Regression analysis of compositional data via linear model with type-II constraints

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Abstract

The restrictive properties of compositional data, that is multivariate data with positive parts that carry only relative information in their components (Aitchison, 1986), call for special care to be taken while performing standard statistical methods, for example, regression analysis. Among the special methods suitable for handling this problem is the total least squares procedure (TLS, orthogonal regression, regression with errors in variables, calibration problem), performed after an appropriate logratio transformation. The difficulty or even impossibility of deeper statistical analysis (confidence regions, hypotheses testing) using the standard TLS techniques can be overcome by calibration solution based on linear statistical models, namely models with type-II constraints (constraints involve in addition to the unknown model's parameters the other unobservable ones), see e.g. (Brown, 1993; Kubáček et al., 1995). This approach can be combined with standard statistical inference, for example, confidence and prediction regions and bounds, hypotheses testing, etc., suitable for interpretation of results. Here, we deal with the simplest TLS problem where we assume a linear relationship between two errorless measurements of the same object (substance, quantity). We propose an iterative algorithm for estimating the calibration line and also give confidence ellipses for the location of unknown errorless results of measurement. An illustrative example from the fields of geochemistry will be presented.

Keywords

Compositional data, Total least squares, Linear model, Calibration line.

References

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