SAMSUNG

# Samsung Innovation Campus

## Artificial Intelligence Course

Together for Tomorrow!
Enabling People
Education for Future Generations

Chapter 6.

# Machine Learning 2
# - Unsupervised Learning

Artificial Intelligence Course

# Chapter Description

## Chapter objectives

- ✓ Be able to apply necessary machine learning techniques according to the established analysis plan.
- ✓ Be able to apply various unsupervised learning techniques for data compression by reducing high-dimension data into low-dimension and data visualization by reducing dimensions.
- ✓ Be able to solve problems by applying various clustering techniques for subject segmentation.
- ✓ Be able to perform matrix decomposition and principal component analysis and applications.

## Chapter contents

- ✓ Unit 1. Unsupervised Machine Learning Algorithm
- ✓ Unit 2. Hierarchical Clustering
- ✓ Unit 3. Non-Hierarchical Clustering
- ✓ Unit 4. Linear Factor Model for Dimensionality Reduction

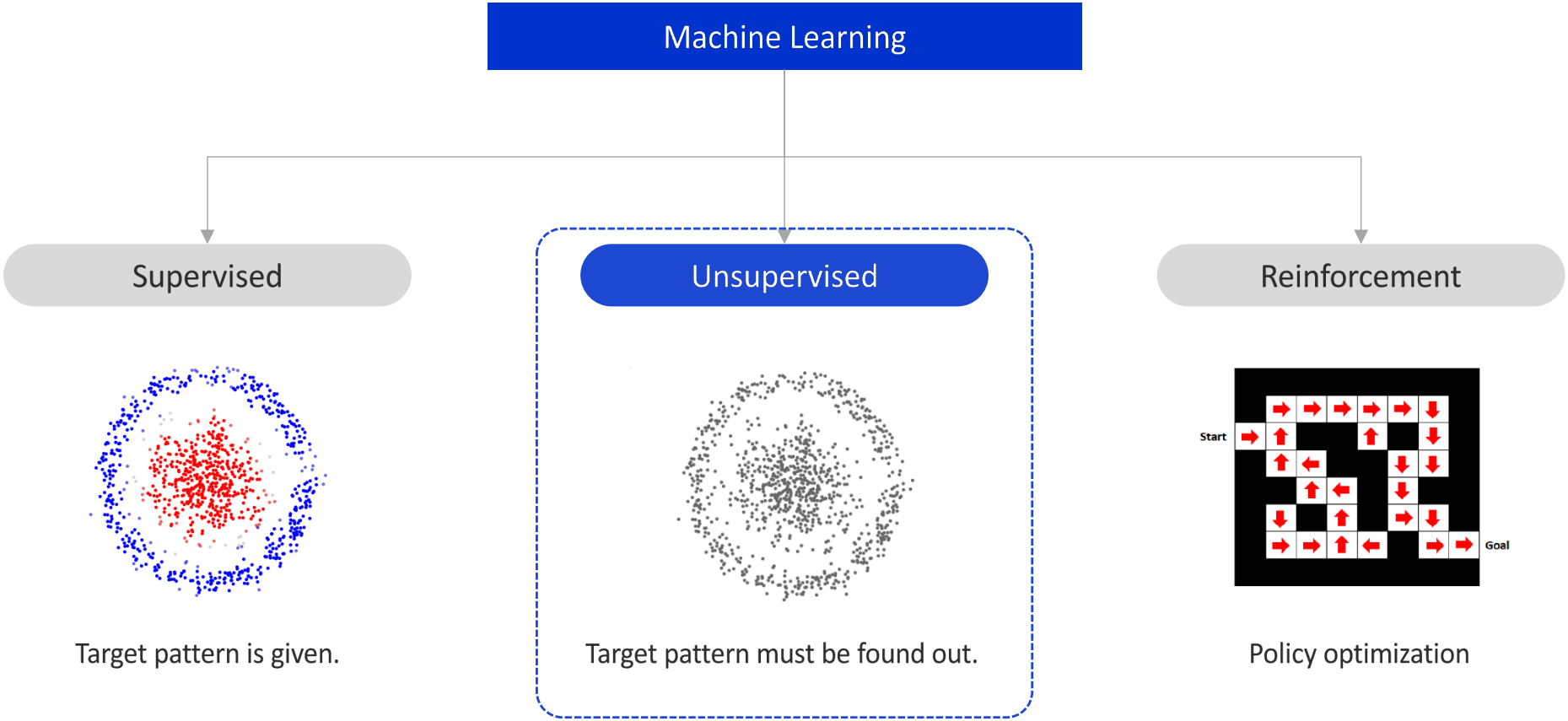
Unit 1.

# Unsupervised Machine Learning Algorithm

1.1. The Concept of Unsupervised Learning

1.2. Clustering Analysis

# Machine Learning Types



# What is unsupervised learning?

## The concept of unsupervised learning

- It is a machine learning technique performed only when a series of variables such as $x_1, x_2, x_3, \ldots x_p$ is given without any objective variables (or response variable Y) in a data set.
- Since no objective variables (or response variables) are associated with explanatory variables, unsupervised learning aims to discover a specific pattern or unknown knowledge from given data instead of making a prediction.

# What is unsupervised learning?

## Machine learning for unsupervised learning

- **Clustering** refers to making groups of similar objects or people according to the analysis purpose and algorithm.
- **Association** refers to uncovering a co-occurrence relationship between specific items in a dataset.
- **Dimensionality reduction** refers to summarizing a given variable set into a smaller number of variables for providing effective explanations.

Unit 1.

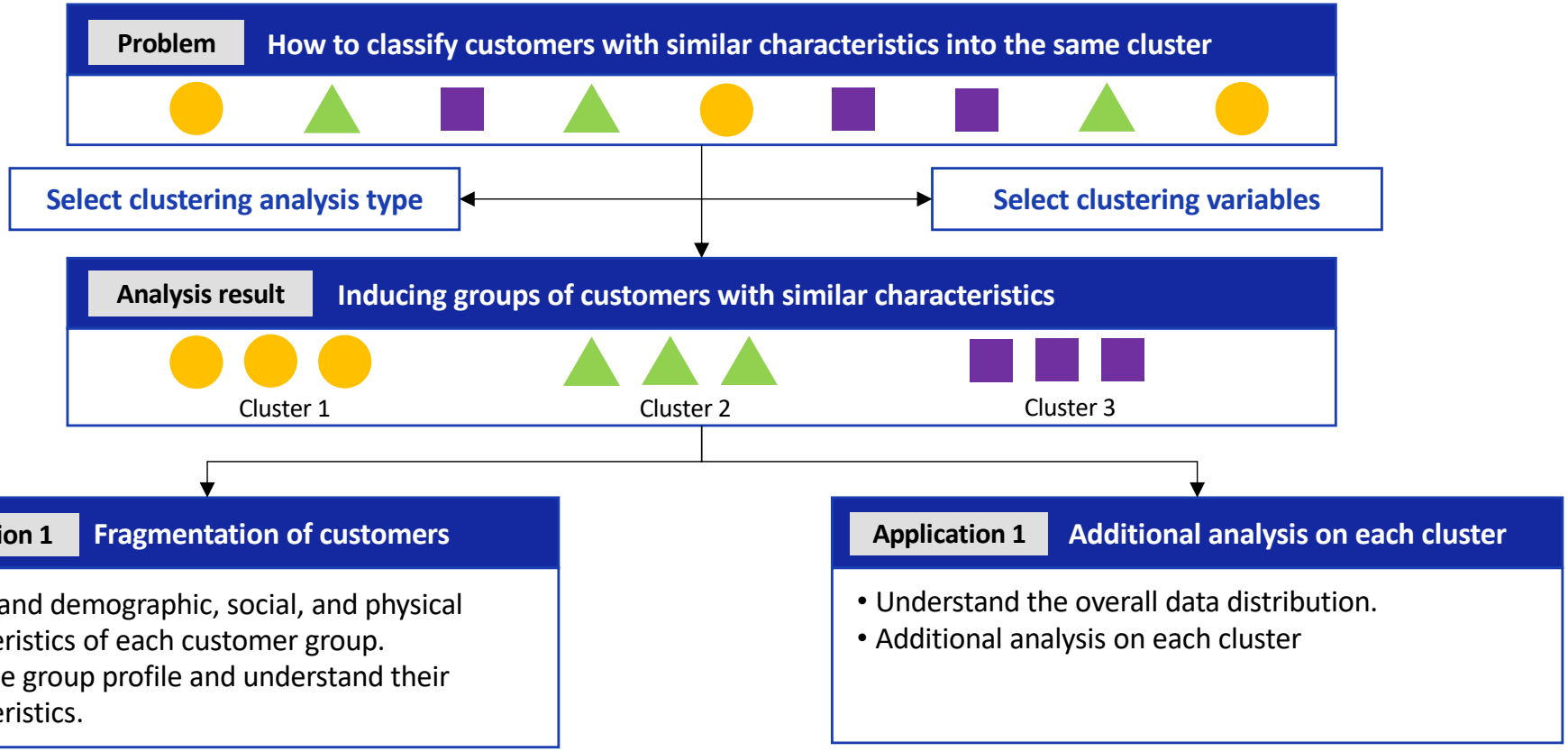
# Unsupervised Machine Learning Algorithm

1.1. The Concept of Unsupervised Learning

1.2. Clustering Analysis

# What is clustering analysis?

Clustering is a technique that divides unlabeled and uncategorized data into similar groups based on the given observed values.

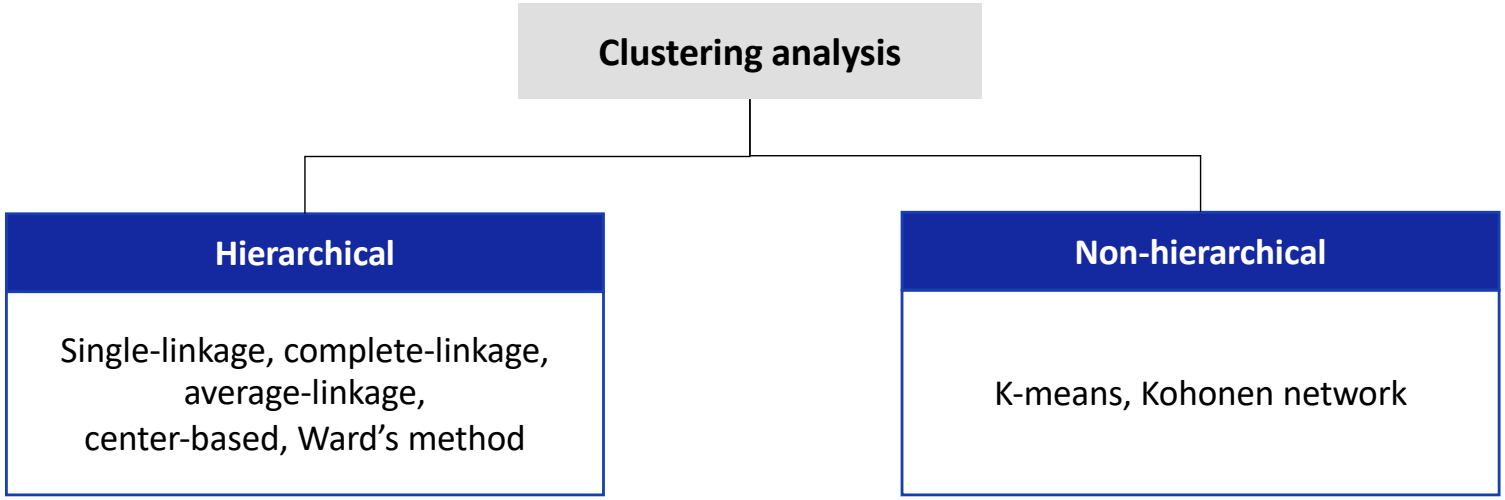


## Clustering analysis

- Clustering technique is the most common type of unsupervised learning. It groups unlabeled data into similar observed values based on suitable criteria.
- Since clustering deals with unknown groups within the data, analysts cannot instruct the computer program what to find.
- Thus, clustering is mainly used to figure out the attributes of different groups and give us insight into the underlying patterns of different groups rather than for making a prediction.

## Types of clustering analysis

- **Hierarchical clustering**: divisive and agglomerative
- **Non-hierarchical clustering**: the number of clusters is determined in advance.



## Types of clustering analysis

- In general, clustering analysis is classified into hierarchical clustering, non- hierarchical clustering, and partition-based clustering.

| | |
|---|---|
| Non-Hierarchical Clustering (Partition-based Clustering) | K-means clustering |
| | K-medoids clustering or PAM (Partitioning Around Method) |
| | DBSCAN (Density Based Spatial Clustering of Application with Noise) |
| | Self Organizing Map |
| | Fuzzy clustering |
| Hierarchical Clustering | Agglomerative or bottom-up clustering |
| | Divisive or top-down clustering |
| Mixture Distribution Clustering | Gaussian Mixture Model |

## Application of clustering analysis

- Identifying the pattern of unknown data groups in financial data analysis
- Detecting any network intrusions (unauthorized penetration activities on a computer network)
- Object and facial recognition from digital images
- Clustering documents, music, or movies into different themes
- Customer segmentation in the marketing field

Unit 2.

# Hierarchical Clustering

## 2.1. Hierarchical method

# Hierarchical method

Hierarchical method is useful for sorting clusters in the natural hierarchy structure. There are two hierarchical clustering methods, which are agglomerative and divisive clustering.

- Agglomerative clustering
  - Bottom-Up
  - It starts with n-clusters to progressively agglomerate similar clusters until one final cluster remains.
- Divisive clustering
  - Top-Down
  - It starts with a single cluster that includes all records and divides it into n-clusters (agglomerative clustering is a mainly used hierarchical method).

