pyrolite: Python for Geochemistry

A set of tools for making the most of your geochemical data.

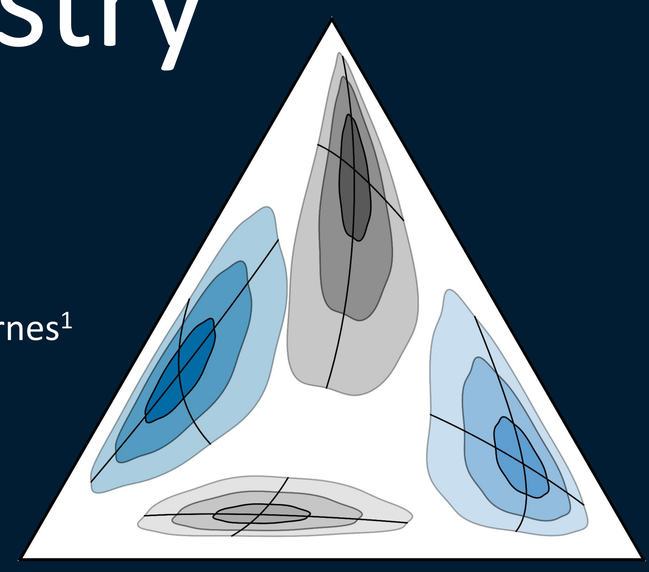
Morgan Williams[1]*, Louise Schoneveld[1], Yajing Mao[2], Jens Klump[1], Hayden Dalton[3], Adam Bath[1] and Steve Barnes[1]

[1]: CSIRO Mineral Resources

[2]: Institute of Geology and Geophysics, Chinese Academy of Geosciences

[3]: School of Earth Sciences, University of Melbourne

* A*uthors listed in reverse alphabetical order.*



- **Free and open source tools for geochemical transformation and visualisation**
- **Community-driven project and repository for reference compositions and models**
- **Beginner friendly and well documented**

MORE INFORMATION

Morgan Williams
Mineral Resources
morgan.williams@csiro.au
@metasomite

PYROLITE DOCUMENTATION

This link will take you to the online documentation for the pyrolite Python package. Here you'll find a getting started guide, examples and detailed API documentation.

pyrolite.readthedocs.io

PYROLITE REPOSITORY

This public repository hosts pyrolite and its documentation.

github.com/morganjwilliams/pyrolite

LIVE EXAMPLES

The pyrolite examples are also distributed as Jupyter notebooks, which you can browse, modify and execute using Binder.

tinyurl.com/pyroliteLiveNotebooks

Open Science, Python & Open Source

The Open Science movement calls for more transparent, cooperative and collaborative scientific research. This encompasses many aspects from open data to open publishing, but requires that the tools and software we use to conduct research are also accessible and transparent. The geochemistry community is increasingly adopting digital approaches to research, but there are few open software options. Using open source software as part of this shift can ensure that our research and tools used to achieve it are accessible to all.

The scientific Python ecosystem provides a 'batteries-included' set of libraries which users can leverage to rapidly prototype and develop data analysis, modelling and visualisation solutions. Using a programmatic approach for data analysis and visualisation enables this aspect of research to be effectively reproduced and versioned, and greatly increases transparency.

pyrolite

pyrolite is an open-source python package built to facilitate data-driven understanding of geological processes using multivariate geochemical data. It has been built with the aim of contributing to more robust and efficient geochemical research through providing an accessible, reproducible and customisable set of tools. It builds on existing packages (matplotlib[1], pandas[2]) to enable geochemists new to Python to hit the ground running, and encourages development of transferable digital skills. Features include:

- **pyrolite.geochem**
  Transforming geochemical data
  Reference compositions for normalisation
- **pyrolite.mineral**
  Mineral endmember recalculation
  Lattice strain calculations[3]
  Rock-forming mineral database
- **pyrolite.comp**
  Compositional data transformations
- **pyrolite.plot**
  Ternary, spider, density diagrams and more.
  Templated plots (e.g. TAS[4], Pearce diagrams[5])
- **pyrolite.util**
  Utilities for scikit-learn[6], plotting, web interfaces, synthetic data, missing data, geological timescale & more

Documentation

Documentation for pyrolite is hosted at pyrolite.rtfd.io, and includes a getting started guide, a set of examples for key features and detailed interface documentation.

