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A study on nuclear binding energy and beta decay energy using deep neural networks

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ABSTRACT

The Artificial Neural Network (ANN) is one of the innovative methods for predicting the structural and dynamic properties of atomic nuclei. In this work, we employed machine learning based on the Deep Neural Network (DNN) technique to find the ground state binding energy and beta decay energy of various nuclei. 3560 experimental nuclear data sets have been used for training and validating the DNN model. Neutron number (N), proton number (Z), the pairing term (δ), a magic number greater than or equal to N and Z, asymmetry factor (a) and promiscuity factor (P) are used as input parameters. The Rectified Linear Unit (ReLU) function and Mean Absolute Error (MAE) are used as activation and Loss functions for the training process. We perform the predictions of ground state binding energy per nucleon and beta decay energies in Zinc and Promethium isotopes using the DNN model, which is in good agreement with experimental results.

1. Introduction

Binding Energy (BE) and Beta-Decay Energy (β-DE) are essential to unravelling the properties of atomic nuclei [1,2]. Theoretical and experimental determination of nuclear properties is significant for both nuclear physics and nuclear astrophysics [3,4]. The recently published AME2020 [5] atomic mass table has provided 3560 sets of experimental nuclear data, which include information about the binding and beta decay energies of atomic nuclei. Despite this, accurately predicting nuclear properties near the driplines remains a challenge. In recent years, several theoretical formalisms have been developed to predict nuclear properties, such as macroscopic-microscopic models like the Finite Range Liquid Drop Model (FRLDM) [6], the Lublin-Strasbourg Model (LSD) [7], the microscopic model, the Hartree-Fock model [8], and mean field models [9]. Additionally, advances in experimental facilities have led to the increased experimental determination of nuclear binding energy and beta decay energies across the entire nuclear landscape [10,11]. Despite these efforts, there is still a gap between the exact theoretical prediction of these nuclear observables and the experimental results obtained. Artificial Neural Networks (ANN) have become a potent tool for studying data analysis. It is employed successfully in numerous applications [12–16]. Nuclear physics is an excellent candidate for research utilizing neural networks because of the rich availability of experimental data [17,18]. Numerous researchers have used neural networks and various algorithmic techniques to predict nuclear features like mass excess, ground state energies, and charge radii [19–23]. This confirms that the neural network is also a method to investigate nuclear properties alongside other theoretical nuclear models. Several ANN models have been created for various applications, including Deep Neural Networks (DNN), Long-Short-Term Memory (LSTM), Recurrent Neural Networks (RNN), Radial Basis Function Neural Networks (RBF), and Convolutional Neural Networks (CNN) [24,15,25]. In this study, we employed the DNN to predict the total binding energy and the beta decay energy of atomic nuclei. We used the neural network technique for training and testing using experimental data from AME2020 [5]. We increased the number of hidden layers to improve the predictions and changed the training to testing data ratio. The effectiveness of this approach is then assessed by comparing our findings with the liquid drop model and experimental results.

2. Methods

Experimental nuclear physics is one of the key research areas with experimental values of nuclear binding energies, and mass excess available for more than 3500 nuclei [26]. Therefore, ANN is a potential tool for studying the nuclear properties of atomic nuclei. We use the DNN technique to estimate the BE and β-DE. The DNN is a feed-forward neural network defined as the ANN with multiple hidden layers, each consisting of a certain number of neurons [27]. Data flow using the DNN can be expressed as,

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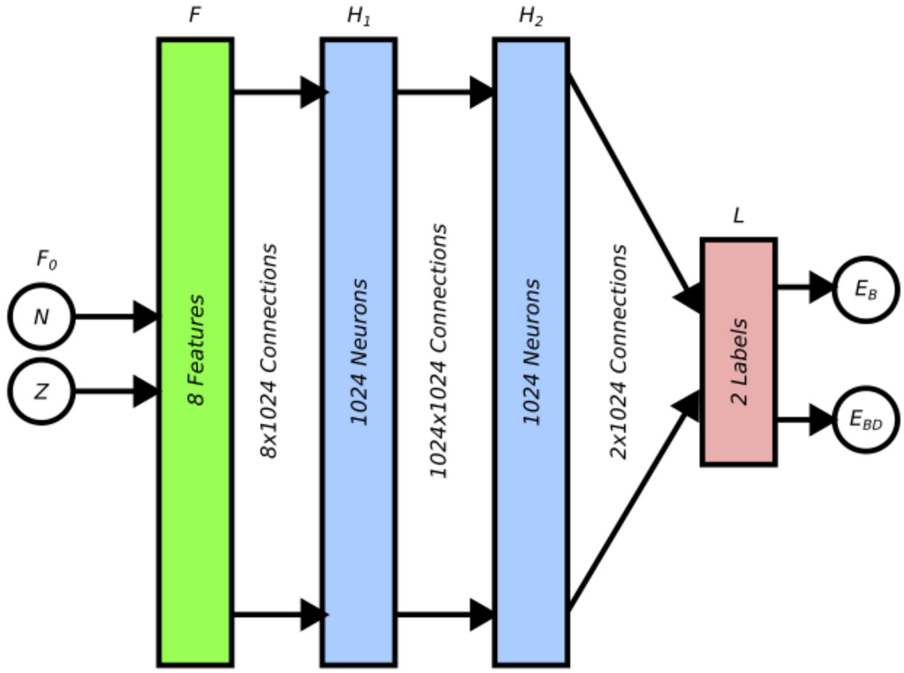

