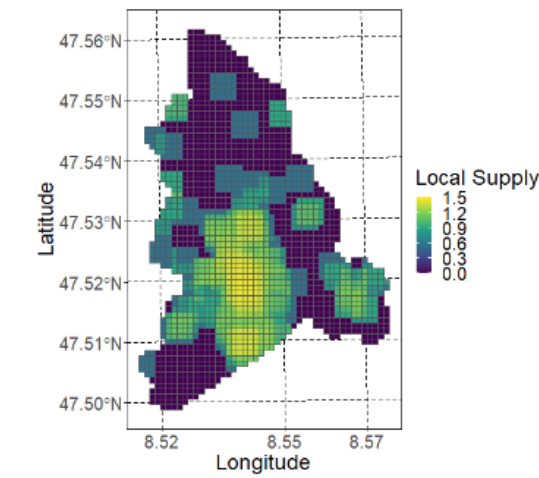


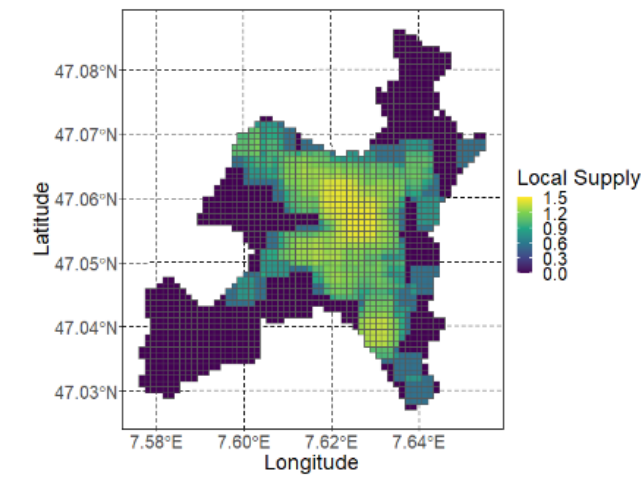
CAS Machine Learning

Unsupervised Learning: Clustering, Anomaly Detection, Dimensionality Reduction and Visualization

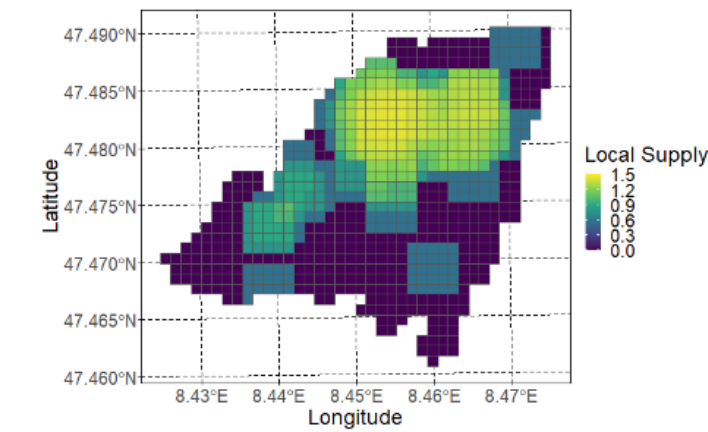
Dr. Yves Staudt
PhD in Actuarial Sciences
yves.staudt@hslu.ch



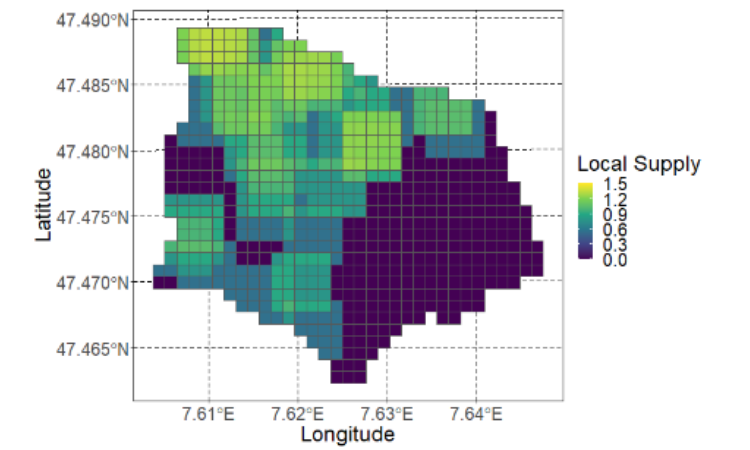
(a)
Grenchen



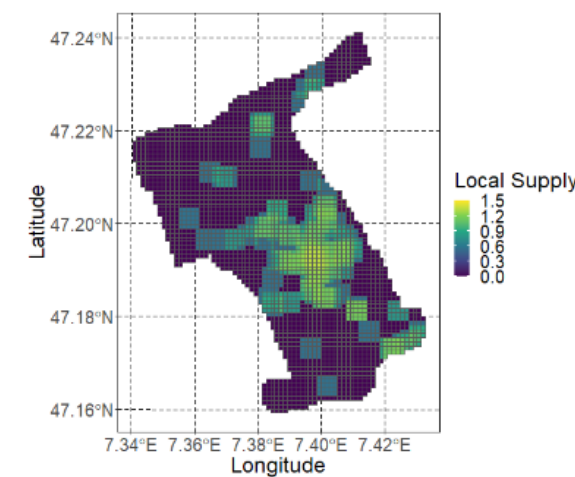
(b)
Oberglatt



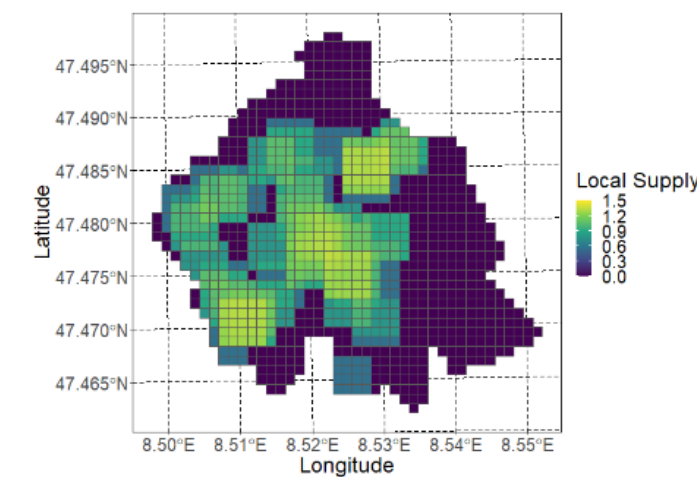
(c)
Reinach



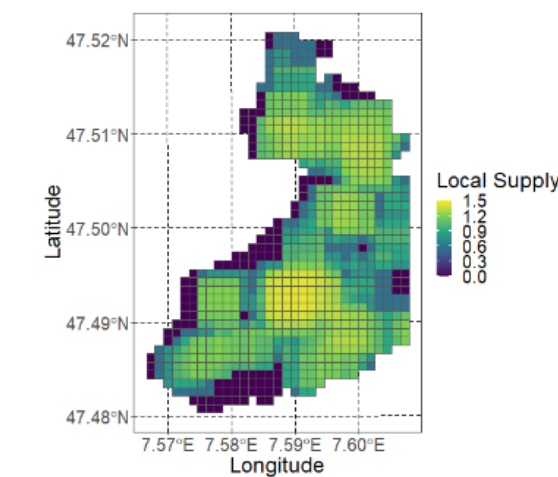
(d)
Rubigen



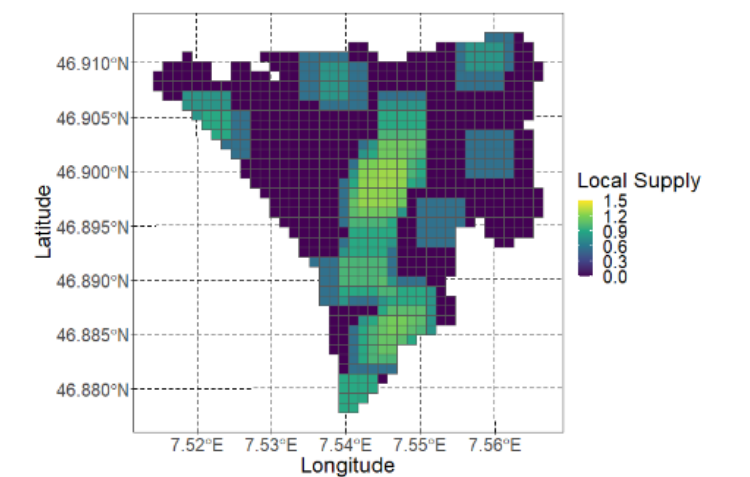
(e)
Buelach



(f)
Burgdorf



(g)
Dielsdorf



(h)
Dornach

Agenda

1. Einführung
2. Kennenlernen Spiel
3. Clustering
4. K-Means Algorithmus
5. Determining Optimal Number of Clusters
6. Hierarchical Clustering Algorithmus
7. Kommunikation der Resultate
8. Dimensions Reduktionsverfahren
9. Principal Components Analysis
10. T-Distributed Stochastic Neighbor Embedding
11. Zusammenfassung

Agenda

1. Einführung

2. Kennenlernen Spiel
3. Clustering
4. Data Preprocessing
5. K-Means Algorithmus
6. Determining Optimal Number of Clusters
7. Hierarchical Clustering Algorithmus
8. Kommunikation der Resultate
9. Dimensions Reduktionsverfahren
10. Principal Components Analysis
11. T-Distributed Stochastic Neighbor Embedding
12. Zusammenfassung

Lernziel

Nach dem Kurs sind die Teilnehmende in der Lage:

- Merkmale nach Gleichheiten und Unterschiede zu bestimmen.
- Unterschiedsmasse zur Messung von Ähnlichkeiten zu beschreiben.
- Cluster Verfahren zu beschreiben, zu unterscheiden und anzuwenden.
- Cluster Resultate zu interpretieren.
- Dimension Reduktionsverfahren zu beschreiben, zu unterscheiden und anzuwenden.

Dozent



Profil: Dr. Yves Staudt

Ursprung: Luxemburg

Erfahrung: Umfangreiche praktische Erfahrung in Datenanalysen, Data-Mining, Machine and Deep Learning

Interesse: Bergen, Fotografie und Kochen

Sozial: Ein sozialer Austausch ist mir wichtig.

Unterrichtsplanung

Uhrzeit	Thema
9:15 – 10:00	Einführung und Unterschiede bestimmen
10:05 – 10:50	Clustering, K-Means and Determining Optimal Number of Classes
11:00 – 11:45	Application Clustering
11:40 -12:35	Hierarchical Clustering Algorithmus
12:35-13:40	Mittagspause
13:40 – 14:25	Kommunikation und Interpretation der Resultate
14:30 – 15:15	Dimension Reduktionsverfahren, Principal Component Analys
15:30 – 16:15	t-Distributed Stochastic Neighbor Embedding
16:15 – 16:45	Zusammenfassung und Abschluss

Code Notebooks

Code Notebooks von Python werden über

- Google Drive oder
- Ilias zur Verfügung gestellt

Bei der Nutzung von Google Drive bitte eine Kopie erstellen.

Lösungen werden Schrittweise auf Ilias hochgeladen

Agenda

1. Einführung

2. Kennenlernen Spiel

3. Clustering

4. Data Preprocessing

5. K-Means Algorithmus

6. Determining Optimal Number of Clusters

7. Hierarchical Clustering Algorithmus

8. Kommunikation der Resultate

9. Dimensions Reduktionsverfahren

10. Principal Components Analysis

11. T-Distributed Stochastic Neighbor Embedding

12. Zusammenfassung

Spielregeln

- Interaktives Spiel
- Wir bewegen uns im Klassenraum
- Fragen zu:
 - Demografie
 - Arbeitsumfeld
 - Kenntnissen in Mathematik

Idee des Spiels: Nach jeder Frage bewegen wir uns so in der Klasse, dass wir uns den Teilnehmenden nähern, welche ähnliche oder gleiche Antworten auf die Frage habe.

Schwierigkeit: In der Fortsetzung der Fragen, versuchen wir die vorher beantworteten Fragen zu berücksichtigen.

Wenn keine Fragen sind dann geht es los.

Frage 1



Wo wohnen Sie?



