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Interpretable Machine Learning at the European XFEL

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The success of experiments at large scale photon sources is strongly connected with the quality of collected data and the information available to scientists during the beamtime. Similarly, streamlined and automated operation of the facility can minimize inefficiencies, thereby boosting the scientific outcome.

The key strategic goal of the Machine Learning program at the European XFEL is to empower scientists through strict information quality control and easily explainable metrics. Each application developed provides a reliability estimate, either through the usage of carefully estimated uncertainties or test statistics designed to verify the trustworthiness of the results. Additionally, the choice of algorithm is guided by a scientific methodology applicable to the situation at hand. The deployment of such methods takes advantage of Karabo, the control system at the European XFEL, which offers a unified point of entry for scientists to monitor and steer the instruments.

In this presentation, we introduce selected applications resulting from the program. We use Bayesian optimization to tune analysis parameters online for serial femtosecond crystallography, based on scientifically relevant metrics. A similar procedure exploits information theory for the automated multi-modular geometry optimization. Another activity exploits machine learning to automate and enhance X-ray spectral diagnostics. Furthermore, a self-supervised approach is used to automatically characterize collected data, so as to highlight interesting data samples. A final contribution includes the research of predictive maintenance methods to identify faults early and react fast, with the aim of preventing a cascade failure and maximizing beamtime efficiency.

The Machine Learning program at the EuXFEL aims to streamline and automate operation of the facility to minimize inefficiencies and boost scientific outcome, and it has been established as a key asset at the European XFEL. Its successful implementation can only be achieved through a strategy of open communication of methods and quality control.

Primary Keyword

bayesian optimization

Secondary Keyword

uncertainty quantification for ML

Tertiary Keyword

failure prediction

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