## How does **agglomerative clustering** work?

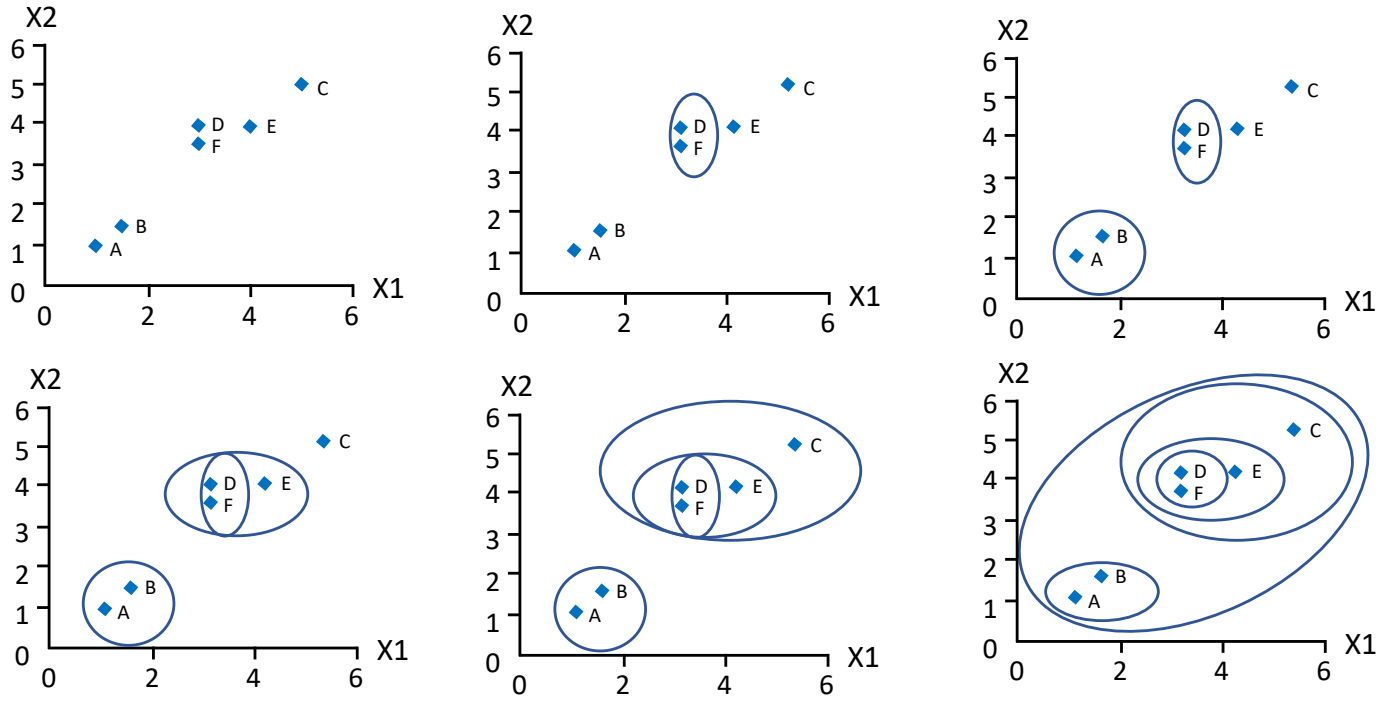
- It starts with single-record clusters.
- Pairs of similar clusters are merged until all clusters are merged into one big cluster containing all records.

## What is **agglomerative clustering algorithm**?

- It starts with n-clusters.
- It merges two closest record clusters into one cluster.
- Two closest clusters are merged in every step. This refers to adding single records to the existing cluster or combining two existing clusters.

## Agglomerative hierarchical clustering

- Start: Each object is an individual atomic cluster.
- Repetition: Repeated merging of two closest clusters
- Finish: Generates a single cluster



# Hierarchical Clustering

## About the hierarchical clustering

- This is a unsupervised learning algorithm; there are only $X$ variables.
- It is also called “agglomerative clustering.”
- Nearest items are gathered to form ever growing clusters.
- Itan be visualized resembling an inverted tree-like structure called “dendrogram.”

## Purpose of the hierarchical clustering

- Cluster the observations into a given number of clusters.

# 2.1. Hierarchical method

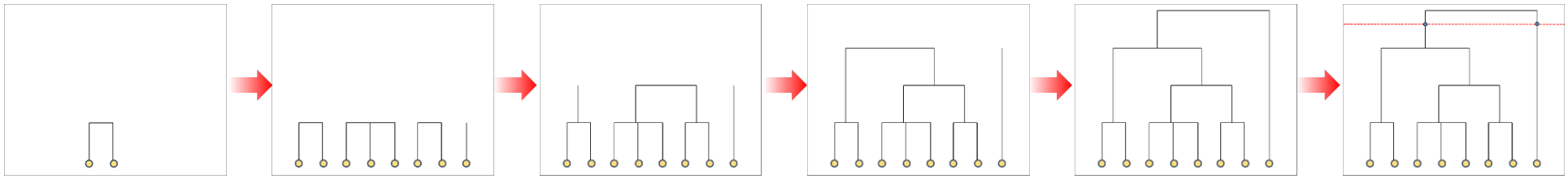
## Pros

- Intuitive interpretation of the results
- Dendrogram that can be further processed to produce a desired number of clusters

## Cons

- A bit more time consuming than k-means

## Hierarchical clustering algorithm



(a) (b) (c) (d) (e) (f)

1) First, group together the nearest observations and get small clusters: (a) ~ (b).

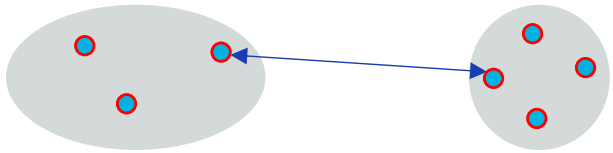
2) Group the nearest clusters together to form larger clusters: (c).

3) Repeat step 2) until all the observations are grouped together into a single cluster: (d) ~ (e).

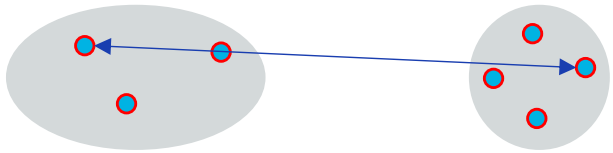
4) Cut the dendrogram at an appropriate height such that we get the desired number of clusters: (f).

## Hierarchical clustering algorithm

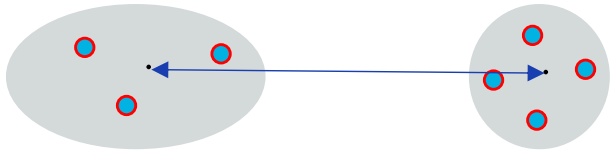
- How do we measure the inter-cluster distances?



Single linkage



Complete linkage



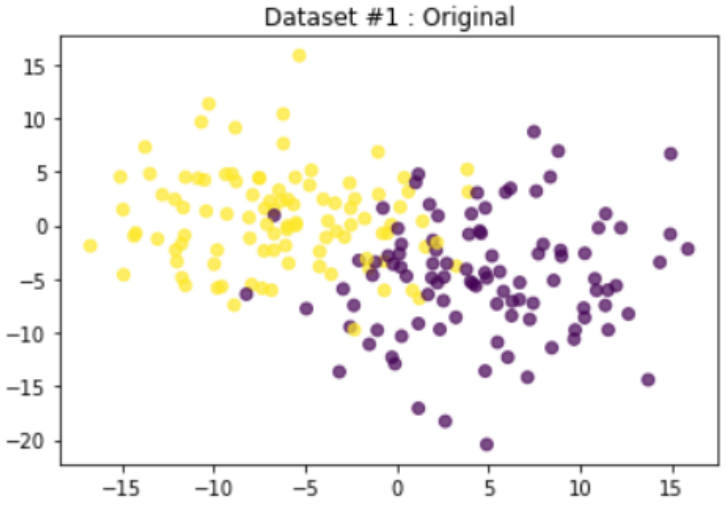
Average linkage

# Apply agglomerative clustering and visualize

## Dataset #1

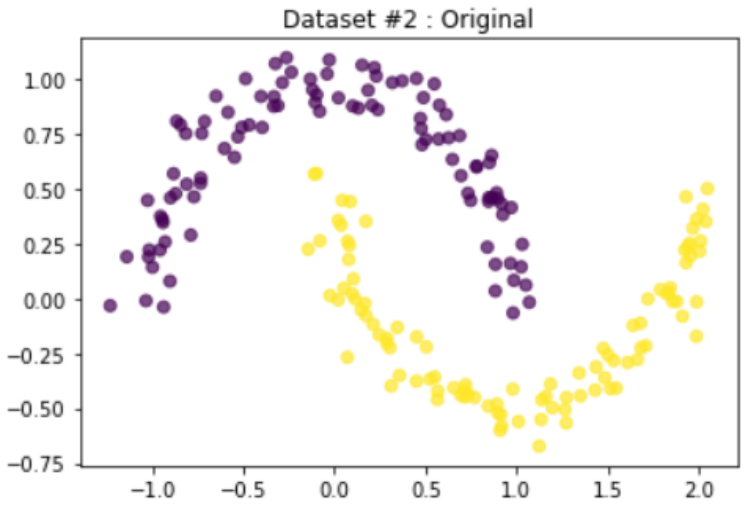
In [1]:
```
from sklearn.datasets import make_blobs, make_moons
import matplotlib.pyplot as plt
```

In [2]:
```
X1, label1 = make_blobs(n_samples=200, n_features=2, centers=2, cluster_std = 5, random_state=123)
plt.scatter(X1[:,0],X1[:,1], c= label1, alpha=0.7 )
plt.title('Dataset #1 : Original')
plt.show()
```



## Dataset #2

In [3]:
```
X2, label2 = make_moons(n_samples=200, noise=0.08, random_state=123)
plt.scatter(X2[:,0],X2[:,1], c= label2, alpha=0.7 )
plt.title('Dataset #2 : Original')
plt.show()
```



## Clusters

In [4]:
```
from sklearn.cluster import AgglomerativeClustering
```

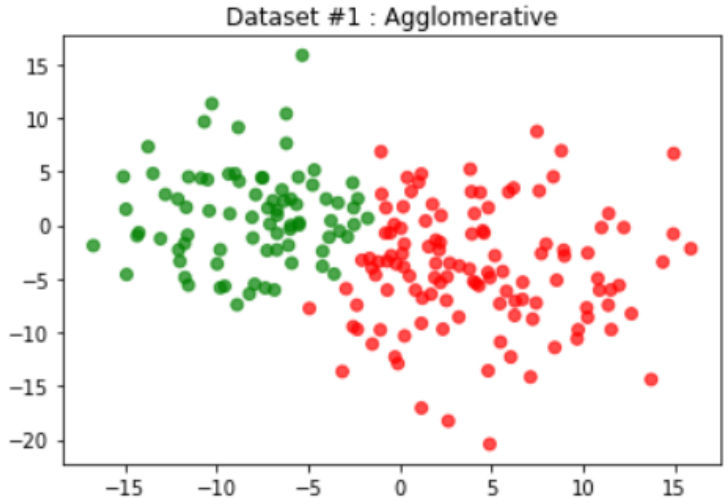
In [5]:
```
import numpy as np
import pandas as pd
```

In [6]:
```
X1
```

Out[6]:
```
array([[ 4.83455936e+00,  1.61209639e+00],
       [-7.19342110e+00,  1.57331116e+00],
       [-1.19919003e+01, -3.38784956e+00],
       [ 8.94965320e+00, -2.34628131e+00],
       [ 5.46630481e+00, -7.33334000e+00],
       [-9.82679362e-01,  2.87439331e+00],
       [ 4.82713114e+00, -1.35870919e+01],
       [-5.95639441e+00, -4.86198432e-02],
       [ 3.25723451e+00, -3.81242660e+00],
       [-1.49388489e+01,  1.46494770e+00],
       [-9.32588959e+00,  4.75039194e+00],
       [ 1.23752259e+00, -6.81998526e+00],
       [ 1.19728386e+01, -5.62837526e+00],
       [-2.58199902e-01, -1.23070271e+01],
       [ 1.49590341e+01,  6.65671714e+00],
       [ 2.25314845e-01, -3.91267708e+00],
       [-5.93898363e+00,  2.41971297e+00],
       [-4.66024882e+00,  5.12509843e+00],
       [-2.49261965e+00,  3.07334679e-02],
       [ 7.73413068e+00, -2.65986906e+00],
       [-5.12306455e-01, -7.42476287e-01],
       [ 1.57887480e+00, -2.01725863e+00],
       [-4.20565001e+00, -2.44769569e+00],
       [-4.00859899e+00,  2.42460873e+00],
       [ 3.91603180e+00,  3.10476808e+00],
       [-1.05722363e+00, -9.77742886e+00],
```

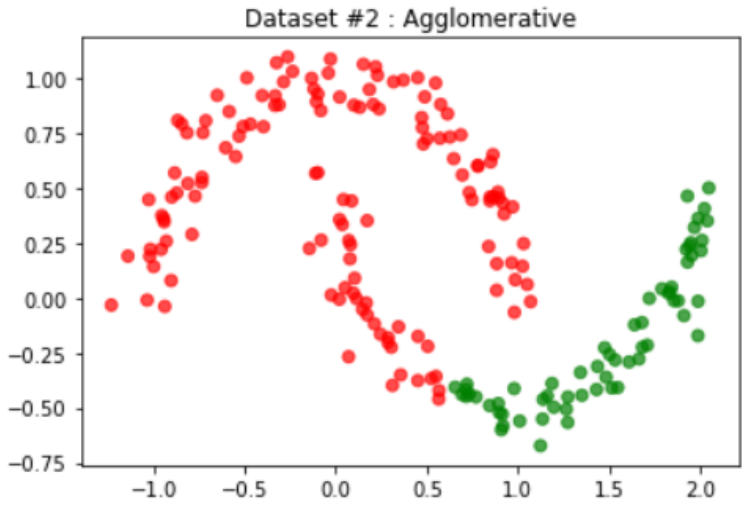
## Dataset #1 and two clusters

In [7]:
```
agglo = AgglomerativeClustering(n_clusters=2)
agglo.fit(X1)
myColors = {0:'red',1:'green'}                                    # Define a color palette: 0~1.
plt.scatter(X1[:,0],X1[:,1], c= pd.Series(agglo.labels_).apply(lambda x: myColors[x]), alpha=0.7 )
plt.title('Dataset #1 : Agglomerative')
plt.show()
```



