Automating SAXS Curve Fitting with Machine Learning: A Scalable Workflow for Nanoscale Structural Analysis

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Small-angle X-ray scattering (SAXS) is a technique used for the characterization of materials at the nanoscale. However, analyzing SAXS data can be time-consuming, particularly when fitting models over large data sets. In this research, I aim to explore the use of machine learning to automate and improve the fitting and interpretation of our SAXS data, thereby reducing workload and potentially predicting outcomes. I used the libraries SciPy for data analysis, such as nonlinear curve fitting and baseline subtraction, and then followed it with PyTorch for predictive modeling based on past measurements. The workflow included training neural networks on experimental SAXS curves, then applying models and past results to predict material parameters such as radius of gyration or Porod's law. The predictive models achieved high accuracy ($R^2 > 0.9$). My analysis demonstrates that neural networks, along with SciPy, can accurately fit SAXS data and even understand data it hasn’t seen yet. This project highlights a scalable approach to SAXS data reduction and interpretation, with future work on improving the model and building a standalone analysis program, as well as exploring physics-informed loss functions and ensemble learning for robustness.