Fission trajectory analysis using ML techniques

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Abstract. This research analyzed trajectories of nuclear fission leading to symmetric or assymmetric mass division, obtained by a four-dimensional Langevin-model, using machine learning models. A hybrid neural network, combining Long Short-Term Memory (LSTM) and Gated Recurrent Unit (GRU), both of which were types of Recurrent Neural Networks (RNN), was utilized to classify whether each Langevin trajectory led to symmetric or asymmetric mass division. It was found that the current model could classify fate of these trajectories before reaching to the final destination (symmetric or assymmetric mode) with an accuracy of over 70%, clearly overestimating the asymmetric data.

1 Introduction

Nuclear fission is a complex phenomenon that produces huge amounts of energy for nuclear power generation for decades. Mechanisms of the nuclear fission has been a hot research topic even though more than eighty years have passed since its discovery due to its complicated nature as a large-amplitude collective motion of a system consisting of finite number of nucleons. A complete understanding of the nuclear fission is difficult because the fission pattern is very sensitive to proton and neutron numbers of fissioning systems. Sometimes, neighboring nuclei in the nuclear chart suddenly show different fission patterns in terms of mass distribution of fission fragments [1]. One good example of such a sudden change can be seen in Fm isotopes.

The dominant fission patterns in nuclear fission among Fm isotopes change from asymmetric to symmetric mass division when the proton and neutron numbers of fission fragments get close to those of the double shell closure, ^{132}Sn. Measured mass distributions of fission fragments of Fm isotopes below ^{256}Fm show two peaks (dominance of the asymmetric mode). In ^{257}Fm, the dominant component is still asymmetric, but a symmetric component is simultaneously observed. At ^{258}Fm, the dominant fission mode suddenly changes to the symmetric one. Then, the symmetric fission is favored towards ^{264}Fm. Our four-dimensional Langevin model can reproduce the continuous and sudden changes in the abovementioned fission modes [2–4], suggesting a strong influence of the shell closure of ^{132}Sn because shape of the heavy fragments turns out to be spherical. Although the four-dimensional Langevin model can explain the nuclear fission of Fm isotopes well, we cannot find any apparent difference in the potential energy surfaces of ^{257}Fm and ^{258}Fm, which affects the Langevin dynamics in a dominant way. Therefore, it is essentially important to understand how the fission process leads the fragment to fall in the symmetric or asymmetric modes driven by a dynamical motion. For such a detailed understanding of dynamics of the nuclear fission, we have analyzed the fission trajectories of our Langevin calculations using a Recurrent Neural Network (RNN) [5]. In this presentation, we will report the common feature in fission trajectories extracted by the RNN.

This study can elucidate unsolved fission mechanisms, such as a predetermining key for each fission mode and the neck radius where the mode freezes. Sudden approximation [6], where the neck rupture suddenly occurs at a finite neck radius, has been applied to fission study as one of the major approaches. The favored neck radius at scission has a considerable ambiguity around 2 fm. A detailed analysis based on the RNN can provide information on the timing when the fission mode freezes. It will provide solid evidence of the reasonable neck radius for the sudden approximation.

2 Computational Methods

2.1 Model

The following describes the machine learning model used in this study. A schematic diagram of the model employed is shown in Figure 1. This model is based on Ref. [7]. As illustrated in Figure 1, data are input into Long Short-Term Memory (LSTM) [8] and its output is then fed into a Gated Recurrent Unit (GRU) [9]. A feature pooling layer is created using the maximum and average values from each of the LSTM and GRU outputs. Finally, a dense layer is introduced with a dropout rate of 10%, which is then connected to the output layer that performs binary classification into either Asymmetry or Symmetry. Scaled Exponential Linear Unit (SELU) [10] is used for the activation

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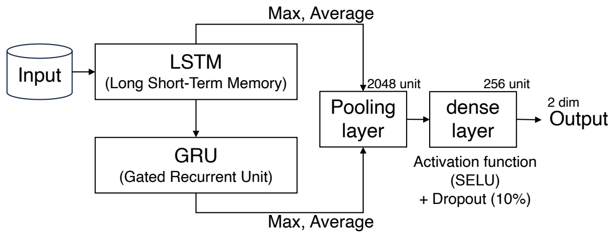

Figure 1. Schematic drawing of the machine learning model.

function of the dense layer. We will implement the above model using the Python library Pytorch [11].

