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Gaussian processes regression for preliminary data evaluation at DNS

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DNS is a polarised diffuse neutron scattering instrument with a time-of-flight inelastic scattering option at MLZ. DNS is particularly useful and powerful for unraveling momentum-, energy-, and neutron-polarisation resolved magnetic correlations in complex magnetic materials and exotic quantum magnets.

The crucial part of DNS data processing workflow is *data reduction*, e.g. correction of the collected data by various experimental artifacts caused by the instrument itself or its environment. This step is necessary for a proper assessment of the measured data and steering the experiment. However, calibration data required to perform the data reduction are not always available at the very beginning of the beam time - the most critical time to define the right setting for a successful neutron experiment.

In our work, we develop a procedure that enables DNS instrument scientists and users to perform a preliminary evaluation of the collected data. This procedure employs a Gaussian processes regression approach to preform a simulation of the calibration data using the set of legacy calibration data collected over the various reactor operation cycles. The simulated data can then be used by the users of the ''DNS Reduction" interface in their preliminary examination of the sample data and, if necessary, adjust some parameters of their experiment during the measurement. Besides being able to use simulated predictions of calibration corrections, the users are also provided with a quantitative estimate of the corresponding uncertainty.

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