Fig. 1. Schematic diagram of DNN model structure used in the present work.

$$h_i = \sigma\left(\sum_j \omega_{ij} x_j + b_i\right) \tag{1}$$

where h_i is the value of the i^{th} neuron in the next layer, x_j is the value of the j^{th} neuron in the previous layer, ω_{ij} and b_i represent weight factors and bias respectively. The neural network model starts with randomly initialized weights and biases for each neuron. During training, the model automatically adjusts its parameters using a stochastic gradient algorithm to optimize its performance on the given task. The input values are multiplied with the corresponding weights and added with the biases, resulting in a linear transformation of the input. The resulting value is then passed through a nonlinear activation function, typically denoted as σ, which introduces nonlinearity to the model. This process is repeated for each neuron in the network. Different activation functions are available in the literature for various applications, including the sigmoid, tangent, and Rectified Linear Unit (ReLU) functions [28]. In this work, we have used the ReLU function as an activation function to build the DNN model.

$$\mathrm{ReLU} = \max(0, x) \tag{2}$$

Our neural network consists of two primary inputs, the neutron number (N) and the proton number (Z). From this, a set of eight secondary inputs, including N and Z, are generated. Other values in this set are pairing term (δ) of N and Z, a magic number greater than or equal to N and Z, asymmetry factor (a) and promiscuity factor (P) [29]. These are defined as,

$$\begin{aligned} \text{Pairing term}(\delta) &= \frac{(-1)^Z + (-1)^N}{2} \\ \text{Asymmetric term(a)} &= \frac{N-Z}{A} \\ \text{Promiscuity factor(P)} &= \frac{v_P v_N}{v_P + v_N} \end{aligned} \tag{3}$$

δ corresponds to nuclear pairing effects that are +1 for even-even nuclei, −1 for odd-odd nuclei and 0 for other nuclei. a corresponds to the quantum effects that emerged from the Pauli exclusion principle, and the P is related to the shell closure effects. P is the difference between a particular proton or neutron number and the nearest magic number of an atomic nucleus. In this work, values $Z = 8, 20, 28, 50, 82, 126$ and $N = 8, 20, 28, 50, 82, 126, 184$ have been taken as magic numbers. It is followed by two hidden dense layers of 1024 neurons each and an output layer producing two outputs: BE and β-DE (both in units of MeV). Internally, a neural network fits data by minimizing a loss function, which in our case is the Mean Absolute Error (MAE),

$$\mathrm{MAE} = \frac{1}{n}\sum_{i=1}^{n} |\hat{Y}_i - Y_i| \tag{4}$$

where $\hat{Y}_i$ represents the value predicted by the DNN model and Y_i represents the true value. 3560 values, taken from AME2020 [5], contain both experimentally obtained values as well as values calculated using the trends from the mass surface in the neighbourhood., which are used for the modelling. Out of this, 50% of randomly selected nuclear data are utilized for training, while the remaining is used to validate the model. After training the model, the best fit for BE and β-DE is found. A schematic diagram of our DNN model is shown in Fig. 1.

3. Results and discussions

In this work, we have predicted the BE and β-DE of the nuclei using the DNN model. The binding energy (BE) of the nucleus is the minimum energy required to disassemble the nucleus of an atom into its constituent protons and neutrons, collectively known as nucleons, where A nucleons consist of Z protons and N neutrons. The semi-empirical mass formula [30] expresses the BE per nucleon (BE/A) in MeV for a given nucleus with A nucleons is defined as,

$$\frac{BE}{A} = a - \frac{b}{A^{1/3}} - \frac{cZ^2}{A^{4/3}} - \frac{d(N-Z)^2}{A^2} \pm \frac{g}{A^{7/4}} \tag{5}$$

where the coefficients are $a = 14.0$, $b = 13.0$, $c = 0.585$, $d = 19.3$, $g = 33.0$ The pairing term is purely empirical, + for even—even nuclei and − for odd—odd nuclei. When A is odd, the pairing term is zero. In a beta decay (β-decay) process, a β particle (energetic electron or positron) is emitted from an atomic nucleus that transforms the original nuclide to an isobar of that nuclide. For the beta decay,

$$^{A}X_Z \rightarrow {}^{A}Y_{Z\pm1} + e^{\mp} + \nu \tag{6}$$

where ν is the electron antineutrino for β^- decay and electron neutrino for β^+ decay. The proton-to-neutron ratio, which represents the relative number of protons and neutrons in the nucleus, is the primary factor determining whether a nucleus undergoes β^+ decay (positron emission)

