Exploring outliers in compositional data with structural zeros

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- **examples**: **(a)** vegetation compositions of various plant species in different survey areas, **(b)** election results of political parties in different regions of a country, **(c)** household expenditures on various costs (housing, foodstuff, etc.) for a sample of households

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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* $\Rightarrow$ the **Aitchison geometry** (AG; EVS of dimension $D-1$)

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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)

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- ***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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× derivation of the likelihood assumes the usual Euclidean geometry, not followed by the original compositions

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⇒ use a **reasonable imputation** of zero parts as an **auxiliary step** to get estimates of parameters (e.g. covariance) from the overall data set (no new information is added to the data structure)

- the resulting estimates are used for an **analysis in the subcompositions resulting from the single zero patterns**

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$$\mathrm{MD}(\mathbf{z}_i) = \left[(\mathbf{z}_i - \mathbf{t})' \mathbf{C}^{-1} (\mathbf{z}_i - \mathbf{t})\right]^{1/2}, i = 1, \ldots, n; \qquad (1)$$

  $\mathbf{t}$ and $\mathbf{C}$ stand for (robust → MCD) location and covariance estimators

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- **MDs are not directly applicable to compositional data with structural zeros**

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

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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**

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- outliers refer to atypical phenomena that occur rarely in the binary matrix of the zero patterns together with frequencies, arising from their occurrence in the data set
- **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

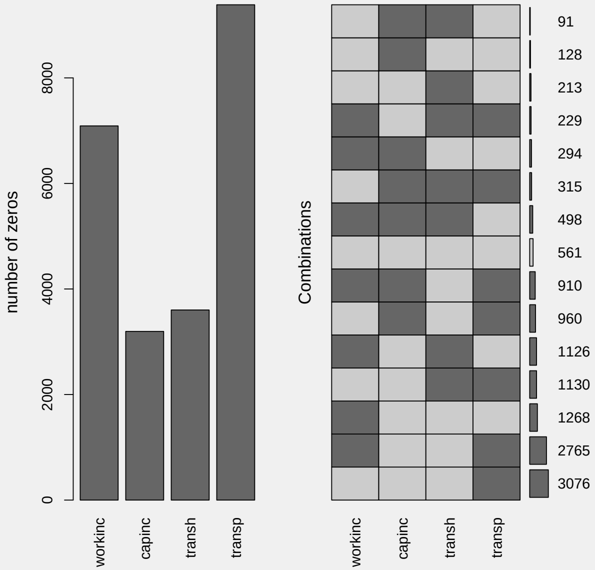
- European Union Statistics on Income and Living Conditions (EU-SILC) is an annual panel household survey conducted in most of European countries, data basis for measuring risk-of-poverty and social cohesion in Europe

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

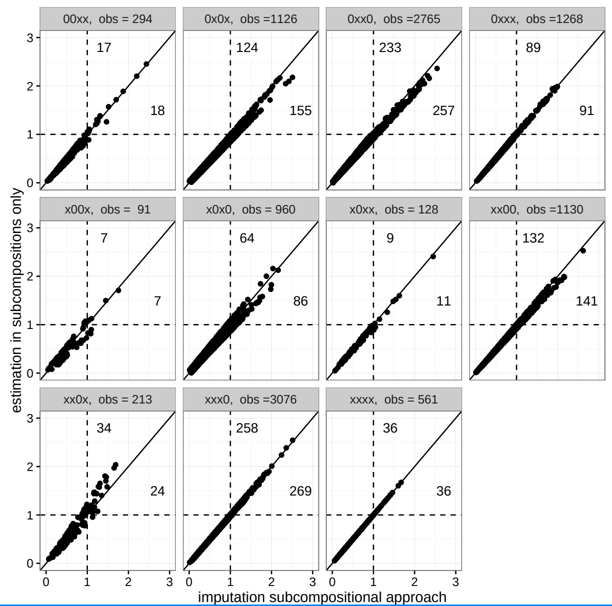
- 14,827 observations from 6,000 households and 28 variables are obtained (data `eusilc` from the R package `laeken`)

- 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



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**

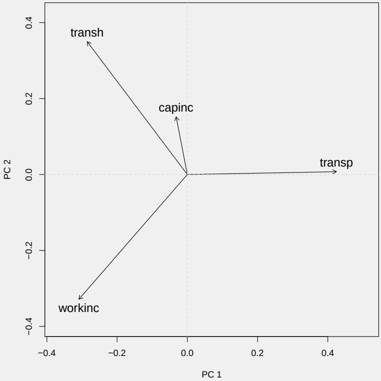
- the imputation approach guarantees that enough sample size is used for robust estimation of MDs in single zero patterns

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

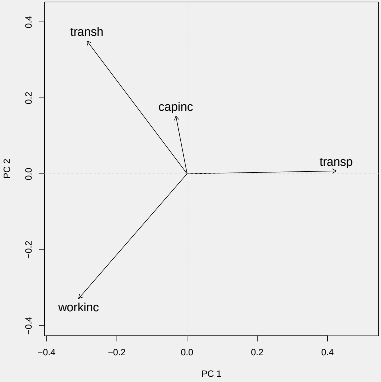
- no clear outlier visible in the scores plot, i.e. none of the zero patterns shows extreme behavior

- 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



Austrian EU-SILC data: PCA for binary data



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

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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

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