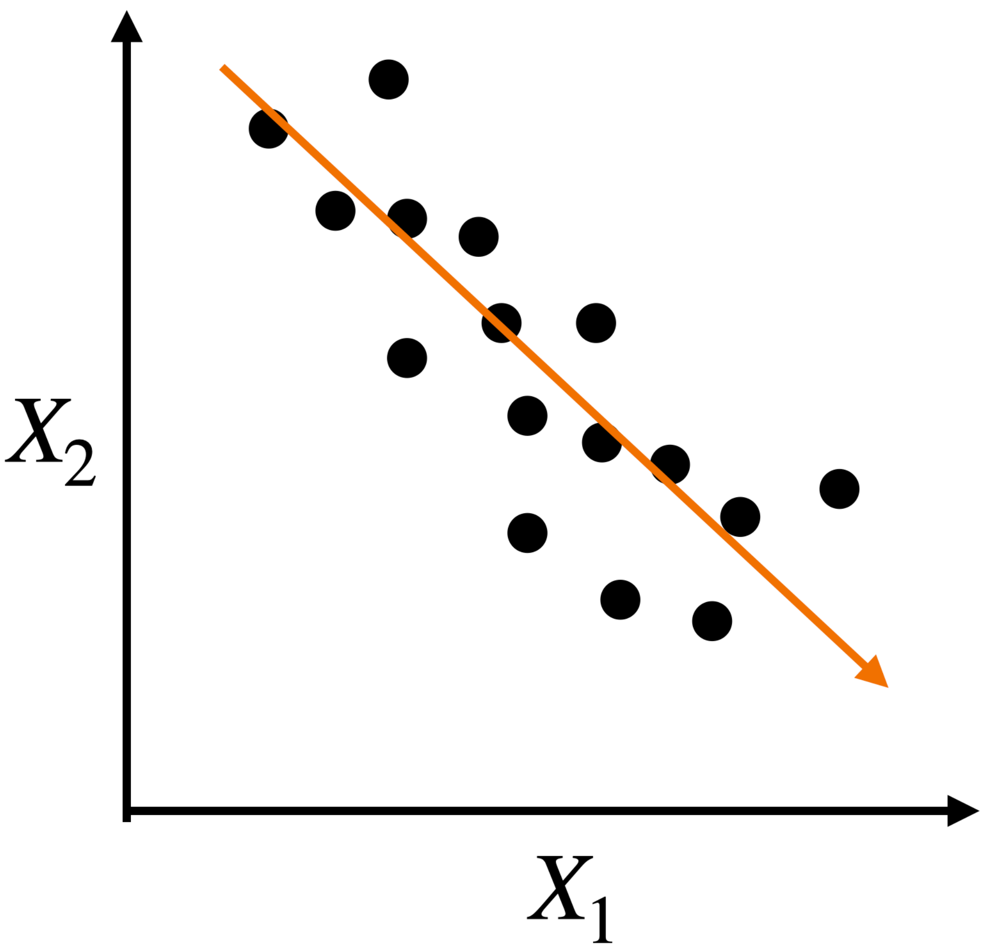
A single predictor X_2 captures much of the spread in the data.



