MONASH
ENGINEERING

MONASH University

Faculty of Engineering
Summer Research Program 2024-2025

Project Title: Bring machine intelligence to materials characterisation

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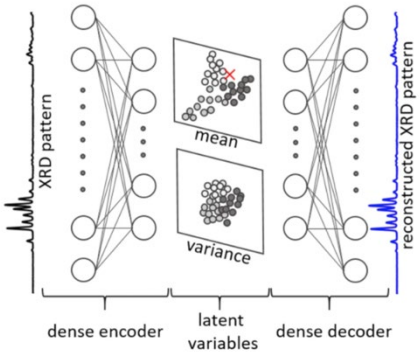
https://www.monash.edu/engineering/departments/materials/about-us/our-people/academic-staff

Objective

Materials characterisation is essential for humans to understand nature, optimise existing materials, and design new materials in a sustainable way. Monash University is a national leader in materials characterisation. The university boasts one of the largest investments in characterisation infrastructure. Monash has a growing focus on real-time characterisation to address critical issues in our generation, e.g. energy, transport, mining, health, and more. We are approaching a stage where our characterisation infrastructure will generate vast amounts of data that human intelligence alone cannot fully analyse. Therefore, we need machine intelligence to augment our capabilities. We invite engineering students to join this initiative, integrating machine intelligence into the materials characterisation workflow and exploring future possibilities together.



Project Details

The student will work with synthetic data of X-ray diffraction patterns generated using a Rietveld analysis program called TOPAS. The students are expected to develop a neural network-based machine learning algorithm using the synthetic data as input to predict the phase fractions as output. The algorithm will then be used to analyse real experimental X-ray diffraction patterns from the Powder Diffraction Round Robin on Quantitative Phase Analysis. We will start by exploring relatively simple convolutional neural networks for the basic classification of different phases. If time allows, we will progress towards more advanced models, such as generative models (e.g., diffusion models). Benchmarking and verification are key aspects of this project. Ultimately, we aim to create a demonstration to show that a carefully developed machine-learning workflow can outperform human analysis.

Prerequisites

- We encourage all students motivated by this project description to apply. The ideal student for this project will need a mixture of expertise in materials science and data science.
- Students with experience in Python programming or other object-oriented programming language, and knowledge of machine learning frameworks (e.g., TensorFlow or PyTorch), will find it easier to get started on the project. A key benefit of this project is that we will provide a subscription to GPT-4 for the year to help the team quickly flatten the learning curve. Students with a good understanding of materials characterisation techniques will easily grasp the materials science aspects.

Additional Information

Please email Dr. Yuxiang Wu (yuxiang.wu@monash.edu) for more details before applying. In your email, please explain (within 200 words): Why this project interests you? Which past experiences/knowledge prepare you for success in this project? Describe a scenario where you solved a hard problem from scratch?