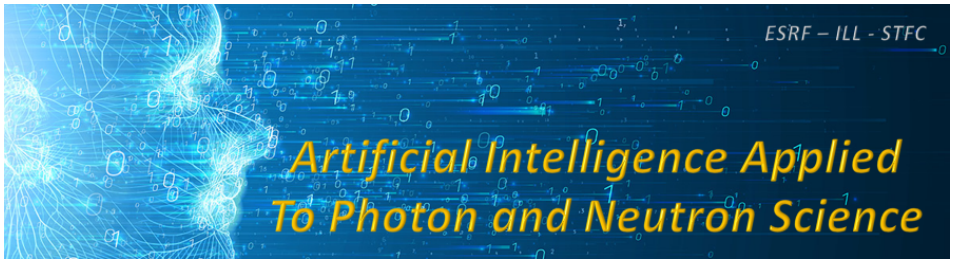

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Machine learning and artificial intelligence in MX

Tuesday, 12 November 2019 17:40 (25 minutes)

In recent years, large-scale facilities such as synchrotrons have encountered a steep increase in demand for computational resources. This is mainly due to very large data rates and volumes and a growing interest by users in real-time feedback during an experiment. Additionally, using X-ray crystallography has gradually become a standard laboratory method rather than a scientific discipline and users now are rarely highly trained experts in the field. Therefore, providing a high-performance computing environment in combination with machine learning applications offers a great opportunity to support and assist users at various key stages during their diffraction experiment.
A series of classification tools has been developed to assist beamline users during decision making when collecting and assessing their X-ray diffraction data. A database, METRIX, was created to hold a default set of training data which is used to train standard base classifiers located at key decision-making steps based on data processing and model statistics. They help the user assess the chances for experimental phasing success and whether a resulting electron density map is of sufficient quality to attempt model building.
The current focus is on data processing and experimental phasing only, but implementations are underway to include data collection and beamline details as well as molecular replacement. Furthermore, including results of other prediction tools, e.g. for secondary structure and contacts, has been considered.

Presenter: Dr VOLLMAR, Melanie (Diamond Light Source)

Session Classification: Afternoon 2