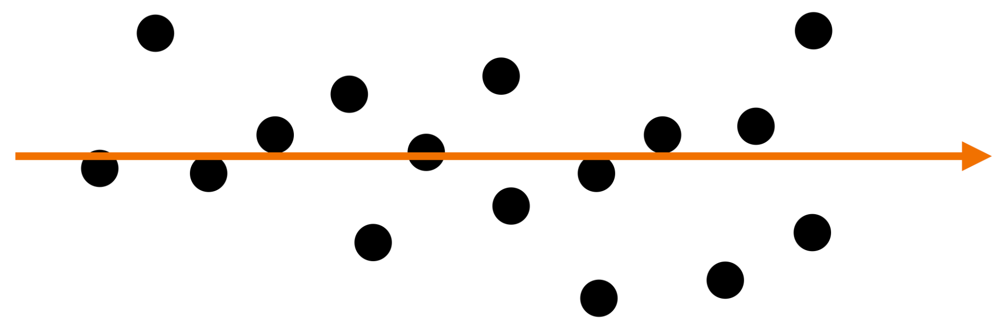
Let’s see another example



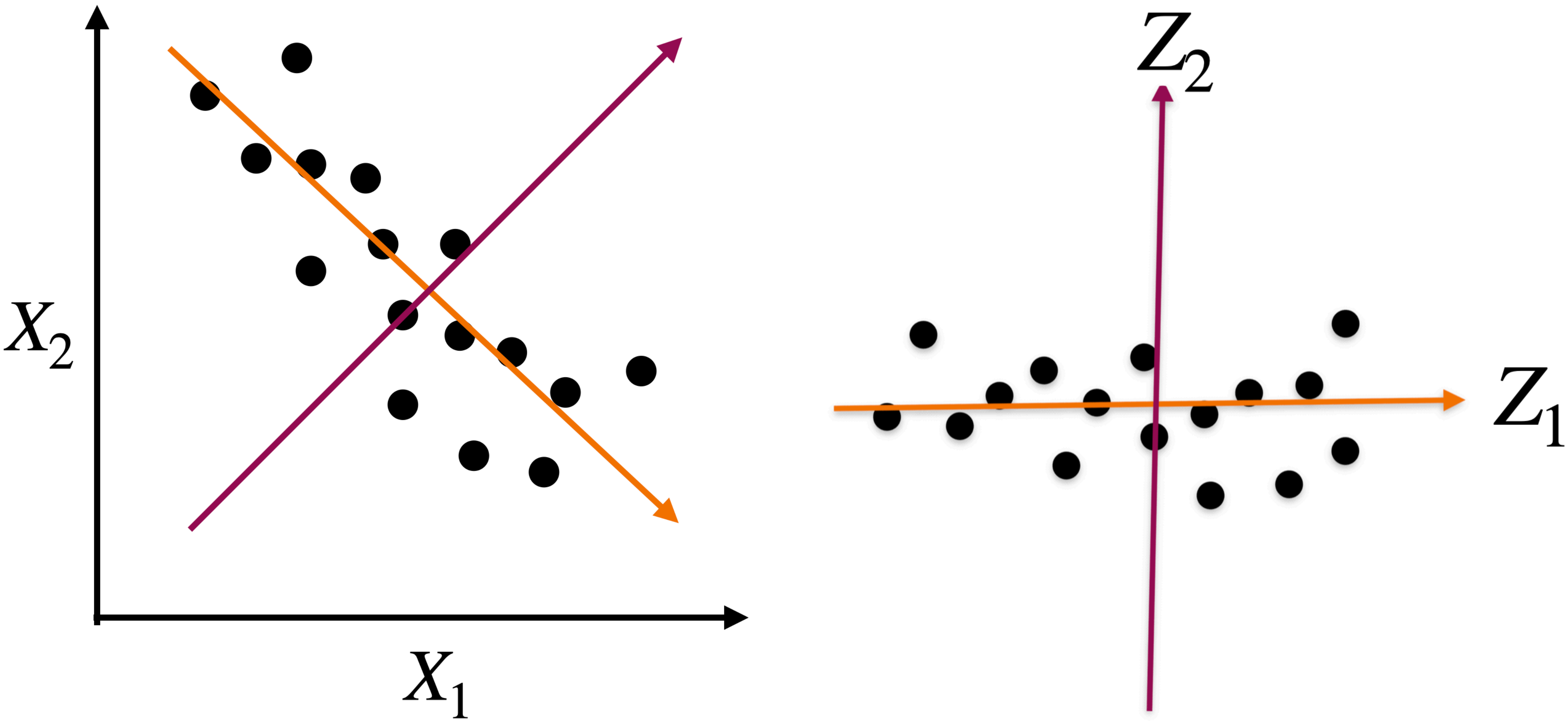
Let’s see another example



A single predictor captures much of the dispersion in the data. In this case, the new predictor has the form $Z_1 = aX_1 + bX_2 + c.$

