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Surrogate Modeling for Fission Cross Sections, Criticality Studies, and Uncertainty Quantification

ABSTRACT

Computational methods have advanced to the point where, in many cases, the main source of uncertainty in neutronics calculations comes from the underlying Nuclear Data (ND). Assessing the impact of the underlying uncertainties can be a challenging and computationally expensive task. Yet, it is critical to understand how ND affect the predicted behavior of nuclear systems. This is the goal of Uncertainty Quantification (UQ) and Sensitivity Analysis (SA), research areas of great interest to nuclear engineering researchers and practitioners alike. The present study considers the sensitivities of the effective neutron multiplication factor (k_{eff}) to multi-group fission cross sections (XS). Machine Learning (ML) techniques are employed to enable and accelerate UQ research beyond the capabilities of current methods.

Adjoint methods are used to examine the sensitivity of a Quantity of Interest (QoI) to perturbations in a model parameter, such as ND. As in the case of this study, computing the sensitivity of k_{eff} to uncertainty in multigroup XS using the adjoint requires only two neutronics calculations. While the adjoint methods are computationally inexpensive, assumptions are made along the way which do not necessarily hold outside of small XS perturbations. Such classical adjoint sensitivities are based on first-order approximations, and cannot capture the true non-linearity of k_{eff}'s response to uncertain XS values. This leads to inaccuracies when evaluating the uncertainty of k_{eff} over the entire uncertain region of the XS.

This study explores a new approach to UQ and SA using data-driven methods. Advances in ML have shown that regression models are able to capture complex non-linear behavior in systems, exhibiting high accuracy and precision in their predictions. Here, we use ML to train surrogate models that map a realization of a XS to the corresponding k_{eff} for a given criticality problem. Once trained, these models can accurately compute k_{eff} across the full uncertain distribution of the XS.

Realizations of the uncertainty in the XS are constructed by sampling from the cross section's multi-group covariance matrix. These samples form a set of inputs which are representative of the uncertainty in the evaluated data. The k_{eff} corresponding to each sample is then computed using a neutron transport code. This set of (XS, k_{eff}) pairs is then used to train, validate, and test the ML models. Performing this analysis using various critical benchmark experiments, multiple nuclides' fission cross sections, and several ML models, the present study then compares the performance of the ML models to each other and to the adjoint solution as a baseline.

Initial results showing the performance of the ML methods on a test set can be seen in Figure 1. Here, Gaussian Process (GP) regression, Support Vector Machine (SVM) regression, Multivariate Adaptive Regression Splines (MARS), and Artificial Neural Networks (ANNs) are

used as surrogates to map the U-235 fission XS to k_{eff} in the Godiva benchmark. The distribution of predicted k_{eff} values is compared to the true distribution in the test set, with the difference (residual) between the two being plotted below. Each method shows strong performance in capturing the full relationship between the multigroup XS and the system criticality, with some showing a mean absolute error in k_{eff} as low as 2 pcm.

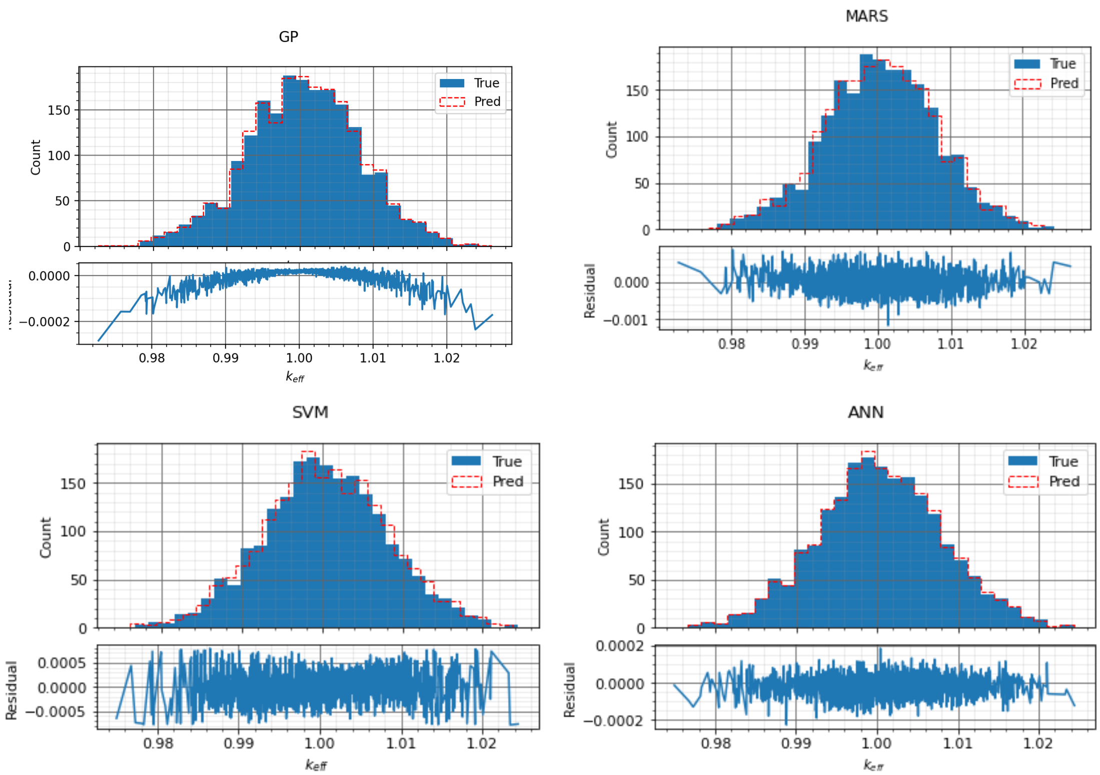

Figure 1. The performance of each regression method for the Godiva problem is shown in the histogram/residual plots above. The models map realizations of the U-235 fission XS to k_{eff}.

This study demonstrates the usefulness of ML in nuclear data applications. Computational costs are often prohibitive in UQ/SA tasks, and perturbation methods designed to avoid these costs involve assumptions which do not always hold true. By building surrogate models which capture the nonlinear relationship between nuclear data and applications such as criticality, UQ and other such studies can be enabled with negligible cost. This study also opens the door to a broad range of future work. Directions for further research include exploring the data requirements for good model performance and implementation of the UQ for more complex QoIs, such as reaction rates, multiphysics effects, and transient system behaviors.