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Advances in Model-Based Clustering

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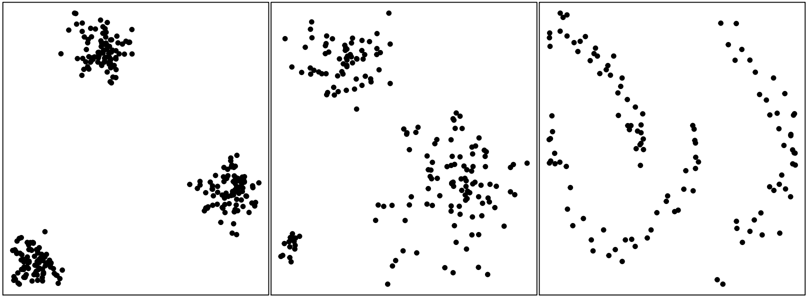
Cluster analysis

- The task of grouping a set of objects such that:
  - Objects in the same group are as similar as possible.
  - Objects in different groups are as dissimilar as possible.
- The aim is to determine a partition of the given set of objects, e.g., to determine which objects belong to the same group and which to different groups.
- Exploratory data analysis tool to detect structure in the data.
- Statistical methods:
  - Heuristic methods: hierarchical clustering, partitioning methods (e.g., k-means).
  - Model-based methods: finite mixture models.

Specifying the cluster problem

- The cluster problem is in general perceived as ill defined.
- Different notions of what defines a cluster exist:
  - Compactness.
  - Density-based levels.
  - Connectedness.
  - Functional similarity.
- Several cluster solutions might exist for a given data set depending on which notion is used.
- The application context is important to define which clusters should be targeted and to assess the usefulness of a clustering solution.

Specifying the cluster problem / 2



Model-based clustering methods

- Model-based clustering embeds the clustering problem in a probabilistic framework.
- This implies:
  - Statistical inference tools can be used.
  - Different cluster distributions can be used depending on the cluster notion.
  - More explicit specification of what defines a cluster required than for heuristic methods.

Finite mixture models

- Generative model for observations $\boldsymbol{y}_i$ given $\boldsymbol{x}_i$, $i = 1, \ldots, n$:
  1. Draw a cluster membership indicator S_i from a multinomial distribution with parameters $\boldsymbol{\eta} = (\eta_1, \ldots, \eta_K)$.
  2. Draw $\boldsymbol{y}_i$ given $\boldsymbol{x}_i$ and S_i from the cluster distribution:

$$\boldsymbol{y}_i | \boldsymbol{x}_i, S_i \sim f_{S_i}(\boldsymbol{y}_i | \boldsymbol{x}_i).$$

- The distribution of $\boldsymbol{y}_i$ given $\boldsymbol{x}_i$ is then given by

$$\boldsymbol{y}_i | \boldsymbol{x}_i \sim \sum_{k=1}^{K} \eta_k f_k(\boldsymbol{y}_i | \boldsymbol{x}_i),$$

  where
  - $\eta_k \geq 0$ for all k and $\sum_{k=1}^{K} \eta_k = 1$.
  - $f_k()$ represents the cluster distribution.

Finite mixture models / 2

Methods differ with respect to:

- Clustering kernel:
  - Specification of cluster distributions.
  - Use of additional variables $\boldsymbol{x}_i$, e.g., for regression.
- Estimation framework:
  - Maximum likelihood estimation.
  - Bayesian estimation.

Finite mixture models / 3

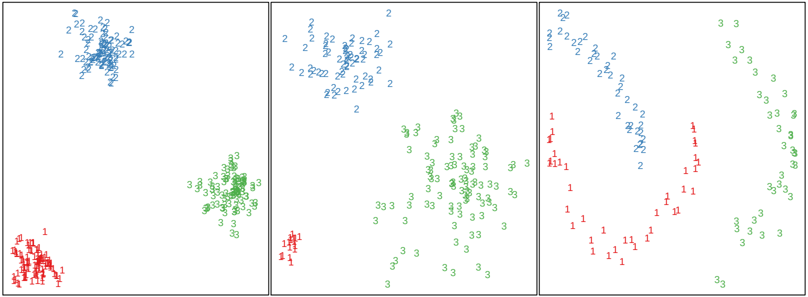
- Cluster membership indicators can be inferred using the a-posteriori probabilities:

$$\mathbb{P}(S_i = k|\boldsymbol{y}_i, \boldsymbol{x}_i) \propto \eta_k f_k(\boldsymbol{y}_i|\boldsymbol{x}_i).$$

- A hard assignment can be obtained by:
  - Assigning to the cluster where this probability is maximum.
  - Drawing from this probability distribution.