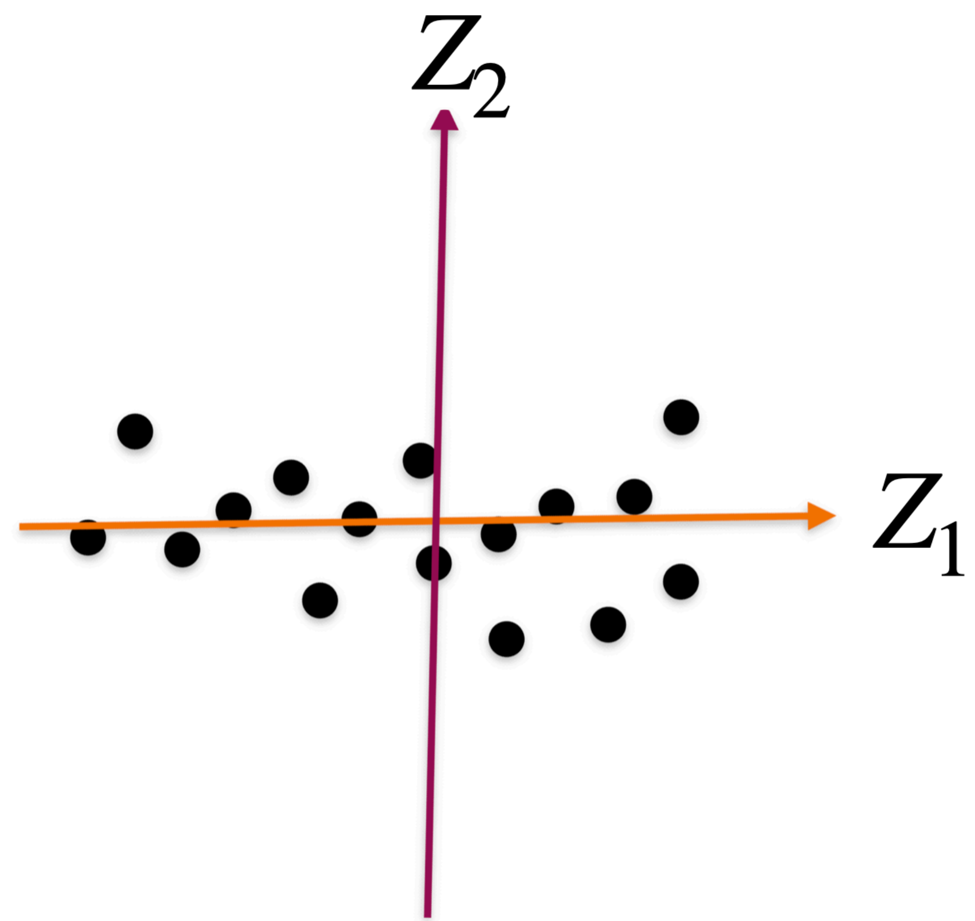


Alternatively, we can use two alternative dimensions to capture the dispersion.


X_2
X_1
Z_2
Z_1

A new coordinate system

- The new coordinate axis is given by two new predictors, Z_1 and Z_2. Both are given by linear equations of the new predictors.
- The first axis, Z_1, captures a large portion of the dispersion, while Z_2 captures a small portion from another angle.
- The new axes, Z_1 and Z_2, are called *principal components*.



Principal Component Analysis

Dimension Reduction

Principal Components Analysis (PCA) helps us reduce the dimension of the data.

- It creates a new coordinate axis in two (or more) dimensions.
- Technically, it creates new predictors by combining highly *correlated* predictors. The new predictors are uncorrelated.

Setup

Step 1. We start with a database with n observations and p predictors.

Predictor 1	Predictor 2	Predictor 3
15	14	5
2	1	6
10	3	17
8	18	9
12	16	11

Step 2. We standardize each predictor individually.

$$\tilde{X}_i = \frac{X_i - \bar{X}}{\sqrt{\frac{1}{n-1}\sum_{i=1}^{n}(X_i - \bar{X})^2}}$$

	Predictor 1	Predictor 2	Predictor 3
	1.15	0.46	-0.96
	-1.52	-1.20	-0.75
	0.12	-0.95	1.55
	-0.29	0.97	-0.13
	0.53	0.72	0.29

	Predictor 1	Predictor 2	Predictor 3
Sum	*0*	*0*	*0*
Variance	*1*	*1*	*1*

IN5148

Step 3. We assume that the standardized database is an $n \times p$ matrix $\mathbf{X}$.

$$\mathbf{X} = \begin{pmatrix} 1.15 & 0.46 & -0.96 \\ -1.52 & -1.20 & -0.75 \\ 0.12 & -0.95 & 1.55 \\ -0.29 & 0.97 & -0.13 \\ 0.53 & 0.72 & 0.29 \end{pmatrix}$$

Algorithm

The PCA algorithm has its origins in linear algebra.

Its basic idea is:

1. Create a matrix $\mathbf{C}$ with the correlations between the predictors of the matrix $\mathbf{X}$.
2. Split the matrix $\mathbf{C}$ into three parts, which give us the new coordinate axis and the importance of each axis.

Correlation matrix

Continuing with our example, the correlation matrix contains the correlations between two columns of $\mathbf{X}$.

Correlation between columns 1 and 1.

$$\mathbf{C} = \begin{pmatrix} \boxed{1.00} & \boxed{0.58} & \boxed{0.11} \\ 0.58 & 1.00 & \boxed{-0.23} \\ 0.11 & -0.23 & 1.00 \end{pmatrix}$$

Correlation between columns 1 and 2.

Correlation between columns 1 y 3.

Correlation between columns 2 y 3.

Partitioning the correlation matrix

The $\mathbf{C}$ matrix is partitioned using the *eigenvalue and eigenvector decomposition method*.

$$\mathbf{C} = \mathbf{B} \quad \mathbf{A} \quad \mathbf{B}^T$$

$$\begin{pmatrix} 1.00 & 0.58 & 0.11 \\ 0.58 & 1.00 & -0.23 \\ 0.11 & -0.23 & 1.00 \end{pmatrix} = \begin{pmatrix} -0.68 & 0.35 & -0.65 \\ -0.72 & -0.13 & 0.68 \\ 0.16 & 0.93 & 0.34 \end{pmatrix} \begin{pmatrix} \boxed{1.60} & 0.00 & 0.00 \\ 0.00 & \boxed{1.07} & 0.00 \\ 0.00 & 0.00 & \boxed{0.33} \end{pmatrix} \begin{pmatrix} -0.68 & -0.72 & 0.16 \\ 0.35 & -0.13 & 0.93 \\ 0.65 & -0.68 & -0.34 \end{pmatrix}$$

