Exploring outliers in compositional data with structural zeros

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Compositional data

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- the constant sum of parts (1, 100) = proper representation of compositions
Geometric aspects of compositional data analysis

- assumptions of a relevant analysis of compositions: *scale invariance, subcompositional coherence, relative scale preserving* ⇒ the **Aitchison geometry** (AG; EVS of dimension $D - 1$)

- most of statistical methods rely on assumption of Euclidean geometry (Eaton, 1983)
Geometric aspects of compositional data analysis

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\(\Rightarrow\) express compositional data in coordinates with respect to an orthonormal basis on the simplex (Egozcue et al., 2003) \(\Rightarrow\) statistical analysis, interpretation (*balances, lack of standard/Carthesian coordinates*)

- **log-ratio analysis** of compositional data (Aitchison, 1986)
Structural zeros are not welcome

- scale invariance principle → all relevant information in compositional data is contained in ratios between parts

- structural zeros - resulting from structural processes (replacement is not meaningful)

- examples:
  (a) plant species that are not able to survive in a given soil type or climate,
  (b) a political party that has no candidates in a region,
  (c) teetotal households that do not have expenditures on alcohol and tobacco
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Strategies for dealing with structural zeros

- **amalgamation** of compositional parts (Aitchison, 1986)
  (tobacco and alcohol parts amalgamated into a new part representing expenditures for both commodities)
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  - derivation of the likelihood assumes the usual Euclidean geometry, not followed by the original compositions
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- the resulting estimates are used for an analysis in the subcompositions resulting from the single zero patterns
Mahalanobis distances for outlier detection

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- given a sample of coordinates \( z_1, \ldots, z_n \in \mathbb{R}^{D-1} \), the MD is defined as

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\text{MD}(z_i) = \left[ (z_i - \mathbf{t})' \mathbf{C}^{-1} (z_i - \mathbf{t}) \right]^{1/2}, \ i = 1, \ldots, n; \quad (1)
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\( \mathbf{t} \) and \( \mathbf{C} \) stand for (robust \( \rightarrow \) MCD) location and covariance estimators

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- MDs are not directly applicable to compositional data with structural zeros
Imputation approach to outlier detection

- the (auxiliary) **imputation strategy** is used to detect outliers in single zero patterns (Templ et al., 2016)
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- **orthonormal (pivot) coordinates** $z = (z_1, \ldots, z_{D-1})'$,

  $$z_i = \sqrt{\frac{D-i}{D-i+1}} \ln \frac{x_i}{\prod_{k=i+1}^{D} x_k}, \quad i = 1, \ldots, D-1$$

  (Fišerová and Hron, 2011), guarantee that the subcomposition $(x_i, \ldots, x_D)'$ is represented by the last $i-1$ coordinates
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- **permutation of parts** and **affine equivariance** of the MCD estimator are used to perform **outlier detection in any subcomposition resulting from the zero patterns**
Outliers according to zero patterns

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- the data are recoded into a binary matrix (non-zeros . . . 1)

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- **the multivariate structure and outlyingness of the zero patterns** are analyzed using **principal component analysis** (PCA) for **binary data** (Leeuw, 2006) → loadings and scores

- results from the previous steps are merged together
Austrian EU-SILC data set

- European Union Statistics on Income and Living Conditions (EU-SILC) is an annual panel household survey conducted in most of European countries, data basis for measuring risk-of-poverty and social cohesion in Europe.

- The Austrian EU-SILC 2006 data set is considered, the data set is simulated from the original (confidential) data with the R package `simPopulation`.

- 14,827 observations from 6,000 households and 28 variables are obtained (data `eusilc` from the R package `laeken`).

- The income components contain (too) many zeros → the parts are amalgamated to obtain the four compositional parts `workinc` (work income), `capinc` (capital income), `transh` (household transfers), and `transp` (personal transfers).
Austrian EU-SILC data: zero structure

Compositional data and their geometry
Dealing with structural zeros
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Real data example
Austrian EU-SILC data: Mahalanobis distances
Austrian EU-SILC data: findings

- MDs results from all patterns are similar → zero patterns do not cause significant changes in covariance structure

- the imputation approach guarantees that enough sample size is used for robust estimation of MDs in single zero patterns

- **PCA biplot**: patterns with observed values in a specific variable (indicated by \(x\)) are located in direction of the respective arrow

- no clear outlier visible in the scores plot, i.e. none of the zero patterns shows extreme behavior

- though, some atypical patterns, located further from the origin, are present, like \(x00x\) (occurs only 91 times)
Austrian EU-SILC data: PCA for binary data

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- the respective R functions (zeroOut, zeroPatterns) from the package robCompositions soon available at CRAN
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Conclusions

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- Since outlier detection already involves the (robust) pattern-individual and joint covariance estimation, it is straightforward to continue with other multivariate analysis methods which are based on the estimated covariance matrices.
**References**


