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ML-based online analysis and autonomous closed-loop experiments at synchrotron beamlines: A case study in x-ray reflectometry

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Modern synchrotron beamlines and neutron instruments have undergone significant changes due to technological advances and newly deployed infrastructure. Thus, experiments are becoming more data-intensive and data-driven and increasingly relying on online data analysis for efficient use of experimental resources. In this regard machine-learning (ML) based approaches of specific importance for real-time decision-making based on online data analysis and connected closed loop feedback applications.

Following recent advances in ML-based analysis of x-ray reflectometry we present both the underlying ML models and concepts as well as the integration into closed loop operation in experiments.

Specifically, we present an approach that incorporates prior knowledge to regularize the training process across broader parameter spaces. This method proves effective in diverse scenarios relying on physics-inspired parameterization of the scattering length density profiles. By integrating prior knowledge, we enhance training dynamics and address the underdetermined (or "ill-posed") nature of the problem. We show that our approach scales well with increasing inverse problem complexity, performing efficiently for an N-layer periodic multilayer model with up to 17 open parameters.

Pithan et al., J. Synchrotron Rad. (2023). 30, 1064
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