MADS-MMS – Mathematics and Multivariate Statistics

Clustering – Overview

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Moodle (SoSe 2025)

Agenda

Motivation

Goals of Clustering

What is Clustering?

Clustering Methods

Ingredients

Outline

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Chapter Goals

- overview on the topic of clustering
- categorization of methodology
- understand motivation and application of clustering

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Goals of Clustering

Goals:

- identify clusters (categories / subsets / groups) in datasets
- instances in the same cluster should be as similar as possible
- instances in different clusters should have low similarity
- (identify instances that belong to no group: outliers, noise)
- NOT: assign instances to known classes

Context:

- detect sets of “comparable/similar/close elements”
- explore and analyze unknown data
- engineer classes / features
- semi-automatic – often data scientist has to “judge” and interprete clusterings
- requires a useful and meaningful distance/similarity function (often individually chosen or designed)

Applications for Clustering

Applications:

- Market segmentation / customer base segmentation
- Pattern recognition
- Community discovery in social networks
- Topic detection in text corpora
- Tracking of evolutional steps
- Identifying common behavior or common interests (e.g. for pdf recommender systems)
- Identifying common physical properties in sensor data
- ...

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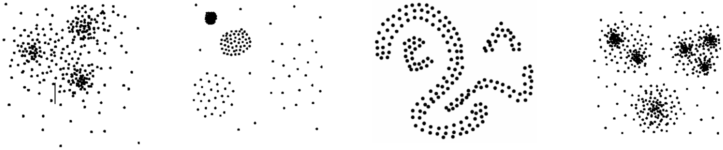
Examples

Clusters of different size, form, density, and hierarchical structure


[1]

[1] Source: [1], Abb. 3-1

Clustering Formally

There is no hard mathematical definition of clustering in general.

Definition 1 (Clustering)

Clustering comprises (machine learning) methods of **unsupervised learning** to collect data instances into **groups, categories, or classes**, called **clusters**. The set of all clusters is called a **clustering**.

Criteria for the grouping can be

intra-class similarity: similarity within a cluster

inter-class dissimilarity: dissimilarity between different clusters

Machine Learning Disciplines

Supervised

- labelled data
- goal: class/prediction of unknown/future data
- idea: Learn by deriving a model from looking at examples
- correctness of the training can be assessed (supervised)
- examples: classification, regression

Unsupervised

- unlabelled data
- goal: Detect patterns (groups, structure) in the data
- learning is unsupervised, no "correct" result that we can compare to
- examples: **clustering**, dimensionality reduction

Clustering Process

Definition 2 (Clustering Process)

A clustering process comprises the following steps:

- representation of the data
- definition of a similarity measure (domain-specific)
- creating the clusters
- optionally abstraction of knowledge
- optionally evaluation of the output

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Classification of Clustering Methods

Partitioning Methods (Hard Clustering)

- determines a partition into disjoint subsets, minimizing a cost function
- typical parameters: number of clusters k, distance function

Density-based Methods

- adds neighbors to clusters, as long as density does not fall below threshold
- distinguishes between the cores of clusters, its borders, and noise
- parameters: minimal acceptable density in a cluster, distance function

Hierarchical Methods

- determine a hierarchy of clusters, fuses most similar clusters
- parameters: distance function

Other Methods (incomplete)

- Soft Clustering (Fuzzy Clustering, Overlapping Clustering)
- Graph-based Methods

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We need:

- a way to express different kinds of data mathematically, and
- a way to measure distance/similarity between points
- all that in many-dimensional realms
- 2D-visualizations despite multidimensional data
- algorithms that cluster
- basic mathematics like logarithms, vector geometry, matrices

📎 Exercises 1

References

M. Ester and J. Sander.
Knowledge Discovery in Databases.
Springer-Verlag, Berlin/Heidelberg, 2000.