## Dataset #2 and two clusters

In [8]:
```
agglo = AgglomerativeClustering(n_clusters=2)
agglo.fit(X2)
myColors = {0:'red',1:'green'}                                  # Define a color palette: 0~1.
plt.scatter(X2[:,0],X2[:,1], c= pd.Series(agglo.labels_).apply(lambda x: myColors[x]), alpha=0.7 )
plt.title('Dataset #2 : Agglomerative')
plt.show()
```

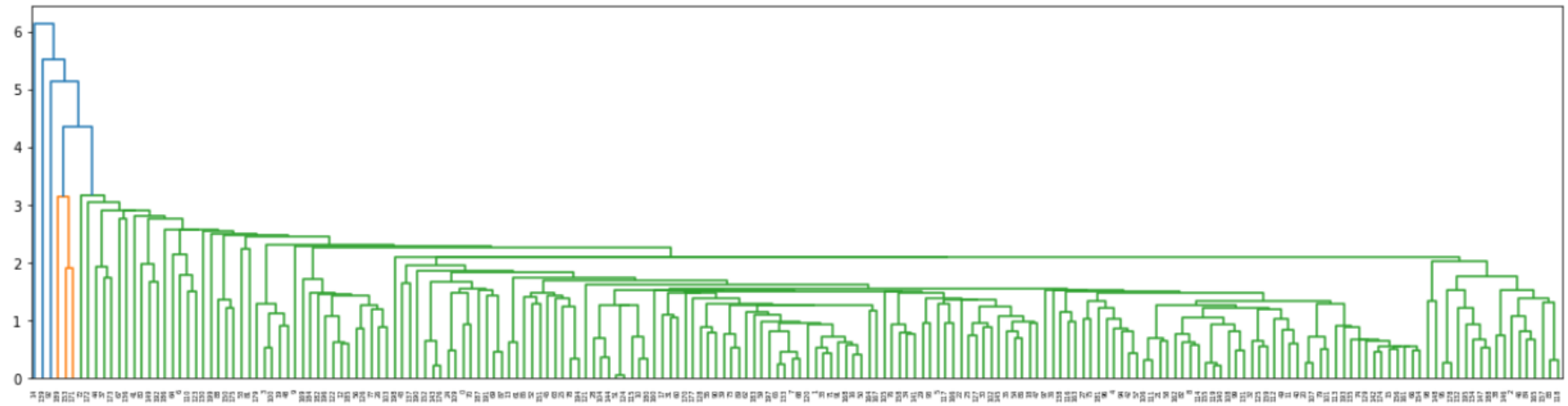


## Applying hierarchical clustering and visualizing

- Dataset #1 and show dendrogram.
- Cluster hierarchically using single linkage

In [9]:
```
from scipy.cluster.hierarchy import linkage, dendrogram, fcluster
```

In [10]:
```
myLinkage = linkage(X1,method='single')
plt.figure(figsize=(20,5))
dendrogram(myLinkage)
plt.show()
```



## Applying hierarchical clustering and visualizing

- Dataset #1 and clusters by cutting the dendrogram
- Cut at the height (distance) = 5 (change this value at will).

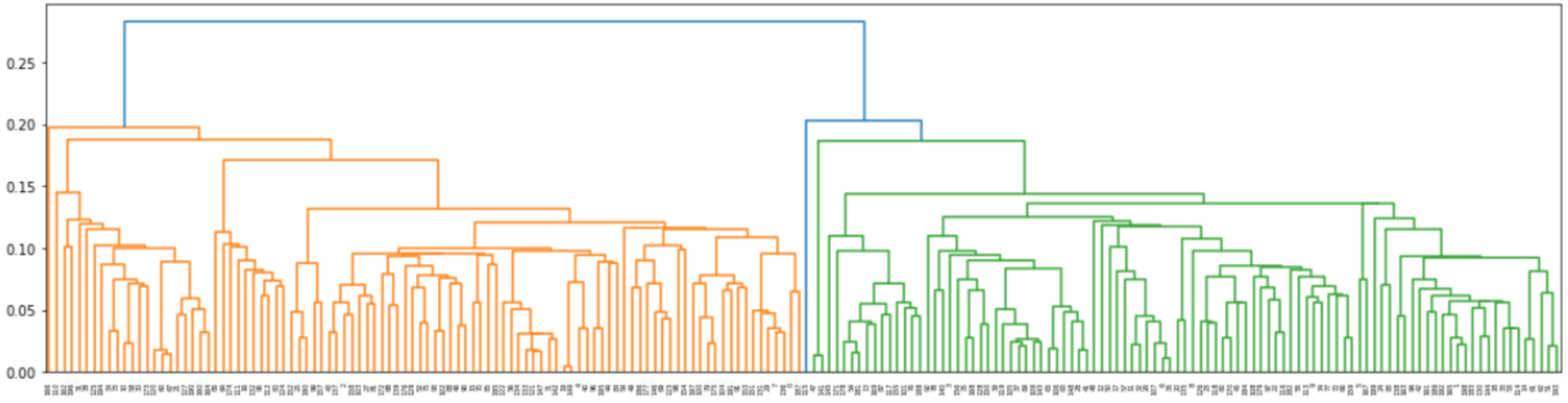
In [11]:
```
labels = fcluster(myLinkage, 5, criterion='distance')
pd.Series(labels).value_counts()
```

Out[11]:
```
1    197
2      1
3      1
4      1
dtype: int64
```

## Applying hierarchical clustering and visualizing

- Dataset #2 and dendrogram
- Cluster hierarchically using single linkage

```
In [12]: myLinkage = linkage(X2,method='single')
         plt.figure(figsize=(20,5))
         dendrogram(myLinkage)
         plt.show()
```



## Applying hierarchical clustering and visualizing

- Dataset #2 and clusters by cutting the dendrogram
- Cut at the height (distance) = 0.23 (change this value at will).

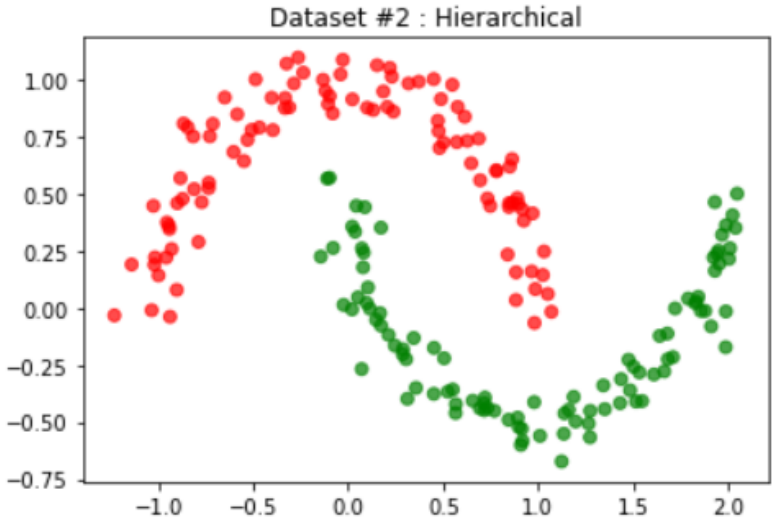
In [13]:
```
labels = fcluster(myLinkage, 0.23, criterion='distance')
pd.Series(labels).value_counts()
```

Out[13]:
```
1    100
2    100
dtype: int64
```

## Applying hierarchical clustering and visualizing

- Define a color palette: 1~2.

In [14]:
```
myColors = {1:'red',2:'green'}
plt.scatter(X2[:,0],X2[:,1], c= pd.Series(labels).apply(lambda x: myColors[x]), alpha=0.7 )
plt.title('Dataset #2 : Hierarchical')
plt.show()
```



## Creating hierarchical clustering

- Use the agglomerative method to create hierarchical clustering.
- Import the iris data.

In [1]:
```
from sklearn.datasets import load_iris
```

In [2]:
```
import pandas as pd
import numpy as np
import matplotlib.pyplot as plt
import math
%matplotlib inline
```

In [3]:
```
iris=load_iris()
```

## Creating hierarchical clustering

In [4]:
```
iris_data=iris.data
iris_data_pd=pd.DataFrame(iris.data, columns=iris.feature_names)
iris_data_pd
```

Out[4]:

| | sepal length (cm) | sepal width (cm) | petal length (cm) | petal width (cm) |
|---|---|---|---|---|
| 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 |
| ... | ... | ... | ... | ... |
| 145 | 6.7 | 3.0 | 5.2 | 2.3 |
| 146 | 6.3 | 2.5 | 5.0 | 1.9 |
| 147 | 6.5 | 3.0 | 5.2 | 2.0 |
| 148 | 6.2 | 3.4 | 5.4 | 2.3 |
| 149 | 5.9 | 3.0 | 5.1 | 1.8 |

150 rows × 4 columns

## Creating hierarchical clustering

In [5]:
```
iris_data_pd.iloc[:,2:4]
```

Out[5]:

| | petal length (cm) | petal width (cm) |
|---|---|---|
| 0 | 1.4 | 0.2 |
| 1 | 1.4 | 0.2 |
| 2 | 1.3 | 0.2 |
| 3 | 1.5 | 0.2 |
| 4 | 1.4 | 0.2 |
| ... | ... | ... |
| 145 | 5.2 | 2.3 |
| 146 | 5.0 | 1.9 |
| 147 | 5.2 | 2.0 |
| 148 | 5.4 | 2.3 |
| 149 | 5.1 | 1.8 |

150 rows × 2 columns

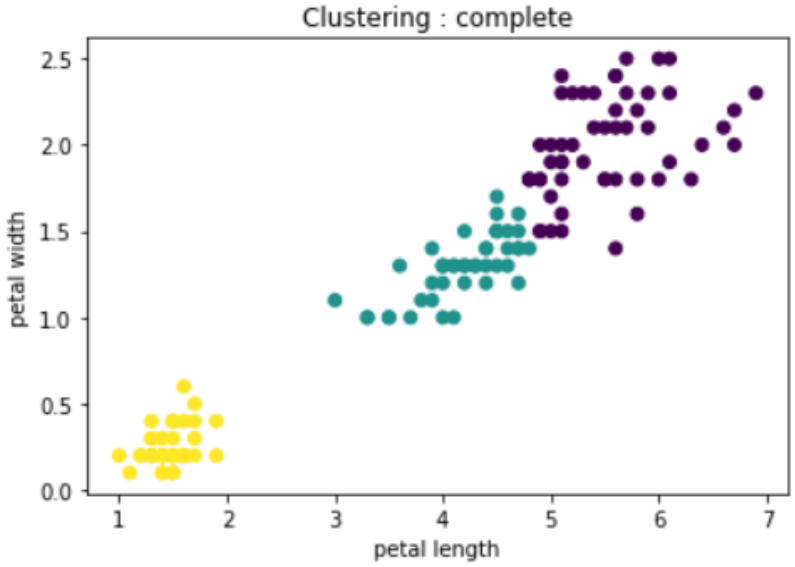
## Creating hierarchical clustering

- To use the 'petal length' and 'petal width' columns, import the sklearn agglomerative clustering, which is supported by the sklearn.clustering package.
- The distance measurement criteria between clustering can be set with the linkage parameter, which only supports ward, complete, and average. Check out how all three cases are used.

In [6]:
```
from sklearn.cluster import AgglomerativeClustering
likage=["complete", "average","ward"]
for idx, i in enumerate(likage):
    plt.figure(idx)
    hier=AgglomerativeClustering(n_clusters=3, affinity='euclidean', linkage=i)
    hier.fit(iris_data_pd.iloc[:,2:4])
    plt.scatter(iris_data_pd.iloc[:,2], iris_data_pd.iloc[:,3],c=hier.labels_)
    plt.title("Clustering : " + i)
    plt.xlabel('petal length')
    plt.ylabel('petal width')
    plt.show()
```

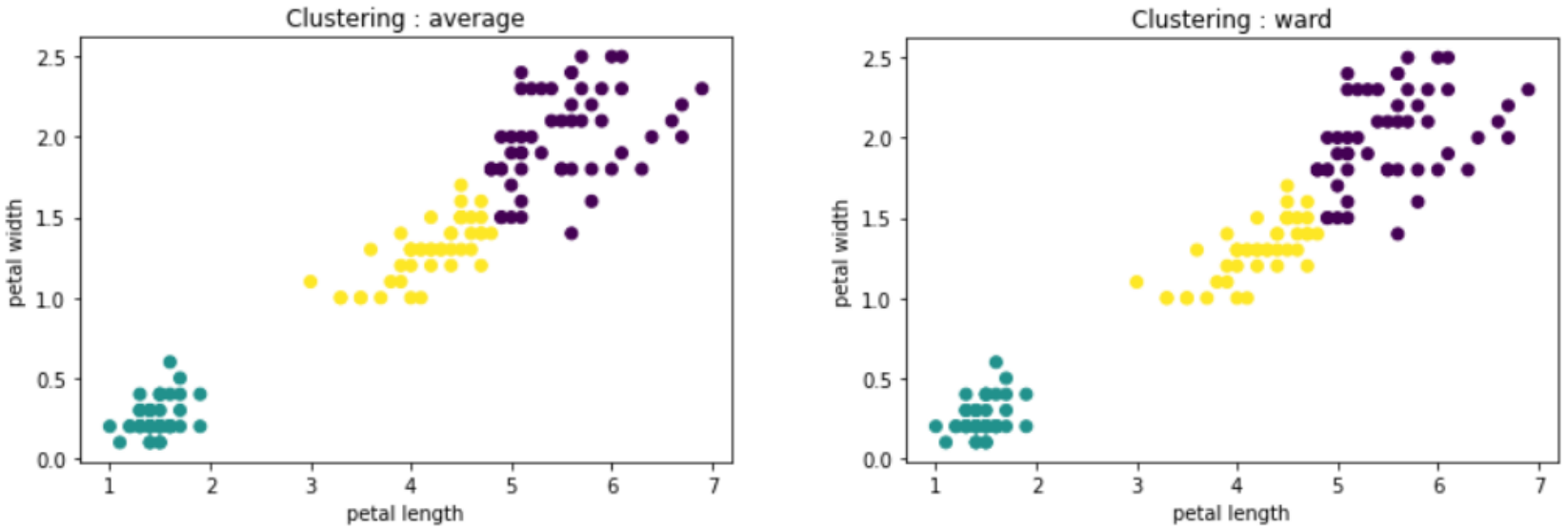
## Creating hierarchical clustering

- To use the 'petal length' and 'petal width' columns, import the sklearn agglomerative clustering, which is supported by the sklearn.clustering package.
- The distance measurement criteria between clustering can be set with the linkage parameter, which only supports ward, complete, and average. Check out how all three cases are used.