Eigen Vectors **Eigen Values**

$$\mathbf{C} = \mathbf{B} \quad \mathbf{A} \quad \mathbf{B}^T$$

$$\begin{pmatrix} 1.00 & 0.58 & 0.11 \\ 0.58 & 1.00 & -0.23 \\ 0.11 & -0.23 & 1.00 \end{pmatrix} = \begin{pmatrix} -0.68 & 0.35 & -0.65 \\ -0.72 & -0.13 & 0.68 \\ 0.16 & 0.93 & 0.34 \end{pmatrix} \begin{pmatrix} \boxed{1.60} & 0.00 & 0.00 \\ 0.00 & \boxed{1.07} & 0.00 \\ 0.00 & 0.00 & \boxed{0.33} \end{pmatrix} \begin{pmatrix} -0.68 & -0.72 & 0.16 \\ 0.35 & -0.13 & 0.93 \\ 0.65 & -0.68 & -0.34 \end{pmatrix}$$

- The columns of $\mathbf{B}$ define the axes of the new coordinate system. These axes are called ***principal components***.
- The diagonal values in $\mathbf{A}$ define the individual importance of each principal component (axis).

Proportion of the dispersion explained by the component

$$\mathbf{A} = \begin{pmatrix} 1.60 & 0.00 & 0.00 \\ 0.00 & 1.07 & 0.00 \\ 0.00 & 0.00 & 0.33 \end{pmatrix}$$

The proportion of the dispersion in the data that is captured by the first component is $\frac{a_{1,1}}{p} = \frac{1.60}{3} = 0.53.$

$$\mathbf{A} = \begin{pmatrix} 1.60 & 0.00 & 0.00 \\ 0.00 & 1.07 & 0.00 \\ 0.00 & 0.00 & 0.33 \end{pmatrix}$$

The proportion captured by the second component is $\frac{a_{2,2}}{p} = \frac{1.07}{3} = 0.36.$

The proportion captured by the third component is $\frac{a_{3,3}}{p} = \frac{0.33}{3} = 0.11.$

Comments

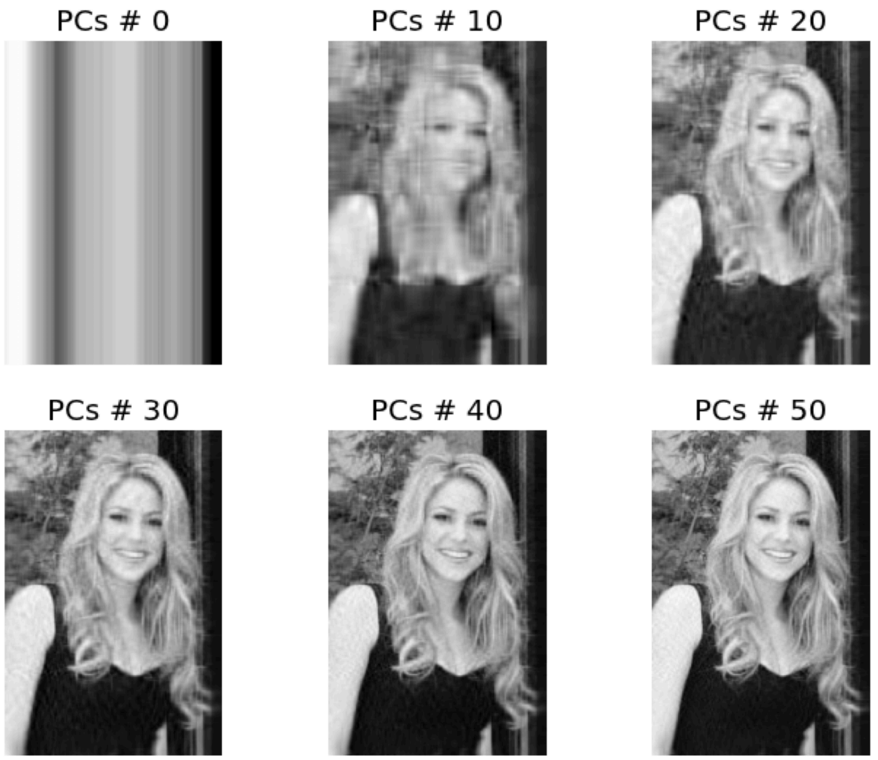
Principal components can be used to approximate a matrix.

