Weighted Pivot Balances: Simulations and Application to Geochemical Mapping

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Abstract

The logratio methodology converts compositional data from their original Aitchison geometry to interpretable real orthonormal coordinates, thereby allowing meaningful statistical processing and visualization (Aitchison, 1986; Pawlowsky-Glahn and others, 2015). However, it must be taken into account that the original concentrations can be flawed by detection limit or imprecision problems. As a consequence, the resulting coordinates can be severely affected. The aim of this contribution is to study the properties of the so-called weighted pivot balances, orthonormal logratio coordinates that capture the relevant relative information about an original component and treat the redundant information in a controlled manner (Filzmoser and Hron, 2015; Hron and others, 2017). Accordingly, weighted pivot balances are logcontrasts endowed with weights that preserve orthonormality of the resulting coordinate system. Weights can be determined, e.g. via simulations. Here a thorough simulation study with real data from a large-scale geochemical survey on the Kola peninsula is presented. A varying number of parts is considered, permuted, and some of the parts are deliberately contaminated, i.e. multiplied by random noise. Within 1000 replications, the first weighted pivot balances of the uncontaminated and contaminated data are computed and such weights are set up that highlight sufficiently the effect of filtering the redundant relative information about the compositional part of interest and provides reliable results in a geochemical context. Finally, weighted pivot balances are applied to the geochemical mapping of catchment outlet sediments from the National Geochemical Survey of Australia further illustrating their advantage over possible alternatives.

References

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