Extensions

Extensions built around pyrolite which provide additional functionality beyond the core scope are also under development:

- **pyrolite-meltsutil**
  An interface for conducting batch alphaMELTS[7] calculations.
- **pyrolite-datasource**
  An interface to get data from common geochemical repositories (e.g. EarthChem[8]; currently a work in progress).

Community: Get Involved

pyrolite is developed for and by the geochemistry community. Contributions to the project are encouraged, and contributions of all forms are welcomed (e.g. code, documentation, bug reports and feature requests). Contributors to the project are recognised in the project contributors list.

pyrolite has an online community forum (gitter.im/pyrolite/community), and we're happy to help you get up and running, answer questions and help with troubleshooting.

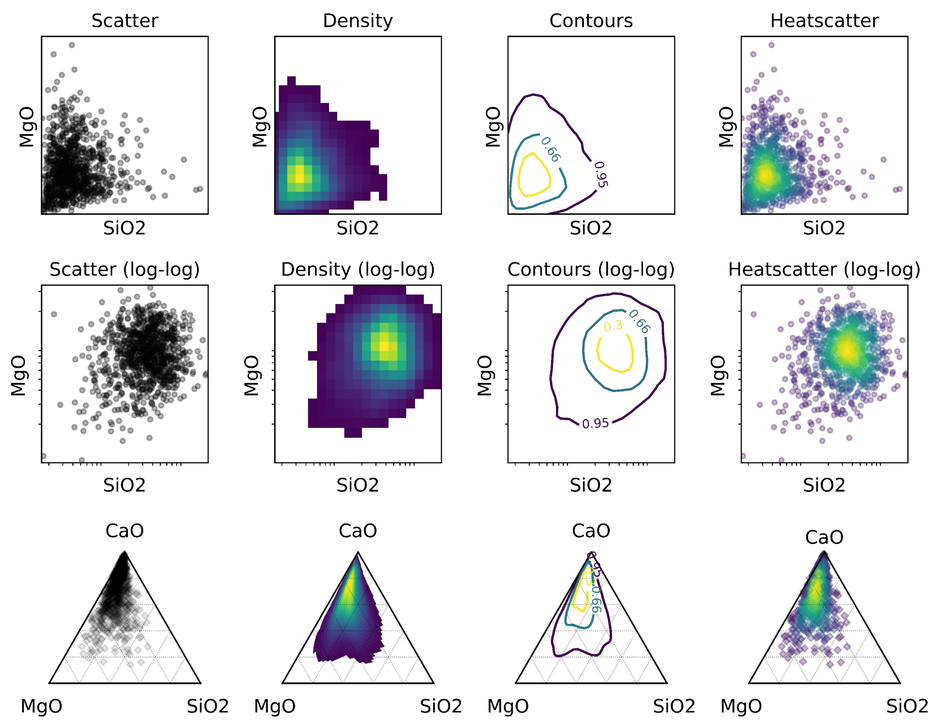


Figure 1: Comparison of various methods for visualising geochemical point data using pyrolite, highlighting different methods to visualise data density. Synthetic data generated using pyrolite.

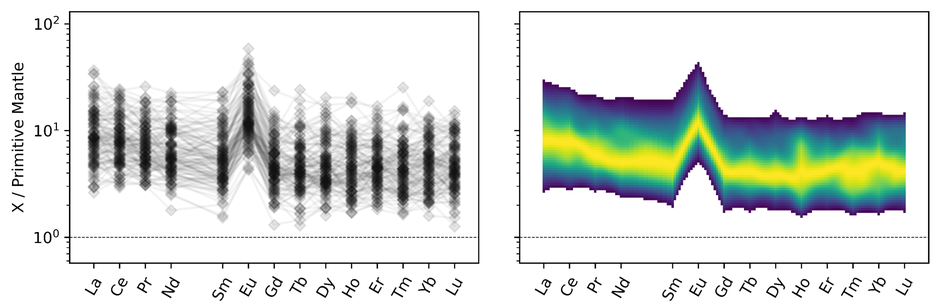


Figure 2: Examples of a simple pyrolite spiderplot and conditional kernel density spiderplot for a synthetic compositional distribution dataset derived from EMORB[9] (with the addition of a synthetic Eu anomaly), normalised to Primitive Mantle[10].

