Learning nuclear mass excess using multi-fidelity deep neural networks

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Introduction

Nuclear mass is a fundamental property of the nucleus, which is directly relevant in extracting nuclear structure information, nuclear effective interactions, nuclear reaction energy in astrophysics etc.[1] Although many nuclear masses have been measured experimentally till date, but predicting these masses based on the theoretical models is difficult due to the inadequate theory for nuclear interactions and quantum many body problem. In recent years great efforts have been made to incorporate prior knowledge in the machine learning algorithms [2]. However very promising field of machine learning is data hungry, which makes it a huge challenge in nuclear physics since high fidelity data (e.g. experimental data) is very sparse and expensive to acquire while low fidelity data (from different sources like empirical models, and microscopic models) is relatively large. In the present study we have tried to overcome such problems by using multi fidelity deep neural networks (MFDNN) [3]. In multi fidelity deep neural networks one tries to leverage from the low fidelity data to train a deep neural network to predict better results for high fidelity neural networks.

Methodology

In this study we have used HFB14 and FRDM predictions for mass excess as low fidelity data and trained a MFDNN on experimental values of mass excess. All the values used in training process were used from RIPL-3 library. A schematic diagram of the neural network architecture used in this study is presented in Fig.1. Number of neutrons (N), number of protons (Z), HFB14 predictions (M1) and FRDM predictions (M2) were used as inputs in the network to learn the experimental data (M). The MFDNN has two parts NNh1 which is a feed forward neural network without an activation function (because it will learn the linear correlations between low and high fidelity data). Other part of the MFDNN is NNh2 which is a feed forward neural network with four hidden layers with 40 neurons each using 'tanh' activation function. The outputs of the NNh1 and NNh2 were combined to give the final output. We have used experimental data (with error < 100 keV) for 1918 nuclei (and their corresponding HFB14 and FRDM predictions) to train the MFDNN. Initial weights and biases were sampled randomly and then used the 'adam' optimizer for 20000 epochs to minimize the loss function. Since the feed forward neural networks are prone to over-fitting therefore L_2 regularisation on NNh2 have been used. A combined loss function presented below was used for the optimisation.

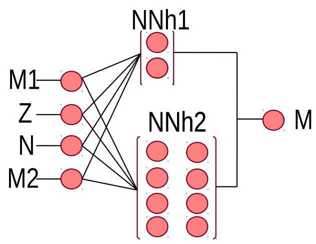

FIG. 1: A schematic representation of the MFDNN.

$$Loss = MSE_M + \lambda \sum \beta_i^2$$

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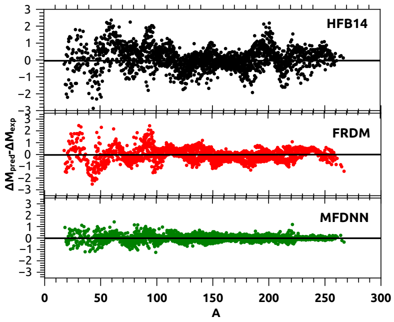

FIG. 2: Difference between predictions of different models and experimental data.

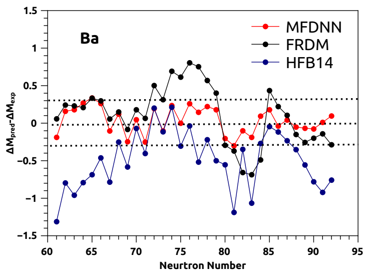

FIG. 3: Comparison of different predictions for isotopes of Ba.

Results

The nuclear mass surface was successfully learned by MFDNN as is clear from Fig.2, where it can be observed that the deviation of the mass excess predictions from experimental data is reduced for MFDNN case in comparison to HFB14 and FRDM. Also the systematic deviation of the theoretical predictions from the experimental results have been learned by present deep neural network. We have also presented the case of Ba isotopes in Fig. 3 and it is clear that MFDNN predictions are better than the HFB14 and FRDM predictions.

We have also predicted mass excess values far from the available experimental data and compared with the HFB14 extrapolations and the results are presented in Fig. 4. It is observed that in the region far from the line

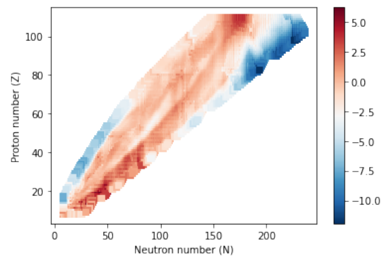

FIG. 4: Difference between the MFDNN predictions and HFB14 data.

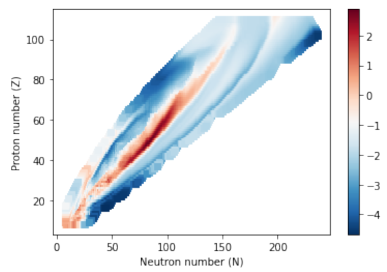

FIG. 5: Results of NNh2 for various nuclei in the nuclear chart.

of stability the HFB14 predictions disagree with the MFDNN results by an order of ≈10 MeV which is less then the difference between FRDM and HFB14 i.e. ≈30 MeV. We have also presented the results from NNh2 for a large number of the nuclei in Fig. 5 and it can be observed that a systematic nonlinear relation between the low fidelity and high fidelity data has been learned.

Acknowledgement

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References

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