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Generative machine learning for scattering and spectroscopy data analysis

Monday 8 April 2024 14:30 (30 minutes)

Supervised machine learning (ML) models are frequently trained on large datasets of physics-based simulations with the aim of being applied for experimental scattering or spectroscopy data analysis. However, ML models trained on simulated data often struggle to perform on experimental data. Two primary challenges are handling data from structures not present in the training database and accounting for experimental data that contains signals not included in the simulated data.

Generative ML can be used to address both challenges by learning the underlying distribution of the data. I will discuss how we use generative ML to solve mono-metallic nanoparticles given pair distribution function data previously unseen by the model and how generative ML can be used to convert a simulated inelastic neutron scattering dataset into one that resembles an experiment, and vice versa.

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