For example, we can approximate the matrix $\mathbf{C}$ by setting the third component equal to zero.

$$\begin{pmatrix} -0.68 & 0.35 & 0.00 \\ -0.72 & -0.13 & 0.00 \\ 0.16 & 0.93 & 0.00 \end{pmatrix} \begin{pmatrix} 1.60 & 0.00 & 0.00 \\ 0.00 & 1.07 & 0.00 \\ 0.00 & 0.00 & 0.00 \end{pmatrix} \begin{pmatrix} -0.68 & -0.72 & 0.16 \\ 0.35 & -0.13 & 0.93 \\ 0.00 & 0.00 & 0.00 \end{pmatrix} = \begin{pmatrix} 0.86 & 0.73 & 0.18 \\ 0.73 & 0.85 & -0.30 \\ 0.18 & -0.30 & 0.96 \end{pmatrix}$$

$$\approx \begin{pmatrix} 1.00 & 0.58 & 0.11 \\ 0.58 & 1.00 & -0.23 \\ 0.11 & -0.23 & 1.00 \end{pmatrix} = \mathbf{C}$$

- Approximations are useful for storing large matrices.
- This is because we only need to store the largest eigenvalues and their corresponding eigenvectors to recover a high-quality approximation of the entire matrix.
- This is the idea behind **image compression**.



Example 1

Consider a database of the 100 most popular songs on TikTok. The data is in the file “TikTok 2020 reduced.xlsx”. There are observations of several predictors, such as:

- Danceability describes how suitable a track is for dancing based on a combination of musical elements.
- Energy is a measure from 0 to 1 and represents a perceptual measure of intensity and activity.
- The overall volume of a track in decibels (dB). Loudness values are averaged across the entire track.

Other predictors are:

- Speech detects the presence of spoken words in a track. The more exclusively speech-like the recording is.
- A confidence measure from 0 to 1 about whether the track is acoustic.
- Detects the presence of an audience in the recording.
- A measure from 0 to 1 that describes the musical positivity a track conveys.

The data

```
tiktok_data = pd.read_excel("TikTok_Songs_2020_Reduced.xlsx")
tiktok_data.head()
```

	track_name	artist_name	album	danceability	ener
0	Say So	Doja Cat	Hot Pink	0.787	0.67
1	Blinding Lights	The Weeknd	After Hours	0.514	0.73
2	Supalonely (feat. Gus Dapperton)	BENEE	Hey u x	0.862	0.63

	track_name	artist_name	album	danceability	ener
3	Savage	Megan Thee Stallion	Suga	0.843	0.74
4	Moral of the Story	Ashe	Moral of the Story	0.572	0.40

Standardize the data

Remember that PCA works with distances, so we must standardize the quantitative predictors to have an accurate analysis.

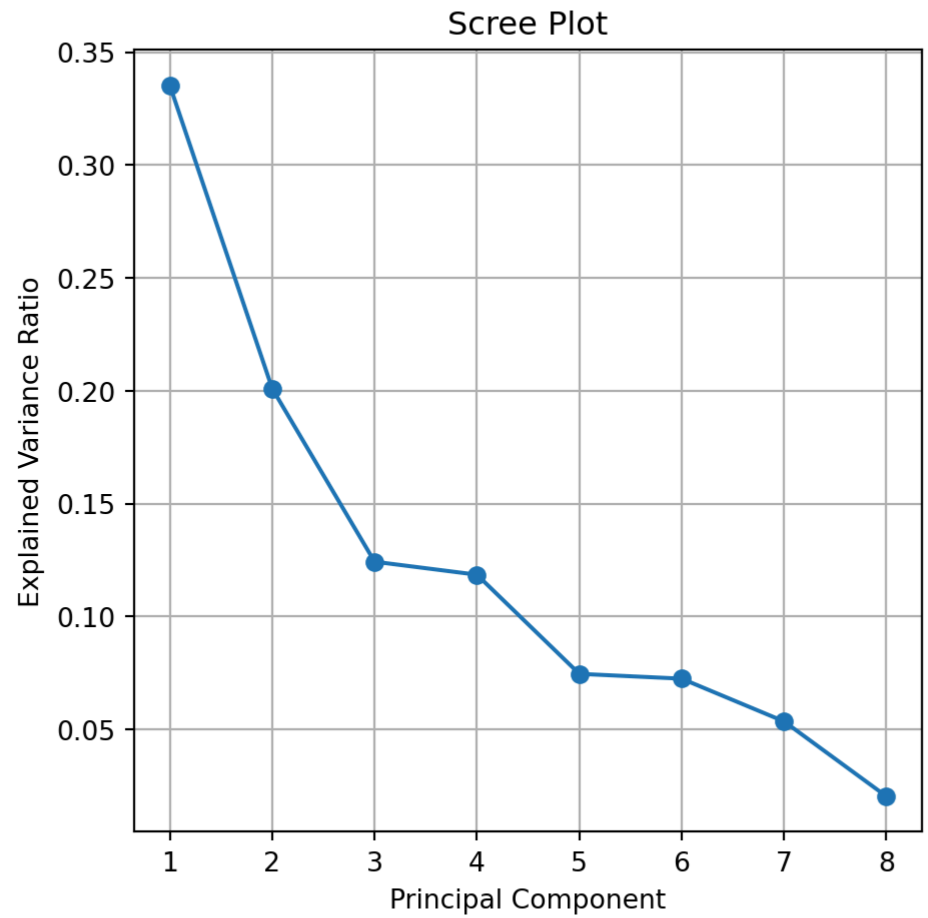
```
# Select the predictors
features = ['danceability', 'energy', 'loudness', 'speechiness',
            'acousticness', 'liveness', 'valence', 'tempo']
X_tiktok = tiktok_data.filter(features)

# Standardize the data
scaler = StandardScaler()
Xs_tiktok = scaler.fit_transform(X_tiktok)
```

