LECTURER: TAI LE QUY

MACHINE LEARNING

UNSUPERVISED LEARNING AND FEATURE ENGINEERING

TOPIC OUTLINE

INTRODUCTION TO UNSUPERVISED MACHINE LEARNING AND FEATURE ENGINEERING	1
CLUSTERING	2
DIMENSIONALITY REDUCTION	3
FEATURE ENGINEERING	4
FEATURE SELECTION	5
AUTOMATED FEATURE GENERATION	6

UNIT 3

DIMENSIONALITY REDUCTION

STUDY GOALS

- Explain **how dimensionality reduction** approaches **work**.
- **Apply** dimensionality reduction approaches.
- **Choose an appropriate** dimensionality reduction **approach** with respect to the challenges and constraints of the dataset.

EXPLAIN SIMPLY

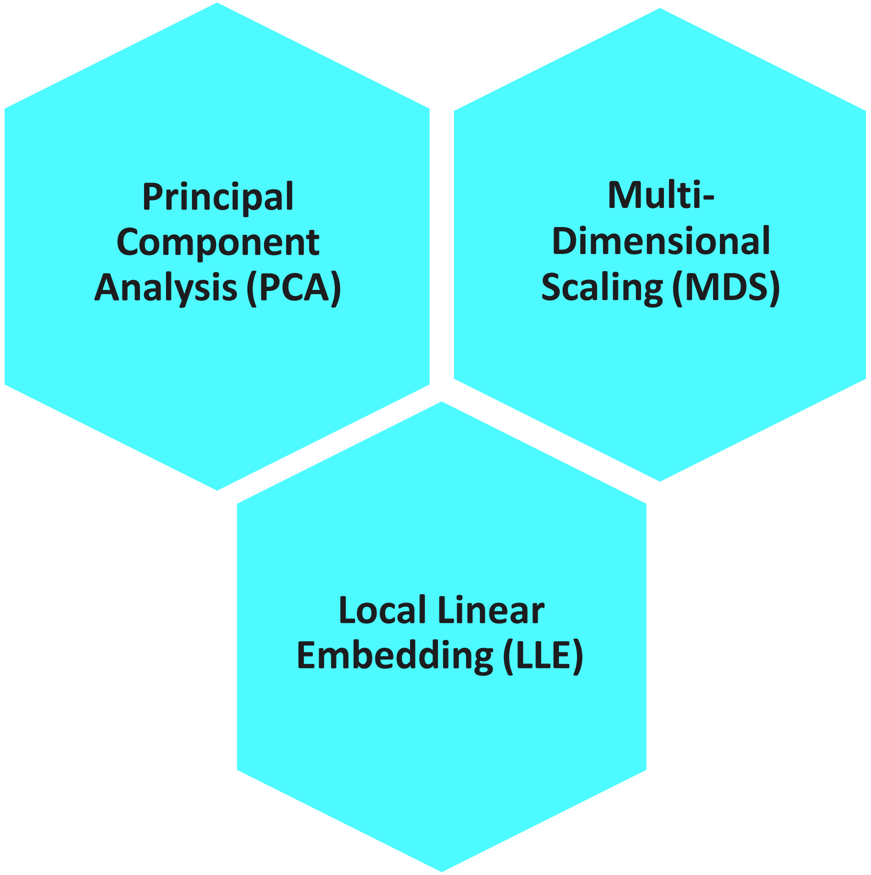
1. Name one **reason** why **dimensionality reduction** is conducted **before clustering** algorithms are applied.

2. Explain what the **curse of dimensionality** is.

3. Explain how dimensionality reduction can be **used during** the **reporting** phase of a project.

UNIT CONTENT

Image 1: Unit content - Dimensionality reduction



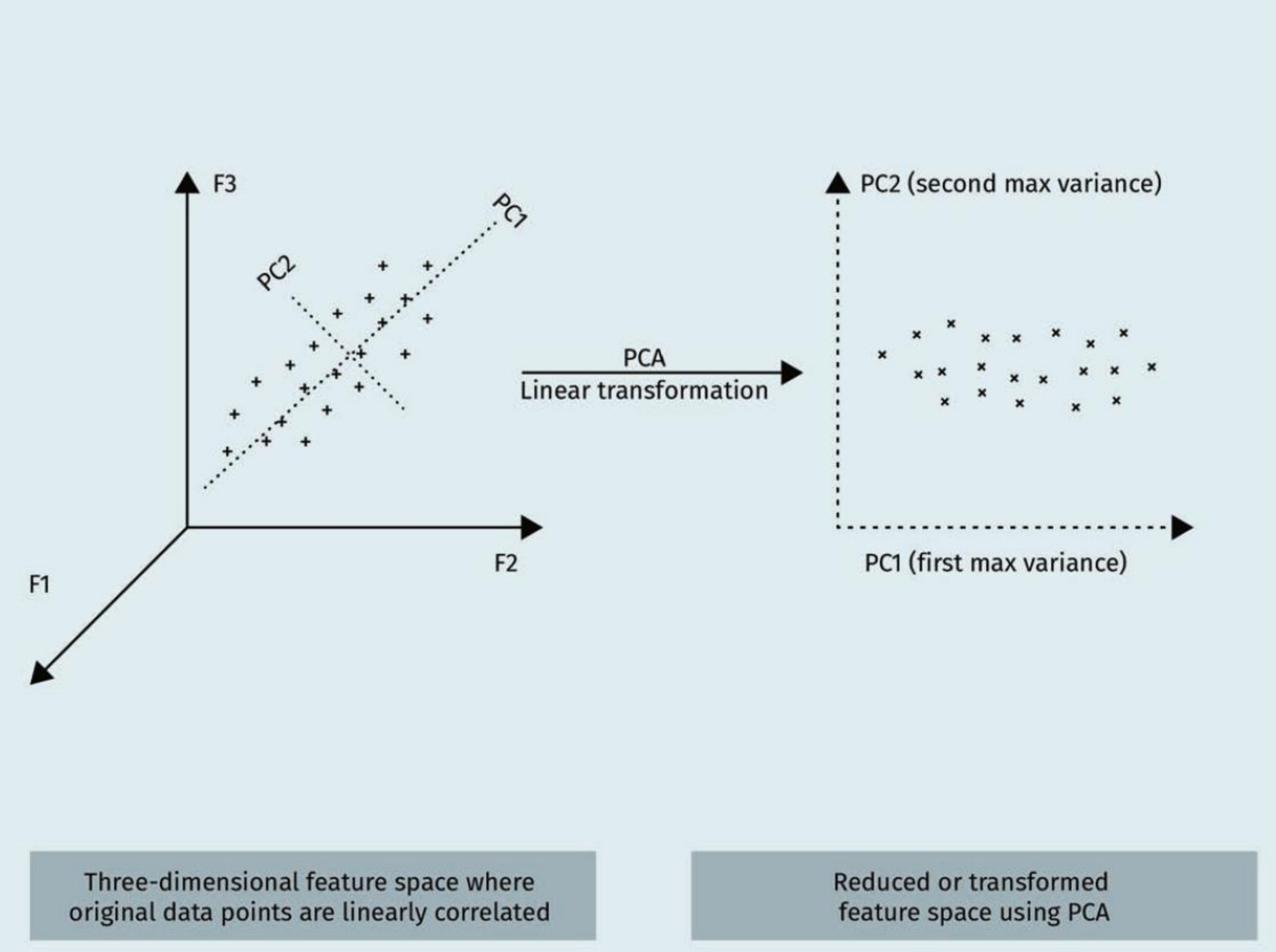
Principal Component Analysis (PCA)

