

Practical aspects of compositional data analysis using regional geochemical survey data

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Government geological surveys and mineral exploration companies collect large amounts of geochemical data, which are used in search for mineral commodities or for determining environmental disturbances. These surveys consist of many thousands of samples (observations) with as many as 50 elements determined for each. Because the nature of the data is compositional, they must be treated according to the protocols established by John Aitchison and others. This contribution details an approach based on the application of the alr, clr and ilr transforms for process discovery and validation. Issues of around the treatment of zeros and/or missing values are complicated due to the stoichiometric nature of the data. Case studies are presented where the use of logratio transforms and the estimation of replacement values for missing data are considered in the context of stoichiometric constraints.