NRDAA: A Machine Learning Algorithm for Fitting Neutron Reflectometry Data

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Neutron reflectometry is a useful technique to analyze the structure of thin films, but the current methods for fitting models to experimental data are time consuming and require significant knowledge of the sample. A thin film sample might have multiple layers, varying thicknesses and chemical compositions, which are the parameters needed to fit experimental data. A machine learning algorithm, Neutron Reflectometry Data Analysis Algorithm (NRDAA), was created to fit neutron reflectometry data by finding and optimizing parameter values. First, NRDAA utilizes weighted k-Nearest Neighbor to rank model types. Then, for a given model, Stochastic Gradient Descent optimizes the individual parameters. Finally, , NRDAA calculates the accuracy of the optimized parameters with sensitivity analysis. NRDAA was incorporated into a graphical user interface (GUI) to provide a user friendly platform. The GUI allows users to easily customize parameters based on their knowledge of the sample. NRDAA was tested with three samples of real neutron reflectometry data to verify its efficacy. NRDAA allows a user with minimal knowledge of their thin film sample to quickly fit experimental neutron reflectometry data.

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