MADS-MMS – Mathematics and Multivariate Statistics

Clustering - Overview

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Agenda

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Goals of Clustering

What is Clustering?

Clustering Methods

Ingredients

Outline

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Chapter Goals

overview on the topic of clustering

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Chapter Goals

- overview on the topic of clustering
- categorization of methodology

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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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- 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)

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Examples

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



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¹Source: [1], Abb. 3-1

Clustering Formally

There is no hard mathematical definition of clustering in general.

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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.

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Criteria for the grouping can be

intra-class similarity: similarity within a cluster

inter-class dissimilarity: dissimilarity between different clusters

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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

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Clustering Process

Definition 2 (Clustering Process)

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- ► optionally abstraction of knowledge
- ▶ optionally evaluation of the output

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- basic mathematics like logarithms, vector geometry, matrices

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References



M. Ester and J. Sander.

Knowledge Discovery in Databases. Springer-Verlag, Berlin/Heidelberg, 2000.