Multi-Dimensional Scaling (MDS)

Local Linear Embedding (LLE)

Source of the image: Müller-Kett, 2021.

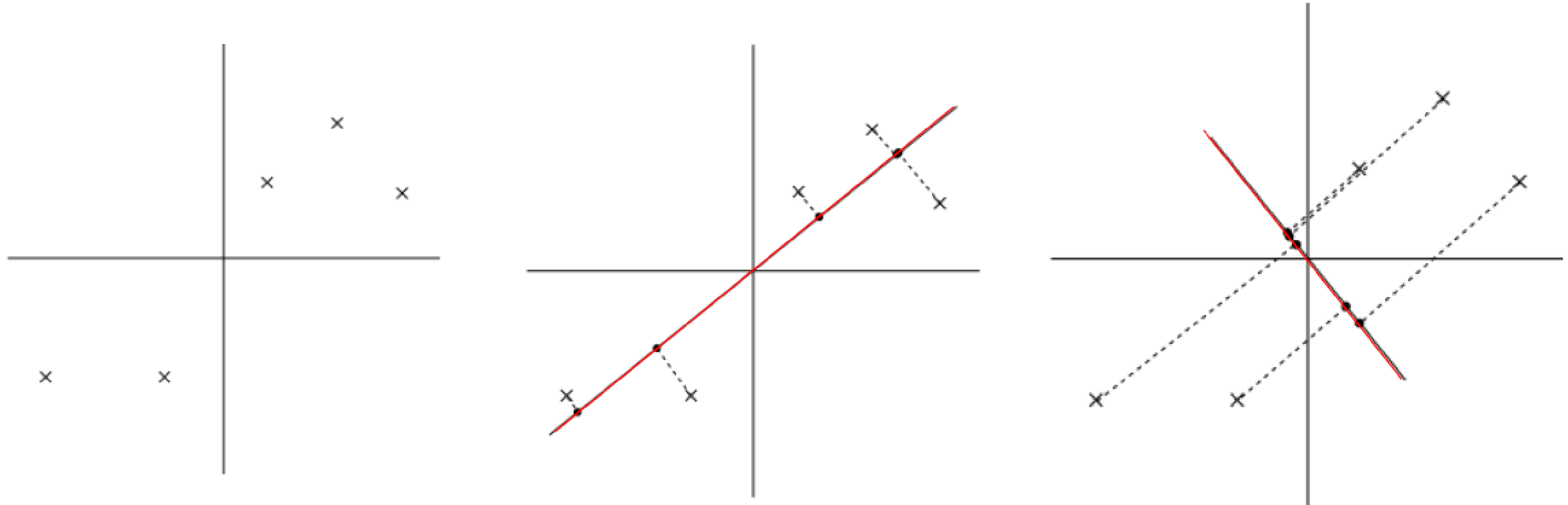
PRINCIPAL COMPONENT ANALYSIS (PCA)


F3
PC1
PC2
F2
F1
PCA
Linear transformation
PC2 (second max variance)
PC1 (first max variance)
Three-dimensional feature space where original data points are linearly correlated
Reduced or transformed feature space using PCA

Source of the image: Müller-Kett, 2021.

PRINCIPAL COMPONENT ANALYSIS (PCA)

- The data has some amount of variance/information. We would like to choose a direction *u* so that if we were to approximate the data as lying in the direction/subspace corresponding to *u*, as much as possible of this variance is still retained.



Initial data

Direction 1

Direction 2

Idea: Choose the direction that maximizes the variance of the projected data

PRINCIPAL COMPONENT ANALYSIS (PCA)

- General form: DV = D’
  - D_{nxd} is the original dataset
  - V_{dxk} is a linear transformation
  - D'_{nxk} is the re-representation of the dataset
  - d: original dimensionality
  - k: reduced dimensionality
  - General form: DV = D’

- Geometrically, *V* is a *rotation* and a *stretch* which transforms *D* into *D’*
  - The eigenvectors are the rotations to the new axes
  - The eigenvalues are the amount of stretching that needs to be done
  - The eigenvectors (principal components) determine the directions of the new feature space
  - The eigenvalues explain the variance of the data along the new feature axes.

- PCA computes the **eigenvalues** and **eigenvectors** of covariance matrix

Source of the image: Müller-Kett, 2021.

PRINCIPAL COMPONENT ANALYSIS (PCA) : Variance - Covariance matrix

– Describes the **variance** of all features (in the diagonal) and feature pairwise correlations/**covariances**

$$D = \begin{pmatrix} v_1 \\ \vdots \\ v_n \end{pmatrix} = \begin{pmatrix} v_{1,1} & \cdots & v_{1,d} \\ \vdots & \ddots & \vdots \\ v_{n,1} & \cdots & v_{n,d} \end{pmatrix} \qquad \Sigma_D = \begin{pmatrix} VAR(X_1) & \cdots & COV(X_1, X_d) \\ \vdots & \ddots & \vdots \\ COV(X_d, X_1) & \cdots & VAR(X_d) \end{pmatrix}$$

- For *d*-dimensional data, *dxd* covariance matrix
- symmetric matrix as *COV(X,Y)=COV(Y,X)*

– Variance is a measure of the spread of the data along a dimension *X*
It measures how far the values of X are spread out from the average X value (μ)

$$VAR(X) = \frac{1}{n}\sum_{i=1}^{n}(x_i - \mu)^2$$

ID	Height
1	100
2	100
3	100
4	100
5	100

Variance =0

ID	Height
1	100
2	100
3	105
4	100
5	100

Small variance (4)

ID	Height
1	100
2	100
3	100
4	200
5	100

Large variance
(1600)

