Classifying Rocks using Geochemistry? Use An Objective Data-Driven Approach

Multivariate Geochemical Tectonic Discrimination: Practical Approaches, Limitations and Opportunities

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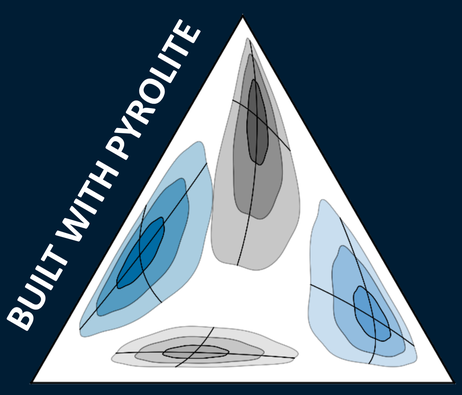

- **A machine learning approach to geochemical discrimination overcomes limitations of classical methods**
- **Free and open source tools for building classifier workflows are readily available**
- **Dimension-reducing techniques are particularly useful for visualisation**

Check out the extended abstract and live examples via links below

ABSTRACT

tinyurl.com/aegc2019MWabstract

LIVE EXAMPLES

tinyurl.com/aegc2019MWlive

This poster is accompanied by a set of examples in Jupyter notebooks, which you can browse, modify and execute using Binder.

REPOSITORY

tinyurl.com/aegc2019MWgithub

This public repository contains the notebooks, abstract and a copy of this poster.

PYROLITE DOCS

pyrolite.readthedocs.io

Much of the tooling for this project is contained within the open source python package pyrolite; this link will take you to the online documentation.

Interpretations regarding the source and tectonic context of magmatic rocks are commonly centred around the abundance of a small number of relatively incompatible trace elements[1,2]. These classic methods for tectonic discrimination have been practically useful, but most underutilise available information, resulting in uncertain classification[3]. Modern public data repositories allow new opportunities for systematic analysis on a previously inaccessible scale, and provide a variety of data with global scope. This study investigates a machine learning approach to the problem of tectonic discrimination, and focuses on the practical elements of building classification systems using geochemistry or other compositional data.

Machine Learning for Tectonic Discrimination

Supervised machine classification models for tectonic discrimination of magmatic rocks improve resolution of geochemical contrast by using more geochemical features[3,4], and use training data from public databases to build classifiers overall accuracies of approximately 90%. The approach used here follows these methods, extends the datasets used and investigates the nature of classification uncertainty.

The majority of the effort required to use machine classification models is for data preparation and pre-processing, but this is often where the largest gains for performance are to be found. Compositional data typically requires transformation prior to the use of any statistical measures (e.g. log ratio transforms), but most transforms are incompatible with missing data. Where datasets have significant missing data, this results in a principal trade-off between the volume of valid training data and dimensionality. Hence the inclusion of compositional features in classification models should be based on the value they add. Training data are also commonly strongly biased towards particular classes, which can result in classification biases; resampling classes prior to training models can minimise this effect.

Tools and Workflows

The classifier workflows used in this study are built around the scikit-learn and pandas python packages, with geochemistry-specific components integrated into a new package, pyrolite. pyrolite is an open-source python package built to facilitate data-driven understanding of geological processes using multivariate geochemical data. It's core functionality is for transformation and visualization of geochemical data. You can find links to the live demonstrations and pyrolite documentation above.

Results and Limitations

- Accurate classifiers for tectonic discrimination problems can be readily constructed using a variety of different classifier models.
- Overall accuracy is rarely above 90%, reflecting the significant geochemical overlap arising through natural variations and similarities in magmatic, metamorphic and alteration processes and sources across multiple tectonic settings. For this reason, beyond certain thresholds, increasing the number of samples does not significantly affect accuracy.
- There are limits to discrimination using a practical subset of elements, and features chosen will limit the future applicability of any classifier.
- Classification probabilities and uncertainties should be quantified or estimated where possible, as these can provide valuable insight into classifier performance.
- The models built here use data for modern tectonic settings, but their applicability in deep time is questionable (given rock-record biases, secular change)

Overcoming Graphical Limitations for Visualisation

One of the historical limitations for geochemical classification methods has been visualisation. The multivariate classifiers effectively exploit the high-dimensional data relationships which remain difficult to visualise directly. One approach to approximating these relationships for visualisation is to use manifold dimensional reduction methods (e.g UMAP[9]), which preserve local scale data structure. When considering classification probabilities, information entropy is a useful measure which can reduce multi-class classification probabilities to singular values related to classification uncertainty.

Implications and Getting Started

- **Know your data, and get it in shape** before you start; with curated datasets, building classifiers is relatively straightforward
- External public data can be useful to **avoid biases** and reduce sensitivities to outliers/novel data, but comes with higher degrees of missingness
- **Start with simple models, and build multiple**
- Accuracy is often not the only objective, and understanding the relative certainty of your predictions is useful; be wary of overfitting
- Know what question you trying to answer, and **adapt to your application;** targeted selection of features can increase the relevance and accuracy of predictions

MORE INFORMATION

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