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Integrating Machine Learning into X-ray Data Analysis: Insights from GRADES at SOLEIL

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In this paper, we present the GRADES team's exploration and implementation of machine learning (ML) techniques at the SOLEIL synchrotron radiation facility in Saclay. Our work encompasses three distinct use cases, each demonstrating the potential of ML to revolutionize data analysis in large-scale photon facilities.

Firstly, we detail the development of an X-ray diffractogram classification tool, which employs ML algorithms to quickly determine lattice types and space groups, thereby enabling faster and high throughput material analysis.

Secondly, we explore the application of large language models in creating an assistant app designed to streamline the management and utilization of SOLEIL's extensive documentation stored in Confluence, JIRA, logbooks, and our experiment databases. This tool aims to significantly improve accessibility and user interaction with critical data.

Lastly, we delve into the use of neural networks for the denoising of spectral images, specifically in the context of Angle-resolved photoemission spectroscopy (ARPES). Our approach demonstrates notable improvements in spectral image quality.

Collectively, these case studies highlight the versatility of ML in various aspects of synchrotron data analysis. We deliver our applications to all our users through our remote data treatment service "DARTS" [1,2].

[1] https://gitlab.com/soleil-data-treatment/soleil-software-projects/remote-desktop/
[2] https://doi.org/10.21105/joss.05562

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