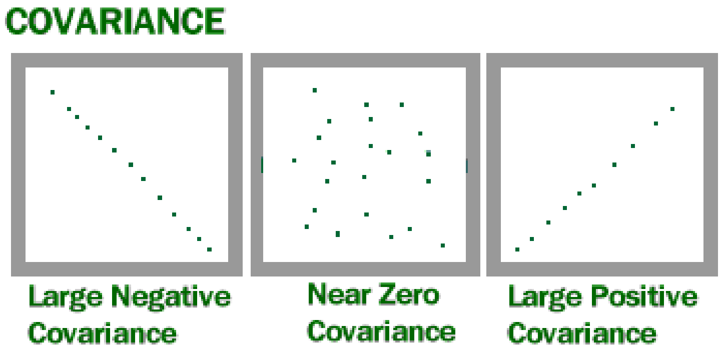
PRINCIPAL COMPONENT ANALYSIS (PCA) : Variance - Covariance matrix

- Covariance provides a measure of the strength of the correlation between two variables X,Y

$$COV(X,Y)=\frac{1}{n}\sum_{i=1}^{n}(x_i-\mu_x)(y_i-\mu_y)$$

- μ_x,μ_y: the means of *X, Y*

- What the covariance values mean
  - Zero value: the variables are uncorrelated.
  - Positive values: both dimensions move together (increase or decrease)
  - Negative values: while one dimension increases the other decreases



PRINCIPAL COMPONENT ANALYSIS (PCA) : Eigenvectors Eigenvectors and eigenvalues formally

- Let Σ be square dxd matrix
- A non-zero vector v is called an *eigenvector* of Σ if and only if there exists a scalar (i.e., a single number) λ such that:

$$\Sigma v = \lambda \mathrm{v}$$

$$I = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$

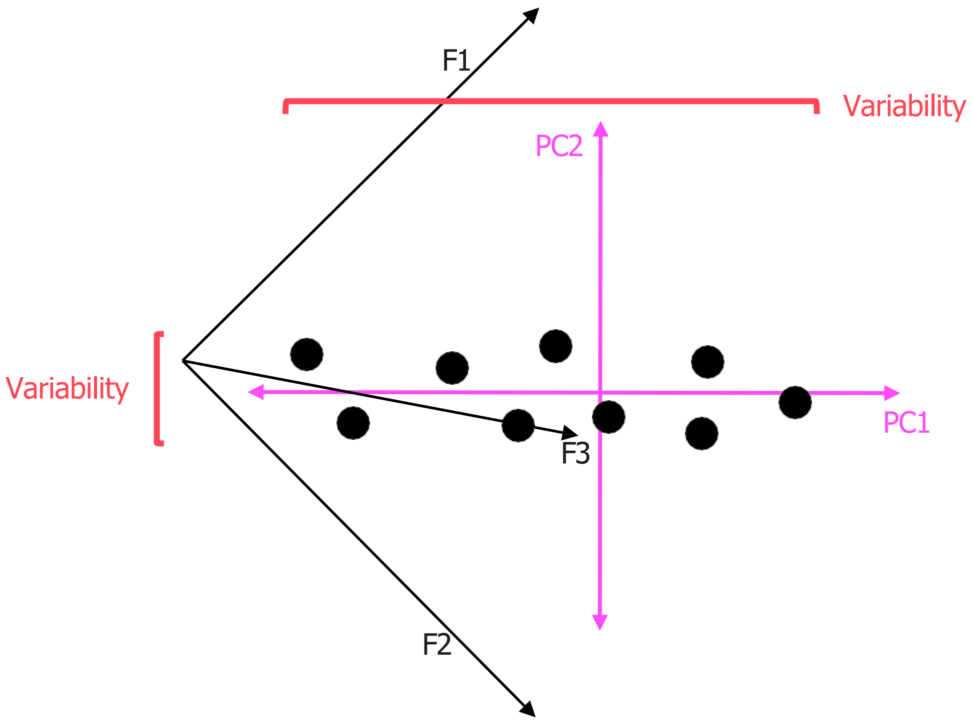
$$|A| = \begin{vmatrix} a & b \\ c & d \end{vmatrix} = ad - bc.$$

- If such a number λ exists it is called and eigenvalue of Σ
- The vector v is call the eigenvector associated with λ
- How to find the eigenvalues/eigenvectors of Σ ?
  - By solving Σv=λv, which can be rewritten as (Σ-λI)v = 0 (I is the identity matrix, 0 is a vector of all zero.
  - From linear algebra, in order for (Σ-λI)v = 0 to hold, the determinant should be zero, i.e., det(Σ -λI)=0
  - Solving det(Σ -λI)=0 we get the eigenvalues λ
  - For each eigenvalue λ we can find the eigenvector by solving: Σv=λv

PRINCIPAL COMPONENT ANALYSIS (PCA)

