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Feature Engineering for Small Angle Scattering ML/AI YUKE WANG, None, TYLER MARTIN, National Institute of Standards and Technology — Small-angle neutron scattering (SANS) is used to measure the thermodynamic and structural properties of materials. In SANS, a neutron beam interacts with a material and produces a scattering pattern depending on the nanostructure of the material. However, finding correlations between scattering patterns and material properties is difficult as the patterns produced are often similar and obfuscated by noise. Machine learning offer the promise of revolutionizing scientific data tasks, including analysis of scattering data. Unfortunately, due to the cost and slow acquisition time from SANS measurements limited data was available. Therefore, some of the most powerful ML techniques (deep learning) was not feasible and training traditional classifiers on the raw data resulted in low accuracy. The goal of this project was to engineer feature inputs for ML algorithms to extract information from small SANS datasets. The feature creation methods considered were manual feature engineering, and transfer learning. By comparing and combining physics based engineered features and learned features from simulations, a protocol was developed for building robust scattering classifiers and regressors. This project was contributing to a larger effort by NIST to develop a ML toolset to partially automate the process of analyzing/interpreting SANS data.

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