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Exploratory data analysis and clustering of multivariate spatial hydrogeological data by means of GEO3DSOM, a variant of Kohonen's Self-Organizing Map

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Abstract. The use of unsupervised artificial neural network techniques like the self-organizing map (SOM) algorithm has proven to be a useful tool in exploratory data analysis and clustering of multivariate data sets. In this study a variant of the SOM-algorithm is proposed, the GEO3DSOM, capable of explicitly incorporating three-dimensional spatial knowledge into the algorithm. The performance of the GEO3DSOM is compared to the performance of the standard SOM in analyzing an artificial data set and a hydrochemical data set. The hydrochemical data set consists of 131 groundwater samples collected in two detritic, phreatic, Cenozoic aquifers in Central Belgium. Both techniques succeed very well in providing more insight in the groundwater quality data set, visualizing the relationships between variables, highlighting the main differences between groups of samples and pointing out anomalous wells and well screens. The GEO3DSOM however has the advantage to provide an increased resolution while still maintaining a good generalization of the data set.

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