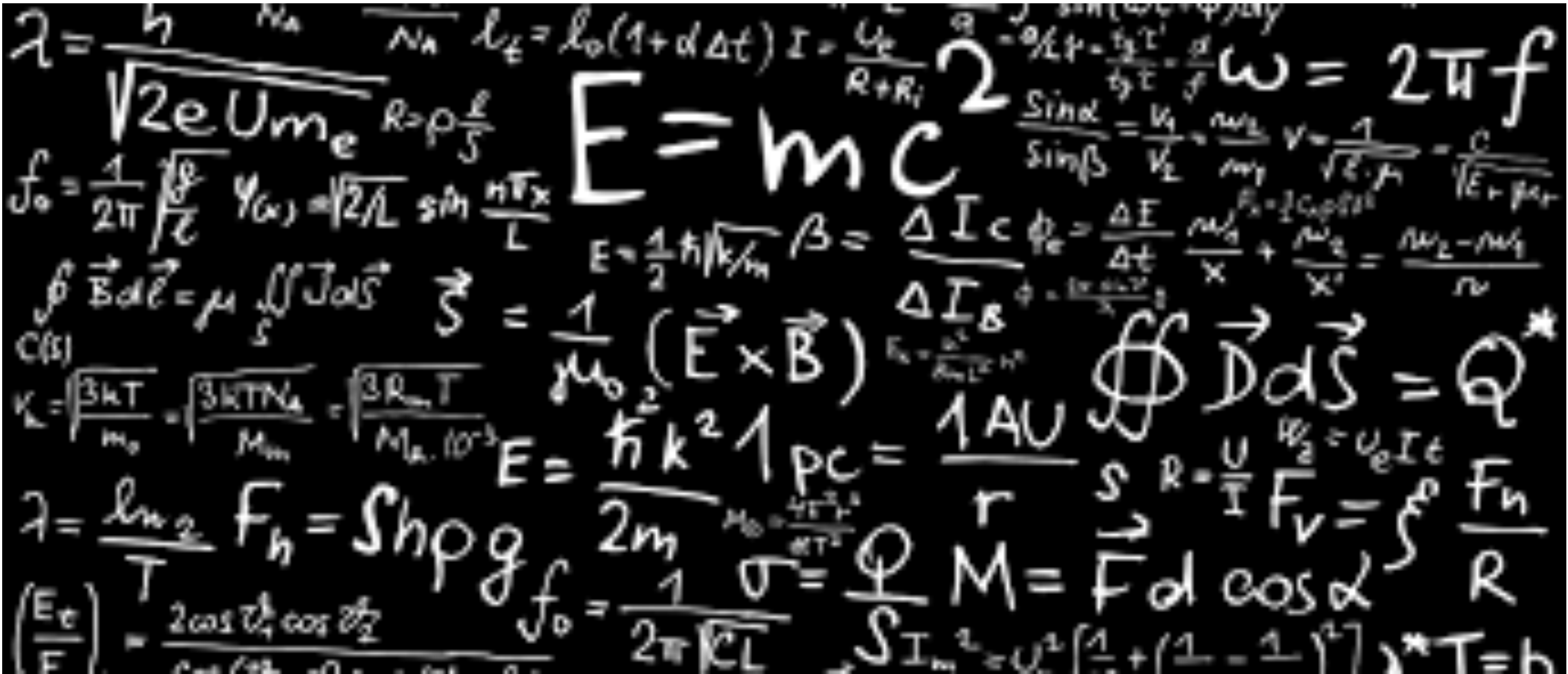
Frage 2



Wie alt sind Sie?



Frage 3



Wie schätzen Sie ihre Mathematikkenntnisse ein?



Erkenntnisse

Wie verbinden Sie das Spiel mit dem Thema des Kurses?

Was sind eure Erwartungen an den Kurs?

Schreiben Sie in einer Gruppe von drei die Erkenntnisse auf (10 Min)

Distances

Euclidean Distance: $\|x - y\|_2 = \sum_{j=1}^n (x_j - y_j)^2$ (Yin et al., 2021)

Simple Matching Distance: $D(x, y) = \begin{cases} 1, & \text{if } x_j \neq y_j \\ 0, & \text{if } x_j = y_j \end{cases}$ (Yin et al., 2021)

Dynamic Time Warping: $DTW(m, n) = |p_m - q_n| + \min \begin{pmatrix} DTW(m-1, n) \\ DTW(m-1, n-1) \\ DTW(m, n-1) \end{pmatrix}$ (Wong and Chung, 2019)

Agenda

1. Einführung

2. Kennenlernen Spiel

3. Clustering

4. K-Means Algorithmus

5. Determining Optimal Number of Clusters

6. Hierarchical Clustering Algorithmus

7. Kommunikation der Resultate

8. Dimensions Reduktionsverfahren

9. Principal Components Analysis

10. T-Distributed Stochastic Neighbor Embedding

11. Zusammenfassung

Statistical analysis of **MULTIVARIATE DATA**

AN ASSORTMENT OF MULTIVARIATE MODELS HELP TO ANALYZE AND DISPLAY n -DIMENSIONAL DATA. SOME MULTIVARIATE TECHNIQUES:

Cluster analysis

SEEKS TO DIVIDE THE POPULATION INTO HOMOGENEOUS SUBGROUPS. FOR EXAMPLE, BY ANALYZING CONGRESSIONAL VOTING PATTERNS, WE FIND THAT REPRESENTATIVES FROM THE *SOUTH AND WEST* FORM TWO DISTINCT CLUSTERS.



Darstellung der Clusteranalyse und deren
Anwendung (Gonick and Smith, 2005).

Goal of Clustering

- The **goal** of **clustering** is to group similar objects or data points together based on their inherent characteristics
- Clustering is a fundamental task in **unsupervised learning**
- Clustering identifies natural groupings or patterns within the data
- Objects within the same cluster are more similar to each other than to those in other clusters
- Clustering algorithms help in understanding the **underlying structure** or organization of the data, revealing insights, and supporting decision-making processes.

Application of Clustering

Clustering has various **applications** across different domains including:

- customer segmentation
- document classification
- anomaly detection
- image analysis
- data mining
- ...

(Generated by Chat GPT 1.1.2023)

Anomaly Detection

The goal of anomaly detection is to identify **unusual** or **anomalous** patterns or observations in a dataset

Unusual patterns deviate significantly from the norm or expected behavior

Anomalies can be indicative of errors, outliers, fraud, or any unexpected behavior that requires attention or investigation

Clustering aims to group **similar** data points together

Anomaly detection focuses on identifying the data points that are **dissimilar** or different from the majority

Clustering can be used as a preprocessing step for anomaly detection

By clustering the data, we can establish a notion of what is considered normal or expected within each cluster

Any data point that does not belong to any cluster or deviates significantly from its assigned cluster can be flagged as an anomaly

Aufgabe 1: Händisches Clustering

- Bilden Sie Gruppen von 2 bis 3 Teilnehmenden
- Gruppieren Sie die Bilder in drei Gruppen
- Dokumentieren Sie in Stichworten wie sie die Gruppierung vorgenommen haben



Aufgabe 2: Merkmale Bestimmen

- Begeben Sie sich in die vorher gegebenen Gruppen
- Dokumentieren Sie für die Bilder vier Merkmale/Variablen für die Bilder
- Dokumentieren Sie ob sich die Gruppierung verändern oder gleich bleibt

Agenda

1. Einführung
2. Kennenlernen Spiel
3. Clustering
- 4. K-Means Algorithmus**
5. Determining Optimal Number of Clusters
6. Hierarchical Clustering Algorithmus
7. Kommunikation der Resultate
8. Dimensions Reduktionsverfahren
9. Principal Components Analysis
10. T-Distributed Stochastic Neighbor Embedding
11. Zusammenfassung

K-means Clustering

Task of clusters: Partitioning the dataset into groups, called clusters.

Goal: To split up the data in such way that points within single clusters are very similar and points in different clusters are different.

Algorithm alternates between **two steps**:

1. Assigning each data point to the closest cluster center.
2. Setting each cluster center as the mean of the data point that are assigned to it.

The algorithm is finished when the assignment of instances to clusters no longer changes.

In k-means clustering the number of clusters k needs to be fixed by the analyst.

(Jamies et al., 2017; Kuhn and Johnson, 2016)

Properties of k-means clustering

Let C_1, C_2, \dots, C_K denote sets containing indices of the observations in each cluster

The sets satisfies the following two properties:

1. $C_1 \cup C_2 \cup \dots \cup C_K = \{1, \dots, n\}$
2. $C_k \cap C_l = \emptyset \forall k \neq l$

(James et al., 2013)

Optimization

Idea: A good clustering is one for which the within-cluster variation is as small as possible.

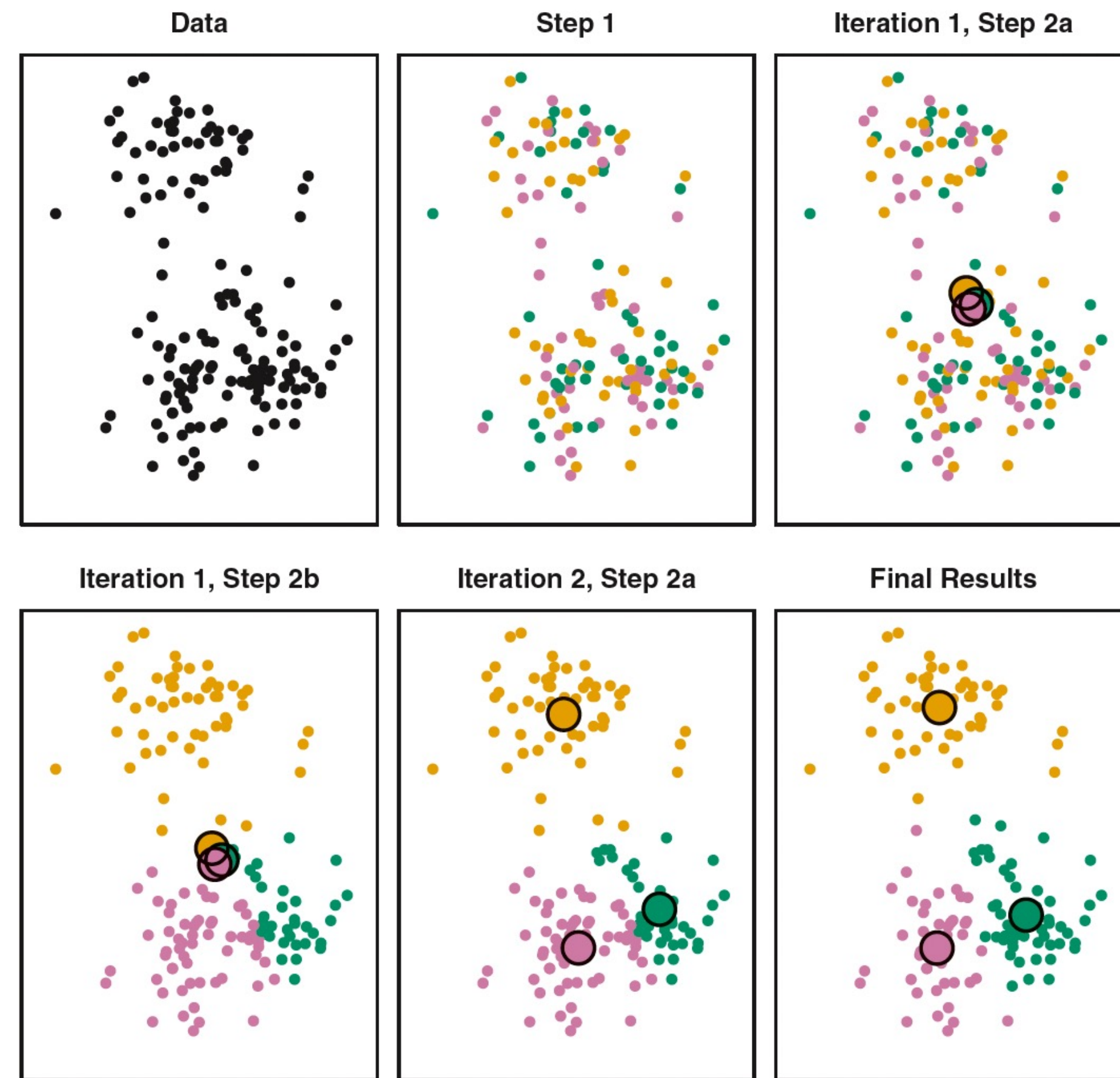
Within-cluster variation for cluster C_k measures the difference between the observations within a cluster.