PCA in Python

We tell Python that we want to apply PCA using the function `PCA()` from **sklearn**. Next, we run the algorithm using `.fit_transform()`.

```
pca = PCA()
PCA_tiktok = pca.fit_transform(Xs_tiktok)
```

- The **Screen or Summary Plot** tells you the variability captured by each component. This variability is given by the *Eigenvalue*. From 1 to 8 components.
- The first component covers most of the data dispersion.
- This graph is used to define the total number of components to use.



The code to generate a scree plot is below.

```python
explained_var = pca.explained_variance_ratio_

plt.figure(figsize=(5, 5))
plt.plot(range(1, len(explained_var) + 1), explained_var,
         marker='o', linestyle='-')
plt.title('Scree Plot')
plt.xlabel('Principal Component')
plt.ylabel('Explained Variance Ratio')
plt.xticks(range(1, len(explained_var) + 1))
plt.grid(True)
plt.tight_layout()
plt.show()
```

Biplot

The code to generate the biplot is lenghty but it can be broken into three steps.

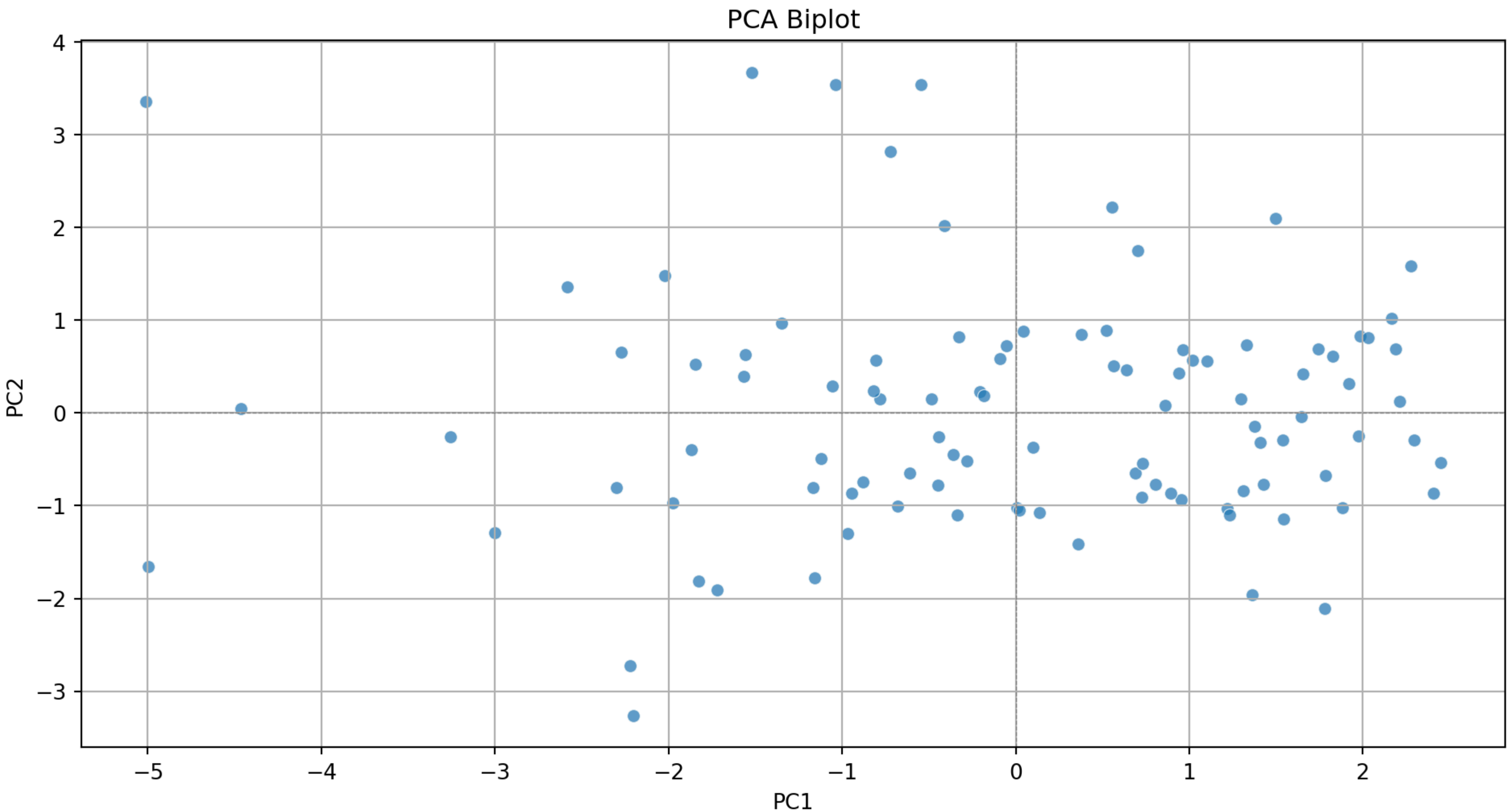
Step 1. Create a DataFrame with the PCA results

```
pca_df = pd.DataFrame(PCA_tiktok, columns=[f'PC{i+1}' for i in range(PCA_ti
pca_df.head()
```