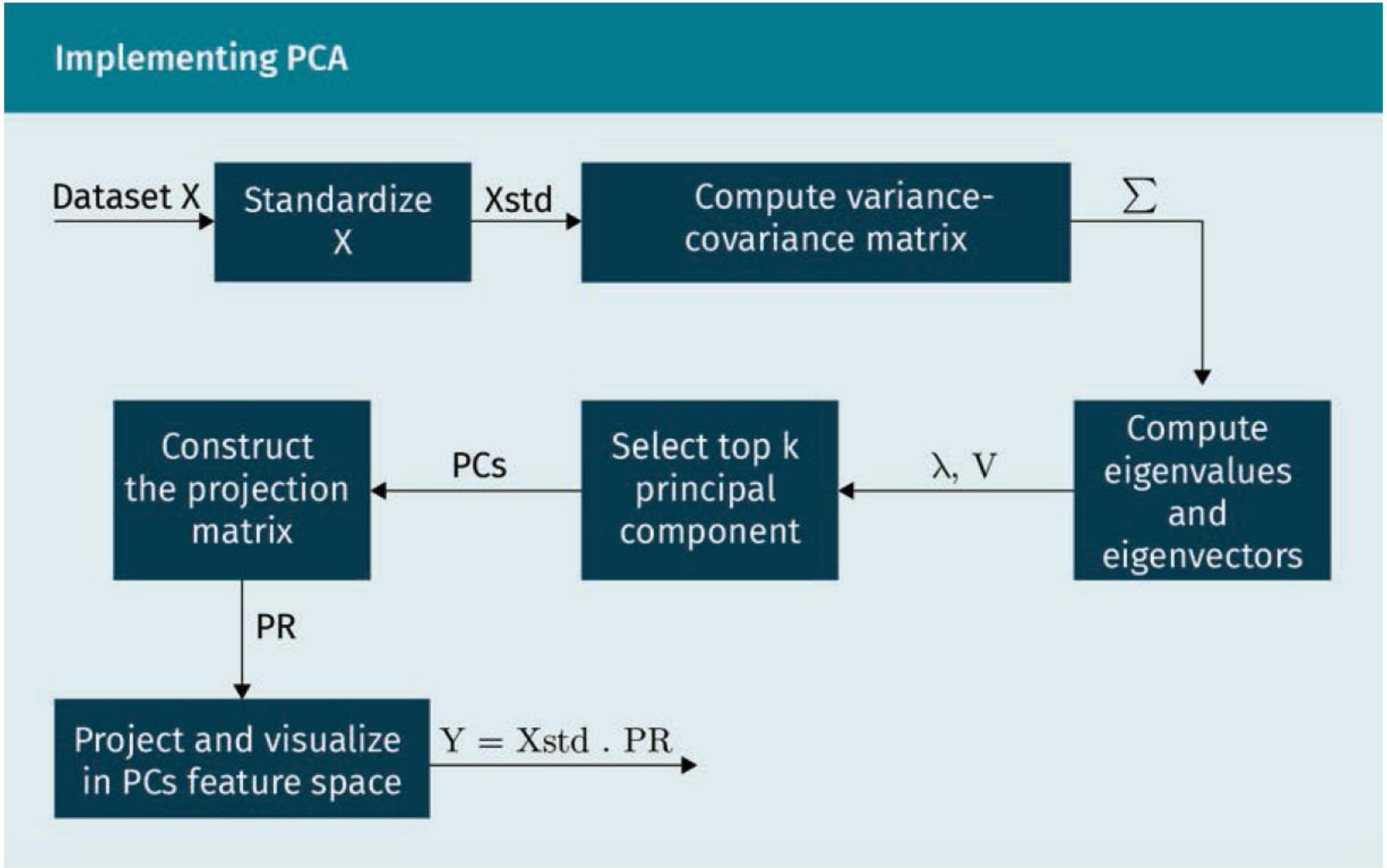
1. **Standardize** the data.
2. Compute the **variance-covariance matrix.**
3. Compute **eigenvalues** and **eigenvectors** (matrix eigen decomposition).
4. **Select** the top k **Principle Components.**
5. Construct the **projection matrix/loading scores.**
6. **Project** the data and **visualize** it in the PC feature space.

Image 2: PCA



Source of the image: Müller-Kett, 2021.

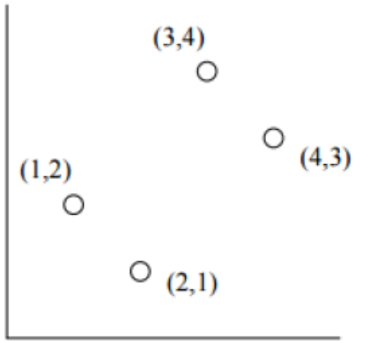
PRINCIPAL COMPONENT ANALYSIS (PCA)


Implementing PCA
Dataset X
Standardize X
Xstd
Compute variance-covariance matrix
Σ
Compute eigenvalues and eigenvectors
λ, V
Select top k principal component
PCs
Construct the projection matrix
PR
Project and visualize in PCs feature space
Y = Xstd . PR

Source of the image: Müller-Kett, 2021.

PRINCIPAL COMPONENT ANALYSIS (PCA): Example of transformation

- Original



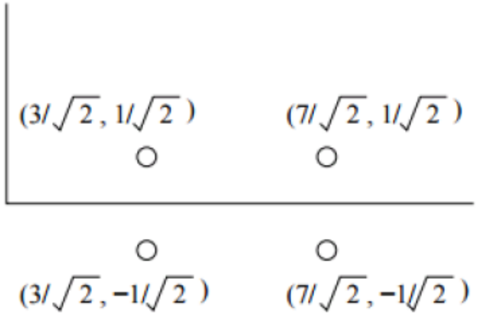
Eigenvectors

$$\boxed{\begin{bmatrix} 1/\sqrt{2} \\ 1/\sqrt{2} \end{bmatrix}} \quad \begin{bmatrix} -1/\sqrt{2} \\ 1/\sqrt{2} \end{bmatrix}$$

- Transformed data

$$\begin{bmatrix} 1 & 2 \\ 2 & 1 \\ 3 & 4 \\ 4 & 3 \end{bmatrix} \begin{bmatrix} 1/\sqrt{2} & -1/\sqrt{2} \\ 1/\sqrt{2} & 1/\sqrt{2} \end{bmatrix} = \begin{bmatrix} 3/\sqrt{2} & 1/\sqrt{2} \\ 3/\sqrt{2} & -1/\sqrt{2} \\ 7/\sqrt{2} & 1/\sqrt{2} \\ 7/\sqrt{2} & -1/\sqrt{2} \end{bmatrix}$$

In the rotated coordinate system



Source: http://infolab.stanford.edu/~ullman/mmds/ch11.pdf

PERCENTAGE OF VARIANCE EXPLAINED BY PCA

- Let *k* be the number of top eigenvalues out of *d* (*d* is the number of dimensions)
- The percentage of variance in the dataset explained by the k selected eigenvalues λ_1 $_{, \dots ,}$ λ_k is:

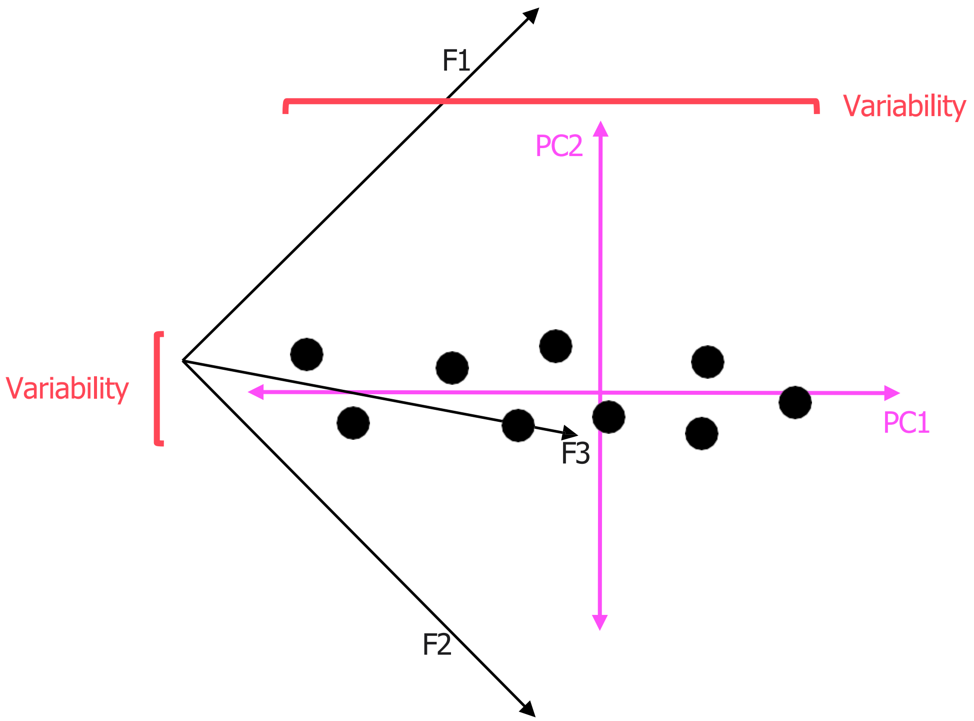
$$\frac{\sum_{i=1}^{k} \lambda_i}{\sum_{i=1}^{d} \lambda_i}$$