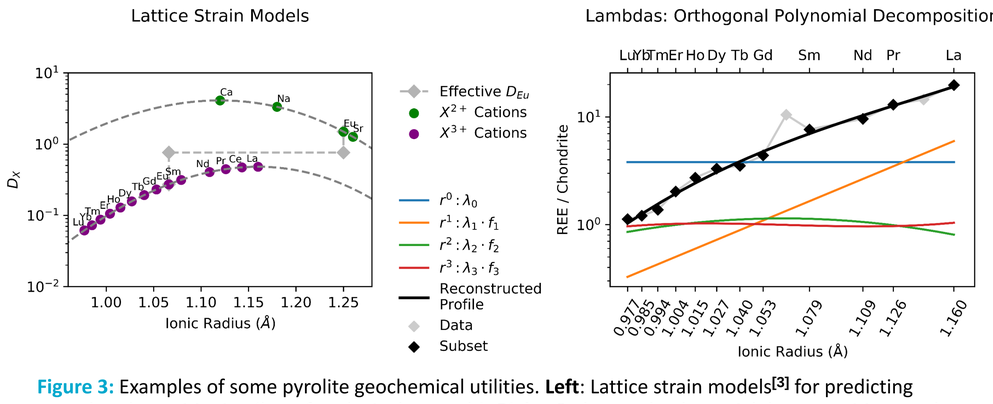


Figure 3: Examples of some pyrolite geochemical utilities. **Left**: Lattice strain models[3] for predicting crystal-melt partitioning (here for plagioclase-melt). **Right**: Orthogonal polynomial decomposition used to parameterise REE profile data using polynomial weights (or 'lambdas'[11]), which can be effectively used to quantitatively compare REE profile 'shapes'.

REFERENCES

[1] Hunter, J.D., 2007. Matplotlib: A 2D Graphics Environment. Comput. Sci. Eng. 9, 90–95. doi.org/10.1109/MCSE.2007.55 **[2]** Wes McKinney, 2010. Data structures for statistical computing in python, in: van der Walt, S., Jarrod Millman (Eds.), Proceedings of the 9th Python in Science Conference. pp. 51–56. **[3]** Blundy, J., Wood, B., 2003. Partitioning of trace elements between crystals and melts. Earth and Planetary Science Letters 210, 383–397. doi.org/10.1016/S0012-821X(03)00129-8 **[4]** Le Bas, M.J., Le Maitre, R.W., Woolley, A.R., 1992. The construction of the Total Alkali-Silica chemical classification of volcanic rocks. Mineralogy and Petrology 46, 1–22. doi.org/10.1007/BF01160698 **[5]** Pearce, J.A., 2008. Geochemical fingerprinting of oceanic basalts with applications to ophiolite classification and the search for Archean oceanic crust. Lithos 100, 14–48. doi.org/10.1016/j.lithos.2007.06.016 **[6]** Pedregosa, F., Varoquaux, G., Gramfort, A., Michel, V., Thirion, B., Grisel, O., Blondel, M., Prettenhofer, P., Weiss, R., Dubourg, V., Vanderplas, J., Passos, A., Cournapeau, D., Brucher, M., Perrot, M., Duchesnay, É., 2011. Scikit-learn: Machine Learning in Python. Journal of Machine Learning Research 12, 2825–2830. **[7]** Smith, P.M., Asimow, P.D., 2005. Adiabat_1ph: A new public front-end to the MELTS, pMELTS, and pHMELTS models. Geochemistry, Geophysics, Geosystems 6. doi.org/10.1029/2004GC000816 **[8]** Lehnert, K., Su, Y., Langmuir, C.H., Sarbas, B., Nohl, U., 2000. A global geochemical database structure for rocks. Geochemistry, Geophysics, Geosystems 1. doi.org/10.1029/1999GC000026 **[9]** Sun, S., McDonough, W.F., 1989. Chemical and isotopic systematics of oceanic basalts: implications for mantle composition and processes. Geological Society, London, Special Publications 42, 313–345. doi.org/10.1144/GSL.SP.1989.042.01.19 **[10]** Palme, H., O'Neill, H.St.C., 2014. Cosmochemical Estimates of Mantle Composition. Treatise on Geochemistry (Second Edition) 3, 1–39. doi.org/10.1016/B978-0-08-095975-7.00201-1 **[11]** O'Neill, H.S.C., 2016. The Smoothness and Shapes of Chondrite-normalized Rare Earth Element Patterns in Basalts. J Petrology 57, 1463–1508. doi.org/10.1093/petrology/egw047