Byrd Polar and Climate Research Center

Fast and accurate identification of minerals in ice cores

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The problem

Analyzing EDS data is slow and prone to error

Scanning electron microscopy (SEM) with energy dispersive spectrometry (EDS) allows us to probe individual particles for their chemical compositions. However, this technique does not identify minerals *directly* and the typical methods for categorizing minerals from EDS data are inefficient and are not probabilistic.

The solution

Improve upon old methods with computerization

There are many classification workflows in the literature, but not all are quantitative and most lack automation. Weber [1] has transcribed three popular SEM-EDS mineral dust classification procedures [2—4] into easy-to-use MATLAB code.

Develop new, robust machine learning models

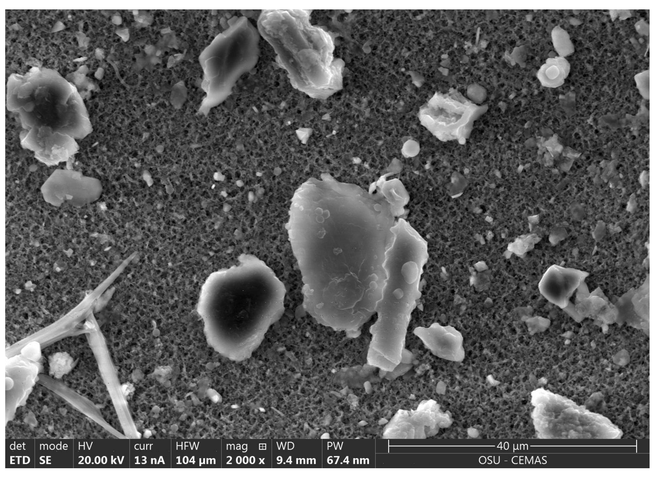
Machine learning (ML) provides a quantitative and probability-based approach of creating classification models. Weber [1] introduces a ML model—trained to recognize 18 minerals commonly found in ice cores—that exhibits an accuracy of 99%!

Methods

Sample preparation for SEM-EDS

- Collect discrete ice core samples
- Decontaminate with scraping/rinsing
- Melt the samples and filter the dust
- Mount the filters on SEM pins
- Carbon coat the samples before analysis

SEM image of an ice core dust sample



Secondary electron image of an ice core mineral dust sample taken at the Center for Electron Microscopy and Analysis (CEMAS) in the College of Engineering at Ohio State University.

Data acquisition

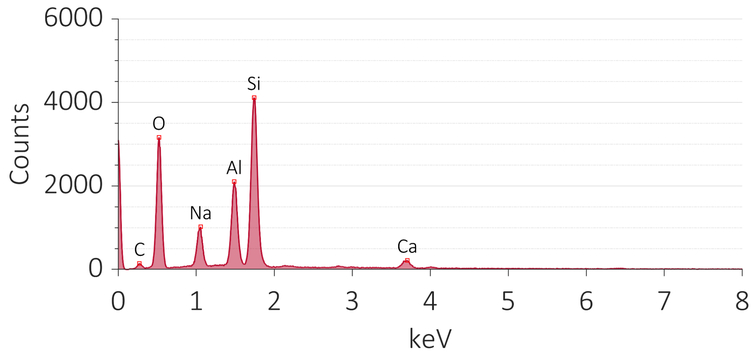
- Run EDS spot analyses for at least 10 s particle^{-1}
- Save x-ray spectra as .msa files
- Use the quantification tool to collect net intensity and atom percent data for the following mineral-forming elements: F, Na, Mg, Al, Si, P, S, Cl, K, Ca, Ti, Cr, Mn, and Fe

Mineral identification by dichotomous key

With the functions by Weber [1], you can visualize EDS spectra (.msa files) in MATLAB. These spectra can be compared to the dichotomous key in Severin [5] to make preliminary mineral identifications.

Visualizing EDS spectra in MATLAB

```
>> spectrum = "plagioclase.msa";
>> plt = xray_plot(spectrum);
>> xray_peak_label(plt,"best");
```



With the `xray_plot` and `xray_peak_label` functions from Weber [1], you can quickly load EDS spectra (.msa files) and identify mineralogy using the Severin [5] dichotomous key.