- Similarly, you can find the variance explained by each principal component
- Rule of thumb: keep enough to explain 85% of the variance

Drawbacks

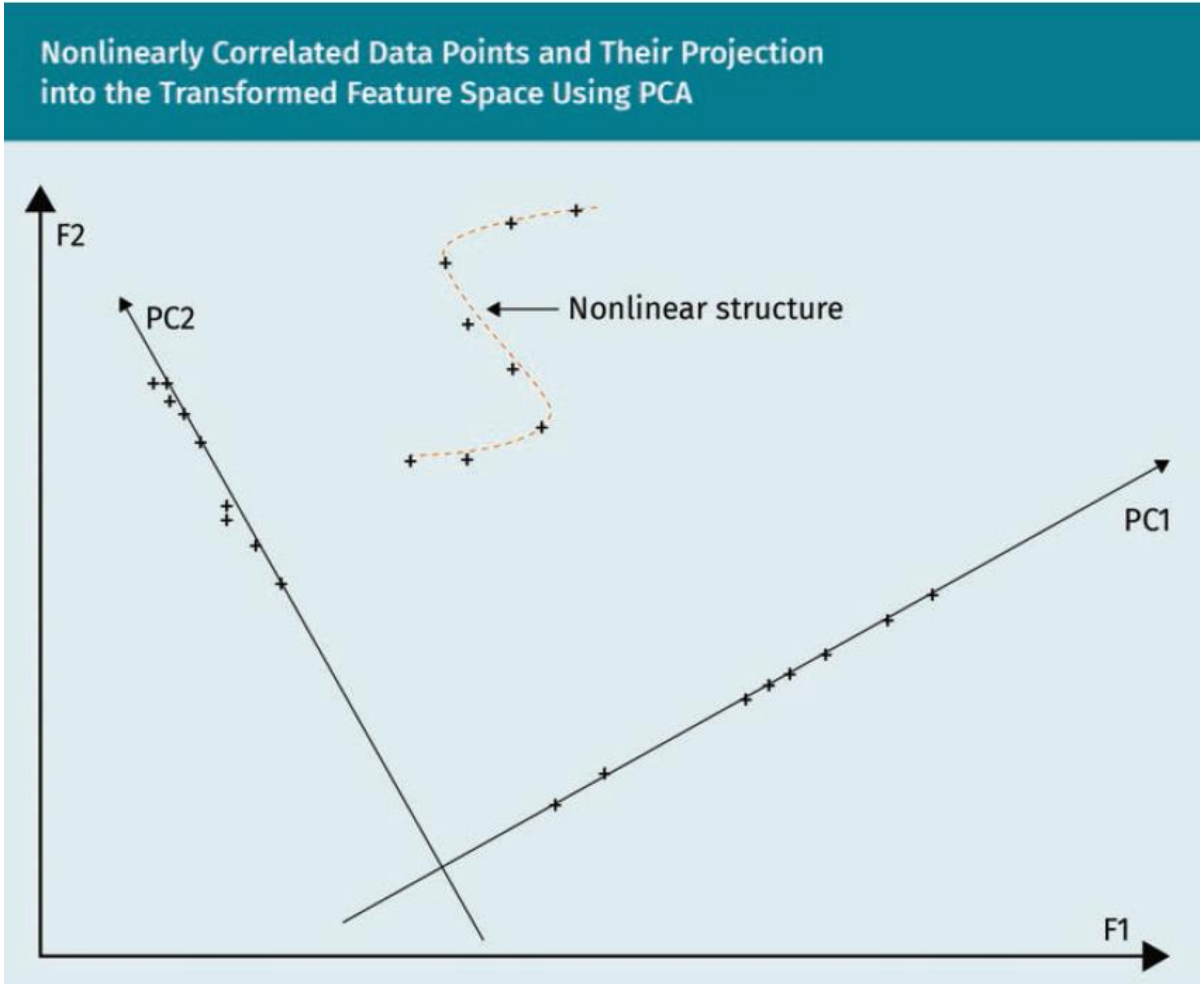
- PCA performs **poorly on non-linearly correlated** data
- **Thresholds** and **PC selection** is highly **use-case specific** and **subjective**
- **Only** for **numerical** features
- **Bad interpretability**

Image 3: PCA



Source of the image: Müller-Kett, 2021.

PRINCIPAL COMPONENT ANALYSIS (PCA)