$\Rightarrow$ Results in a partition of the data.

Finite mixture models / 4



Estimation of finite mixtures with fixed K

- Maximum likelihood estimation:
  - Expectation-Maximization (EM) algorithm.
  - General purpose optimizers.
  - Hybrid approaches.
- Bayesian estimation:
  - Markov chain Monte Carlo (MCMC) sampling with data augmentation by adding S_i, $i = 1, \ldots, n$.
  - General purpose Gibbs samplers can be used, e.g., JAGS available in R through package **rjags** (Plummer, 2019).

Determining the number of clusters

- No generally accepted solution available.
- Suggested methods include:
  - Maximum likelihood estimation:
    - Information criteria: AIC, BIC, ICL.
    - Likelihood ratio test with distribution under the null determined using sampling methods.
  - Bayesian estimation:
    - Marginal likelihoods.
    - Posterior of the number of clusters in the data partitions, in particular for overfitting mixtures with sparsity inducing priors.
    - Transdimensional sampling schemes with a prior on K.

Clustering kernel

- **Components corresponding to clusters:**
  Use parametric distributions for the components and thus also for the clusters.
  - Multivariate continuous data.
  - Multivariate categorical data.
  - Multivariate mixed data.
  - Multivariate data with regression structure.
- **Combining components to clusters:**
  Use mixture distributions as cluster distributions.
  - Two-step procedures.
  - Simultaneous estimation using constraints or informative priors.

Multivariate continuous data

- The standard model is a mixture of multivariate Gaussians.
- The model-based clustering model is given by

$$\boldsymbol{y}_i \sim \sum_{k=1}^{K} \eta_k \phi(\boldsymbol{y}_i | \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k).$$

- For K clusters and d-dimensional observations $\boldsymbol{y}_i$ the number of estimated parameters corresponds to

$$K \cdot (d + d(d+1)/2) + K - 1.$$

Multivariate continuous data / 2

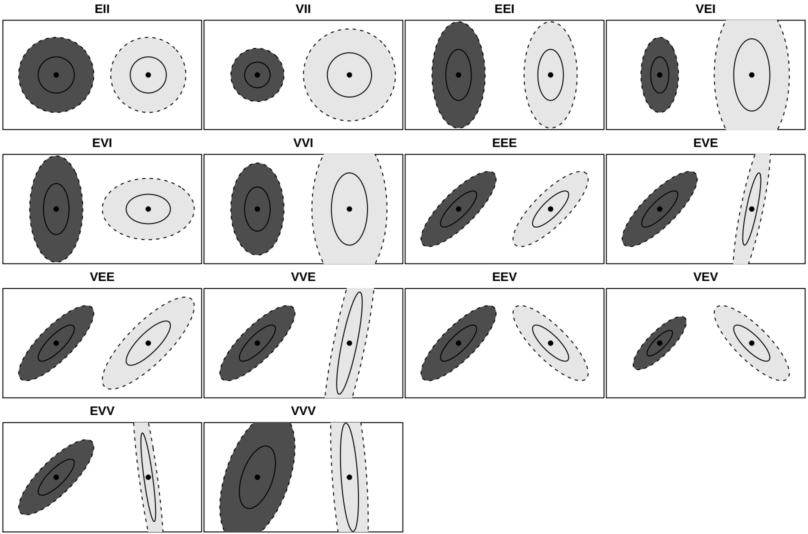
- Parsimony is achieved based on the decomposition of the variance-covariance matrix into
  - Volume λ
  - Shape A
  - Orientation D

  given by

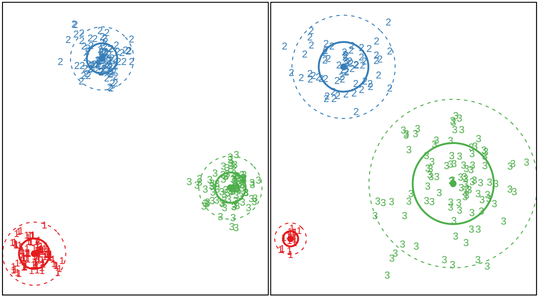
$$\Sigma_k = \lambda_k D_k A_k D_k^\top .$$