Algorithms for SEM-EDS mineral dust classification

An all-in-one function

- Aggregate the EDS data into a spreadsheet with a column for each chemical element.
- Load the data into MATLAB with the `readtable` function and use the `eds_classification` function from Weber [1] to analyze the data:

```
minerals = eds_classification(data,...
        Algorithm="Name");
```

- where "Name" can be set to "Weber" (default), "Donarummo" [2], "Kandler" [3], or "Panta" [4].

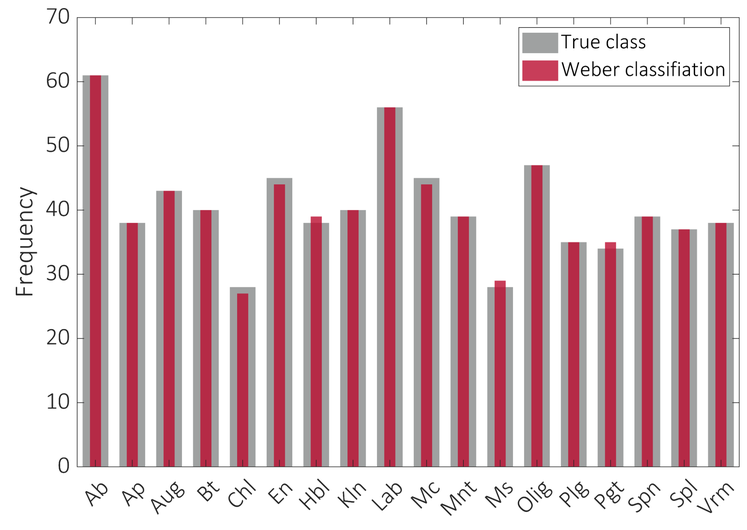
Individual functions

- Each algorithm has its own function, and some have additional outputs. For example:

```
[minerals,groups,scores] = ...
 weber_classification(data);
```

- where the `groups` output returns a list of mineral groups and the `scores` output returns a table of probability estimates for each identified mineral.

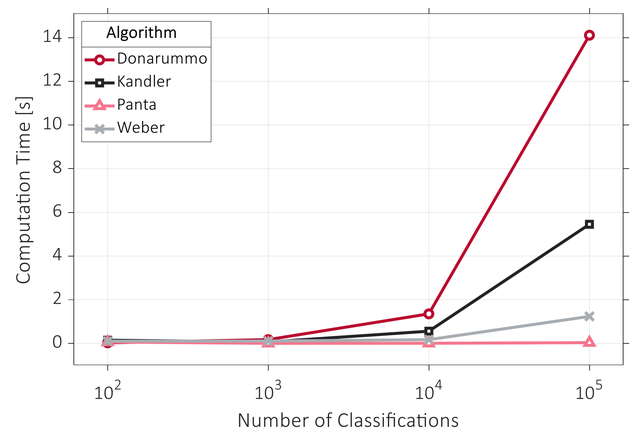
The Weber classification algorithm is up to 99% accurate!



The accuracy of the ML algorithm is ~99% (N=731) for 18 minerals.

Algorithmic identification has been optimized for speed!

- Classify EDS data for tens of thousands of mineral particles in seconds.



The speed of each mineral identification algorithm was tested using multiple synthetic data sets for each order of magnitude. The figure above illustrates the median computation times.

Conclusions

- Don't rely on the old, slow methods of identifying mineral particles in ice cores. Try this new, computer-optimized approach instead!
- Scan the QR code to view the software repository on GitHub or to read the related publication in the *Journal of Open Source Software* [1].

References

[1] Weber (2025). *JOSS*, *10*(107), 7533.
[2] Donarummo *et al.* (2003). *Geophys. Res. Let.*, *30*(6).
[3] Kandler *et al.* (2011). *Tellus B*, *63*(4), 475—96.
[4] Panta *et al.* (2023). *Atmos. Chem. Phys.*, *23*(6), 3861—85.
[5] Severin (2004). Kluwer Academic Publishers.

Acknowledgements

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https://github.com/weber1158/eds-classification