A Nuclear Data Evaluation Pipeline for the Fast Neutron Energy Range - using heteroscedastic Gaussian processes to treat model defects

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Abstract: In this paper, we discuss the development of a nuclear data evaluation pipeline, created at Uppsala University. The pipeline focuses on the evaluation of the fast neutron energy range, above the resolved resonances. The evaluation methodology is based on the Levenberg-Marquardt algorithm, a natural extension of the Generalized Least Squares method to non-linear models. The nuclear model code TALYS is combined with relevant experimental data to produce nuclear data evaluations. A strong focus in the development lies on automation and reproducibility to enable rapid testing of new algorithms and modified assumptions. Several novel concepts for nuclear data evaluation methodology are implemented in the pipeline. This includes automated procedures to identify and correct unrecognized sources of uncertainty in experimental data. Additionally, ways to treat model defects using Gaussian processes on energy-dependent model parameters are implemented.

A particular problem in evaluating the neutron-induced reaction cross-section using optical and statistical models, as implemented in TALYS, relates to the intermediate energy range. While TALYS only predicts the smooth average cross-section, experiments reveal unresolved resonance-like structures. We explore ways to treat this type of model defect using heteroscedastic Gaussian processes to automatically determine the distribution of experimental data around an arbitrary, smooth cross-section curve. We will discuss the practical implementation of these concepts in the context of a tentative evaluation of ^{52}Cr neutron-induced reaction cross-sections.