

Robust Factor Analysis for Compositional Data

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Factor analysis as frequent technique for multivariate data inspection is widely used also for compositional data analysis. The usual way is to use a centered logratio (clr) transformation to obtain the random vector \mathbf{y} of dimension D . The factor model is then

$$\mathbf{y} = \mathbf{\Lambda}\mathbf{f} + \mathbf{e} \quad (1)$$

with the factors \mathbf{f} of dimension $k < D$, the error term \mathbf{e} , and the loadings matrix $\mathbf{\Lambda}$. Using the usual model assumptions (see, e.g., Basilevsky, 1994), the factor analysis model (1) can be written as

$$\text{Cov}(\mathbf{y}) = \mathbf{\Lambda}\mathbf{\Lambda}^T + \mathbf{\Psi} \quad (2)$$

where $\mathbf{\Psi} = \text{Cov}(\mathbf{e})$ has a diagonal form. The diagonal elements of $\mathbf{\Psi}$ as well as the loadings matrix $\mathbf{\Lambda}$ are estimated from an estimation of $\text{Cov}(\mathbf{y})$.

Given observed clr transformed data \mathbf{Y} as realizations of the random vector \mathbf{y} . Outliers or deviations from the idealized model assumptions of factor analysis can severely effect the parameter estimation. As a way out, robust estimation of the covariance matrix of \mathbf{Y} will lead to robust estimates of $\mathbf{\Lambda}$ and $\mathbf{\Psi}$ in (2), see Pison et al. (2003). Well known robust covariance estimators with good statistical properties, like the MCD or the S-estimators (see, e.g. Maronna et al., 2006), rely on a full-rank data matrix \mathbf{Y} which is not the case for clr transformed data (see, e.g., Aitchison, 1986).

The isometric logratio (ilr) transformation (Egozcue et al., 2003) solves this singularity problem. The data matrix \mathbf{Y} is transformed to a matrix \mathbf{Z} by using an orthonormal basis of lower dimension. Using the ilr transformed data, a robust

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covariance matrix $C(\mathbf{Z})$ can be estimated. The result can be back-transformed to the clr space by

$$C(\mathbf{Y}) = \mathbf{V}C(\mathbf{Z})\mathbf{V}^T$$

where the matrix \mathbf{V} with orthonormal columns comes from the relation between the clr and the ilr transformation. Now the parameters in the model (2) can be estimated (Basilevsky, 1994) and the results have a direct interpretation since the links to the original variables are still preserved.

The above procedure will be applied to data from geochemistry. Our special interest is on comparing the results with those of Reimann et al. (2002) for the Kola project data.

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