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A flexible open-source toolbox for robust end-member modelling analysis - The R-package EMMAgeo

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Interpreting geomorphological and sedimentological processes from grain-size data in environmental archives typically runs into problems when source- and process-related grain-size distributions become mixed during deposition. A powerful approach to overcome this ambiguity is to statistically "unmix" the samples. Typical algorithms use eigenspace decomposition and techniques of dimension reduction.
This contribution presents a package for the free statistical software R. Some of the great advantages of R and R-packages are the open code structure, flexibility and low programming effort. The package contains a series of flexible, ready-to-use functions to perform different tasks of data tests, preparation, modelling and visualisation. The package originated from a recently presented Matlab-based end-member modelling algorithm (Dietze et al., 2012, SedGeol). It supports simple modelling of grain-size end-member loadings and scores (eigenspace extraction, factor rotation, data scaling, non-negative least squares solving) along with several measures of model quality. The package further provides preprocessing tools (e.g. grain-size scale conversions, tests of data structure, weight factor limit inference, determination of minimum, optimum and maximum number of meaningful end-members) and allows to model data sets with artificial or user-defined end-member loadings. EMMAgeo also supports inferring uncertainty estimation from a series of plausible model runs and the determination of robust end-members.
The contribution presents important package functions, thereby illustrating how large data sets of artificial and natural grain-size samples from different depositional environments can be analysed to infer quantified process-related proxies.