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Autonomous experiments in neutron scattering

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We investigate new concepts for enhancing the data acquisition efficiency of scanning type instruments exploring a multidimensional feature space. We test machine-learning algorithms and probabilistic methods in order to minimize the number of experimental data points, which are required to determine models and model parameters down to precisions defined by the scientists. Data acquisition, interpretation and modeling are part of a closed loop, typical of the concept of Autonomous Experimentation [1]. This approach is opposite to data-driven methods [1], which try to maximize the amount of experimental data and to extract data patterns and physical information with the help of neural networks or similar AI techniques.

Taking classic triple-axis spectrometers (TAS) as representative for scanning type instruments, we develop data acquisition strategies on TAS to explore a scattering function S(Q,⍰) in a four-dimensional feature space, spanned by the momentum space, Q, and the neutron energy transfer axis, $\hbar\omega$. In the context of experimental design, each invested measuring point reduces the initially available experimental budget, i.e. the total available measuring time, which has to be carefully balanced against the gain of information from this measurement. At present the ubiquitous data acquisition method in TAS experiments is grid scanning (so-called const-Q or const-E-scans). However, we were recently able to show that a non-parametric algorithm like Gaussian Process Regression (GPR) has the potential to steer information more efficiently [2-4]. Based on these recent advances, we anticipate a further gain in efficiency by replacing model-independent strategies (as GPR) with physics informed machine learning. This discipline is very recent and rapidly progressing in various domains of science, where sparse data are combined with machine-learning techniques [5]. Policies need to be worked out in order to locate those points in the feature space which have the highest impact on the differentiation of possible available models and which lead to the fastest convergence in the model parameter space.

References

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