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Algorithms for mineral dust classification using SEM-EDS

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The mineralogical compositions of atmospheric particles (i.e., “dust”) have significant implications for environmental, glaciological, and climatological research. One of the most common techniques for characterizing mineral dust is the use of a scanning electron microscope equipped with an energy dispersive x-ray detector (SEM-EDS). However, while SEM-EDS is an effective way for scientists to identify the elemental compositions of individual dust particles, it is often difficult to accurately reconstruct the particles’ mineralogical classifications from the elemental data alone. Presently, numerous algorithms exist in the literature that can aid users in classifying mineralogical compositions from EDS data, ranging from relatively simple sorting schemes that distinguish minerals based on elemental peak intensity ratios [1] to more complex sorting schemes [e.g., 2-3], and, more recently, a random forest model (Qmin) [4] trained with data collected with electron probe microanalyzers (EPMA). Thus far, the sorting scheme algorithms in particular are limited in their ability to provide probabilistic estimates in their final mineralogical assignments. These algorithms are also only written in print and are not available as functional programmatic code, making it extremely difficult for scientists to re-use the algorithms in an efficient manner. Moreover, the Qmin model is limited in that it was trained using elemental weight percent data collected with EPMA instruments, which is more difficult to acquire than elemental peak intensity data derived from SEM-EDS analyses. To address these algorithmic limitations, several sorting scheme algorithms have been transcribed or are in the process of being transcribed from the literature into functionally optimized MATLAB (licensed software) code and Julia (open-source software) code, while more robust machine learning algorithms, similar to Qmin, are currently under development, designed specifically for mineral particle classification using data collected via SEM-EDS. These algorithms are to be made publicly available along with clear documentation on the necessary data collection methods and how each algorithm can be utilized.

[1] Donarummo *et al*. (2003), *Geophysical Research Letters* 30(6), 1269.

[2] Kandler *et al*. (2011), *Tellus B* 63(4), 475-596.

[3] Panta *et al*. (2023), *Atmospheric Chemistry and Physics* 23(6), 3861-3885.

[4] da Silva *et al*. (2021), *Computers & Geosciences* 157, 104949.