

GROUPING GEOLOGICAL SAMPLES WITH MATHEMATICAL METHODS

by

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The dissertation consists of two parts. The first is essentially methodological. It contains short descriptions of the most important multivariate methods used for clustering geological samples (cluster analysis, ANDREWS function plot, principal component analysis, principal coordinates analysis, ZAHN's graph-theoretical method, correspondence analysis, non-linear mapping, non-metric multidimensional scaling, Q-type factor analysis, RODIONOV's automatic clustering, eigenvector biplot, special graphic representations, variation diagrams) and their comparison and evaluation in respect to their possibilities in geology. Then a sort of analysis of the relevant (to clustering) properties of geoscience data (like cluster-structures of great complexity, variables of different types etc.) is given. The concept of *clusters derived from one another* is introduced and investigated. It is pointed out that in geological researches one often encounters groups, classes or types of objects that, as results of successive stages of one or more processes, can be originated one from another. At last, a *data analysing strategy* for processing geological data is developed: applying hierarchical agglomerative cluster analysis and nonlinear mapping jointly for detecting incorrectly classified samples, erroneous groupings, outliers, well-separated, touching, derived from one another and of special form clusters.

The second part comprises four studies of real geological questions using the data analysing strategy developed in the first part. In the first one, petrochemical types (alkaline-rich, K-rich, Mg-rich and average types) of

Transdanubian young alkaline basalts are revealed and for their interpretation a Mg-rich-average-K-rich differentiation trend is proposed. In the second, the Árpádtető (Mecsek-Mts.) *Coenothyris vulgaris* (SCHLOTHEIM) (an Anisian Brachiopoda-species) shells are investigated and existence of three morphotypes (Alpine, German, juvenile) is proved. The third one states and shows that the granite-pluton of the Velence Mts. is petrochemically rather uniform with a slightly more homogeneous and basic central part. In the fourth study lithochemical-lithogenetic types of karst bauxites from Némethánya and a formation-controlled variation in their compositions are showed.

It is stressed that in geological scientific researches only little-automized, expert-controlled clustering can lead to good results.

As a non-primary part of the theses, some written by the author FORTRAN 77 source program listings, including cluster-analysis methods and non-linear mapping, are also given.