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On the potential for the Partial Triadic Analysis to grasp the spatio-temporal variability of groundwater hydrochemistry

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The Luxembourg sandstone aquifer is of major relevance for the national supply of drinking water in Luxembourg. The city of Luxembourg (20% of the country's population) gets almost 2/3 of its drinking water from this aquifer. As a consequence, the study of both the groundwater hydrochemistry, as well as its spatial and temporal variations, are considered as of highest priority. Since 2005, a monitoring network has been implemented by the Water Department of Luxembourg City, with a view to a more sustainable management of this strategic water resource. The data collected to date forms a large and complex dataset, describing spatial and temporal variations of many hydrochemical parameters. The data treatment issue is tightly connected to this kind of water monitoring programs and complex databases.

Standard multivariate statistical techniques, such as principal components analysis and hierarchical cluster analysis, have been widely used as unbiased methods for extracting meaningful information from groundwater quality data and are now classically used in many hydrogeological studies, in particular to characterize temporal or spatial hydrochemical variations induced by natural and anthropogenic factors. But these classical multivariate methods deal with two-way matrices, usually parameters/sites or parameters/time, while often the dataset resulting from qualitative water monitoring programs should be seen as a datacube parameters/sites/time. Three-way matrices, such as the one we propose here, are difficult to handle and to analyse by classical multivariate statistical tools and thus should be treated with approaches dealing with three-way data structures.

One possible analysis approach consists in the use of partial triadic analysis (PTA). The PTA was previously used with success in many ecological studies but never to date in the domain of hydrogeology. Applied to the dataset of the Luxembourg Sandstone aquifer, the PTA appears as a new promising statistical instrument for hydrogeologists, in particular to characterize temporal and spatial hydrochemical variations induced by natural and anthropogenic factors. This new approach for groundwater management offers potential for 1) identifying a common multivariate spatial structure, 2) untapping the different hydrochemical patterns and explaining their controlling factors and 3) analysing the temporal variability of this structure and grasping hydrochemical changes.