Algorithms for SEM-EDS Mineral Dust Classification

Austin M. Weber ![ORCID] [1,2]

1 Byrd Polar and Climate Research Center, Columbus, Ohio **2** School of Earth Sciences, The Ohio State University, Columbus, Ohio

Summary

Mineral dust plays an important role in governing Earth's energy balance and also accelerates the melting of glaciers. The most common analytical method for studying mineral dust is scanning electron microscopy (SEM) with energy dispersive x-ray spectrometry (EDS). The primary benefit of SEM-EDS over alternative techniques is that it allows researchers to select and measure the elemental compositions of individual particles. However, elemental composition alone is often not enough to confidently infer mineralogy because many unrelated minerals are comprised of the same elements. Identifying minerals from SEM-EDS data has also historically been a labor intensive task because automated procedures are not readily available. To address these limitations, a repository of MATLAB functions has been assembled to work with SEM-EDS data, with the objective of providing researchers with tools to quickly and accurately determine the mineral compositions of dust particles. The repository includes a machine learning classifier and three additional sorting algorithms that have been transcribed from the peer-reviewed literature, as well as functions for importing and visualizing x-ray energy spectra.

Statement of need

The mineral classification of single particles (i.e., dust) has major implications for atmospheric and glaciological research. For instance, there is a great need for building mineral dust datasets that can be used to improve the predictive ability of climate models (Gieré, 2010). Mineral dust observations are also severely limited in many glaciated mountain regions, meaning that the dust's radiative impact on glacier melt rates cannot be easily determined (Gilardoni et al., 2022).

One of the most common methods for reconstructing the mineral dust history of a location or region has been the use of scanning electron microscopy with energy dispersive x-ray spectrometry (SEM-EDS) to analyze single particles extracted from ice cores (Donarummo Jr et al., 2003; Nagatsuka et al., 2021; Wu et al., 2016). SEM allows researchers to examine particles individually while an EDS detector measures the particles' elemental compositions as they emit x-rays under the influence of an electron beam. However, the process of classifying single particles from EDS data is highly laborious and prone to error due to the complexity of certain minerals' elemental signatures. The adoption of numerous classification techniques is typically required to improve the certainty of the classifications before finalizing the results. Many have used the dichotomous key in Severin (2004) to compare EDS spectra to that of mineral standards, but this protocol requires access to a physical or digital copy of the book and cannot be automated. Others have used published sorting algorithms like the one by Donarummo Jr et al. (2003), but these algorithms are limited in the number of minerals that they can identify and, to the author's knowledge, each of these algorithms is only available in print and not as a functional computer program.

Therefore, to satisfy the needs of Earth and atmospheric scientists seeking to rapidly classify

43 mineral particles from EDS data with a high degree of certainty, an open-source repository
44 of functions for implementing different mineral classification algorithms has been developed
45 for MATLAB (along with several homologous functions written in the Julia programming
46 language). This library of functions gives users the tools to work with SEM-EDS data and to
47 perform mineral classification with ease.

Methods

Mineral Dust Classification

50 The function library introduces a supervised machine learning model (the "Weber algorithm")
51 that is trained to recognize 18 common minerals from EDS net intensity data and exhibits
52 an overall accuracy exceeding 99% (see Supplemental Information). The library also includes
53 functions for three non-machine learning algorithms that have been painstakingly transcribed
54 from the literature into MATLAB and Julia code. This includes the sorting algorithm from
55 Donarummo Jr et al. (2003) which can be used to classify 16 unique aluminosilicate minerals
56 based on EDS net intensity data, the Panta algorithm (Panta et al., 2023) which can be used
57 to classify 17 unique minerals and 6 mineral groups based on EDS atom percent data, and the
58 Kandler algorithm (Kandler et al., 2011) which can be used to categorize EDS atom percent
59 data into broad mineral groups, classes, and refractive indexes.

60 The four mineral classification algorithms are available as individual functions (`weber_classification`,
61 `donarummo_classifiation`, `panta_classifiation`, and `kandler_classification`) as well
62 as packaged together in a single function (`eds_classification`). Each function has clearly
63 written documentation that can be viewed using the MATLAB `help` or `doc` commands. The
64 general syntax, however, is very basic:

```
minerals = eds_classifiation(data,Algorithm="Name")
```

65 where `data` is a table of EDS data and `"Name"` specifies the desired algorithm; i.e., `"Weber"`
66 (default), `"Donarummo"`, `"Kandler"`, or `"Panta"`. The output `minerals` is a categorical vector
67 containing the mineral assignments for each row in the input table.

Visualizing EDS Spectra

69 For individuals who want to compare the EDS spectra of their single particle measurements to
70 the standard spectra in Severin (2004), it will be necessary to visualize each energy spectrum
71 along with labels for the major characteristic x-rays. Most EDS software save x-ray energy data
72 in the EMSA (`.msa`) file format which is compiled differently depending on the software and
73 therefore makes it difficult to simply import the data using a base MATLAB function such as
74 `readtable`. While methods for visualizing EDS spectra are available for the Julia programming
75 language (Ritchie, 2022) and as a desktop Java application (see DTSA-II), there are currently
76 no simple alternatives to perform these tasks in MATLAB.

