Study of (n,2n) reaction cross section of fission product based on neural network and decision tree models

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Abstract. The neutron induced nuclear reaction cross sections of fission products are related with the neutron flux and the reactor burnup, which are important for the accurate of nuclear engineering design. To predict the (n,2n) reaction cross section, especially those lack of experimental measurements, we analyzed the relevant features and establish the experimental data set on the basis of sorting out the experimental data recorded in EXFOR library. The back propagation artificial neural network (ANN) and decision tree (DT) models are built to learn the experimental data set, respectively, adopting PyTorch and XGBOOST toolboxes. we report that machine learning models are applied to analysis and predicate (n,2n) reaction cross section.

1 Introduction

The study and understanding of the characteristics of atomic nuclei is the foundation for the development of nuclear energy and technology. Nuclear data involves various properties such as nuclear structure and decay, nuclear reactions and interactions. The design of nuclear reactors require precise nuclear data to ensure the safety and economy. Meanwhile, nuclear data is crucial for improving the accuracy of neutron metrology and the effectiveness of nuclear medicine. In order to meet the demand for nuclear data, both experimental and theoretical research play important roles in providing reliable nuclear data. However, due to the expensive and complex nature of nuclear experimental facilities, as well as the limitations of theoretical models and computational resources, we rely on the nuclear data evaluation for provide complete and accurate nuclear data[1–3].

Nuclear data evaluation is a complex and important process that requires professional researchers to provide complete recommended values through the analysis of experiments, and the establishment of physical models. The latest evaluation techniques have overcome some limitations of traditional methods, such as the assumption of perfect models, linear error propagation, and the normal distribution of uncertainty, making the evaluation results more objective and accurate. Among them, the total Monte Carlo method is an effective method for incorporating the integral benchmarks into the evaluation process. And on the basis of fully

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considering physical constraints, the Bayesian network can provide an automated and visual evaluation tool. In the process of long-term accumulation, the main international evaluation libraries have provided users with a large amount of valuable information and general nuclear data[4–7]. As a representative example, the CENDL-3.2 library provides a complete set of neutron data for 272 materials, and is improved continuously.

On the other hand, theoretical prediction is one of the foundations of nuclear data evaluation[3]. High precision models imply the complexity, which may lead to unreliable extrapolation ability. The current suite of predictive neutron reaction model is only accurate to within approximately 20% for light particle emission channels where a large body of experimental measurements currently exist. While in cases where few data exist, these codes often exhibit discrepancies anywhere within a factor of 2–50. Appropriately, machine learning are driving a significant expansion of the role of computing in nuclear data. For example natural language learning technology may be adopted to extract knowledge from original document. Physics-aware model may provide robust extrapolation of observables. More and more automatic evaluation implement quantifies the amount of the theoretical model defects and measurements discordant.

In this work, we report that machine learning is making progress in the field of nuclear data to predict the nuclear reaction cross section of fission product. We analyzed the relevant features and establish the experimental dataset on the basis of sorting out the experimental data of (n,2n) reaction cross section in EXFOR library. The back propagation artificial neural network (ANN) and decision tree (DT) models are built to learn the experimental data set, respectively, adopting PyTorch and XGBOOST toolboxes. Draw lessons from the Variational Auto-encoder, a network containing 2 sub-networks with the same internal structure, are designed to learn the mean and variance respectively. The results show that both ANN and DT models not only describe the experimental cross sections data well, but also has a certain predictive ability.

2 (n,2n) Cross section dataset

The neutron induced nuclear reaction cross sections of fission products are related with the neutron flux and the reactor burnup. There are numerous kinds of fission products with proton numbers ranging from Z=31 to Z=68, and the complete list includes more than 500 nuclei, of which less than 300 kinds can be found in the current nuclear reaction evaluation libraries. The theoretical predictions for cross section are crucial especially when the neutron-rich unstable nuclei lack of experimental measurements. As the foundation of machine learning, a dataset containing 5294 (n,2n) reaction cross section measurement points was established based on the nuclear reaction experiments database EXFOR. The dataset contains the target nucleus from sodium to bismuth, covering the complete fission product nuclear region.