The predictions obtained in Figure 1 are evaluated for their deviation from the correct labels using the Cross-Entropy Error. The Cross-Entropy Error used in the loss function is shown in Equation 1,

$$\text{Loss} = -\sum_{t}\sum_{\text{class}} y^{(t)}_{\text{class}} \log \hat{y}^{(t)}_{\text{class}}\,, \tag{1}$$

where $y^{(t)}_{\text{class}}$ represents the correct data, while $\hat{y}^{(t)}_{\text{class}}$ denotes the predicted output from the model's output layer. In addition, t is the number of data, and class is calculated as binary values, symmetric and asymmetric. The learning process is conducted to minimize the value of Equation 1.

Next, the data used in this study is described. In this research, nuclear fission path data obtained through four-dimensional Langevin calculations are utilized as the training data. Our Langevin model describes a compound nuclear shape with the two-center model [12]. The time evolution of the compound nuclear shape corresponds to the fission path from the initial state to scission on a certain potential surface. In our calculation, the scission is defined as a status with a neck radius of a compound nucleus that becomes zero. Each event features eight variables: the mass asymmetry α, the elongation of the compound nucleus ZZ_0, the deformation of the right fragment δ_{right}, the deformation of the left fragment δ_{left}, and each momentum.

Examples of the Langevin trajectories are shown in the left panel of Figure 2. We can notice that most fission paths stall behind the saddle and show a stochastic behavior for a long time. We can observe the difference in the fission path for symmetric/asymmetric only around $ZZ_0 = 2.0$. However, the fate of the fission might be determined in a much earlier phase of the fission process. Once we successfully make an excellent RNN model to estimate the fission results with enough accuracy, we can examine the condition that fates the fission paths beyond human eyes. Based on such an idea, we have made the RNN model.

The data are labeled according to whether the fission path results in symmetric or asymmetric fission. For the training data, a total of 4000 events, consisting of 1000 events each of symmetric and asymmetric fission paths for ^{236}U and ^{258}Fm, are used. Similarly, for testing purposes, an additional 4000 events without known labels, comprising 1000 events each of symmetric and asymmetric fission paths for ^{236}U and ^{258}Fm, are employed.

2.2 Data preprocessing

The nuclear fission path data obtained from the Langevin calculations vary in the number of steps to fission for each event, making them difficult to handle directly in machine learning. Therefore, by performing the data preprocessing shown below, the data can be made more manageable, and their essential properties can be extracted for analysis. In each event, the segments of 10,000 steps prior to the timestep at which the elongation of the compound nucleus, ZZ_0, becomes 2.0 are extracted. This process allows for the alignment of the length of time series and narrows down to only the ranges that are difficult to classify based on mass asymmetry α.

Figures before and after preprocessing the time series are shown in the left and right panels of Figure 2. Figure 2 plots 30 events each of symmetric and asymmetric fission for ^{236}U. The left figure represents before preprocessing, and the right figure represents after preprocessing. It can be observed that preprocessing enables narrowing down to an extremely short range.

In addition to the aforementioned processing, when inputting data into the machine learning model, standardization is performed for each variable. This means that data with a mean of 0 and a variance of 1 are used as inputs for each variable.

