MS35 Artificial intelligence in photon and neutron crystallography, data mining, machine learning

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Improve neutron measurements performances with AI and machine learning

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Abstract

Artificial Intelligence and machine learning are, nowadays, powerful methods to increase the performances of neutron scattering experiments, both in terms of data collection strategy and in instrument parameters optimization. In the present talk we will present two different use-cases covering both aspects. Small Angle Neutron Scattering (SANS) is a growing technique especially in biology and it is characterized by short measuring time and, therefore, high throughput of samples per experiment. This high-volume data contains rich scientific information about structure and dynamics of materials under investigation. Deep learning could help researchers better understand the link between experimental data and materials properties. We applied deep learning techniques to evaluate the quality of experimental neutron scattering images [1], which can be influenced by instrument configuration, sample and sample environment parameters. Sample structure can be deduced on-the-fly during data collection that can be therefore optimised. The neural network model can predict the experimental parameters to properly setup the instrument and derive the best measurement strategy. A three-axis neutron spectrometer represent the opposite situation in terms of quantity of collected data although an experiment last typically several days. With the aim to optimize the beam-time usage, it is therefore very important to concentrate the data acquisition in those regions of the reciprocal space where a maximum of information on our physical system can be acquired. Autonomous data acquisition becomes increasingly important for the execution and analysis of ever more complex experiments. In autonomous learning, algorithms learn from a comparatively little amount of input data and decide themselves on the next steps to take in a closed-loop. We have performed a series of experiments fully driven by the computer without any human intervention. The used algorithm was able to explore the reciprocal space and fully reconstruct the signal without any prior knowledge of the physics case under study. Thanks to autonomous learning gpCAM [2], developed by Marcus Noack of the CAMERA team at Berkeley Lab, estimates the posterior mean and covariance and uses them in a function optimization to calculate the optimal next measurement point. The posterior is based on a prior Gaussian probability density function, which is repeatedly retrained on previously measured points. The main advantage of such an approach is clearly the possibility to drastically reduce the number of measurements with respect to a classical grid scan (i.e. const- Q, const-E scans) and therefore optimize the beam-time usage [3]. In this talk we will compare these new experimental approaches and compare them to traditional data acquisition. We try to show a perspective of the future possibilities and howthe scientific measurements could evolve in conjunction with modern algorithms.

References

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