Data features serve as the building blocks for training machine learning algorithms, so the physical quantities associated with the cross sections are analyzed. The reaction cross section, which is determined by the interaction between the neutron and the target nucleon, varies continuously with the incident neutron energy. For reaction channels with threshold energies, such as the neutron proliferation (n,2n) channel, the cross section always increases first as the incident energy increases and then reach the plateau. Although the cross section shapes of different target nuclei are similar, the value of the cross section is related to the properties of the target nucleus. Firstly, the nucleus is a strongly interacting system that is self-bound, so the nucleon number is the most important property. In general, the greater the nucleon number, the greater the reaction cross section. Secondly, the finite size nuclei exhibit significant shell effects, causing periodic oscillations of the single neutron and single proton separation energies, and the Casten factor. The Casten factor, i.e. the product of the number

of valence neutrons and valence protons, is derived based on the nucleon magic number (2, 8, 20, 28, 50, 82, 126) and is an indicator of collective motion. Finally, the compound nucleus system is in an excited quasi bound state before the particle is emitted, so the cross section is dependent on the energy level density. In summary, the features of the dataset include 8 physical inputs: proton number, mass number, single neutron/proton separation energy, Casten factor, energy level density parameter and pair correction, incident neutron energy.

In order to improve the efficiency of machine learning, generally a uniformly distributed data set is desirable. Unfortunately, the datasets cannot be considered as a uniform distribution. From Figure 1, it can be found that the structural materials nuclei such as copper, nickel, and zirconium have more abundant experimental measurements. At the same time more than half of the incident neutron energies are concentrated near 14 MeV, while measurements are very sparse for regions greater than 20 MeV energies. In addition, there are divergence cross sections coming from different measured results for the same target nucleus and similar incident energies.

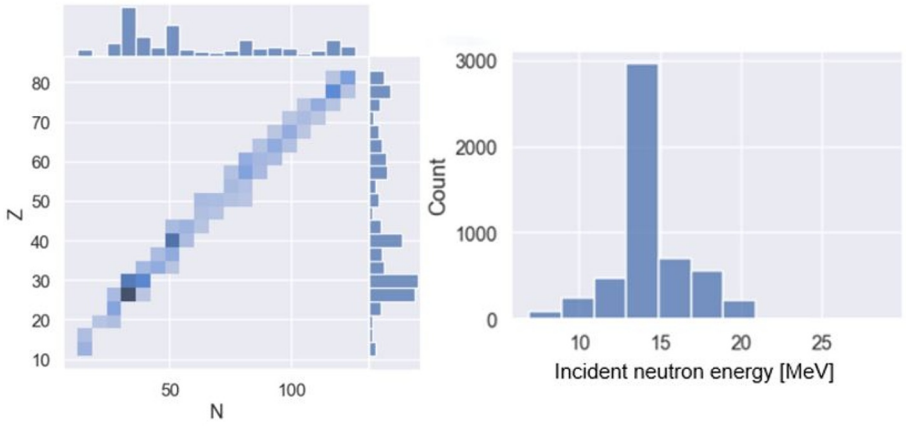

Figure 1. Distribution of measurement points in the dataset with response to mass (left) and incident energy (right).

3 Training of neural network and decision tree models

Artificial neural network (ANN) is a complex network of a large number of simple nodes interconnected, with a capable of complex logical operations and non-linear relation implementations. The goal of the ANN model is to discover the mapping relationship between the features and outputs. This is similar to physical models predicting observables based on parameters, but the structure of the neural network is more complex and ideally capable of simulating any mapping relationship. By adjusting the threshold of the neurons and the weights between the neurons, and selecting an appropriate activation function to account for the non-linear, the loss function of ANN is minimized to get the optimal result.