## Creating hierarchical clustering

- To use the 'petal length' and 'petal width' columns, import the sklearn agglomerative clustering, which is supported by the sklearn.clustering package.
- The distance measurement criteria between clustering can be set with the linkage parameter, which only supports ward, complete, and average. Check out how all three cases are used.



## Creating hierarchical clustering

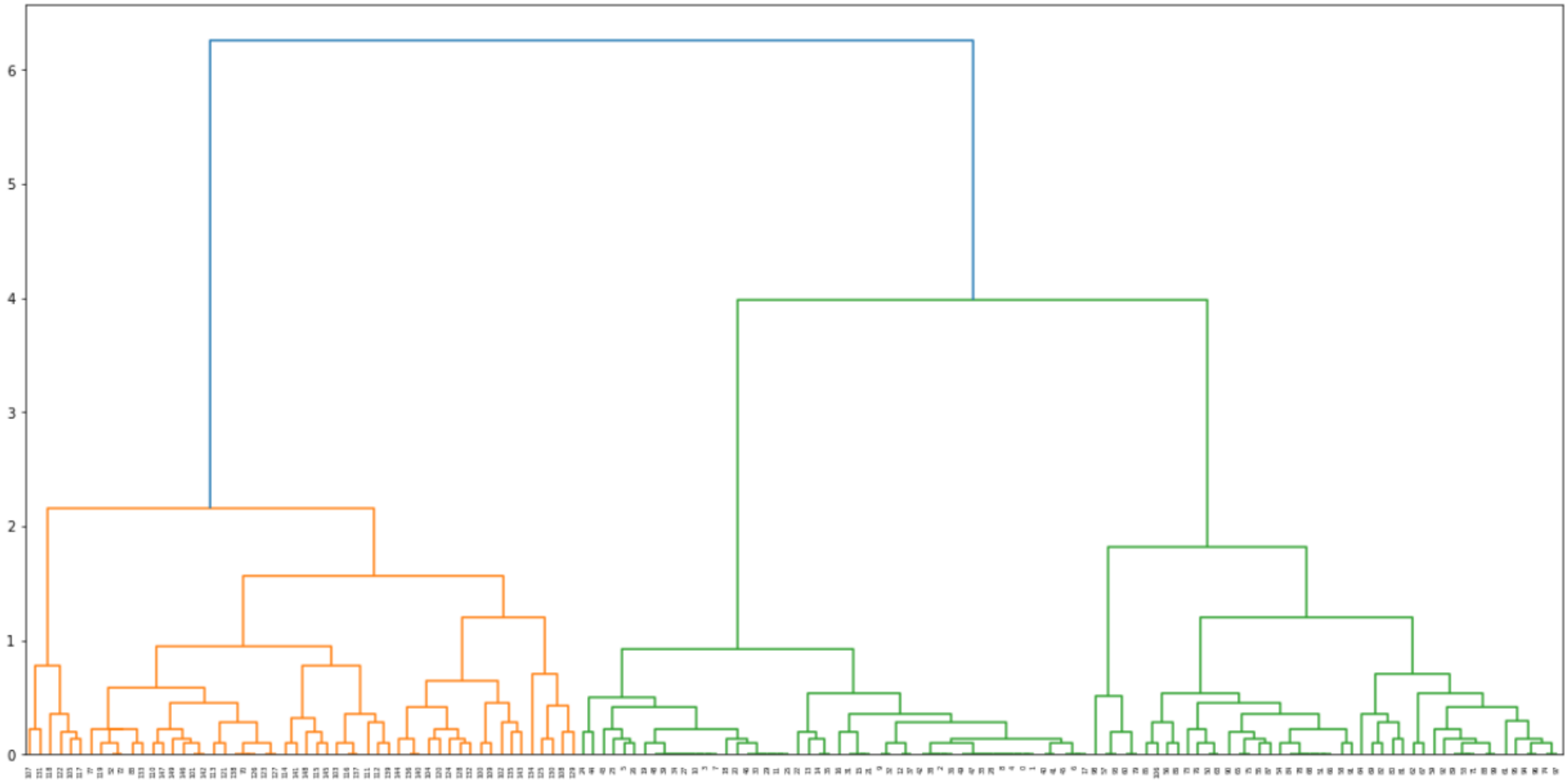
- Use Scikit-learn to confirm the clustering result. You may want to check how the tree is created, but this package does not provide this function.
- Instead, use the Scipy package for clustering and drawing a tree.
- As provided previously, implement the complete linkage.

## Creating hierarchical clustering

In [7]:
```
from scipy.cluster import hierarchy
```

In [8]:
```
hierar=hierarchy.linkage(iris_data_pd.iloc[:,2:4],'complete')
plt.figure(figsize=(20,10))
dn=hierarchy.dendrogram(hierar)
```

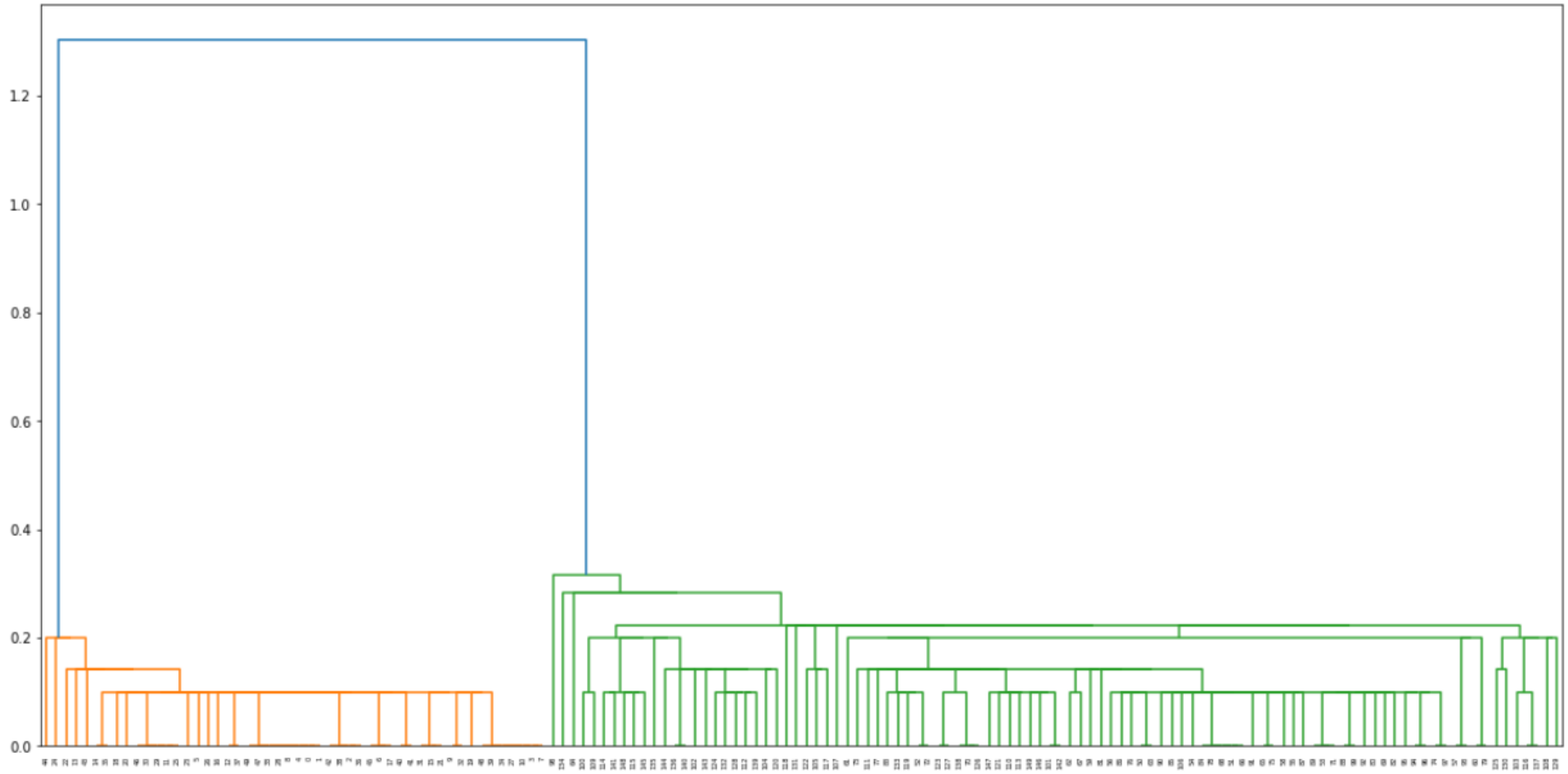
## Creating hierarchical clustering



## Creating hierarchical clustering

In [9]:
```
hierar=hierarchy.linkage(iris_data_pd.iloc[:,2:4],'single')
plt.figure(figsize=(20,10))
dn=hierarchy.dendrogram(hierar)
```

## Creating hierarchical clustering



## Creating hierarchical clustering

- Unlike complete linkage, **single linkage creates hierarchical clustering from the closest elements**. It is highly different from K-means, such that the single linkage creates a tree-shaped hierarchical cluster.
- It is important to select an appropriate linkage type to create a suitable model for the data condition.

Unit 3.

# Non-hierarchical Clustering

3.1. K-means clustering

3.2. Other clustering methods

# K-Means Clustering

## About the k-means clustering

- There is one ore more explanatory variables $X1$ , $X2$ , …, $Xd$.
- There is no response variable. Hence, this is a unsupervised learning algorithm.

## Purposes of the k-means clustering

- Cluster the observations in $k$ clusters.
- Find the centroids (cluster means) that characterize the clusters.

## Pros

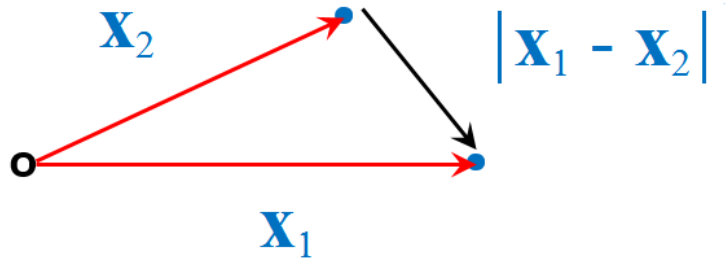
- Intuitive interpretation of the results
- Quick and easy

## Cons

- Sensitive to the noise and outliers
- Cluster boundaries can only be linear.

## Distance metric

- Euclidean distance: it is the modulus of the difference between two position vectors.




$$|X_1 - X_2| = \sqrt{(x_{11} - x_{21})^2 + (x_{12} - x_{22})^2 + \cdots + (x_{1d} - x_{2d})^2}$$

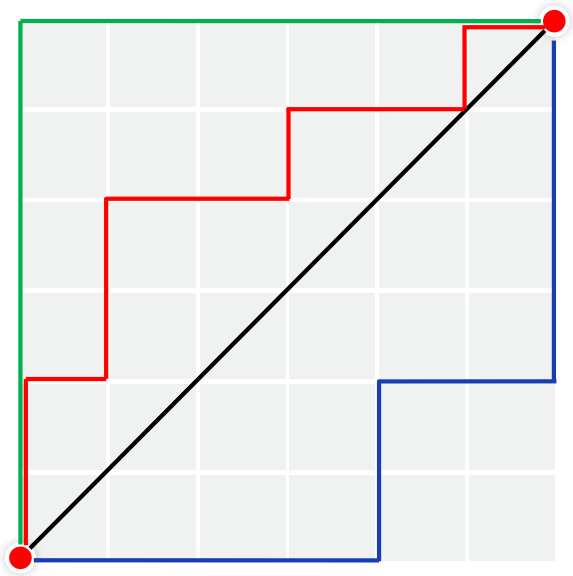
## Distance metric

- For numeric variables:

  Euclidean, Standardized, Mahalanobis, Chebyshev, Canberra, Manhattan, Minkowski, etc.

- For categorical variables:

  Jackard, etc.



Black: Euclidean / Colored: Manhattan

## Standard algorithm

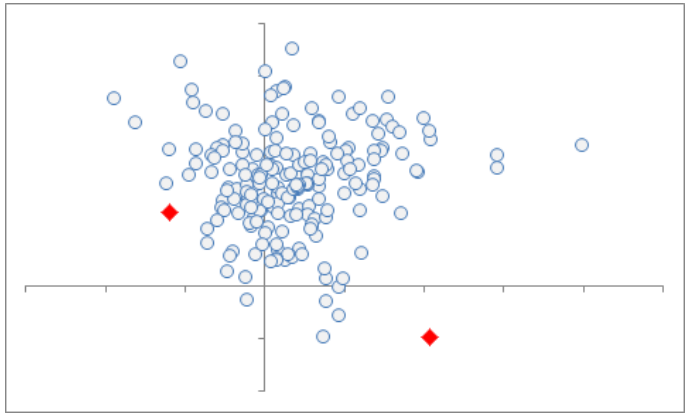
1) Let's suppose a dataset composed of $n$ observations:

$\boldsymbol{x}_1, \boldsymbol{x}_2, \cdots, \boldsymbol{x}_n$

- Each observation $\boldsymbol{x}i$ is a vector of $d$ components ($d$ = number of variables) .

2) Suppose that we target two ($k$=2) clusters, denoted as $C_1$ and $C_2$.

3) Two centroid positions are randomly initialized: $\mu_1$ and $\mu_2$.



