Nuclear data evaluation using machine learning approach - A preliminary effort

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Nuclear data is an intricate collection of information of different properties of the nuclei along with their interactions with other particles, such as neutrons, protons, and photons. It has applications in energy and non-energy domains, however, its acquisition poses a significant challenge. There is a need for a meticulous approach due to the complexities in experiment and the intricacies present in the analysis of the nuclear data.

The traditional Nuclear Data Evaluation (NDE) methods are often complicated and time-consuming. These processes are evaluator-dependent as it requires manual tuning. Hence are prone to uncertainties and bias. By using vast experimental data available in EXFOR [1] in Machine Learning (ML) techniques for NDE could improve cross-section evaluations. In 2021, Vicente et al [2], developed NucML: A Python-toolbox for ML-augmented Nuclear Data Evaluations.

In this work, we attempt to generate neutron-induced reaction cross-section for ^{233}U using NucML and validate them with Jezebel critical assembly benchmark using OpenMC code [3]. NucML provides utilities to download large set of experimental data from EXFOR and Atomic Mass Evaluation (AME) and also convert them to ML-friendly formats, such as CSV, JSON, and HDF5. These large datasets undergo feature engineering and processing which involves filtering essential features and/or adding new features along with necessary transformations like one-hot encoding and normalization. The dataset is split into a training, validation and testing set in the ratio 80-10-10, before applying any feature processing. We use the dataset with the features like, 'Energy', 'Cross-section', 'Z', 'N', 'A', 'MT' (reaction rate index number, see evaluated nuclear data file (ENDF) 102 formats manual [4]), 'Center-of-Mass Flag', 'Element Flag', 'Atomic Mass', 'Nucleus radius', and 'Neutron Nucleus Radius Ratio'.

In this work, we use Random Forest (RF) model, a ensemble learning method that combines multiple decision trees to improve regression accuracy by averaging their predictions. Overfitting is avoided by fine tuning parameters of the model given in Table I. The geometry of the ^{233}U Jezebel critical assembly, fabricated and operated at Los Alamos laboratory, was modelled and the effective multiplication factor, k_{eff}, which determines the neutron density within a critical assembly is calculated using OpenMC particle transportation code. This benchmark is chosen for its simple and nearly mono-isotopic nature, making it an ideal candidate for evaluating nuclear data of ^{233}U. This assembly consists of a bare 16.535kg

Parameters	Range of Values
n_estimators (NE)	[100-500]
max_depth (MD)	[10, 30, 5]
min_samples_split (MSS)	[2, 5, 10]
min_samples_leaf (MSL)	[1, 3, 5]

TABLE I: Parameters for training of RF model

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Isotope	Density (atoms/barn-cm)
^{233}U	4.6712×10^{-2}
^{234}U	5.9026×10^{-4}
^{235}U	1.4281×10^{-5}
^{238}U	2.8561×10^{-4}

TABLE II: Atomic densities of ^{233}U Jezebel Critical Assembly

of ^{233}U metal spherical assembly (5.9838 cm radius and 18.424 g/cm^{3} density) at room temperature having atomic densities as specified in Table II. The International Criticality Safety Benchmark Evaluation Project (ICSBEP) [5] reference to this benchmark is 233U-MET-FAST-001 and its experimental k_{eff} is 1.000±0.001. Note that this benchmark is insensitive to resonance and thermal region data but sensitive to ≈ 100 keV-10 MeV range.

The trained RF models were used to predict nuclear cross sections for reactions such as (n,t), (n,g), (n,n'), (n,el), (n,nonelastic), and (n,f) for the ^{233}U. Predictions of the fission cross section (MT = 18) were compared with the data available in the basic evaluated nuclear data file (ENDF / B- VIII.0) in a compact ENDF (ACE) format, as shown in Figure 1. The bottom panel displays the percentage deviation of the ML model relative to ENDF. The RF model parameters are NE = 300, MD = 25, MSS = 2, and MSL = 1.

The values of k_{eff} calculated using the ^{233}U Jezebel benchmark for RF model and ENDF/B-VIII.0 data are given in Table III. The trained RF model performs well with ^{233}U Jezebel benchmark with a very low **pcm** (per cent mille, 1 pcm = 0.00001 in Δk_{eff}) of 4. The results were obtained with minimal human interventions. To further validate the ML

Library	k_{eff}
ENDF	1.00187 ± 0.00137
RF	1.00004 ± 0.00117

TABLE III: k_{eff} values calculated using Open MC for ENDF/B-VIII.0 and RF model.

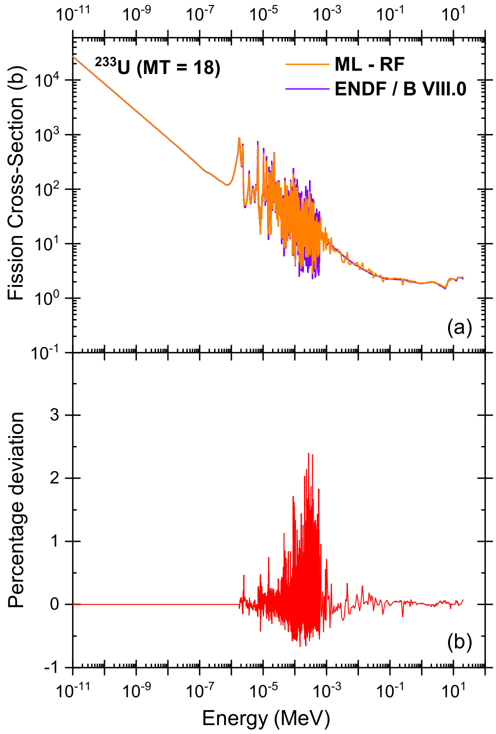

FIG. 1: (a) Comparison of RF model and ENDF/B-VIII.0 fission cross-sections of ^{233}U (b) Percentage deviation RF model relative to ENDF.

model, additional benchmark studies with different features are needed.

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References

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