Goal: To minimize the within-cluster variation

$$\begin{aligned} & \text{minimize}_{C_1, \dots, C_K} \left\{ \sum_{k=1}^K W(C_k) \right\} \\ & \text{minimize}_{C_1, \dots, C_K} \left\{ \sum_{k=1}^K \frac{1}{|C_k|} \sum_{i, i' \in C_k} \sum_{j=1}^p (x_{ij} - x_{i'j})^2 \right\} \end{aligned}$$

(James et al., 2013)

Representation of the k-means algorithm



Representation of the K-means algorithm (James et al. 2013)

Algorithm k-means clustering

The algorithm is explained with the help of three clusters (**k = 3**)

1. Initialization: Declaring three ($k=3$) data points randomly as clusters center.
2. Assign Points: Each data point is assigned to the cluster center it is closest to. (Using similarity measure)
3. Cluster centers are updated to the mean of the assigned points (Recompute Centers)
4. Stop when no assignments are done anymore.

(Jamies et al., 2013; Kuhn and Johnson, 2013)

Impact of scale

The scale of the variables has a huge impact in the algorithm.

To scale the data before application of k-means.

Exercise

- Begeben Sie sich in Gruppen von 2 bis 3 Teilnehmenden
- Öffnen Sie das Code Notebook "clustering_k_means_exercise.ipynb"
- Führen Sie für den gegebenen Datensatz das k-Means Clustering für $k=3$ durch
- Dokumentieren Sie was Ihnen aufgefallen ist

Agenda

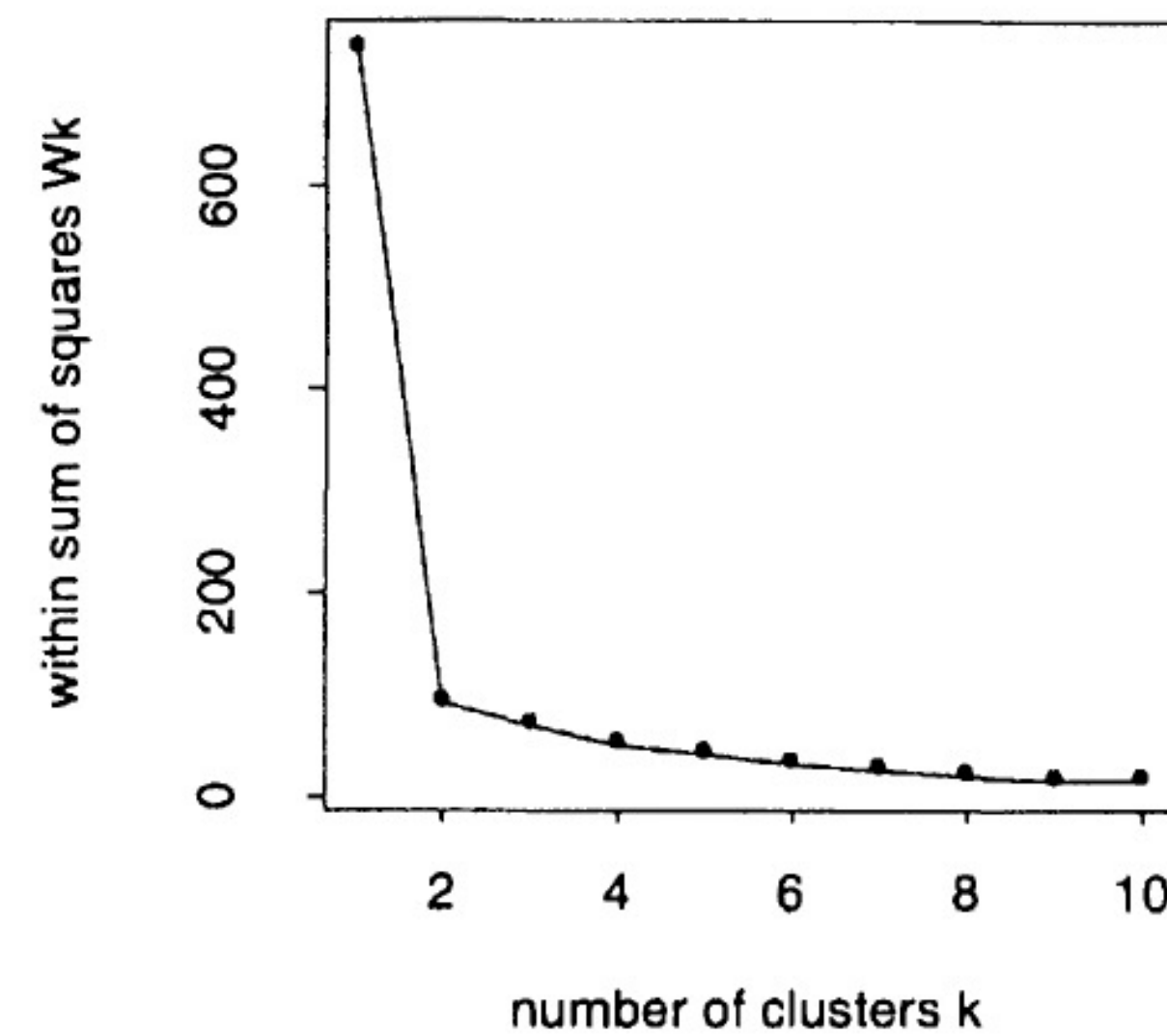
1. Einführung
2. Erwartungen an den Kurs
3. Clustering
4. K-Means Algorithmus
- 5. Determining Optimal Number of Clusters**
6. Hierarchical Clustering Algorithmus
7. Kommunikation der Resultate
8. Dimensions Reduktionsverfahren
9. Principal Components Analysis
10. T-Distributed Stochastic Neighbor Embedding
11. Zusammenfassung

How to select optimal number of clusters

- But how determine the number of clusters?
- The seen methods from Machine Learning cannot be applied
- There exists several methods to assess optimal number of clusters
- We treat three methods
 1. Elbow method
 2. Silhouette
 3. GAP Statistic

Elbow Method

- Most popular method
- Idea: Calculating the Within-Cluster-Sum-of Squared (WSS) for different number of clusters
- Elbow method decrease with increasing k



(b)

Representation of the elbow method (Tibshirani et al. 2001)

Silhouette

- Silhouette coefficient tells us if individual points are correctly assigned to their clusters.
- Silhouette Coefficient for an observation i is defined as follows

$$S(i) = \frac{b(i) - a(i)}{\max\{a(i), b(i)\}}$$

- where $b(i)$ is the smallest average distance of point i to all points in any other cluster
- and $a(i)$ is the average distance of i from all other points in its cluster

The Silhouette Coefficient for the data set is the average of the Silhouette Coefficient of individual points.

Meaning of $S(i)$:

- $S(i)$ close to 0 means that the observation is between two clusters
- $S(i)$ close to -1 than the point should be assigned to the other cluster
- $S(i)$ close to 1, than the point belongs to the correct cluster

GAP Statistic

Idea: To compare the cluster results with a null reference distribution of the data

The optimal number of cluster is the value of k for which $\log(W_k)$ falls the farthest below the curve of the reference distribution

$$Gap_n(k) = E_n^*\{\log(W_k)\} - \log(W_k)$$

- where W_k is the within-cluster variation
- and $E_n^*\{\log(W_k)\}$ the expectation under a sample of size n from the reference distribution

The optimal \hat{k} is obtained by maximizing $Gap_n(k)$

We assume a null model of a single component and reject it in favour of a k -component model

For each feature a uniformly distributed variable over the range of the observed values is created as reference distribution.

Exercise

- Begeben Sie sich in Gruppen von 2 bis 3 Teilnehmenden
- Öffnen Sie das Code Notebook "clustering_k_means_optimizing_exercise.ipynb"
- Bestimmen Sie die optimale Anzahl Clusters
- Dokumentieren Sie ihre Resultate

Feedback

Vielen Dank für euer Feedback auf folgender Seite
<http://www.evaluationszielscheibe.ch/?disc=2a68db>.

Agenda

1. Einführung
2. Kennenlernen Spiel
3. Clustering
4. K-Means Algorithmus
5. Determining Optimal Number of Clusters
- 6. Hierarchical Clustering Algorithmus**
7. Kommunikation der Resultate
8. Dimensions Reduktionsverfahren
9. Principal Components Analysis
10. T-Distributed Stochastic Neighbor Embedding
11. Zusammenfassung

Disadvantage k-means

- Number of clusters needs to be fixed

Dendrogram

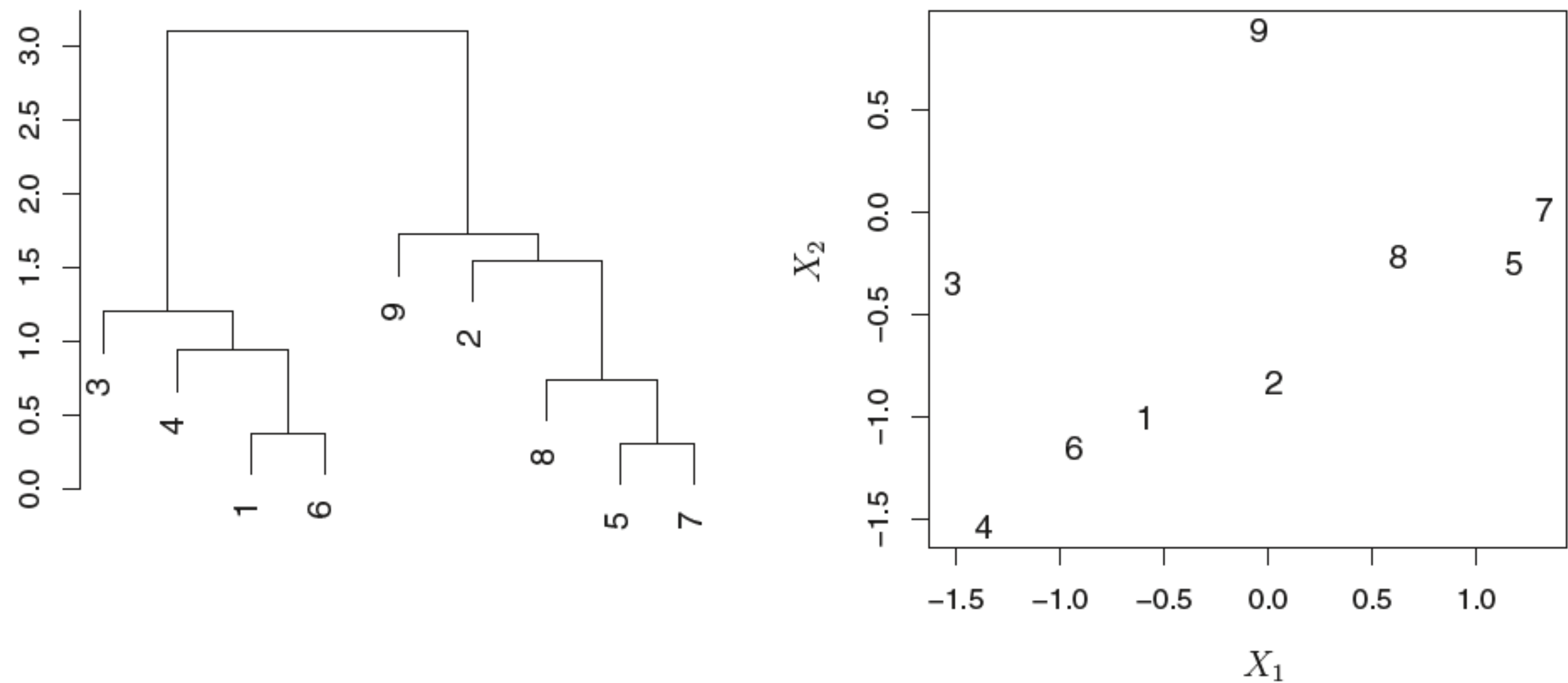


Illustration of a dendrogram applied to a simple application (James et al., 2013).