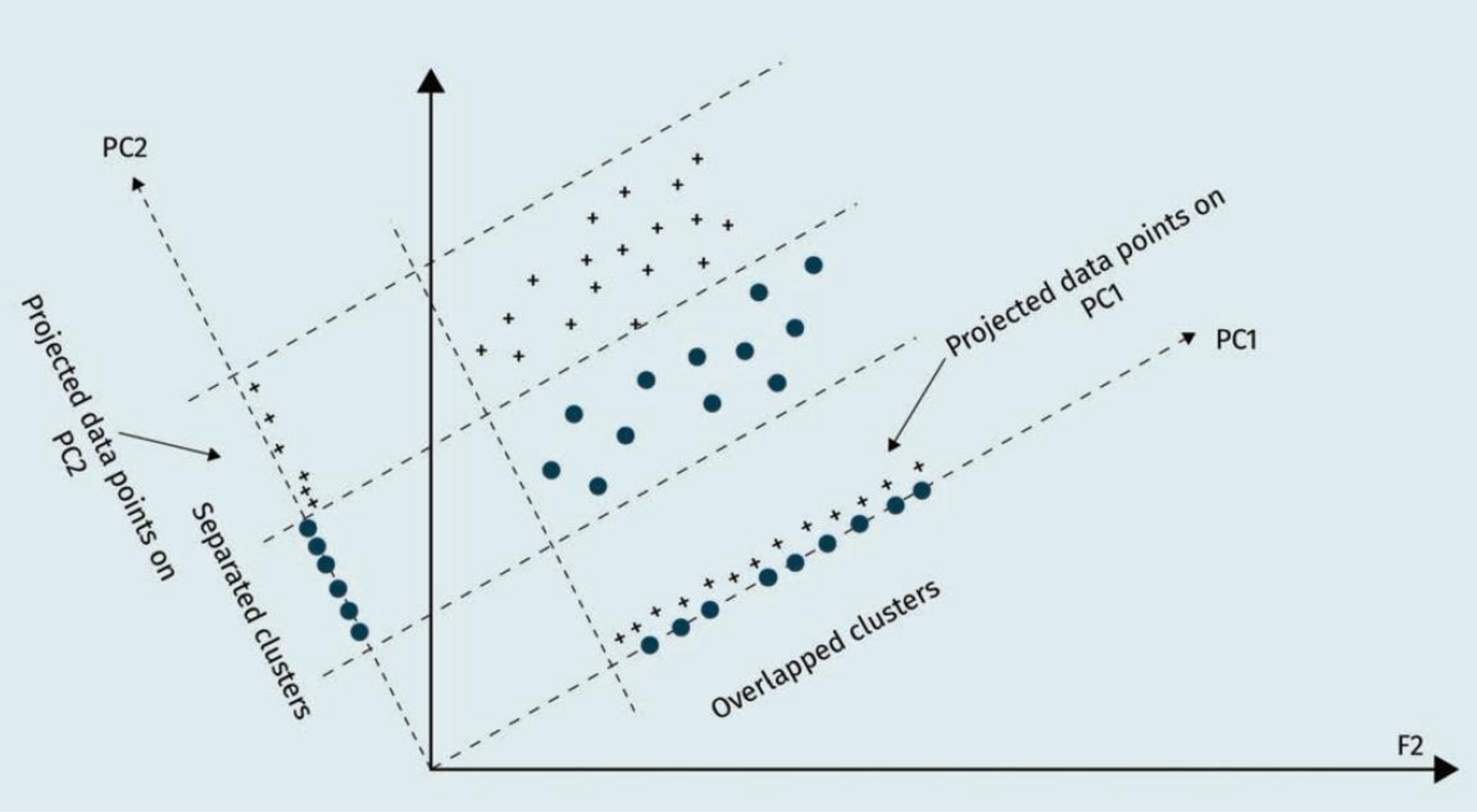


Nonlinearly Correlated Data Points and Their Projection into the Transformed Feature Space Using PCA

Source of the image: Müller-Kett, 2021.

PRINCIPAL COMPONENT ANALYSIS (PCA)

- Vector loadings:
  - The vector loadings are the eigenvectors multiplied by the square root of eigenvalues.
  - They represent the correlations between the original variables and the eigenvectors.



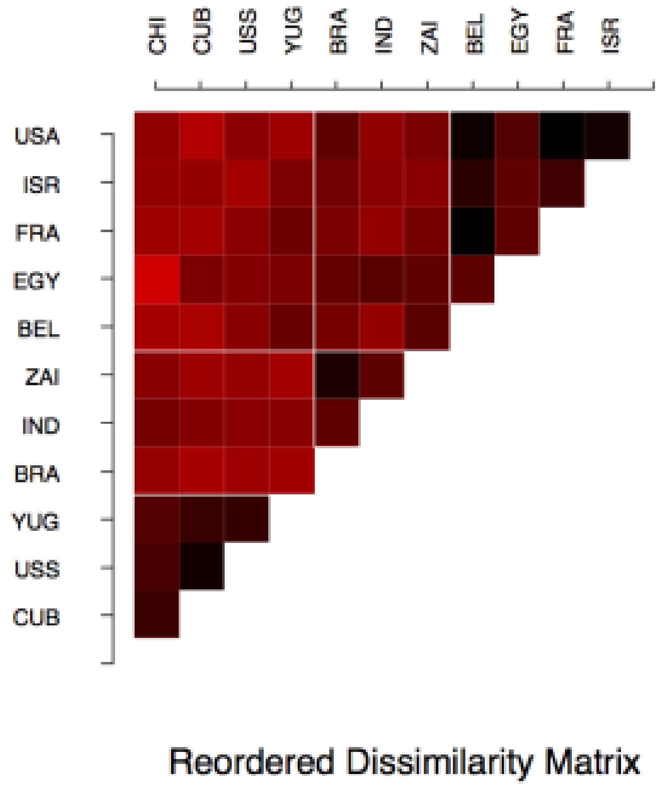
Source of the image: Müller-Kett, 2021.

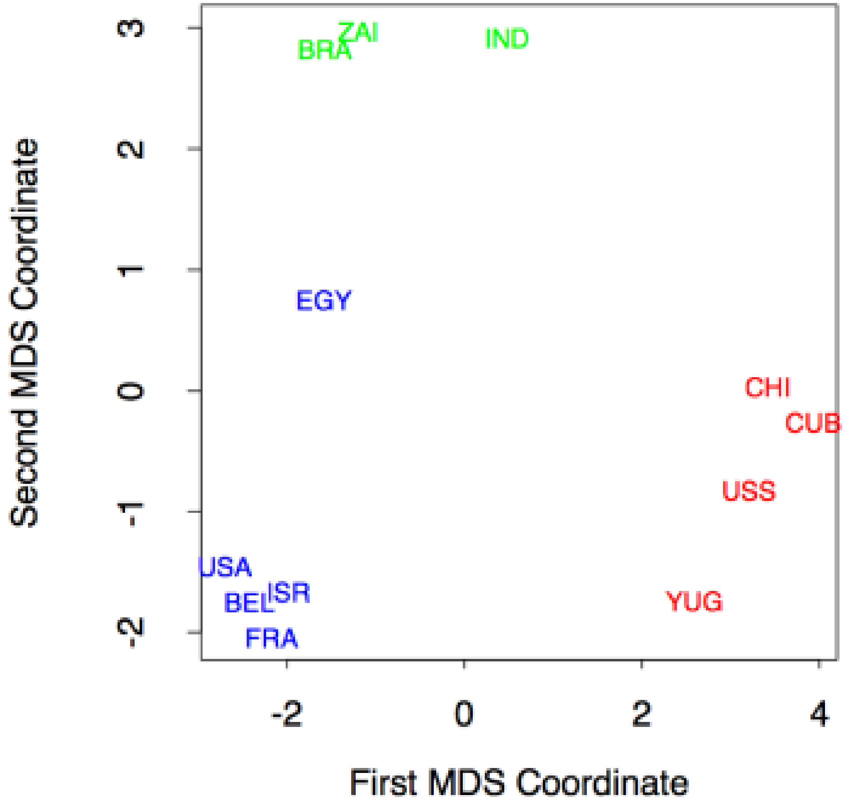
MULTI-DIMENSIONAL SCALING (MDS)

- Similar to PCA
- Instead of maximizing the variance, MDS **preserves pairwise similarities**…
- …by **minimizing the difference** between **distances in the original and reduced feature spaces.**
- Based on a **dissimilarity matrix**
  - **Metric MDS** for numeric data
  - **Non-Metric MDS** for categorical data

Source of the text: Buja et al., 2008.