## Standard algorithm

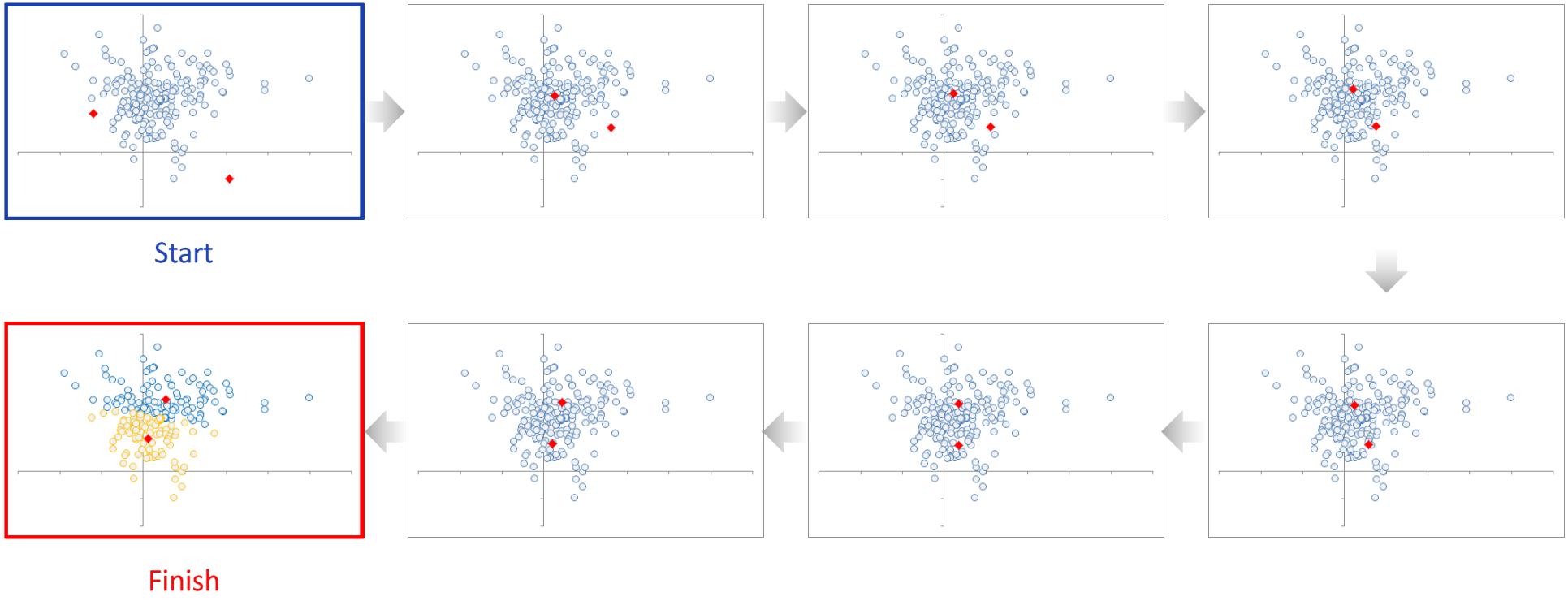
4) Assign the observations to the nearest centroids.

5) Update the centroid positions, such that the sum of square distances between the observations and the nearest centroids gets smaller.

$$minimize \sum_{i=1}^{k} \sum_{x \in C_i} |\boldsymbol{x} - \boldsymbol{\mu}_i|^2$$

6) Repeat from step 4) until the centroids converge to their final positions.

## Standard algorithm

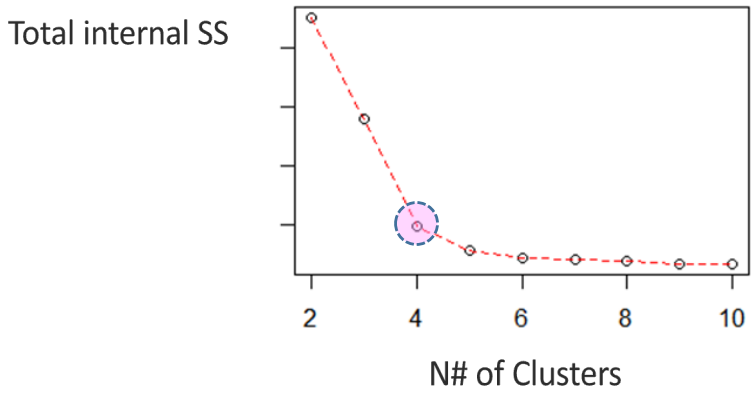


## Standard algorithm

- A question: how do we find the optimal number of clusters?
- Let's define the sum of square distances between the observations and the nearest centroids as:

$$Total\ internal\ sum\ of\ squares = \sum_{i=1}^{k} \sum_{x \in C_i} |\boldsymbol{x} - \boldsymbol{\mu}_i|^2$$

- Plot the "Total internal sum of squares" vs "N# of clusters" and find the inflexion point. ← "Elbow"



Unit 3.

# Non-hierarchical Clustering

3.1. K-means clustering

3.2. Other clustering methods

# Other clustering methods

## K-medoids clustering

- K-medoids clustering is the advanced version of the K-means clustering method. It uses all types of similarity and dissimilarity measures. Moreover, it is advantageous for noise or outlier processing because it designates the cluster center using actual data set values rather than random dots on plane coordinates.

## DBSCAN (Density Based Spatial Clustering of Application with Noise)

- K-means clustering method calculates the average of K-clusters and distances between each data point for clustering. On the other hand, DBSCAN applies density to create the same group of data sets linked with constant density. It is a clustering method that is advantageous for identifying noise and outliers.

## Gaussian Mixture Model

- It is a probability-based clustering analysis that predicts the parameter using the EM (Expectation Maximization) or MCMC (Markov Chain Monte Carlo) algorithms.

# Density-based spatial clustering of applications with noise (DBSCAN)

## About the DBSCAN

- The most common algorithm in density clustering is the Density-based Spatial Clustering of Applications with Noise (DBSCAN) algorithm. Similar to K-means clustering, DBSCAN clustering is affected by data distribution.
- While K-means clustering creates clusters according to the distribution using the standard data, the DBSCAN clustering is affected by the density of each data. In other words, it assumes that the data included in the same cluster would have high density.
- We are going to look at how the DBSCAN determines density.

## About the DBSCAN

- This is a unsupervised learning algorithm; there are only $X$ variables.
- It was developed in 1996.
- It allows density-based clustering.

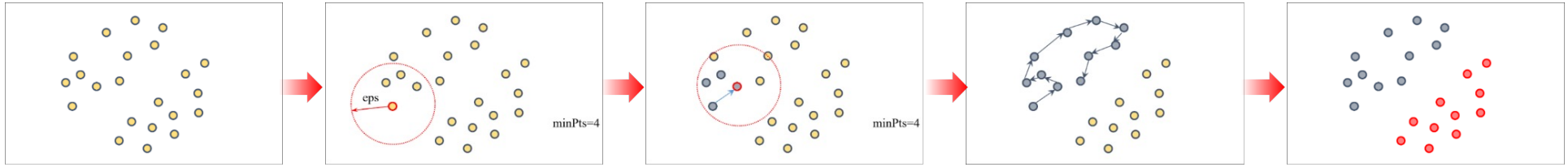
## Pros

- It can reveal structures that the k-means and hierarchical clustering cannot

## Cons

- Hyperparameters eps and minPts must be specified.
- It is hard to get stable clusters in case the dense regions overlap.

## DBSCAN algorithm




(a) (b) (c) (d) (e)

1) Suppose that the observations are distributed as in (a).

2) From a point, count the points within a radius eps and look around: (b).

3) If there are more than minPts points within the circle, include them in the same cluster: (b).

4) Then move on to the next point and repeat from step 2) until all the points are exhausted: (c)~(d).

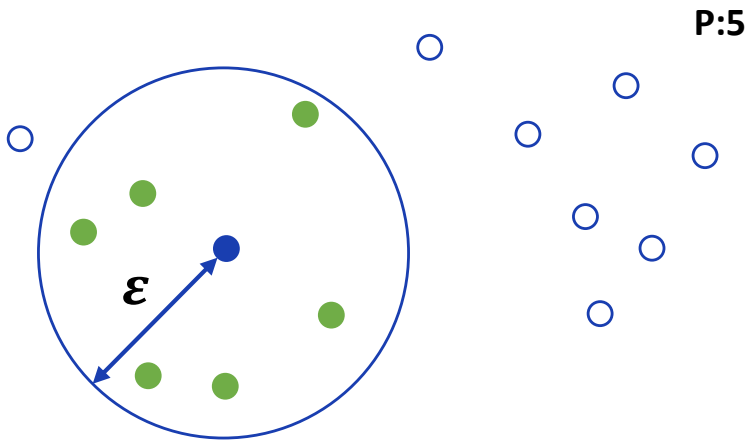
5) Move on to another point that has not been clustered yet. Repeat from step 2): (e).

## How to determine density for DBSCAN algorithm

- Check the following parameters to determine the density for DBSCAN algorithm.

1. $\varepsilon$ as the radius of the circle with the element in the center
2. P as the minimum number of elements that exist within the radius. The radius distance is measured with the Euclidian distance method.

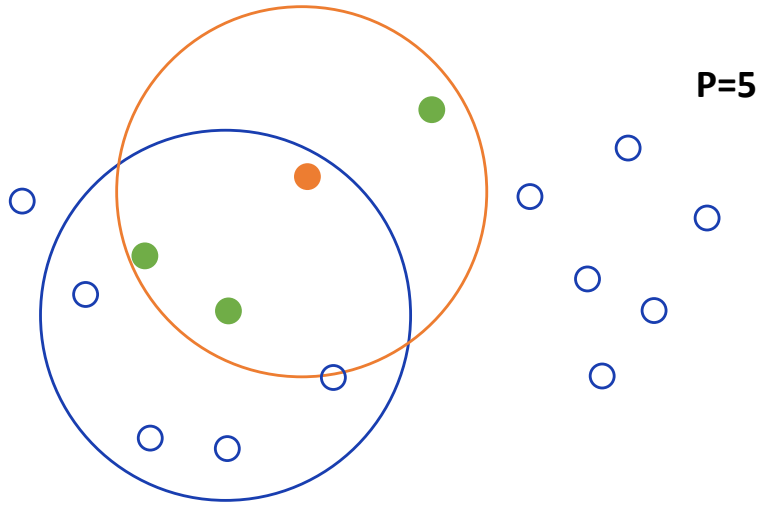
- Look at the following figure. First, select a random point.



## How to determine density for DBSCAN algorithm

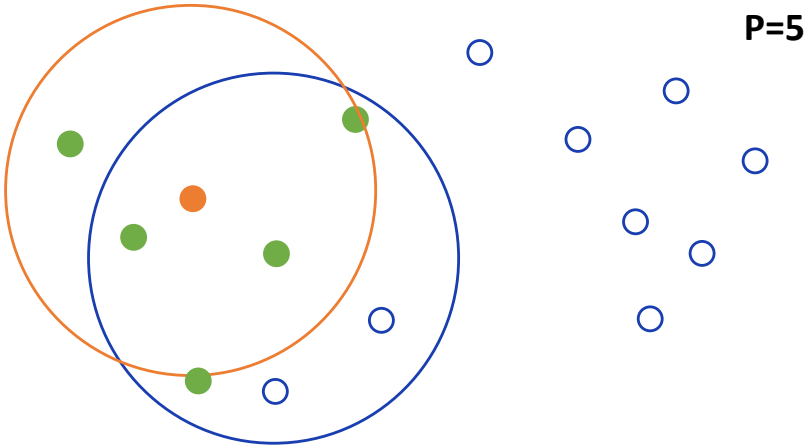
- The randomly selected point is designated at a red dot, as shown in the figure in the previous slide.
- The circle is centered on the red dot and has a radius of ε. Check if the number of elements inside the circle is the same as P or greater than P.
- If it is the same or greater than P, then the red dot becomes a core object, and the circle is created as a cluster. If the value is smaller than P, the red dot is defined as noise.
- In the figure, the elements in the red circle are six green dots. P equals 5, so the minimum number of elements that should exist within the radius is satisfied.
- Thus, the rod dot becomes a core object, and the red circle becomes a cluster. Now, move on to other elements. Select one of the elements in the circle other than the core object.
- Let’s look at the new dot in the next figure.

## How to determine density for DBSCAN algorithm



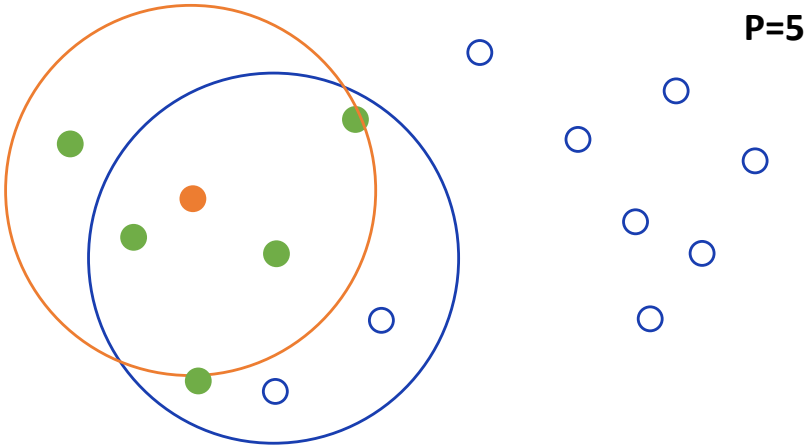

- Blue circle is the existing cluster, and a new dot is designated within the radius. When creating a circle with the red dot in the center, only three elements are inside it.
- The P value is 5, so the number of elements inside the circle is less than P. Thus, this dot cannot become the core object. Instead, it is defined as noise.
- Move on to another dot within the radius.