	PC1	PC2	PC3	PC4	PC5
0	1.103065	0.558086	-0.800688	0.446496	0.605944
1	0.805080	-0.766973	1.580513	-2.215856	0.359655
2	1.330433	0.728161	-0.288982	0.376298	0.786185
3	1.496277	2.095014	1.351398	-0.621691	0.390949
4	-1.973362	-0.966108	-0.302071	-1.266269	0.41463[illegible]

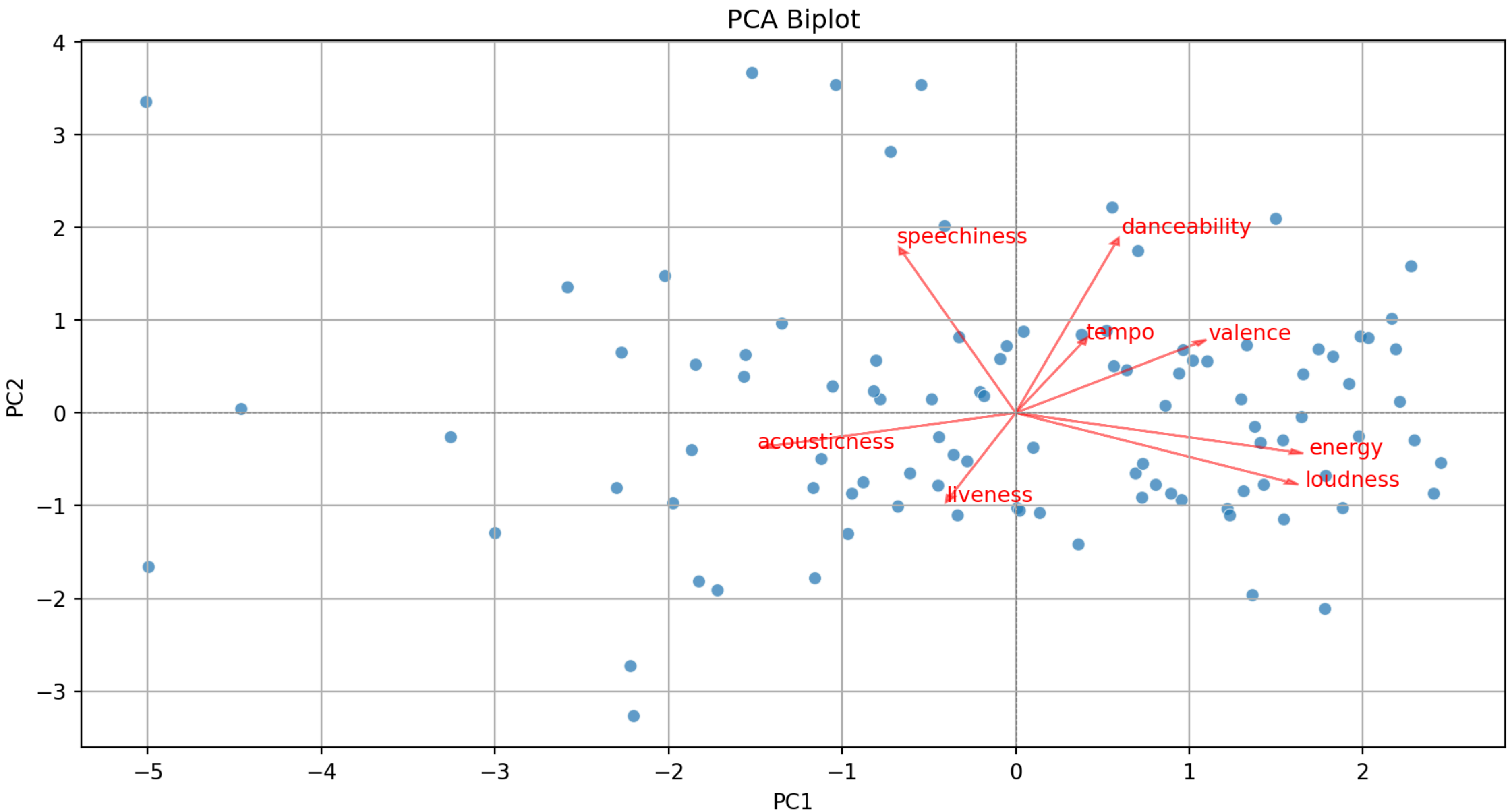
Step 2. Create biplot of first two principal components

