PROJECT TITLE: Integrating Machine Learning into Spectroscopic Data Analysis for Environmental Research

University of Bristol Theme: Data and Digitalisation
Research Group(s): Marine and Terrestrial Environments (MATES)
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Funder: University of Bristol Scholarship

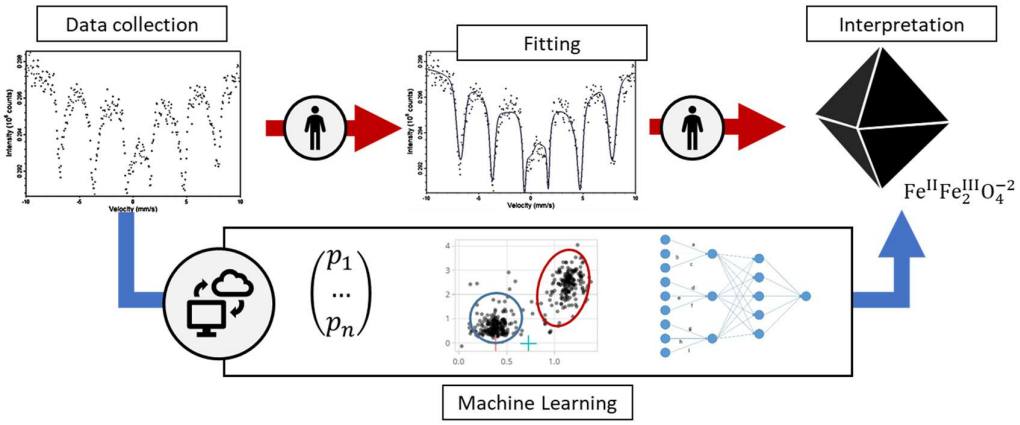

Figure 1 – The traditional data analysis pipeline (red) requires manual data fitting, followed by interpretation supported by personal knowledge. In contrast, using supervised and unsupervised machine learning methods (blue) supported by databases will enable automated, impartial, replicable analysis.

Project Background

The continuing and growing relevance of earth and environmental sciences is resulting in an explosion of experimental data. Analysis of this data seeks to address specific environmental questions, such as how soil bacteria are connected to the release of greenhouse gases, or how changes in geochemistry influences the release of pollutants into drinking water. Accumulation of this information raises challenging questions about how to efficiently store, analyse, and share the data especially in the era of open science. Spectroscopy data is often analysed manually, with domain expertise used to interpret and eventually publish results. This approach works for specialists or experienced researchers; however, it creates an invisible barrier to new adopters or more general users such as those working in multidisciplinary contexts. To overcome this barrier and advocate for an open culture in data analysis, this project will focus on implementing machine learning to provide semi- and fully automated fitting routines for spectroscopic data, especially focusing on those data which are relevant to environmental sciences.

Project Aims and Methods

This cutting-edge project will deliver a framework to accelerate the analysis and interpretation of data via a combination of supervised and unsupervised machine learning methods. The outcome will then be incorporated into a larger web-based platform which will make data analysis available to researchers across the world. This work will focus on three key aspects: (a) automated data interpretation tools to assist with analysis; (b) validation of the concept through analysis of complex environmental samples as part of a case study; (c) simplification of learning approaches used for spectral analysis to encourage more widespread uptake of different techniques. The project will initially focus on just a few techniques, including Moessbauer spectroscopy and X-ray diffraction, but will be expanded into a range of analytical methods. The resulting platform will thus cater to a range of research fields, including (bio)geochemistry, geophysics, paleomagnetism, geomicrobiology, and astrobiology amongst countless others.

Candidate

This project would be well suited to a student with a passion for combining mathematical thinking with real world applications. A strong numerical background in either chemistry, physics, statistical, environmental, or another Earth Science related field (preferably to MSc-level) would be preferred. Highly motivated multi-disciplinary students from other backgrounds will also be considered. The work will provide the student with the opportunity to plan and design their models, develop their computational skillset, in addition to experimental work collecting data with state-of-the-art instruments such as at a UK based or international synchrotron. They will work under the guidance of the supervisory team, and give presentations in group seminars and at conferences, as well as write publications together with supervisors. The PhD student will attend training workshops to learn new techniques where appropriate. We welcome and encourage student applications from under-represented groups. We value a diverse research environment.

Training

The student will be trained in relevant techniques including advanced Python, statistical methods, machine learning, and data-app development. Collaborating with the supervisory team, the student will gain paper-writing and science-communication skills. The candidate will also be given the opportunity to collect data on their own samples and use different advanced analytical techniques for which they will receive appropriate training. They will be encouraged to participate in external training courses and be able to access opportunities from Bristol such as lectures within BSc/MSc courses. Funding is provided for the student to present their research at high-profile international conferences and will be encouraged to apply for grants that support further travel opportunities.

Background reading and references

Byrne, J.M. MinSight – a new concept for fitting and interpreting Mössbauer spectroscopy data. *Interactions* **246**, 111 (2025). https://doi.org/10.1007/s10751-025-02331-7

Useful links

https://www.bristol.ac.uk/earthsciences/postgraduate/
https://www.bristol.ac.uk/science-engineering/postgraduate-research/pgr-scholarships/
https://www.bristol.ac.uk/directory/visas/student-visa/apply/money
https://www.minsight.org

Eligibility

UK and International students are eligible for University of Bristol Postgraduate Research Scholarships. These are funded for 4 years and cover university fees, living expenses at the UKRI standard rate, and an allowance towards research expenses. Scholarships do not cover visa or NHS surcharge costs. See links above for details.

Application

During application select "**University of Bristol Scholarship**" for funding source and "**Geology (PhD)**" for programme. If you are applying this specific project upload this PDF as the "research statement". All studentships must have a September 2026 start date.