## How to determine density for DBSCAN algorithm



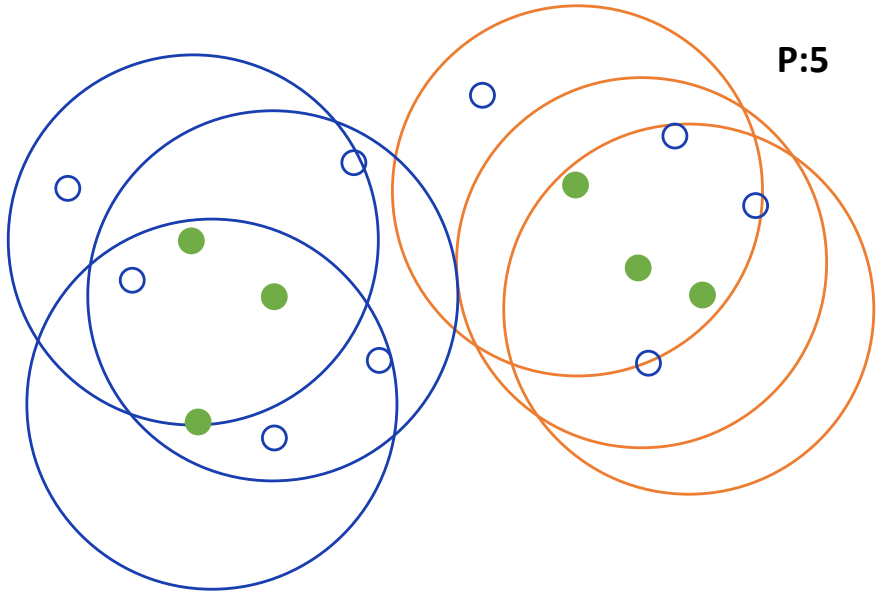

- Now, there are 5 elements in the red circle. It is the same as the P value, so this red dot is recognized as a core object.
- It is possible to create a cluster, but make sure to consider if this element was included in the previous cluster, as it is now classified as a new core object.
- If included in the previous cluster, do not create a new cluster but expand the existing cluster. If it is not relevant to the previous cluster, a new cluster will be created using the red dot as a new core object.
- In the figure, the red dot is an element presented in the blue circle, which is the previous cluster. Since it is included in the previously created cluster, the previous cluster is expanded without making a new cluster.

## How to determine density for DBSCAN algorithm




- This is the expanded cluster.
- The DBSCAN algorithm aims to check every dot by repeating the same process over and over. After completing all processes, the data cluster looks as follows.

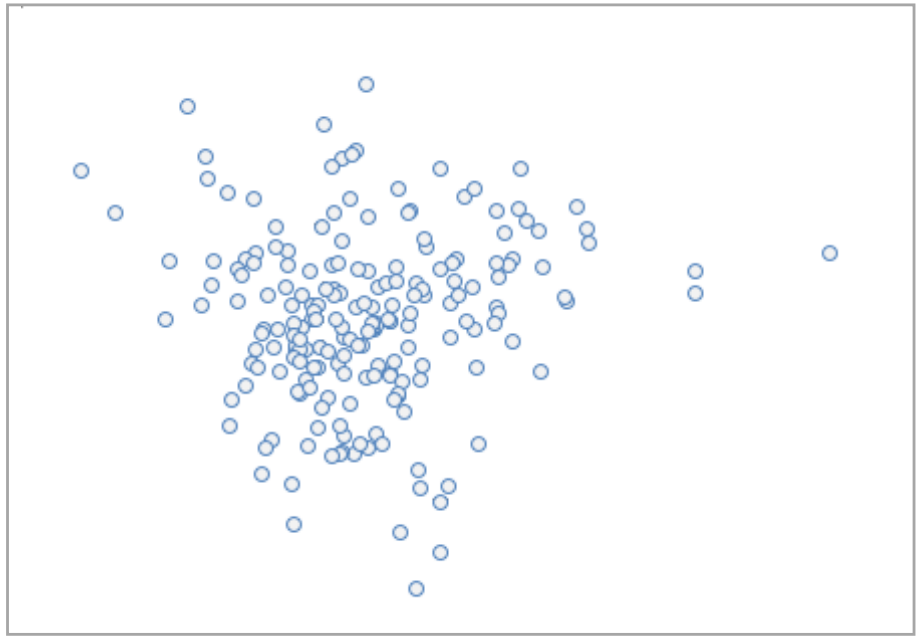
## How to determine density for DBSCAN algorithm



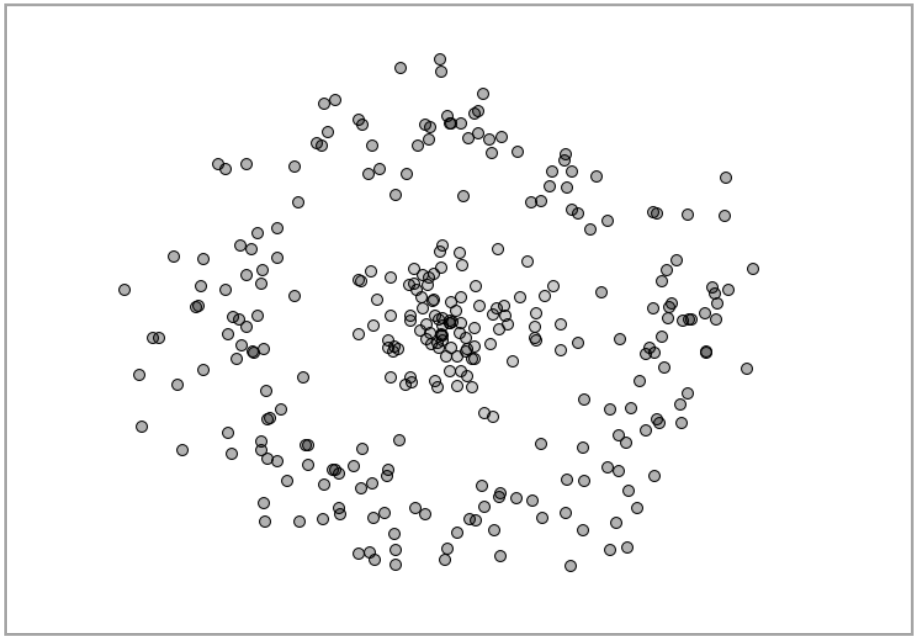

- The black dots are the core objects.
- Likewise, the DBSCAN takes only two parameters and uses them to create a cluster.
- Thus, no other parameters are required besides ε and P values. This is how the density is determined in the DBSCAN algorithm.

# Clustering

Question: which clustering algorithms are suitable for the following cases?



(a)



(b)

Unit 4.

# Linear Factor Model for Dimensionality Reduction

4.1. Principal Component Analysis

4.2. Applications of Principal Components

# Principal Component Analysis

## Purposes of the principal component analysis (PCA)

- Transform a set of correlated variables into another set of uncorrelated variables.
- Get a new set of orthogonal vectors (principal components or PCs).
- Order the new variables from the largest to the smallest variance.

## Pros

- Many data science applications: preprocessing, modeling, dimensional reduction, visualization, etc.

## Cons

- It is difficult to interpret because PCs are obtained by linear combinations of the original features.

## Terminology

a) Loading

- Normalized principal component (PC)
- There are as many loading vectors as the number of variables.

b) Variance $\sigma$^2 (or standard deviation $\sigma$)

- The principal components have associated variances.

c) Transformed scores

- Raw scores (original observations) represented using the PCs as new coordinate axes.

## Principal components

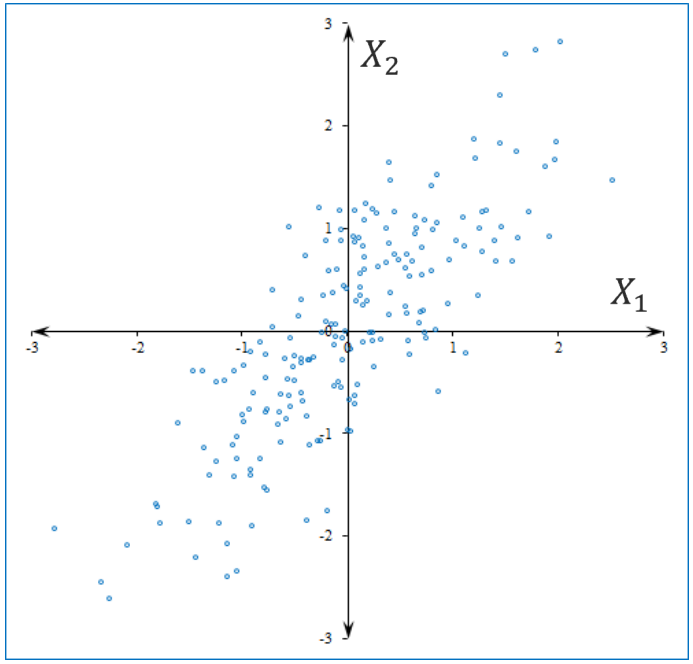
- Let's suppose that there are $k$ variables or features $X1$ , $X2$ , …, $Xk$.
- Then, the $PC1$ , $PC2$ , …, $PCk$ are linear combinations of the original features:

  $PCi$=$\alpha$1, $iX$1+$\alpha$2, $iX$2+…+$\alpha k$, $iXk$
- Conversely, the original features can be expressed in terms of the PCs:

  $Xi$ = $\beta$1, $iPC$1 + $\beta$2, $iPC$2+…+$\beta k$, $iPCk$

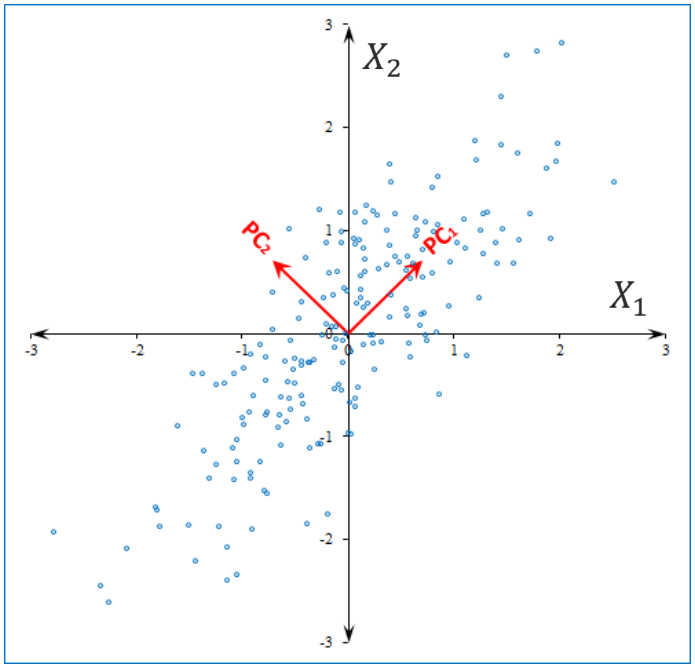
## Principal component and variance

- Suppose a dataset with two variables that can be conveniently visualized on a plane:



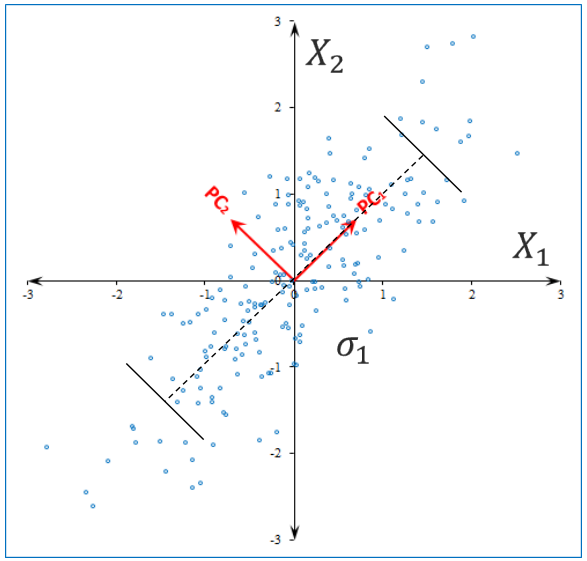
## Principal component and variance

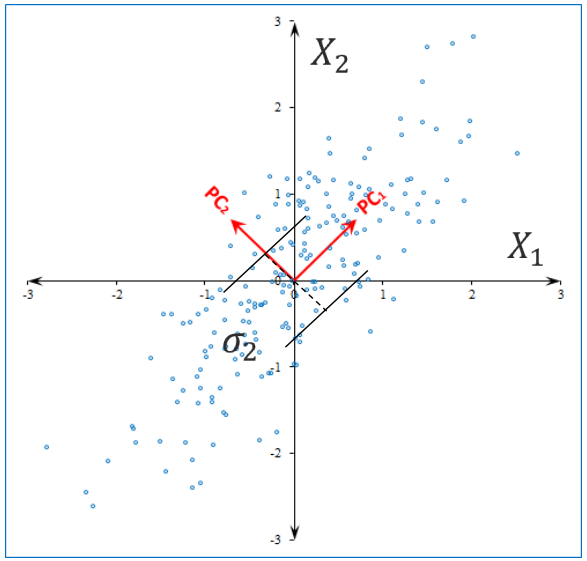
- We can find the $PC1$ and $PC2$ that are orthogonal to each other.



## Principal component and variance

- $PC1$ is the direction of the largest variance, while $PC2$ is the direction of the next largest variance.

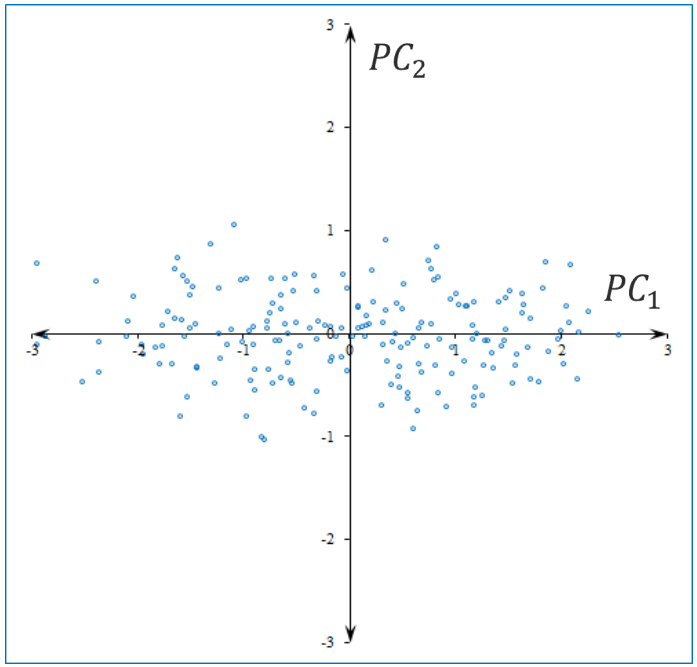



- So, we have $\sigma_1 > \sigma_2$.

