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Enhancing Neutron Scattering Experimentation: A Data Science and Machine Learning Approach to Predict Background Scattering

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In the field of neutron scattering experimentation, the use of complicated sample environments containing strong magnets introduces significant challenges. The inclusion of substantial material within the experimental structure is necessary in order to withstand the large magnetic forces, which eventually influences the experimental outcome through events of multiple neutron scattering. This project leverages data science and machine learning techniques to investigate and predict background scattering due to multiple scattering that takes place in the complex sample environment.

Utilizing the McStas neutron ray-trace simulation package, a detailed model of the 15 T magnet for the BIFROST spectrometer at the European Spallation Source (ESS) was developed. The model was parameterised to cover different experiment setups with a number of simulation parameters, generating a substantial amount of simulation results. A comprehensive database of 24000 simulation results was constructed, and analysed to uncover underlying patterns and relationships between the experimental setup parameters and the observed background scattering. Subsequently, machine learning models were trained, fine-tuned and tested, and their predictive accuracy was assessed.

This project contributes to the field of neutron scattering by providing a novel approach to addressing the challenges of background prediction due to multiple scattering in complex sample environments and can serve as an introduction to a new method of background recognition, paving the way for the development of automated background prediction tools that can be used within a wide range of instruments, with combinations of simulated and experimental data in the future. It also exemplifies the potential of data science in advancing experimental physics.

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