Algorithm Hierarchical Clustering

Algorithm 10.2 *Hierarchical Clustering*

1. Begin with n observations and a measure (such as Euclidean distance) of all the $\binom{n}{2} = n(n-1)/2$ pairwise dissimilarities. Treat each observation as its own cluster.
2. For $i = n, n-1, \dots, 2$:
 - (a) Examine all pairwise inter-cluster dissimilarities among the i clusters and identify the pair of clusters that are least dissimilar (that is, most similar). Fuse these two clusters. The dissimilarity between these two clusters indicates the height in the dendrogram at which the fusion should be placed.
 - (b) Compute the new pairwise inter-cluster dissimilarities among the $i-1$ remaining clusters.

Illustration of the hierarchical clustering (James et al., 2013).

Linkage functions in hierarchical clustering

linkage : {'ward', 'complete', 'average', 'single'}, default='ward'

Which linkage criterion to use. The linkage criterion determines which distance to use between sets of observation. The algorithm will merge the pairs of cluster that minimize this criterion.

- 'ward' minimizes the variance of the clusters being merged.
- 'average' uses the average of the distances of each observation of the two sets.
- 'complete' or 'maximum' linkage uses the maximum distances between all observations of the two sets.
- 'single' uses the minimum of the distances between all observations of the two sets.

New in version 0.20: Added the 'single' option

Illustration of the different linkage functions applied in hierarchical clustering in Scikit-Learn.

<i>Linkage</i>	<i>Description</i>
Complete	Maximal intercluster dissimilarity. Compute all pairwise dissimilarities between the observations in cluster A and the observations in cluster B, and record the <i>largest</i> of these dissimilarities.
Single	Minimal intercluster dissimilarity. Compute all pairwise dissimilarities between the observations in cluster A and the observations in cluster B, and record the <i>smallest</i> of these dissimilarities. Single linkage can result in extended, trailing clusters in which single observations are fused one-at-a-time.
Average	Mean intercluster dissimilarity. Compute all pairwise dissimilarities between the observations in cluster A and the observations in cluster B, and record the <i>average</i> of these dissimilarities.
Centroid	Dissimilarity between the centroid for cluster A (a mean vector of length p) and the centroid for cluster B. Centroid linkage can result in undesirable <i>inversions</i> .

Illustration of the different linkage functions applied in hierarchical clustering (James et al., 2013).

Application example

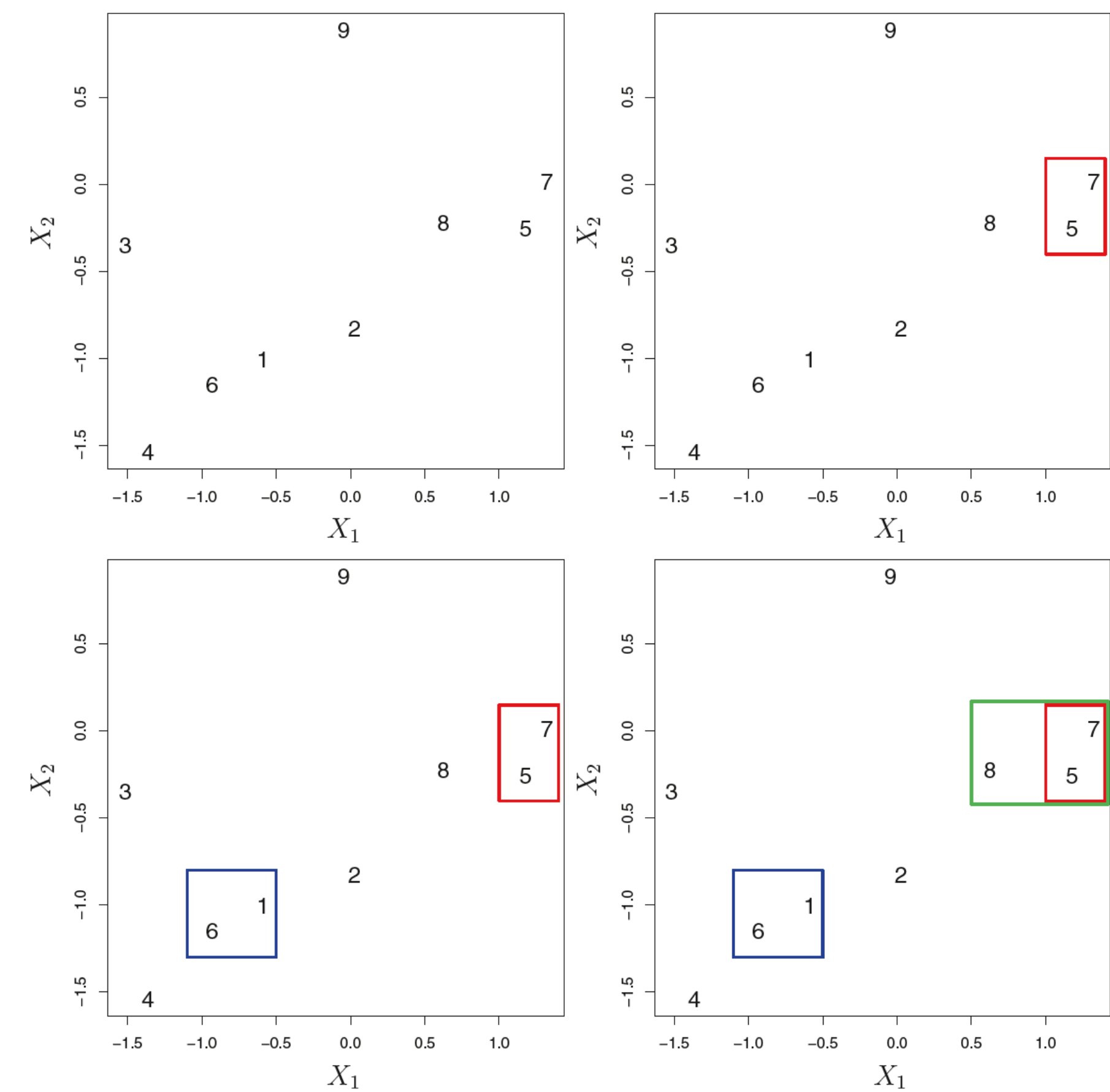


Illustration of an application of the hierarchical clustering algorithm (James et al., 2013).

Difference due to the linkage function

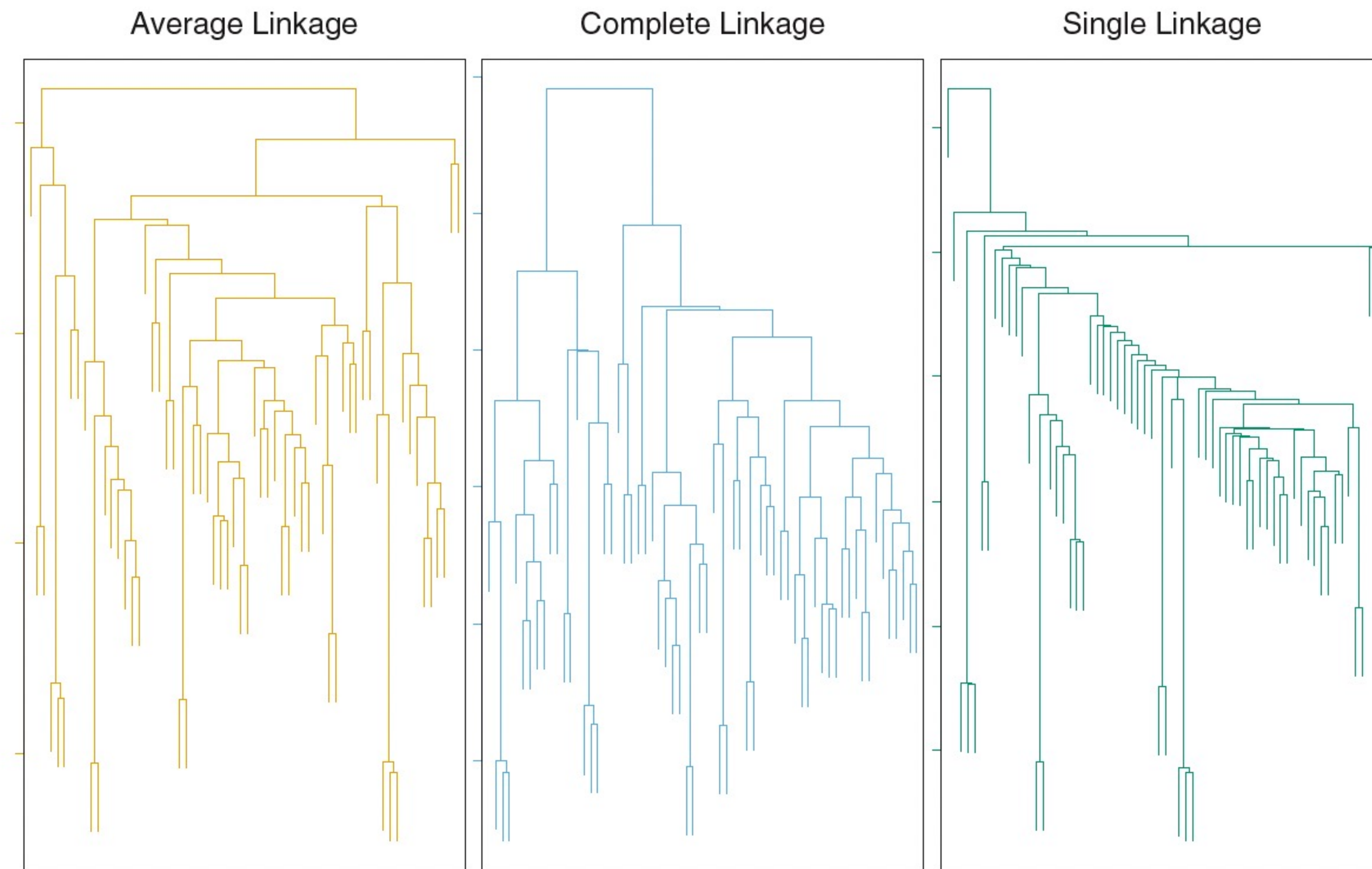


Illustration of differences in the dendrogram due to the linkage function (James et al., 2013).

Small Decisions with Big Consequences

- Standardization of data
- Use of dissimilarity measure
- Use of linkage
- Number of clusters

Exercise

- Begeben Sie sich in eine Gruppe von 2 bis 3 Teilnehmenden
- Öffnen Sie das Codenotebook "hiearchical_clustering_exercise.ipynb"
- Führen Sie das Hierarchical Clustering vorherigen optimale Clusteranzahl durch
- Dokumentieren Sie ihre Erkenntnisse

Agenda

1. Einführung
2. Kennenlernen Spiel
3. Clustering
4. K-Means Algorithmus
5. Determining Optimal Number of Clusters
6. Hierarchical Clustering Algorithmus
- 7. Kommunikation der Resultate**
8. Dimensions Reduktionsverfahren
9. Principal Components Analysis
10. T-Distributed Stochastic Neighbor Embedding
11. Zusammenfassung

Wieso?



Wie unterscheiden sich die Gruppen?