## Transformed scores

- The observations can be represented using the $PC1$ and $PC2$ as new coordinate axes.



## Cumulative variance

- As the principal components can be regarded as independent variables, the total variance is:

$$\sigma_{total}^2 = \sigma_1^2 + \sigma_2^2 + \sigma_3^2 + \cdots$$

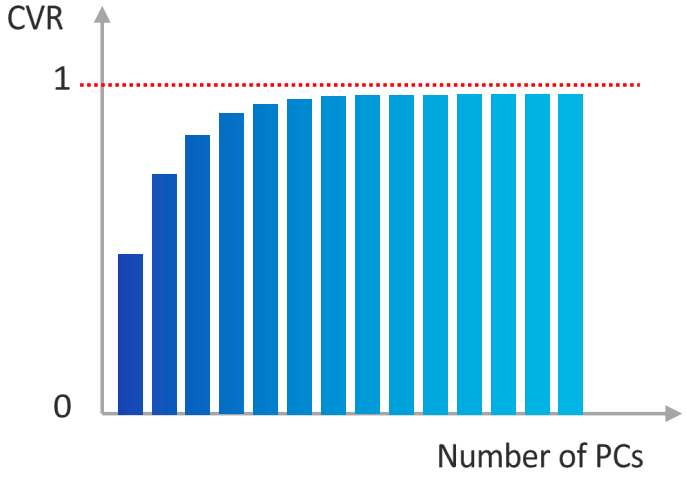
- So, we can calculate the cumulative variance ratios (CVRs):

$$CVR_1 = \frac{\sigma_1^2}{\sigma_{total}^2}$$

$$CVR_2 = \frac{\sigma_1^2 + \sigma_2^2}{\sigma_{total}^2}$$

$$CVR_3 = \frac{\sigma_1^2 + \sigma_2^2 + \sigma_3^2}{\sigma_{total}^2}$$

$$\vdots$$



## Calculating the principal components

- The PCs can also be obtained by eigenvalue decomposition (ED) of the covariance matrix.
- The PCs can be calculated by singular value decomposition (SVD) of the data matrix.
- If we standardize the variables, we would have the correlation instead of the covariance.

**Ex** A covariance matrix and a correlation matrix

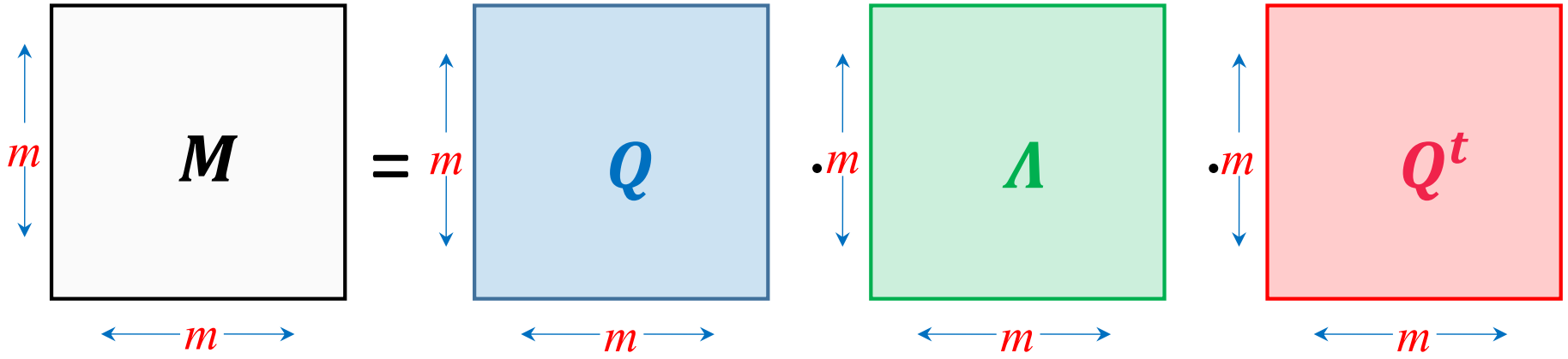
$$\begin{bmatrix} \sigma_1^2 & \sigma_{12} & \sigma_{13} & \sigma_{14} \\ \sigma_{21} & \sigma_2^2 & \sigma_{23} & \sigma_{24} \\ \sigma_{31} & \sigma_{32} & \sigma_3^2 & \sigma_{34} \\ \sigma_{41} & \sigma_{42} & \sigma_{43} & \sigma_4^2 \end{bmatrix} \qquad \begin{bmatrix} 1 & \rho_{12} & \rho_{13} & \rho_{14} \\ \rho_{21} & 1 & \rho_{23} & \rho_{24} \\ \rho_{31} & \rho_{32} & 1 & \rho_{34} \\ \rho_{41} & \rho_{42} & \rho_{43} & 1 \end{bmatrix}$$

“In the next few slides, let’s make a detour and review the ED and SVD in detail.”

# Matrix Decompositions

## Eigenvalue decomposition (ED)

- A square matrix $\boldsymbol{M}$ is decomposed as $\boldsymbol{M}=\boldsymbol{Q}\,\boldsymbol{\Lambda}\,\boldsymbol{Q}^{t}$.
- All the matrices have the same size: $Size(\boldsymbol{M})=Size(\boldsymbol{Q})=Size(\boldsymbol{\Lambda})=m\times m$.



## Eigenvalue decomposition (ED)

- A square matrix $\boldsymbol{M}$ is decomposed as $\boldsymbol{M}=\boldsymbol{Q}\,\boldsymbol{\Lambda}\,\boldsymbol{Q}^{t}$.
- Here, $\boldsymbol{\Lambda}$ is a diagonal matrix that contains the “eigenvalues.”

$$\boldsymbol{\Lambda}=\begin{bmatrix}\lambda_1 & 0 & \cdots & 0\\ 0 & \lambda_2 & & 0\\ \vdots & & \ddots & \vdots\\ 0 & 0 & \cdots & \lambda_m\end{bmatrix}$$

## Eigenvalue decomposition (ED)

- A square matrix $\boldsymbol{M}$ is decomposed as $\boldsymbol{M}=\boldsymbol{Q}\,\boldsymbol{\Lambda}\,\boldsymbol{Q}^{t}$.
- The columns of $\boldsymbol{Q}$ are the so-called "eigenvectors."

$$\boldsymbol{Q}=\begin{bmatrix}\uparrow & \cdots & \uparrow\\ \boldsymbol{q_1} & \cdots & \boldsymbol{q_m}\\ \downarrow & \cdots & \downarrow\end{bmatrix}$$

- Between an eigenvector and its eigenvalue, we have the following relation:

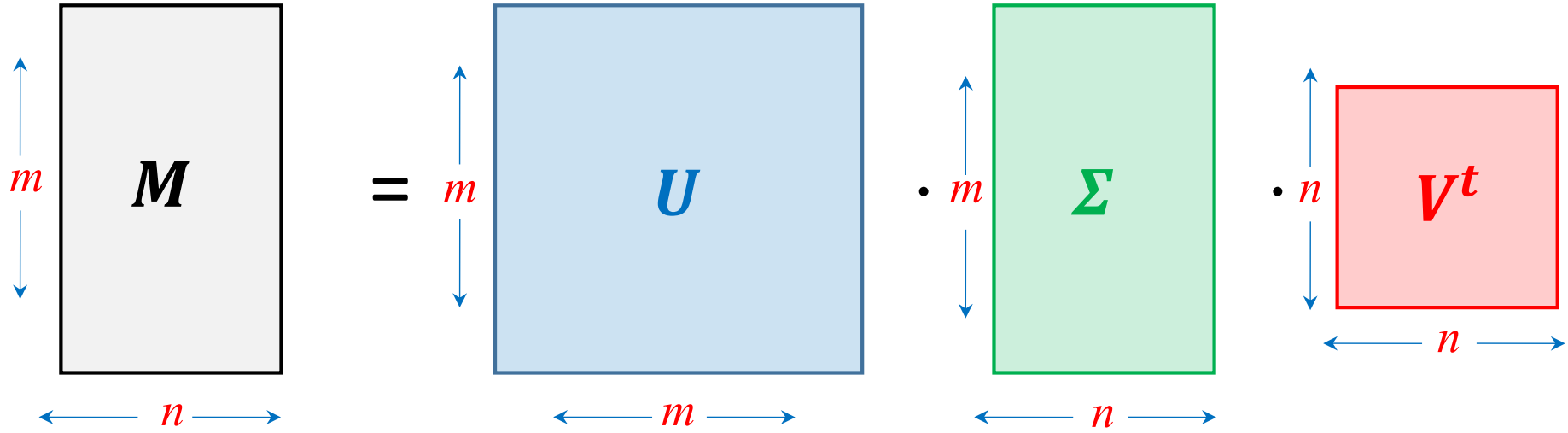
$$\boldsymbol{M}\boldsymbol{q_i}=\lambda_i\,\boldsymbol{q_i}$$

- Between any two eigenvectors, we have the following orthogonality condition:

$$\boldsymbol{q_i}\cdot\boldsymbol{q_j}=\delta_{ij}\quad\Leftrightarrow\quad\boldsymbol{Q}\boldsymbol{Q}^{\boldsymbol{t}}=\boldsymbol{Q}^{\boldsymbol{t}}\boldsymbol{Q}=\boldsymbol{I}$$

## Singular value decomposition (SVD)

- A matrix $\boldsymbol{M}$ is decomposed as $\boldsymbol{M}=\boldsymbol{U}\boldsymbol{\Sigma}\boldsymbol{V}^{t}$.



## Singular value decomposition (SVD)

- A matrix $\boldsymbol{M}$ is decomposed as $\boldsymbol{M}=\boldsymbol{U}\boldsymbol{\Sigma}\boldsymbol{V}^t$.
- Here, $\boldsymbol{\Sigma}$ contains the singular values as diagonal elements.
- These singular values are ordered from the largest to the smallest: $\sigma_1>\sigma_2>\ldots>\sigma_m$

$$\boldsymbol{\Sigma} = \begin{bmatrix} \sigma_1 & 0 & \cdots & 0 & 0 \\ 0 & \sigma_2 & & 0 & 0 \\ \vdots & & \ddots & \vdots & \\ 0 & 0 & \cdots & \sigma_m & 0 \end{bmatrix}$$

## Singular value decomposition (SVD)

- A matrix $\boldsymbol{M}$ is decomposed as $\boldsymbol{M}=\boldsymbol{U\Sigma V^t}$.
- The columns of $\boldsymbol{U}$ are the "left singular vectors."
- The columns of $\boldsymbol{V}$ are the "right singular vectors."

$$= \begin{bmatrix} \uparrow & \cdots & \uparrow \\ \boldsymbol{u_1} & \cdots & \boldsymbol{u_m} \\ \downarrow & \cdots & \downarrow \end{bmatrix} \qquad \boldsymbol{V} = \begin{bmatrix} \uparrow & \cdots & \uparrow \\ \boldsymbol{v_1} & \cdots & \boldsymbol{v_n} \\ \downarrow & \cdots & \downarrow \end{bmatrix}$$

- Between a set of the left and right singular vectors and their singular value, we have:

$$= \boldsymbol{M}\, \boldsymbol{v_i} = \sigma_i\, \boldsymbol{u_i}$$

- Between any two singular vectors, we have the following orthogonality condition:

$$\boldsymbol{v_i} \cdot \boldsymbol{v_j} = \delta_{ij} \quad \Leftrightarrow \quad \boldsymbol{V V^t} = \boldsymbol{V^t V} = \boldsymbol{I}$$
$$\boldsymbol{u_i} \cdot \boldsymbol{u_j} = \delta_{ij} \quad \Leftrightarrow \quad \boldsymbol{U U^t} = \boldsymbol{U^t U} = \boldsymbol{I}$$

## Relation between ED and SVD

1) If $\boldsymbol{X}$ is a matrix composed of standardized scores, then we can apply SVD: $\boldsymbol{X}$=$\boldsymbol{U\Sigma Vt}$.

2) Using the decomposed form, we can express the covariance matrix as following:

$$\boldsymbol{M = X\,X^t = U\Sigma V^t (U\Sigma V^t)^t}$$

$$\left.\begin{aligned} &= \boldsymbol{U\Sigma V^t\, V\Sigma^t U^t} \\ &= \boldsymbol{U\Sigma\Sigma^t U^t} \end{aligned}\right\} \text{By orthogonality } \boldsymbol{V^tV = I}$$

- We can see that $\boldsymbol{\Sigma\Sigma^t}$ is a diagonal matrix with elements equal to $\sigma i^2$.
- Thus, $\boldsymbol{\Sigma\Sigma^t}$ is the same as the eigenvalue matrix $\boldsymbol{\Lambda}$.
- Also, we can see that the left singular matrix $\boldsymbol{U}$ is the same as the eigenvector matrix $\boldsymbol{Q}$.

## Relation between ED and SVD

- Let's summarize in the following table.

| ED | SVD |
|---|---|
| $X X^t = Q \Lambda Q^t$ | $X X^t = U \Sigma \Sigma^t U^t$ |
| $\Lambda = \Sigma \Sigma^t$ | |
| $Q = U$ | |

# Principal Component Analysis

## Calculating the principal components

- Finally, let us summarize the PCA in terms of the matrix decompositions.

| | ED | SVD |
|---|---|---|
| Decomposition Target | Covariance matrix $\boldsymbol{XX^t}$ | Data matrix $\boldsymbol{X}$ |
| $\boldsymbol{PCs}$ | Columns of the $\boldsymbol{Q}$ matrix | Columns of the $\boldsymbol{U}$ matrix |
| $\boldsymbol{\sigma_i^2}$ or $\boldsymbol{\sigma_i}$ | Diagonal elements of the $\boldsymbol{\Lambda}$ matrix are the $\boldsymbol{\sigma_i^2}$. | Diagonal elements of the $\boldsymbol{\Sigma}$ matrix are the $\boldsymbol{\sigma_i}$. |

Unit 4.