▶ Code



Step 3. Add more information to the biplot.

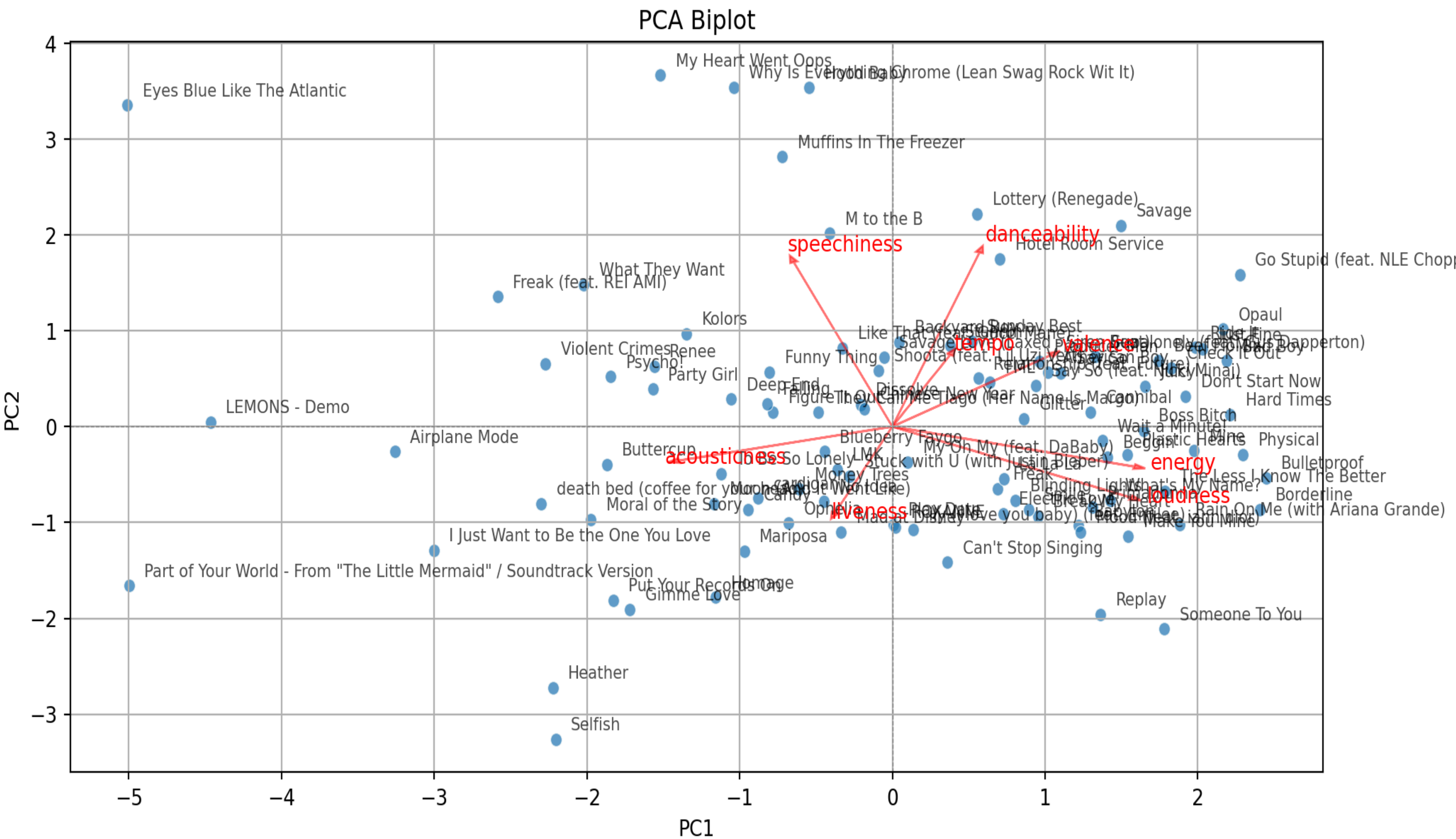
- Code



IN5148

With some extra lines of code, we label the points in the plot.

▶ Code



IN5148

Return to main page