

A new clustering method for geochemical data using spatial contextual information: GEOFCM

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Geochemical data from geological samples show compositional trends that reflect the material differentiation and assimilation occurred during certain geological processes. These trends often comprise groups in a multidimensional compositional space and are distributed in real space as geological units ranging from millimeters to kilometers in scale (e.g., Ueki and Iwamori, 2017). Therefore, spatial contextual information combined with chemical affinities could provide fundamental information about the sources and generation processes associated with the samples.

However, conventional clustering algorithms such as *k*-means and fuzzy c-means (FCM) cluster analysis do not fully utilize the spatial distribution information of geologic samples. In this study, we propose a new clustering method for geochemical datasets with location coordinates. A spatial FCM algorithm originally constructed for image segmentation was modified to deal with a sparse and unequal-spaced dataset. The proposed algorithm evaluates the membership function modified using a weighting function calculated from neighboring samples within a certain radius.

We applied new algorithm to a geochemical dataset of granitoids in the Ina-Mikawa district of the Ryoke belt that was compiled by Haraguchi et al. (2017), showing that samples collected from the same geological unit are likely to be classified as the same cluster. Moreover, overlapping geochemical trends are classified consistently with spatial distribution, and the result is robust against noise addition compared with standard FCM analysis.

The proposed method can be calculated in the “GEOFCM” Excel® sheet provided as supplementary material and on our website (<http://dsap.jamstec.go.jp>). Geological datasets with precise location coordinates are becoming increasingly available, and the proposed method can help find overviews of complicated multidimensional data structure.

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