- 14 different models emerge by imposing different constraints on the variance-covariance matrices within or across clusters.
- Available packages in R, e.g.,
  - **mclust** (Scrucca et al., 2016),
  - **mixture** (Pocuca et al., 2021),
  - **Rmixmod** (Lebret et al., 2015).

Multivariate continuous data / 3



Multivariate continuous data / 4



Multivariate continuous data / 5

- Alternative approaches to achieve parsimonity are mixtures of factor analyzers.
  - E.g., package **pgmm** (McNicholas et al., 2019) in R.
- If the cluster shapes are not symmetric and light tailed, alternative cluster kernels are:
  - *t*-distributions (e.g., package **teigen**; Andrews et al. 2018).
  - Skewed and / or heavy tailed distributions: e.g.,
    - **mixsmsn** (Prates et al., 2013),
    - **MixSAL** (Franczak et al., 2018).

Multivariate categorical data

- Often also referred to as latent class analysis.
- Clusters induce a dependency between variables, while variables are independent within clusters.
  $\Rightarrow$ Local independency assumption.
- The model-based clustering model is given by

$$\boldsymbol{y}_i \sim \sum_{k=1}^{K} \eta_k \left[\prod_{j=1}^{d} \text{Multinomial}(y_{ij} | \pi_k^j) \right]$$

  for d-dimensional observations.
- Available packages in R: e.g.,
  - **poLCA** (Linzer and Lewis, 2011)
  - **Rmixmod** (Lebret et al., 2015)

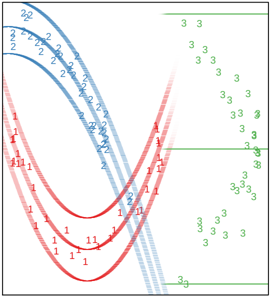
Multivariate data with regression structure

- Often also referred to as clusterwise regression.
- The model-based clustering model is given by

$$\boldsymbol{y}_i | \boldsymbol{x}_i \sim \sum_{k=1}^{K} \eta_k f(\boldsymbol{y}_i | \boldsymbol{\mu}_k(\boldsymbol{x}_i), \phi_k).$$

- Different regression models possible:
  - Generalized linear models.
  - Generalized linear mixed-effects models.
- Available packages in R: e.g.,
  - **flexmix** (Leisch, 2004; Grün and Leisch, 2008)
  - **mixtools** (Benaglia et al., 2009)

Multivariate data with regression structure / 2



Combining components to clusters

- Two-step procedures:
  1. Fit a mixture model as semi-parametric tool for density estimation.
  2. Combine components of the mixture model to form clusters based on some criterion.

  Available packages in R, e.g.:
  - **mclust** uses entropy or connectedness of components as criterion (Baudry et al., 2010; Scrucca, 2016).
  - **fpc** (Hennig, 2020) provides several variants as proposed in Hennig (2010).
- Simultaneous estimation using informative priors in Bayesian estimation can be used in combination with standard estimation methods.

Applications of model-based clustering

- Modeling unobserved heterogeneity:
  - Density approximation / semi-parametric modeling.
  - Continuous versus discrete heterogeneity.
- Extensibility:
  - Any statistical model can be used as cluster-specific model.
  - Model-specific estimation methods can be re-used.
- Challenges:
  - Selecting the clustering base: variable selection.
  - Assessing and comparing different clustering solutions.

Summary

- Model-based clustering is a versatile method for clustering.
- Different variants exist depending on
  - Clustering kernel.
  - Estimation approach.
- A large number of R packages are available covering different kinds of models.
- For more information see the CRAN Task View: Cluster Analysis & Finite Mixture Models:
  `https://CRAN.R-project.org/view=Cluster`

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