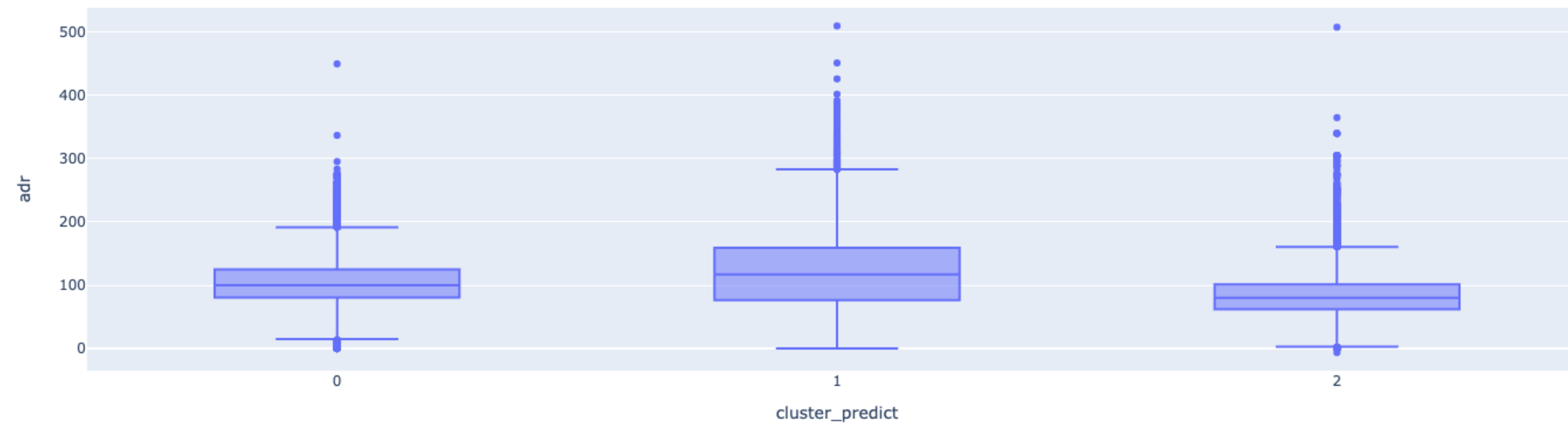
Wie kann ich die Gruppen am besten unterscheiden?

Welche Schwierigkeit ist Ihnen aufgefallen?



Möglicher Weg

- Die Resultate werden auf den skalierten Daten angezeigt
- Wir würden aber gerne den Bezug zu den Ursprungsdaten herleiten
- Lösung: Erhalten Cluster mit den Ursprungsdaten verbinden
- Cluster nach Merkmalen analysieren
- Beste Möglichkeit: Visualisierung und Deskriptive Statistiken



Exercise

- Begeben Sie sich in Gruppen von 2 bis 3 Teilnehmenden
- Beschreiben Sie die Clusters
- Dokumentieren Sie wie sie die Gruppen beschreiben würden

Agenda

1. Einführung
2. Erwartungen an den Kurs
3. Clustering
4. K-Means Algorithmus
5. Determining Optimal Number of Clusters
6. Hierarchical Clustering Algorithmus
7. Kommunikation der Resultate
- 8. Dimensions Reduktionsverfahren**
9. Principal Components Analysis
10. T-Distributed Stochastic Neighbor Embedding
11. Zusammenfassung

Challenge

- Many Machine Learning problems involve **thousands** or even **millions** of features for each training instance
- High number of dimensionality can have several **drawbacks**
 - ❖ High dimensionality makes training extremely **slow**
 - ❖ High dimensionality makes it harder to find a **good** solution
 - ❖ High dimensionality makes it harder to **interpret** the results
- The high dimensionality problems are known as **curse of dimensionality**
- Dimensionality reduction reduce the **number of features** considerably
- Dimensionality reductions turns an **intractable** problem into a **tractable** problem
- Dimensionality reduction is extremely useful for **data visualization**

Drawbacks of Dimensionality Reduction

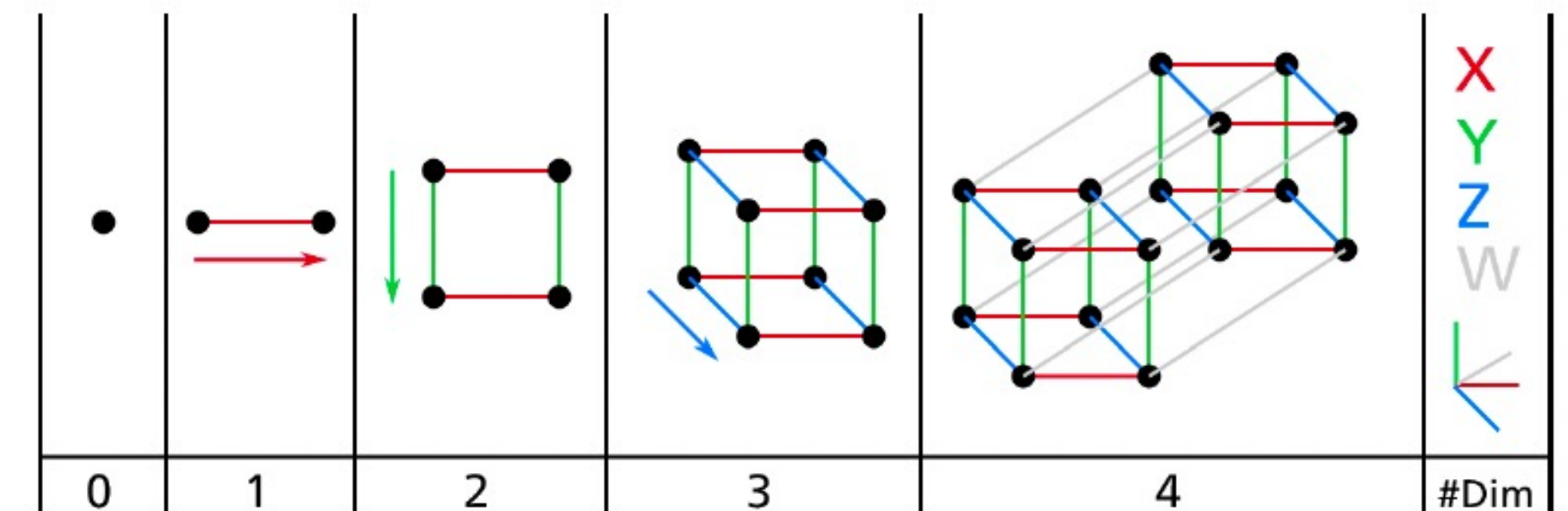
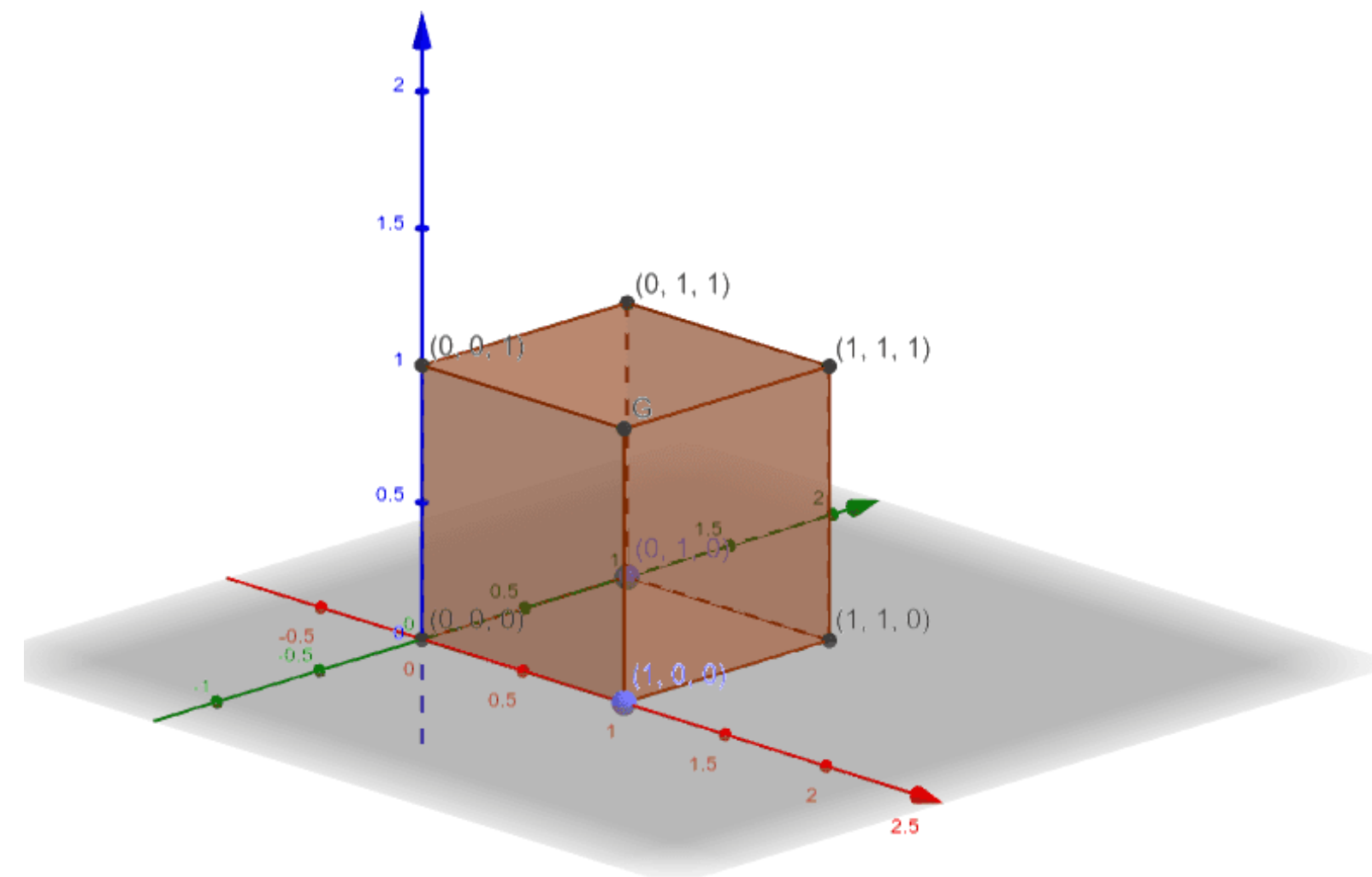
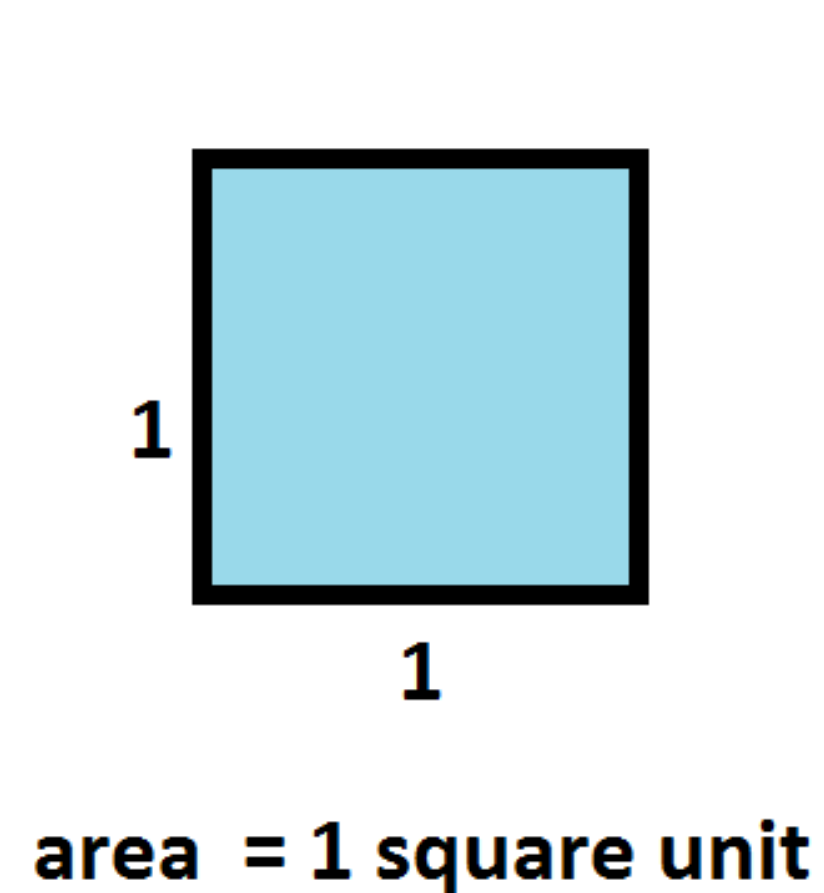
- Through reducing dimensionality, we **lose** some information
- The dimensionality reduction can speed up training, however, lead to a slightly **worse** performance
- In some cases, dimensionality reduction of the training data may filter out some **noise** and unnecessary details
- When dimensionality reduction filter out noise, we get a gain in performance
- This gain of performance is not always given
- Always should first try to train system on the **original** data

Curse of Dimensionality

If you pick two points randomly in a **unit square** the distance between these two points will be, on average, roughly **0.52**

If you pick two points randomly in a **unit 3D cube**, the average distance will be roughly **0.66**