MULTI-DIMENSIONAL SCALING (MDS)





Source of the image:https://www.stat.pitt.edu/sungkyu/course/2221Fall13/lec8_mds_combined.pdf

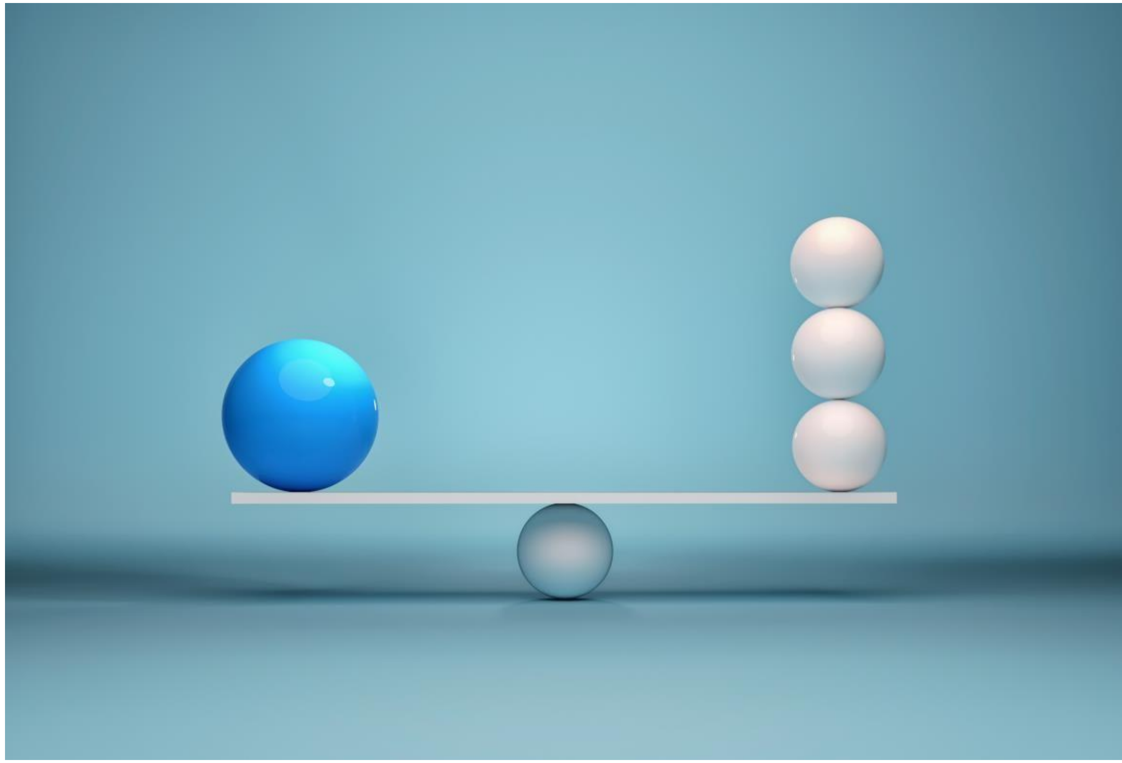
Advantage over PCA

- Can be used for **non-linear correlations.**

Disadvantage

- **Computationally expensive** compared to PCA.

Image 4: Pros and cons



Source of the image: Microsoft Archive.

LOCAL LINEAR EMBEDDING (LLE)

- Preserves **local geometries** of the "manifold‟.

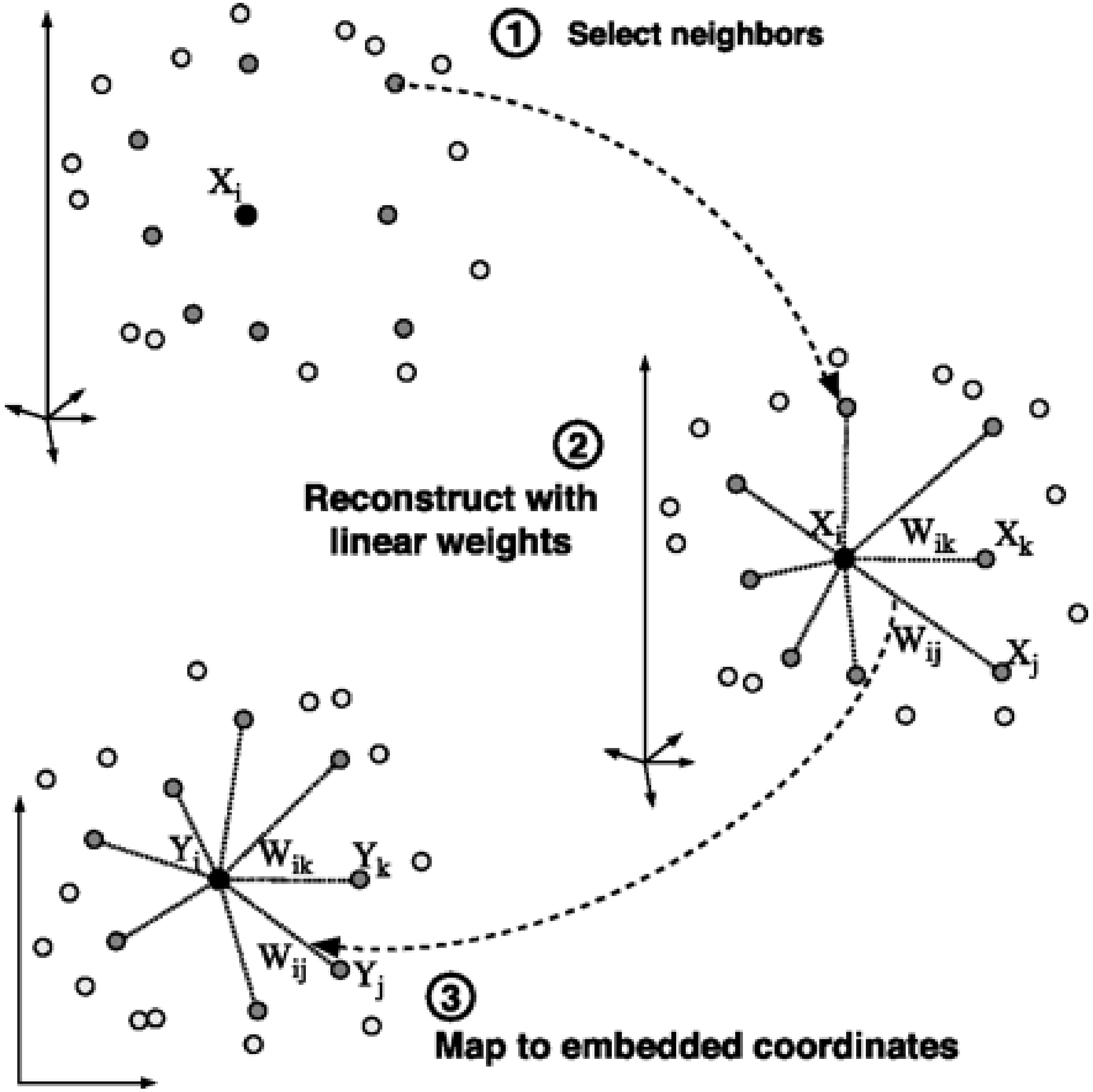
1. For each sample, choose **k nearest neighbors.**