This work is based on the PyTorch deep learning framework[8] to quickly implement network construction and to learn reaction cross section dataset. After determining the network structure, the training dataset is used to perform training on the model to find network parameters that perform well by adjusting super parameters such as the learning rate. The mean square error MSE of the predicted value to the data set is used as the objective function

for model optimization, then the loss function adopts

$$L(\theta) = \frac{1}{M}\sum_{M}(Y_{out} - Y_{exp})^2. \tag{1}$$

This is the loss function form most commonly used in regression problems. The weight and threshold optimization problems are solved by employing the Adam optimizing algorithm and the error back propagation principle, which mainly includes the feed forward and back processes. At last, the network is verified, which guarantees that it has good prediction ability and can control the over fitting phenomenon. The constructed network includes 2 sub-networks with the same internal structure, which contains 128 neurons in 2 hidden layers. Draw lessons from the Variational Auto-encoder[9], the outputs of sub-network are designed to learn the mean and variance respectively.

$$Y_{out} = Y_1 + e^{Y_2}, \tag{2}$$

where Y_1 and Y_2 indicate the sub-networks. The parameters of the hidden layer are adjusted in turn from the output to the input.

The reasonable hyper-parameter enables good predictive power not only for known data but also for unknown data. The dataset errors given by the loss function are criteria for model selection. In general, the training set error is less than the test set error, and both the error decrease simultaneously as the model complexity increases. But if the training error is too small, far less than the test error, it may indicate that the model is too complex to easily cause overfitting. In this work, the errors of the test set and the training set have a comparable downward trend, and the learning curve remains stable after multiple iterations, indicating that the selected model is reasonable and well trained.

Decision trees are another common class of machine learning algorithms, especially the ensemble tree model represented by the XGBOOST[10], an extreme gradient lifting tree, which plays a major role in processing tabular data. It simulates the process of human decision making, making decisions from the root node depending on data characteristics, constantly making new decisions based on existing decisions until the final decision is made. The model training is divided into two main steps: first, the samples are divided into trees for tree generation, and then the trees are pruned with validation data. For regression problems, the tree model expression is

$$f(x) = \sum_{m=1}^{M} c_m I(x \in R_m), \tag{3}$$

where the regression space is divided into M cells, and the optimal value c_m of each cell is the mean of the outputs. Traverse all the inputs until the optimal variable is found such that the loss function is minimized.

4 Results and discussion

Once machine learning models are trained, they have the ability to reproduce experimental cross section well. Overall the predictions with a mean absolute percentage deviation of less than 10% from the experimental data account for more than 85%. As a example, Fig. 2 shows a comparison of experimental measurements of the ^{23}Na(n,2n) reaction cross-section with evaluation data and machine learning results. Due to the needs of the sodium cooled fast reactor, and the interest in theoretical model research on the transition area from light to medium heavy nuclei, there are many experimental attempt on sodium. From the figure

it can be seen that the results of H. Liskien *etal*. in 1965 and Xu Zhizheng *etal*. in 1991 are significantly larger than other measurements, differing by about 2 times. The ENDF/B-VIII.0 evaluation is closer to these two measurements above, but the other recommended results support lower values. It is obvious that the measurement and evaluation results of the ^{23}Na(n,2n) reaction cross section are divergent. Interestingly, the ANN model predicts the relatively low cross sections.