If you pick randomly two points in a **1'000'000-dimensional hypercube**, the average distance will be roughly about **408.25**



Curse of Dimensionality

High dimensional datasets are very **sparse**

Most training instances are likely to be far **away** from each other

New instance will likely be far away from any training instance

Prediction for new instance will be **less reliable** in high dimension than in lower dimension

More dimensions the training set has, the greater the risk of **overfitting**

One solution to the curse of **dimensionality** could be to increase the size of the training set to reach a sufficient density of training instances

In practice, it is generally unfeasible to increase the training instances as required

Main Approaches for Dimensionality Reduction

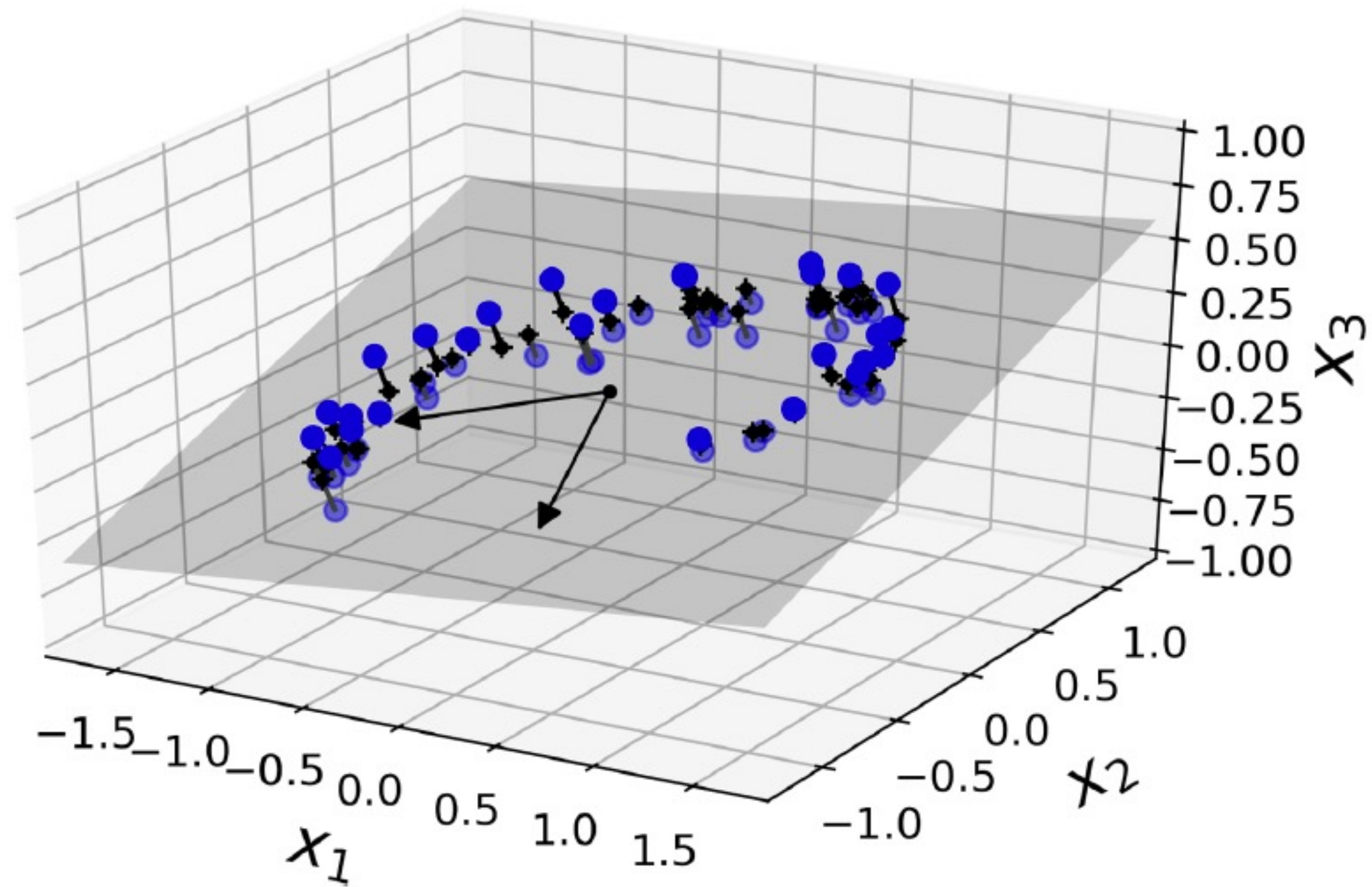
Two main approaches to reducing dimensionality:

- Projection
- Manifold Learning

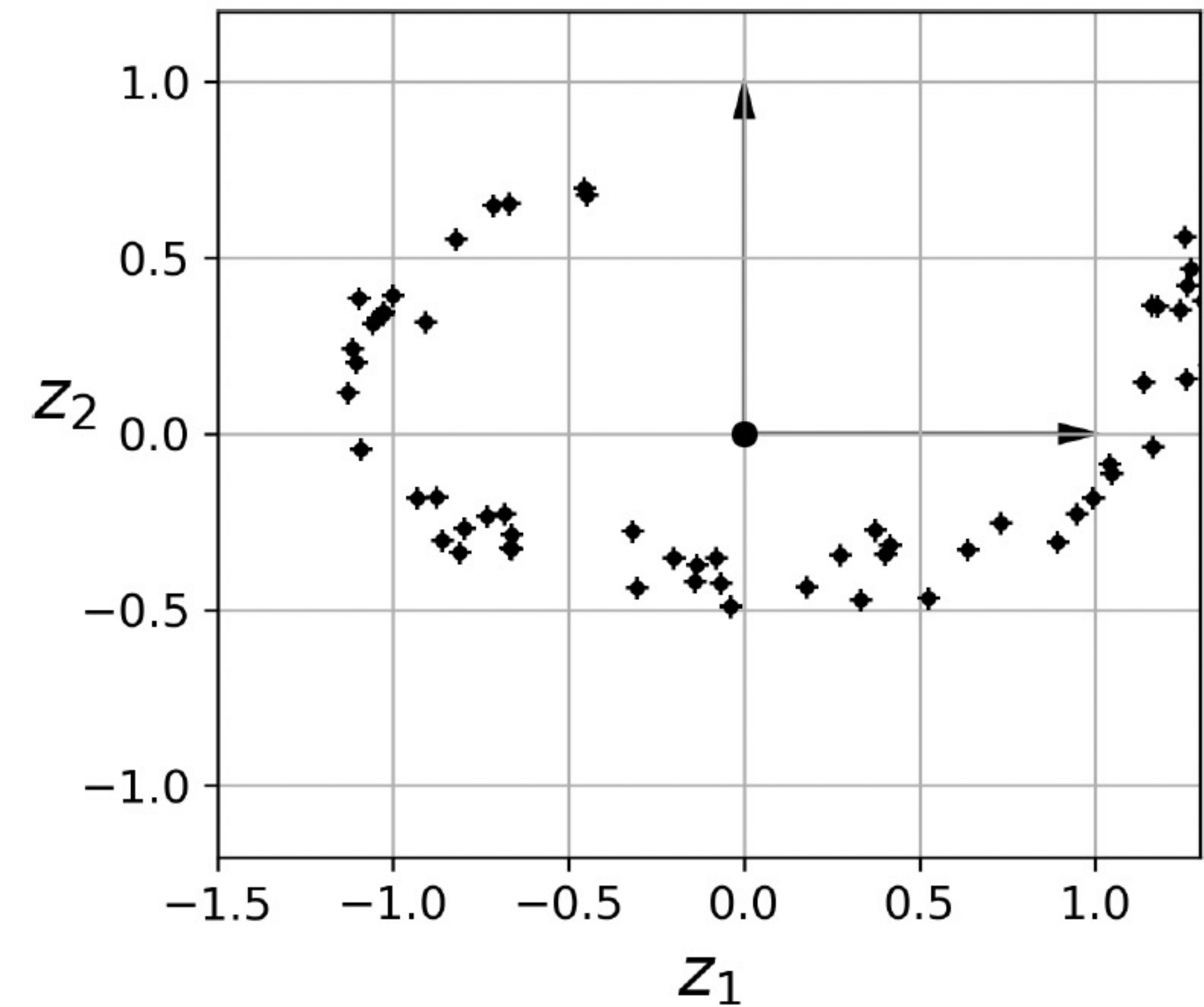
Importance of dimensionality reduction

- In real-world problems, training instances are not spread uniformly across all dimensions
- Many features are constant or highly correlated
- All training instances mostly lie within a much lower-dimensional subspace of the high-dimensional space

Projection

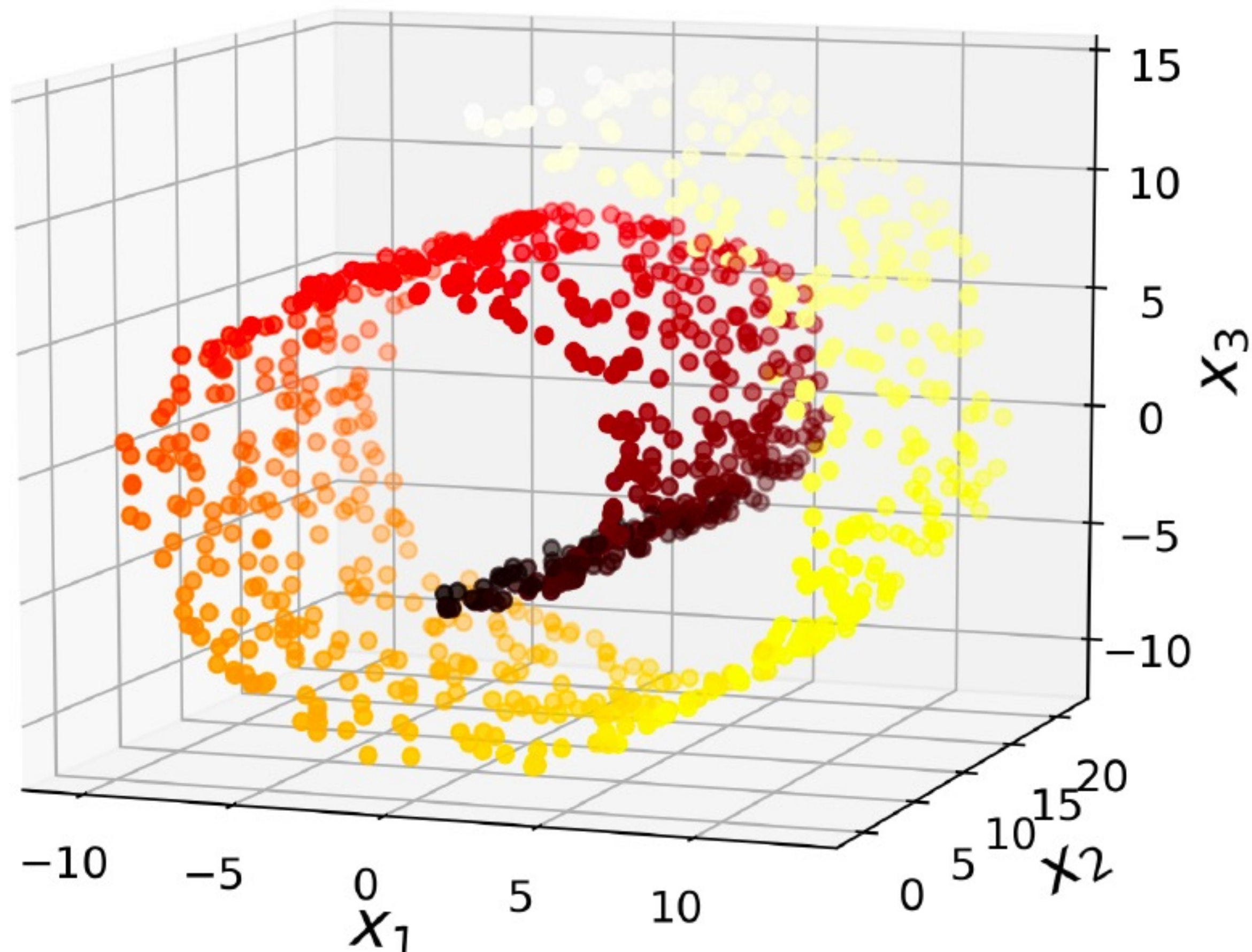


Representation of a 3D dataset (Géron, 2019)