2. Find **weights** that, when being multiplied with the neighbors, **reconstruct the sample** in question.

3. Use the optimized weights to find an **embedding vector** containing the coordinates in the reduced feature space.

Source of the text: Saul & Roweis, 2000.

LOCAL LINEAR EMBEDDING (LLE)



Source: https://cs.nyu.edu/~roweis/lle/algorithm.html

LOCAL LINEAR EMBEDDING (LLE)

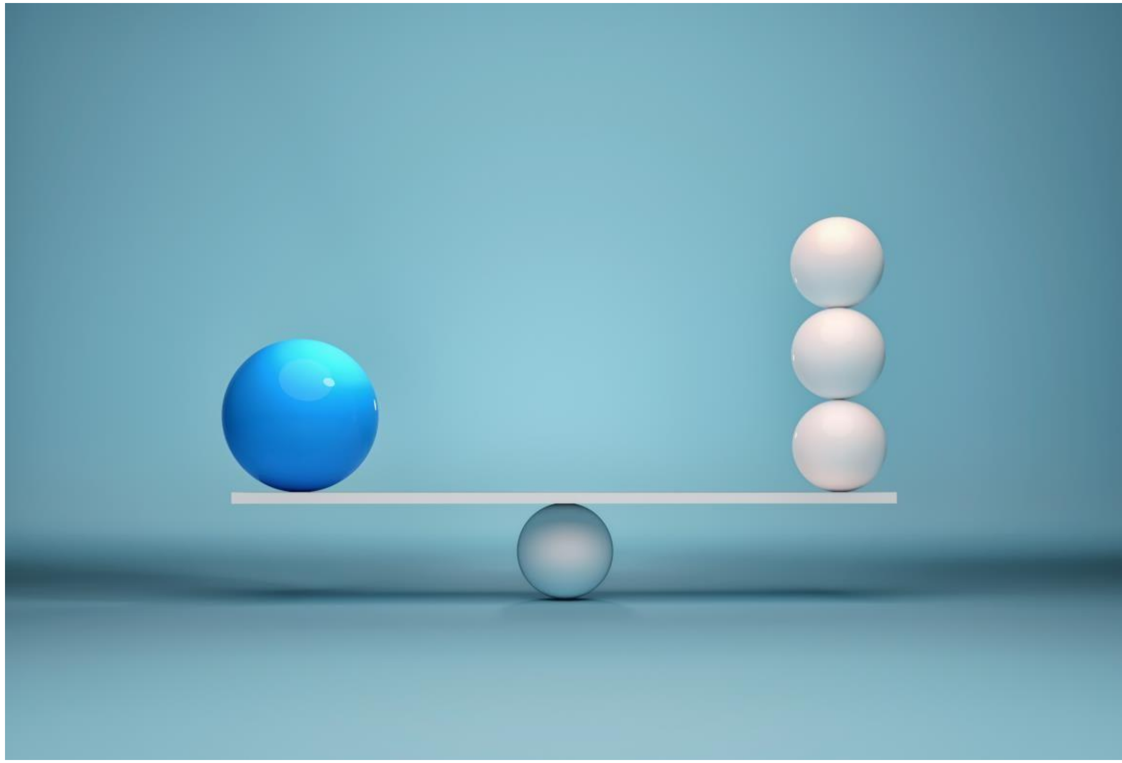
Advantage

- **Computationally cheaper** than MDS

Disadvantages

- **Susceptible to outliers**

Image 4: Pros and cons



Source of the image: Microsoft Archive

REVIEW STUDY GOALS

- Explain **how dimensionality reduction** approaches **work**.
- **Apply** dimensionality reduction approaches.
- **Choose an appropriate** dimensionality reduction **approach** with respect to the challenges and constraints of the dataset.

SESSION 3

TRANSFER TASK

TRANSFER TASKS

A start-up that sells **sustainable products in smaller stores** has been very successful in recent years. As a result, more stores are to be opened worldwide.

To keep an **overview of the offered products**, you and your team of Data Scientists are tasked to **define homogeneous groups of products** to facilitate ordering, marketing, and distribution. For this purpose, you create **data visualizations** that show product groups as data points close to each other.

After some exploratory trials, you realize that the products seem to be **grouped in irregular shapes** in the original feature space. Also, your team is relatively new and still waiting for big PCs, so you still **work on your laptop**.

Discuss which **method** is **appropriate** for this use case. In your reasoning, also explain why other methods are not suitable in this context.

TRANSFER TASK
PRESENTATION OF THE RESULTS

Please present your results.

The results will be discussed in plenary.

LEARNING CONTROL QUESTIONS

1. Which of the following propositions is correct regarding principal component analysis (PCA)?
   a) Eigenvectors form the axes in the reduced feature space.
   b) Eigenvalues represent the overall variance in the entire dataset.
   c) Eigenvalues form the axes in the transformed feature space.
   d) Eigenvectors represent the proportion of explained variances according to each Eigenvalue.

2. Which of the following does MDS seek to preserve during dimensionality reduction?

a) the variance and distance between data samples
b) the variance between data samples
c) the variance-covariance between data samples
d) the distance between data samples

LEARNING CONTROL QUESTIONS

3. In which of the following is it recommended to use LLE?

   a) in datasets with noise and outliers
   b) in small datasets
   c) in large datasets
   d) in data samples with linear correlations

LIST OF SOURCES

Text

Buja, A., Swayne, D. F., Littman, M. L., Dean, N., Hofmann, H., & Chen, L. (2008). Data visualization with multidimensional scaling. Journal of Computational and Graphical Statistics, 17(2), 444—472. https://doi.org/10.1198/106186008X318440

Saul, L. K., & Roweis, S. T. (2000). An introduction to locally linear embedding. [Unpublished article]. https://cs.nyu.edu/~roweis/lle/papers/lleintro.pdf

Images

Müller-Kett, 2021.

Microsoft Archive.