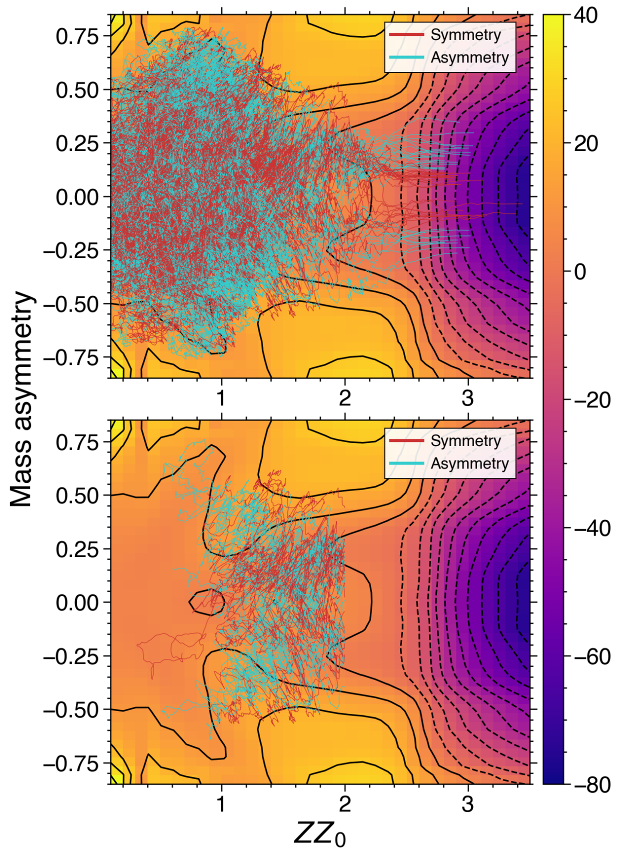

Figure 2. Preprocessing of fission trajectories. The figure shows preprocessed and plotted fission trajectories for 30 events of ^{236}U. The left panel is before preprocessing and the right panel is after preprocessing.

2.3 Evaluation method

In this study, the evaluation method employed is k-Fold Cross Validation. This technique involves dividing the training data into k parts, using $(k-1)$ parts for training and one part for validation. This process is repeated in k patterns, and the average of each pattern's scores is taken as the Cross Validation Mean Score to determine the final accuracy. By evaluating the model's performance with multiple different training datasets through k-Fold Cross Validation, it is possible to prevent overestimating a single result, thereby enhancing the reliability of the outcomes. Furthermore, this approach can also prevent overfitting. In this study, $k = 5$ will be used for learning and evaluation.

3 Results and Discussion

The learning outcomes of the machine learning model are presented below. Figure 3 shows one of the results from the 5-fold Cross Validation. It can be observed that the learning progresses stably without any problems, even as the number of epochs increases. Furthermore, the fact that there is no significant divergence between Train and Valid for both Accuracy and Loss indicates that overfitting has not occurred. The average (Cross Validation Mean Score) and standard deviation of the results from the 5-fold Cross Validation were 70.12% and 0.54%, respectively. From this, it is evident that the current model, variables in the introduced data, and preprocessing achieve a prediction accuracy in the vicinity of 70%, with a variation of approximately 0.54% standard deviation across the models from each of the 5 splits.

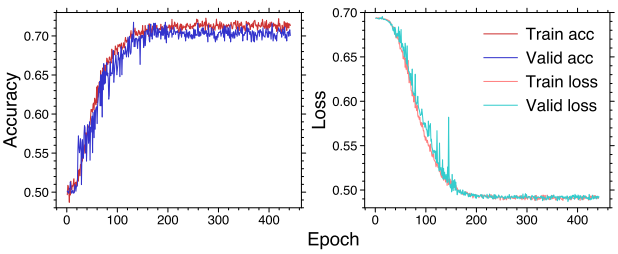

Figure 3. One of the accuracy and loss from the 5-Fold Cross Validation.

Next, the predictions for unknown data are described. The Confusion Matrix of the prediction results for the test data is shown in Table 1. It is evident that asymmetric fission is overestimated by approximately 2.5 times. Since the accuracy of classifying asymmetric fission as asymmetric fission is 91.65%, it becomes clear that predicting symmetric fission is notably challenging. The accuracy for identifying symmetric fission is recorded at 46.10%, which does not significantly differ from the accuracy of purely random classification. Therefore, it can be inferred that the learning process for symmetric fission has not progressed well, suggesting the need for a different approach, such as employing an alternative model or applying weights to the data for symmetric fission. Consequently, it is considered that for ^{236}U and ^{258}Fm, even with $ZZ_0 < 2.0$, asymmetric and symmetric fission possess distinct characteristics.

Table 1. Confusion matrix of predicted results for the test data.

		Prediction label	
		Asymmetry	Symmetry
Actual label	Asymmetry	1833	167
	Symmetry	1078	922
Total		2911	1089

4 Concluding remarks

In this study, we used a hybrid model that combines LSTM and GRU, which are types of RNN, to analyze the four-dimensional Langevin model. We predicted whether a portion of the nuclear fission path would lead to symmetric or asymmetric fission. The results indicated that asymmetric fission, in particular, was overestimated, and predicting symmetric fission was more challenging compared to asymmetric fission. Future work may involve analyzing the features of the machine learning model using feature extraction libraries to elucidate the mechanism of nuclear fission.

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