77 To address this limitation, the EDS mineral dust classification library also provides functions
78 for importing `.msa` files into MATLAB and for visualizing the EDS spectrum contained in a file.
79 Just use the `xray_plot` function to view the spectrum and the `xray_peak_label` function to
80 label the characteristic x-rays with the most likely element (**Fig.1**).

```
plt = xray_plot('spectrum.msa');
xray_peak_label(plt)
```
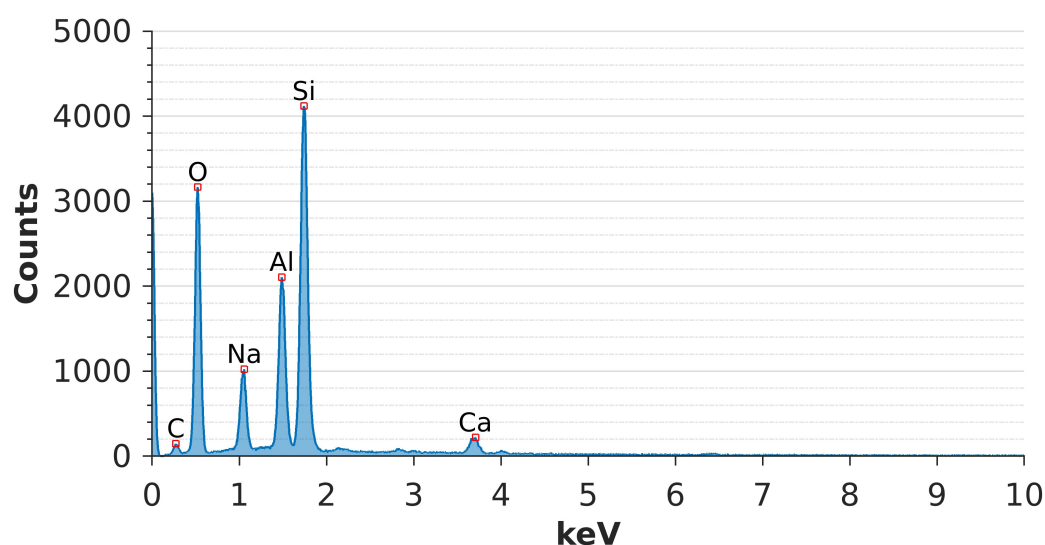
Figure 1: EDS spectrum visualization.

Acknowledgements

Copyrights

The software repository is made available under a MIT license, meaning that users are free to modify and distribute the software without restriction. However, the *intellectual copyrights* for the Donarummo, Kandler, and Panta algorithms belong to their original creators. If you use any of these algorithms in your research, **please** also cite the original references as appropriate.

References

Donarummo Jr, J., Ram, M., & Stoermer, E. F. (2003). Possible deposit of soil dust from the 1930's US dust bowl identified in Greenland ice. *Geophysical Research Letters*, *30*(6). https://doi.org/10.1029/2002GL016641

Gieré, R. (Ed.). (2010). Atmospheric Particles. *Elements*, *6*(4). https://www.elementsmagazine.org/atmospheric-particles/

Gilardoni, S., Di Mauro, B., & Bonasoni, P. (2022). Black carbon, organic carbon, and mineral dust in South American tropical glaciers: A review. *Global and Planetary Change*, *213*, 103837. https://doi.org/10.1016/j.gloplacha.2022.103837

Kandler, K., Lieke, K., Benker, N., Emmel, C., Küpper, M., Müller-Ebert, D., Ebert, M., Scheuvens, D., Schladitz, A., Schütz, L., & others. (2011). Electron microscopy of particles collected at Praia, Cape Verde, during the Saharan Mineral Dust Experiment: Particle

chemistry, shape, mixing state and complex refractive index. *Tellus B: Chemical and Physical Meteorology*, *63*(4), 475–496. https://doi.org/10.1111/j.1600-0889.2011.00550.x

Nagatsuka, N., Goto-Azuma, K., Tsushima, A., Fujita, K., Matoba, S., Onuma, Y., Dallmayr, R., Kadota, M., Hirabayashi, M., Ogata, J., & others. (2021). Variations in mineralogy of dust in an ice core obtained from northwestern Greenland over the past 100 years. *Climate of the Past*, *17*(3), 1341–1362. https://doi.org/10.5194/cp-17-1341-2021

Panta, A., Kandler, K., Alastuey, A., González-Flórez, C., González-Romero, A., Klose, M., Querol, X., Reche, C., Yus-Díez, J., & Pérez García-Pando, C. (2023). Insights into the single particle composition, size, mixing state and aspect ratio of freshly emitted mineral dust from field measurements in the Moroccan Sahara using electron microscopy. *Atmospheric Chemistry and Physics*, *23*(6), 3861–3885. https://doi.org/10.5194/acp-23-3861-2023

Ritchie, N. W. M. (2022). Reproducible Spectrum and Hyperspectrum Data Analysis Using NeXL. *Microscopy and Microanalysis*, *28*(2), 478–495. https://doi.org/10.1017/S143192762200023X

Severin, K. P. (2004). *Energy Dispersive Spectrometry of Common Rock Forming Minerals*. Kluwer Academic Publishers. https://doi.org/10.1007/978-1-4020-2841-0

Wu, G., Zhang, X., Zhang, C., & Xu, T. (2016). Mineralogical and morphological properties of individual dust particles in ice cores from the Tibetan Plateau. *Journal of Glaciology*, *62*(231), 46–53. https://doi.org/10.1017/jog.2016.8