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Active-learning assisted neutron spectroscopy: challenges and perspectives

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Neutron three-axis spectrometers (TAS) provide the opportunity to model lattice dynamics and magnetic interactions by measuring the energy loss of neutron while interacting with material, and applying physical knowledge on the results. In result, the forces forming chemical structures, the origin of magnetic order and the reasons for hybridized excitation modes can be determined qualitatively and quantitatively.

While the technique kept its importance for more than 70 years, it suffers from being expensive and slow, and the very limited availability of beamtime. Therefore, usage of modern techniques is requested to increase efficiency and make better use of given beamtime. Multiplexing is an opportunity for some kinds of experiments, pre-experiment simulations could improve searching strategies (on digital twins as well as theoretical calculations), and the use of advanced computing methods provides alternative experimental strategies.

An active-learning approach based on log-Gaussian process regression was successfully developed for TAS mapping mode measurements (ARIANE, see Nat. Comm. (2023) 14:2246). Here we present our approach and discuss challenges we need to address and perspectives for further developments.

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