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Scaling and nonlinear dynamics in water systems

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Water systems dynamics deals with chemical reactions driven by nonequilibrium conditions. The knowledge of such dynamics has significant implications in management of water resource. From this point of view, the study focuses on the development of tools to investigate the variability structure of aqueous chemical compositions by using the CoDA (Compositional Data Analysis) approach (Aitchison, 1982). In multispecies systems, as the aqueous ones, the CoDA approach appears to be particularly suitable since it allows to look into the whole composition and to investigate the dynamics of the system governed by the relationships between the parts (variables). In order to obtain indications about the nature of geochemical processes, the frequency distribution analysis of compositional indices was evaluated. Such indices were extracted from the compositional matrix of D parts by applying a method recently proposed by Martín-Fernández et al. (2017). Following an approach similar to that used in the Principal Component Analysis, D-1 indices are searched, so that each one explains a part of the total variance of the geochemical system in decreasing order. On the other hand, with the aim of exploring the spatial variability and stability of geochemical variables (as parts of a composition) in the correct sample space, compositional multivariate analysis tools were applied.
Results show differences in the behaviour of geochemical indices that have a various spatial stability and continuity, revealing interesting features about the dynamics of the solutes in terms of their adaptive capacity and resistance to changes. Furthermore, multivariate analysis highlighted a scale of processes (for example: anthropogenic and geogenic ones) that are overlapped and hierarchically ordered according their amount of variability.
The hierarchal structure of the variability could be due to different kinetics of each geochemical variable. In particular, variables standing at the top behave as a sink (trap) by capturing great part of the variability inside the composition and making harder the investigation of the contribution of other sources.
To sum up, in a water monitoring perspective, it is fundamental taking into account different spatial and time scales in the variability of chemical components, in order to identify indices able to be a first sentinel in case of compositional regime shifts in complex nonlinear geochemical systems.

Aitchison J. 1982. The statistical analysis of compositional data (with discussion). J. R. Stat. Soc. B, 44 (2), 139–177.

Martín-Fernández J.A., Pawlowsky-Glahn V., Egozcue J.J. & Tolosana-Delgado R. 2017. Advances in principal balances for compositional data. Math. Geosci., 50, 273-298.