# Linear Factor Model for Dimensionality Reduction

4.1. Principal Component Analysis

4.2. Applications of Principal Components

# Dimensional Reduction

## About the dimensional reduction

- The number of principal components (PCs) is equal to the number of variables, say $k$.
- The original variables $X_i$ can be expressed in terms of the PCs:

$$X_i = \beta_{1,i}PC_1 + \beta_{2,i}PC_2 + \cdots + \beta_{k,i}PC_k$$

- The PCs are ordered by variance: $\sigma_1^2 > \sigma_2^2 > \sigma_3^2 > \cdots > \sigma_k^2$
- Thus, we can reduce dimension starting from the last PC, ($q < k$):

$$X_i \approx \beta_{1,i}PC_1 + \beta_{2,i}PC_2 + \cdots + \beta_{q,i}PC_q$$ "Reduced dimension input"

## Pros

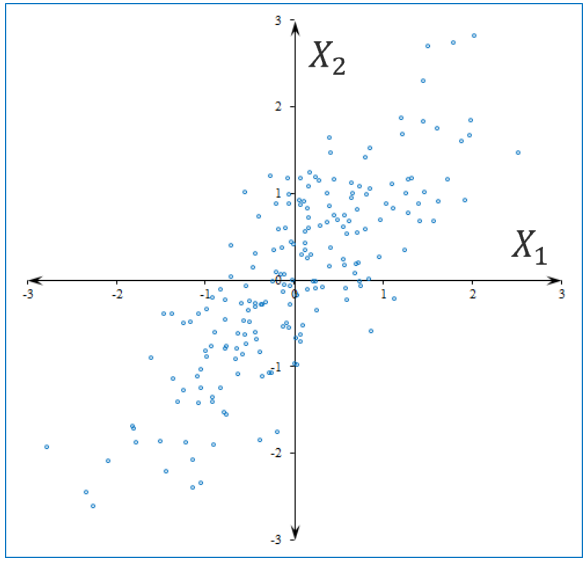
- We can simplify the data and reduce overfitting error.
- We get only the most salient features.

## Cons

- Loss of details
- It is difficult to interpret intuitively.

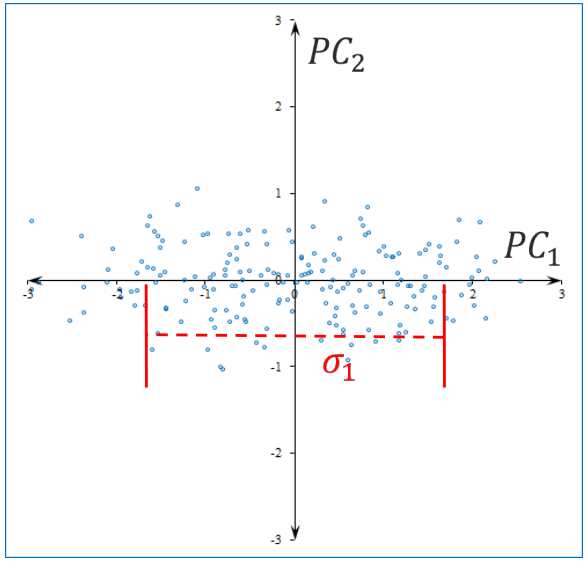
## Dimensional reduction

- Suppose a dataset with two variables that can be conveniently visualized on a plane:



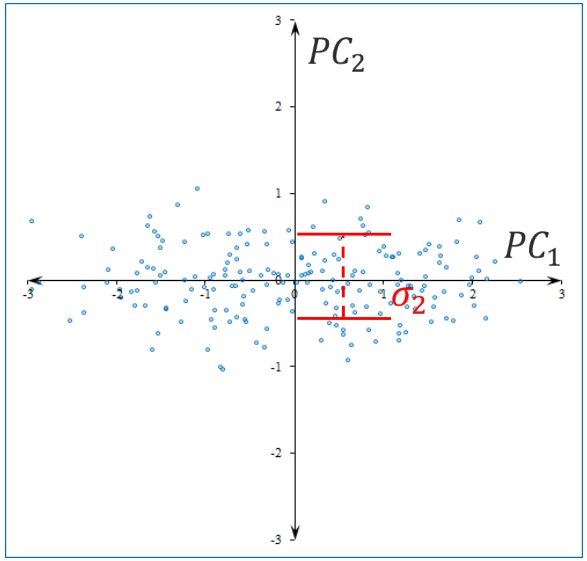
## Dimensional reduction

- The observations can be represented using the $PC_1$ and $PC_2$ as new coordinate axes:



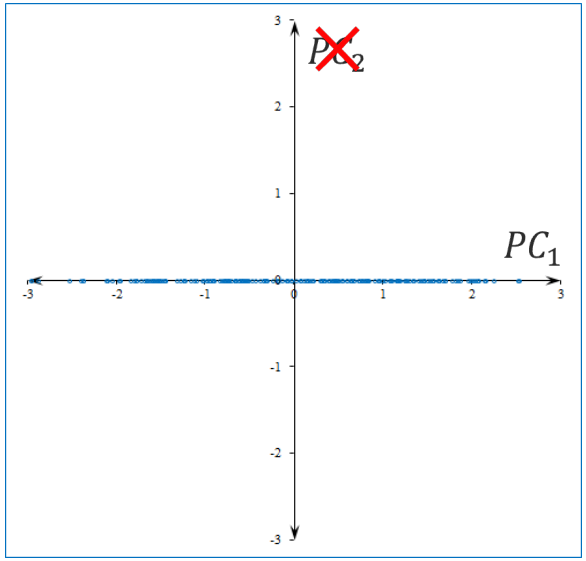
## Dimensional reduction

- The observations can be represented using the $PC_1$ and $PC_2$ as new coordinate axes:



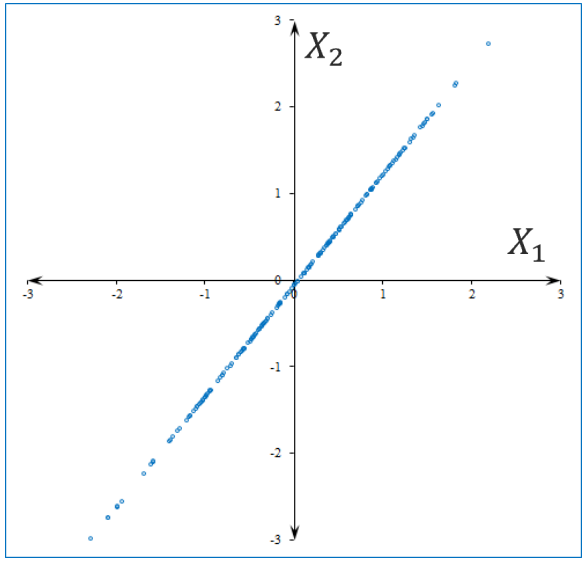
## Dimensional reduction

- We can eliminate the direction represented by $PC_2$ that corresponds to the smaller variance:



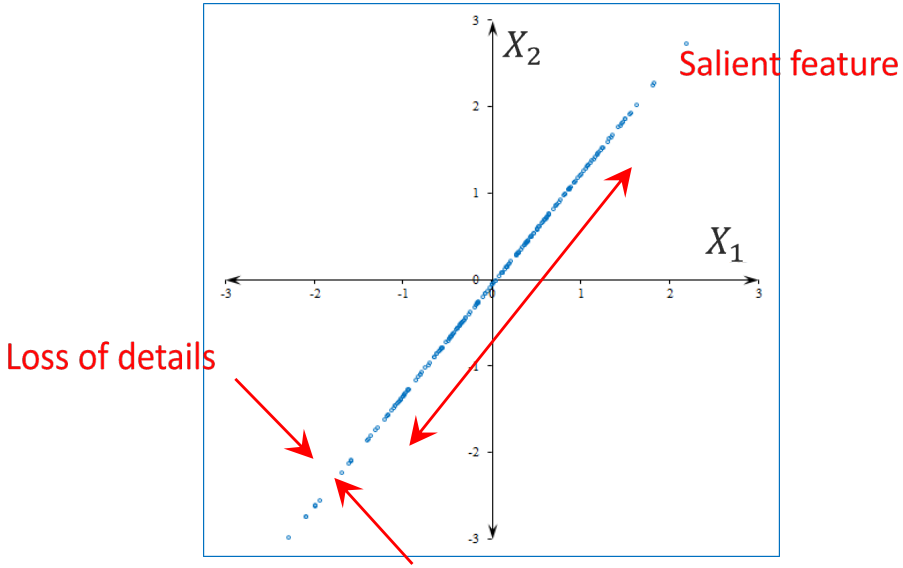
## Dimensional reduction

- Now, we can go back to the original coordinate system and show the “reduced dimensional input”:



## Dimensional reduction

- Now, we can go back to the original coordinate system and show the “reduced dimensional input”:




- We can notice that details have been lost leaving only the most salient feature.

## Dimensional reduction

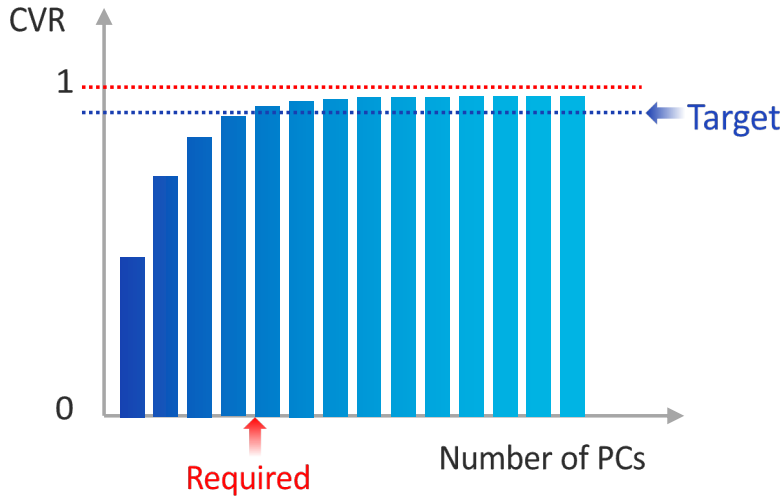
- The total variance is: $\sigma_{total}^2 = \sigma_1^2 + \sigma_2^2 + \sigma_3^2 + \cdots + \sigma_k^2$
- Then, we can calculate the cumulative variance ratios:

$$CVR_1 = \frac{\sigma_1^2}{\sigma_{total}^2}$$

$$CVR_2 = \frac{\sigma_1^2 + \sigma_2^2}{\sigma_{total}^2}$$

$$CVR_3 = \frac{\sigma_1^2 + \sigma_2^2 + \sigma_3^2}{\sigma_{total}^2}$$

$$\vdots$$

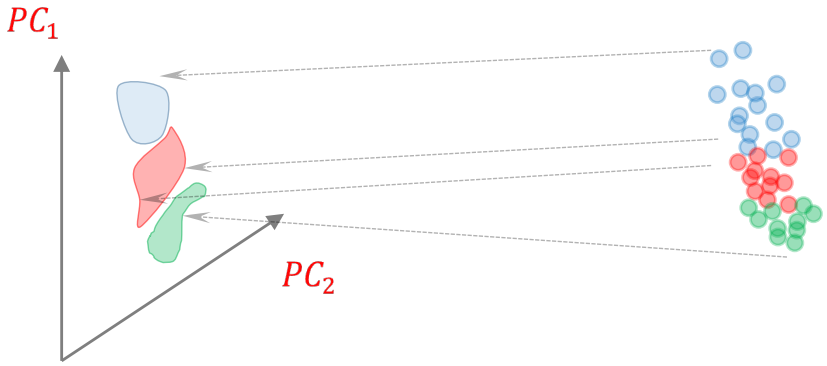



- We can set a target CVR and determine the required number of PCs.

# High Dimension Visualization

## High dimension visualization

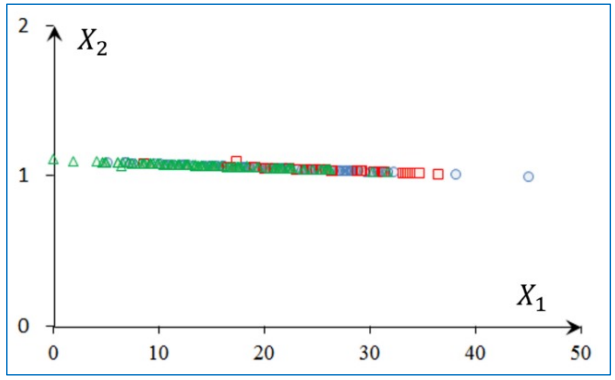
- $PC_1$ and $PC_2$ are the directions of the largest and the second largest variance.
- $PC_1$ and $PC_2$ define the most spread out plane on which to project the high dimensional coordinates.

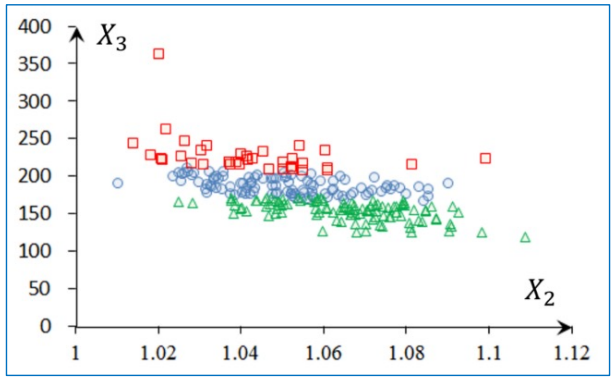



- It is easy to implement as it uses only the first two components of the transformed scores.

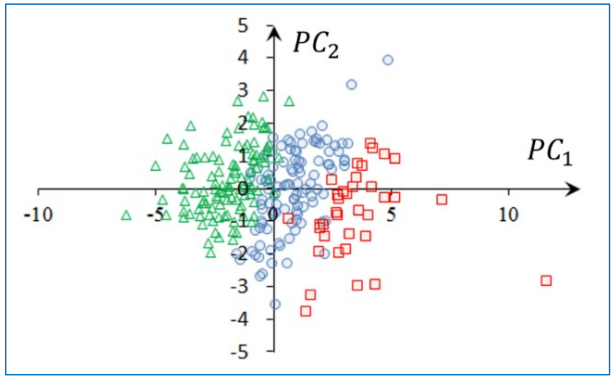
## High dimension visualization

**Ex**




Projected onto the original variable set




Projected onto the plane defined by $PC_1$ and $PC_2$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Document

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