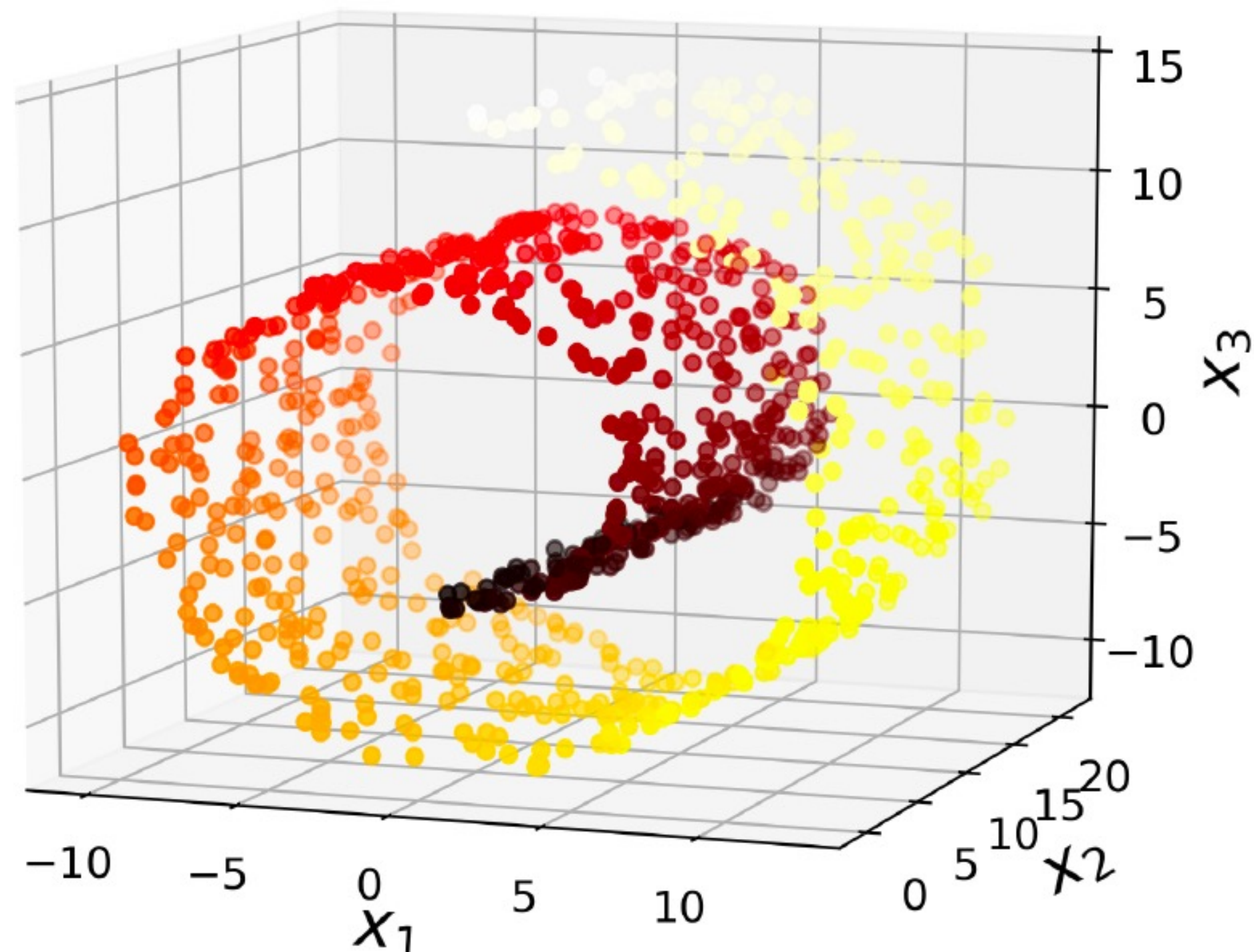
Representation of a 2D project (Géron, 2019)

Possible Drawbacks of Projection

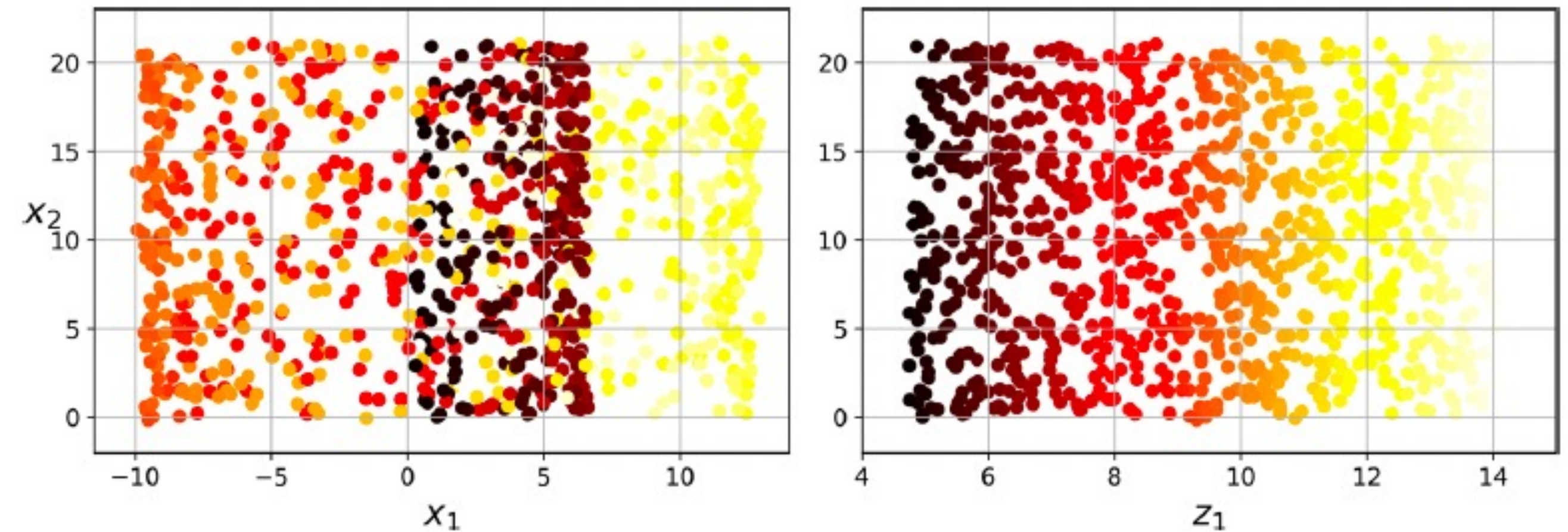


Visualization of the Swiss roll dataset (Géron, 2019)

Possible Drawbacks of Projection



Visualization of the Swiss roll dataset (Géron, 2019)



Visualization of the Swiss roll dataset: Left projection on the plane, right unrolling Swiss roll (Géron, 2019)

Manifold Learning

2D manifold is a 2D shape that can be bent and twisted in higher-dimensional space

d-dimensional manifold is a part of a n-dimensional space (where d-dimensional space)

Manifold Learning reduces the the dimensionality of the training instances by modeling the manifold on which the training instances lies

Agenda

1. Einführung
2. Kennenlernen Spiel
3. Clustering
4. K-Means Algorithmus
5. Determining Optimal Number of Clusters
6. Hierarchical Clustering Algorithmus
7. Kommunikation der Resultate
8. Dimensions Reduktionsverfahren
- 9. Principal Components Analysis**
10. T-Distributed Stochastic Neighbor Embedding
11. Zusammenfassung

Principal Component Analysis

Goal: to find a low representation that captures as much of the information as possible (James et al., 2017)

Let X_1, X_2, \dots, X_p be the p features with n observations.

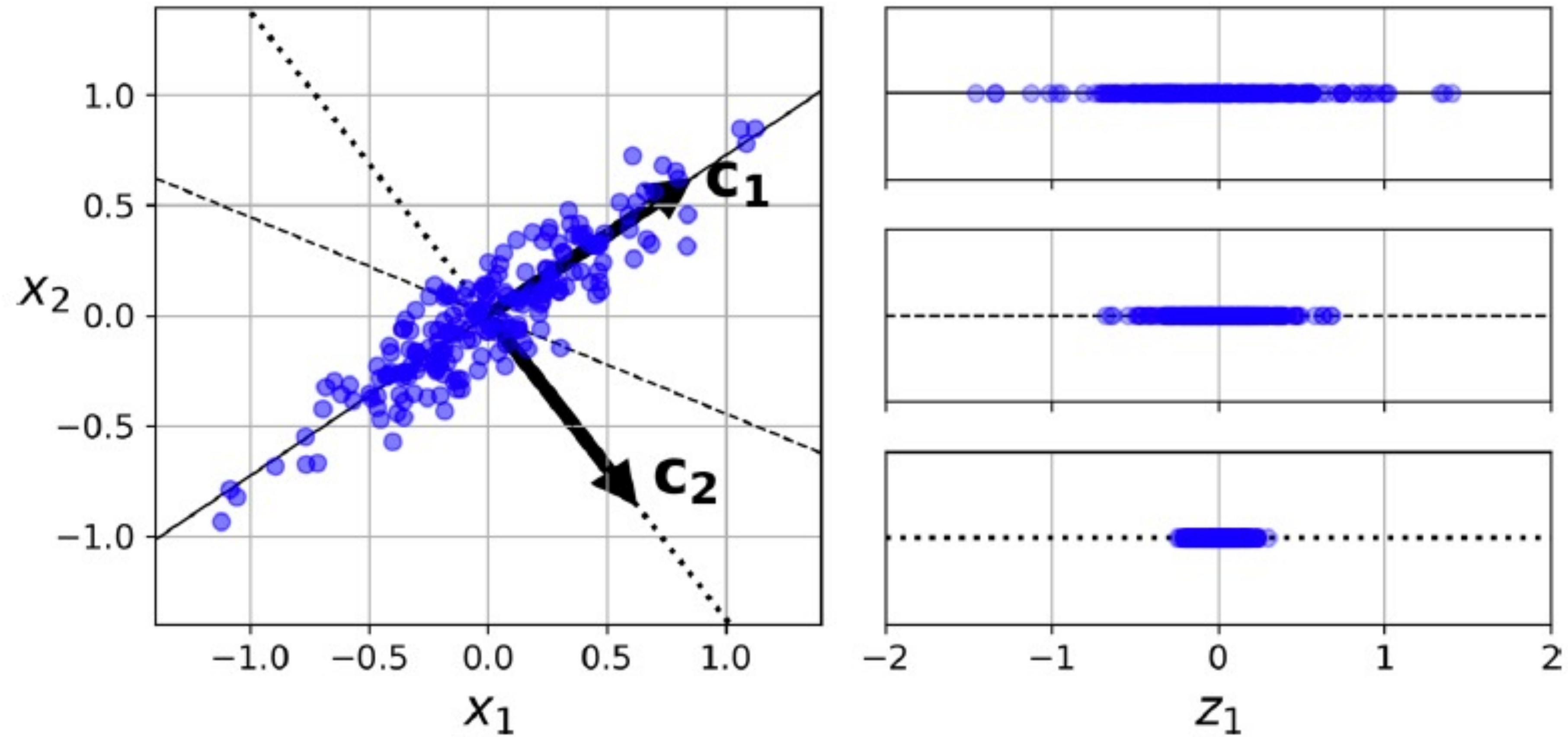
First principal component: $Z_1 = \phi_{11}X_1 + \phi_{21}X_2 + \dots + \phi_{p1}X_p$

- with largest variance and $\sum_{j=1}^p \phi_{j1}^2 = 1$
- ϕ_{j1} are the loadings and z_{i1} are the scores.