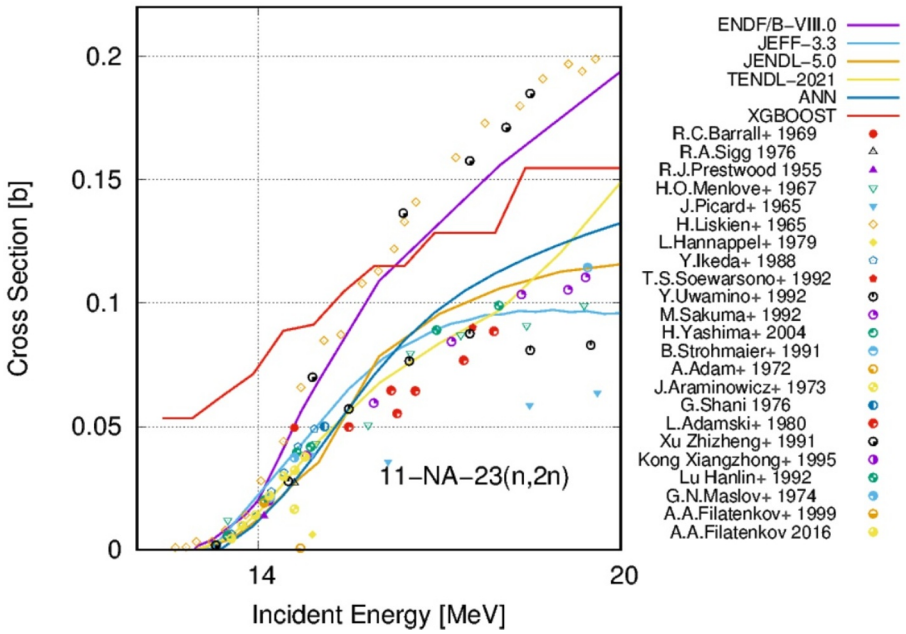

Figure 2. Comparison between machine learning and evaluation data based on experimental measurements of ^{23}Na(n,2n) reaction cross section.

Through analysis of other relevant measurements, discovering potential patterns is a way to solve the data divergence problem. In the case of (n,2n) reaction cross sections, the Levkovskii type formula for systematically describing the cross sections around 14 MeV incident energy of various target nuclei is written as

$$\sigma = r_0^2(A^{1/3} + 1)^2 \exp[3.5(N - Z)/A]. \quad (4)$$

The coefficient before the exponential function denotes the non-elastic cross section. For the light nuclei (Z<30), the cross section is strongly correlated with the isospin asymmetry; For the medium heavy mass nuclei, the isospin dependence of the cross section is weaker. By comparing with a large number of experimental data with neutron incident energies from 14 to 15 MeV, the empirical formula can reproduce most of the cross sections with a factor of 0.5 to 1.5. However, the empirical formula is biased from the experiment near the closed shell and lacks a continuous variation of the cross section with incident neutron energy. Encouragingly, the well trained neural network model greatly improves the prediction ability of the reaction cross section.

The decision tree model not only predicts the cross section, but also ranks the importance of features. According to the entropy increasing principle, the more times a certain feature appears in the decision-making process, the more important the feature is. Fig. 3 shows the

importance score for 8 features in the fission product nuclear (n,2n) reaction cross section dataset. The characteristic importance scores from high to low are nuclear mass number A, energy level density parameter a, single neutron separation energy, incident neutron energy, pair correlation, atomic number Z, single proton separation energy, Casten parameter.

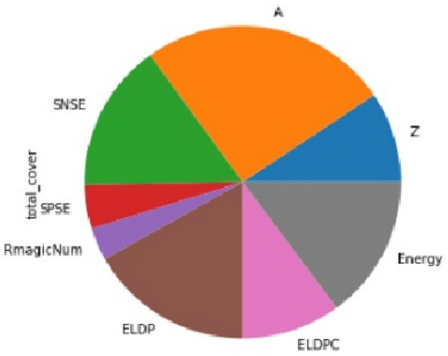

Figure 3. Rank of feature importances based on decision tree model.

Finally we hope more and more experimental measurements in the future, clarifying differences and expanding more nuclei. The activation method provides accurate reaction cross section measurements, but for cases where the half-life of the residual nucleus is too long or short, only direct methods such as measuring the outgoing coincidence neutrons, measuring the recoil of the residual nucleus can be used to determine the cross section. Therefore, the divergence of experimental measurements is promising to be further reduced.

5 Conclusion

Machine learning algorithm provides an alternative to the traditional evaluation methods of nuclear reaction cross section. The outputs indicate that the model can effectively predict the nuclear reaction cross section of a large number of nuclei without the requirement for manual and careful parameter optimization. Machine learning may help evaluator have more time to focus on physical issues. In future we will carry out further work to improve the automation level of nuclear data pipeline.

6 Acknowledge

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