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Reflectorch: A machine learning application for reflectometry data analysis

We present a machine learning approach for automatized analysis of X-ray (XRR) and neutron reflectivity (NR) data that. The method utilizes prior knowledge to regularize the training process over larger parameter spaces. [1-2] We demonstrate the effectiveness of our method in various scenarios, including multilayer structures with box model parametrization and a physics-inspired special parametrization of the scattering length density profile for a multilayer structure. In contrast to previous methods, our approach scales favorably when increasing the complexity of the inverse problem, working properly even for a several layer multilayer model and an N-layer periodic multilayer model with up to 20 open parameters. We will also discuss autonomous experiments enabled by machine-learning-based online data analysis in synchrotron beamline environments. [3]

[1] V. Munteanu, V. Starostin, A. Greco, L. Pithan, A. Gerlach, A. Hinderhofer, S. Kowarik, F. Schreiber, Neural network analysis of neutron and X-ray reflectivity data incorporating prior knowledge
J. Appl. Cryst. 57 (2024) 456

[2] V. Starostin, M. Dax, A. Gerlach, A. Hinderhofer, Á. Tejero-Cantero, F. Schreiber, Fast and reliable probabilistic reflectometry inversion with prior-amortized neural posterior estimation
Sci. Adv. (2025), in print

[3] L. Pithan, V. Starostin, D. Marecek, L. Petersdorf, C. Völter, V. Munteanu, M. Jankowski, O. Konovalov, A. Gerlach, A. Hinderhofer, B. Murphy, S. Kowarik, F. Schreiber, Closing the loop: Autonomous experiments enabled by machine-learning-based online data analysis in synchrotron beamline environments
J. Synchrotron Rad. 30 (2023) 1064

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