Optimization Problem for first principal component:

$$\max_{\phi_{11}, \phi_{21}, \dots, \phi_{p1}} \left\{ \frac{1}{n} \sum_{i=1}^n \left(\sum_{j=1}^p \phi_{j1} x_{ij} \right)^2 \right\} \text{ with } \sum_{j=1}^p \phi_{j1}^2 = 1$$

Selecting the subspace to project on

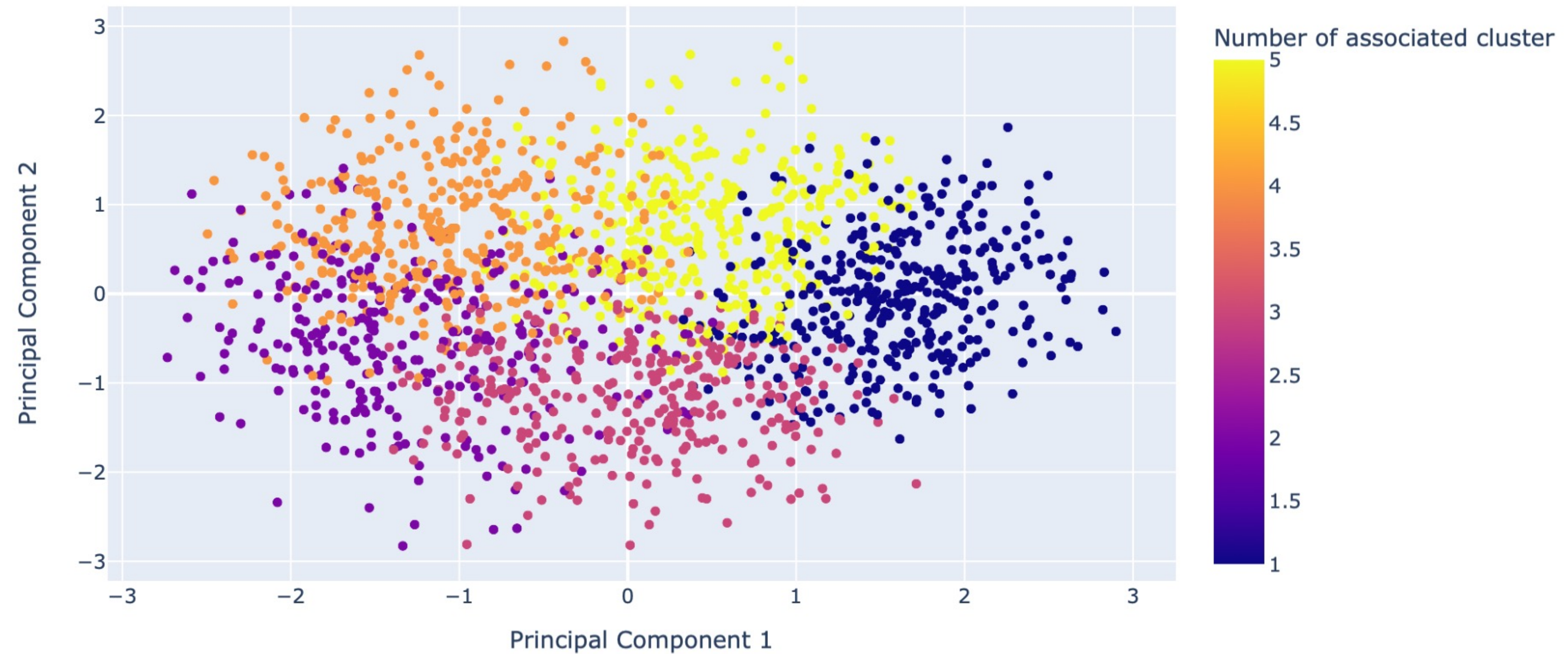


Principal Component Analysis

- When the first principal component Z_1 of the features has been determined, we can find the second principal component Z_2 (James et al., 2017; Kuhn et al., 2016).
- Z_2 uncorrelated with Z_1

Example of PCA

Representation of the two first principal components of PCA



18. November 2023

Exercise

- Begeben Sie sich in ein Gruppe von 2 bis 3 Teilnehmenden
- Öffnen Sie das Code Notebook "dimension_reduction_pca_exercise.ipynb"
- Reduzieren Sie den "Feature" Raum auf zwei Dimensionen
- Dokumentieren Sie ihr Vorgehen und ihre Resultate

Agenda

1. Einführung
2. Kennenlernen Spiel
3. Clustering
4. K-Means Algorithmus
5. Determining Optimal Number of Clusters
6. Hierarchical Clustering Algorithmus
7. Kommunikation der Resultate
8. Dimensions Reduktionsverfahren
9. Principal Components Analysis
- 10. T-Distributed Stochastic Neighbor Embedding**
11. Zusammenfassung

t-Distributed Stochastic Neighbor Embedding (t-SNE)



Video: Design at Large – Laurens van der Maaten,
Visualizing Data Using Embeddings
<https://www.youtube.com/watch?v=EMD106bB2vY>

Video explain t-SNE

Idea of the method is explained from time 11:15 to
24:00

T-SNE (Stochastic Neighbor Embedding)

Data: data set $\mathcal{X} = \{x_1, x_2, \dots, x_n\}$

Cost function parameters: perplexity (perp)

Optimization Parameters:

- Number of iterations T ,
- Learning rate η ,
- Momentum $\alpha(t)$

Result: Low-dimensional data representation $\mathcal{Y}^t = \{y_1, y_2, \dots, y_n\}$

(van der Maaten and Hinton, 2008)

Pseudo Code T-SNE

Begin

Compute pairwise affinities $p_{j|i} = \frac{\exp(-\|x_i - x_j\|^2 / (2\sigma_i^2))}{\sum_{k \neq i} \exp(-\|x_i - x_k\|^2 / (2\sigma_i^2))}$ with perplexity $Perp(P_i) = 2^{H(P_i)}$

where $H(P_i)$ is the Shannon entropy $H(P_i) = -\sum_j p_{j|i} \log_2 p_{j|i}$

Set $p_{ij} = \frac{p_{j|i} + p_{i|j}}{2}$

Sample initial solution $\mathcal{Y}^0 = \{y_1, y_2, \dots, y_n\}$ from $\mathcal{N}(0, 10^{-4}\mathfrak{T})$

For t = 1 to T do

 Compute low dimensional affinities $q_{ij} = \frac{(1 + \|y_i - y_j\|^2)^{-1}}{\sum_{k \neq l} (1 + \|y_k - y_l\|^2)}$

 Compute gradient $\frac{\partial \mathcal{C}}{\partial y} = 4 \sum_j (p_{ij} - q_{ij})(y_i - y_j) (1 + \|y_i - y_j\|^2)^{-1}$

 Set $y^t = y^{(t-1)} + \eta \frac{\partial \mathcal{C}}{\partial y} + \alpha(t)(y^{(t-1)} - y^{(t-2)})$

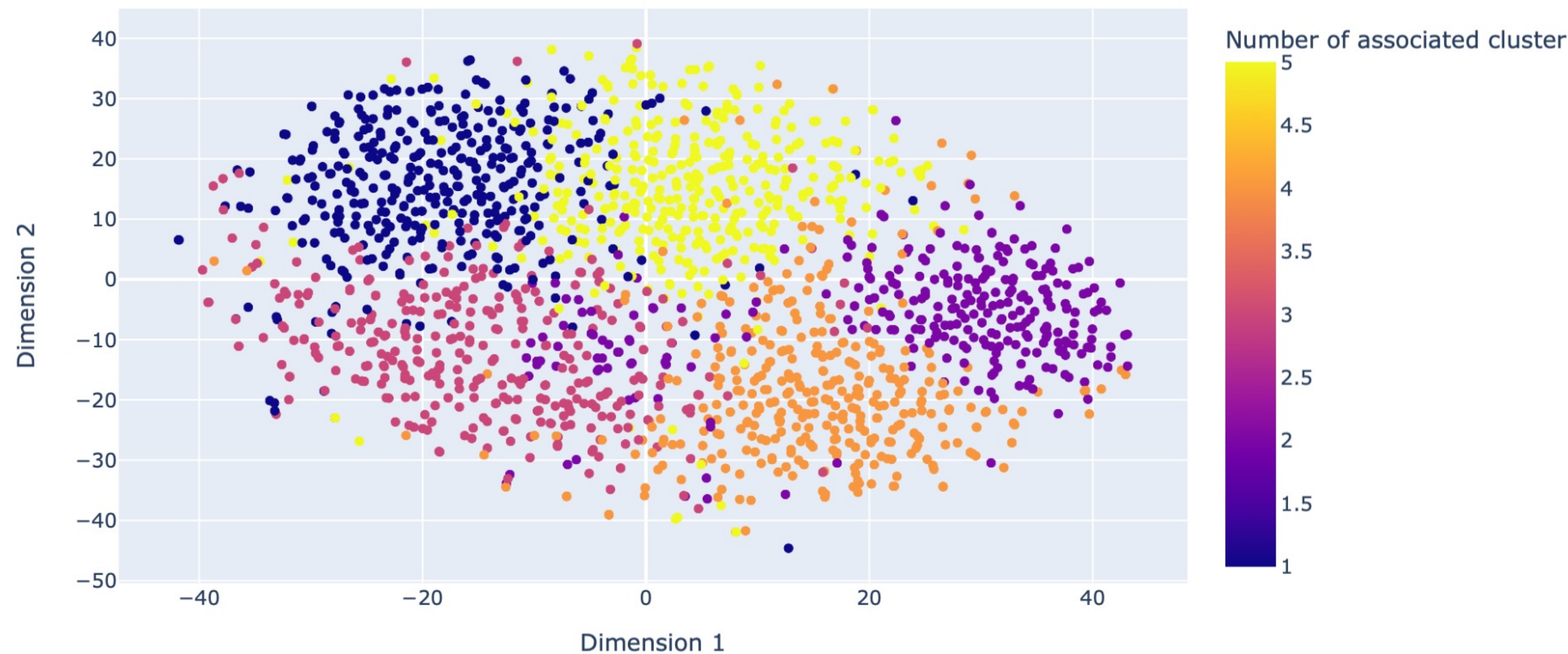
end

End

HSLU
(van der Maaten and Hinton, 2008)

Example of T-SNE

Representation of the dimension reduction by t-SNE



18. November 2023

Exercise

- Begeben Sie sich in ein Gruppe von 2 bis 3 Teilnehmenden
- Öffnen Sie das Code Notebook “dimension_reduction_tsne_exercise.ipynb”
- Reduzieren Sie den Raum
- Dokumentieren Sie ihr Vorgehen und ihre Resultate

Agenda

1. Einführung
2. Kennenlernen Spiel
3. Clustering
4. K-Means Algorithmus
5. Determining Optimal Number of Clusters
6. Hierarchical Clustering Algorithmus
7. Kommunikation der Resultate
8. Dimensions Reduktionsverfahren
9. Principal Components Analysis
10. T-Distributed Stochastic Neighbor Embedding

11. Zusammenfassung

Zusammenfassung

Was haben wir gelernt?

Feedback

Vielen Dank für euer Feedback auf folgender Seite

<http://www.evaluationszielscheibe.ch/?disc=7ebb64>

Fragen



Darstellung eines Fragesymbol aufgerufen von der Webseite <https://www.qnigge.de/news/detail/modul-v/#images> am 12.07.2021.

Referenzen

Galli, S. (2017). Feature Engineering for Machine Learning, <https://github.com/solegalli/feature-engineering-for-machine-learning>, Accessed on 15.09.2022.

Géron, A. (2019). Hands-On Machine Learning with Scikit-Learn and TensorFlow

Gonick, Larry and Woollcott Smith. 2005. The Cartoon Guide to Statistics. HarperCollins Publishers.

Huang, Z. (1997), Clustering Large Data Sets With Mixed Numeric And Categorical Values, Computer Science.

James, G., Witten, D., Hastie, T. and Tibshirani, R. (2013). An Introduction to statistical learning with Applications in R. Springer.

Kuhn, M. and Johnson, K. (2013). Applied Predictive Modeling. Springer.

Staudt, Y. and Wagner, J. (2022). Assessing the Performance of Random Forests for Modeling Claim Severity in Collision Car Insurance. Risks. Vol 9. No. 53. DOI: 10.3390/risks9030053

Tibshirani, R., Walther, G. and Hastie, T. (2001). Estimating the number of clusters in a data set via the gap statistic.

Wong, K. Y., and Chung, F., 2019; Visualizing Time Series Data with Temporal Matching Based t-SNE.

Yin, S., Gan, G., Valdez, E and Vadiveloo, J. (2021). Applications of Clustering with Mixed Type Data in Life Insurance, arXiv.

Danke!

Datum