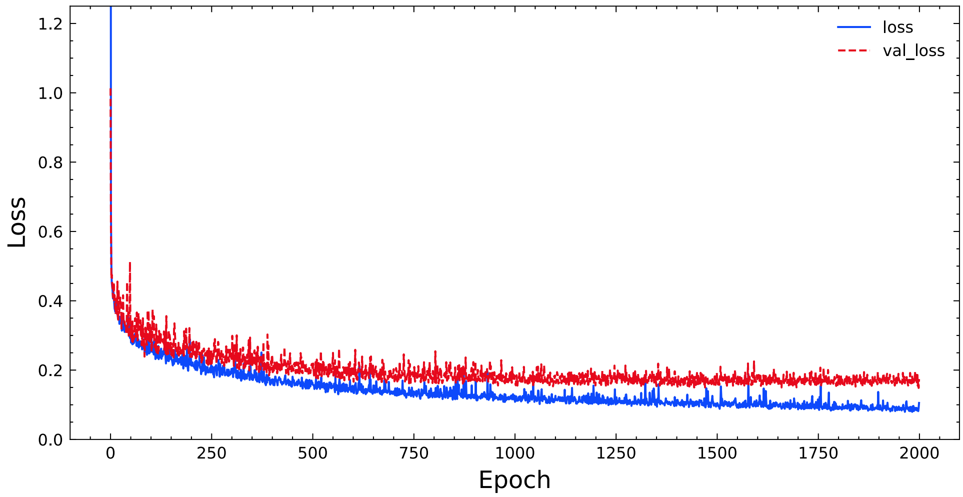

Fig. 2. Plot of Mean Absolute Error (MAE) against epoch for the training and validation datasets. The blue line represents the MAE for the training set and the dashed red line represents the MAE for the validation set. (For interpretation of the colours in the figure(s), the reader is referred to the web version of this article.)

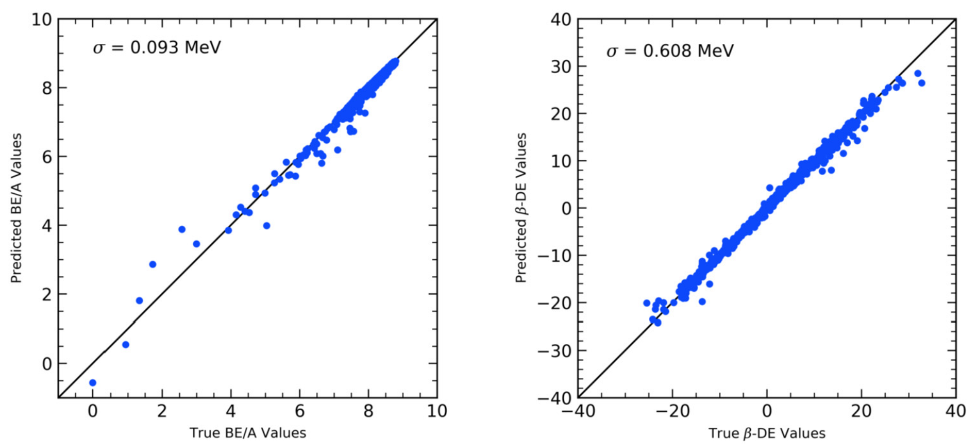

Fig. 3. A comparison of the values predicted by the neural network and known experimental values. σ is the MAE error in the predictions. (a) represents the comparison of predicted BE/A with experimental values and (b) represents the comparison of predicted β-DE with experimental results on the entire nuclear landscape.

or β^- decay (electron emission). When the nucleus has excess neutrons, it tends to undergo β^- decay to increase the proton-to-neutron ratio. Conversely, when the nucleus has excess protons, it undergoes β^+ decay to decrease the proton-to-neutron ratio. Although other factors, such as the stability of the nucleus and the energy levels of the particles involved, can also play a role in determining which type of decay occurs, the proton-to-neutron ratio is the fundamental determining factor.

The total energy released/absorbed during the reaction or Q-value is

$$Q = \left[m(A,Z) - m(A,Z \pm 1) - m_e - m_\nu\right] c^2 \tag{7}$$

Q value must be positive for the electron/positron emission to be energetically possible.

It is observed that data predicted by our DNN model is consistent with available experimental results. We figured out the loss function at different training epochs. Fig. 2 represents the loss function of our DNN model. The model underwent a training process for 5000 epochs, during which the loss function gradually decreased until it attained a minimum value. This minimum value represented the point of convergence, indicating that the model had learned all it could from the training data. Subsequently, the model was utilized to generate predictions based on the minimum loss value attained. Upon training, the value of the loss function converged to 0.049 for the training data and 0.155 for the validation data.

Fig. 3 compares the predicted values of BE/A (a) and $\beta-$DE (b) with known experimental results taken from AME2020. The mean absolute error of our prediction is found to be 0.093 MeV for BE/A and 0.608 MeV for $\beta-$DE. Most experimental observations on binding energy per nucleon are concentrated in the vicinity of approximately 8 MeV, with a limited number of deviations from this value. As a result, more precise predictions for binding energy can be made in the medium and high mass regions, compared to the lower mass region of nuclei.

The predictions of BE and β-DE of the entire nuclear landscape plotted against Z and N are presented in Fig. 4. Our model can predict values in areas where experimental data are absent. Furthermore, our model can accurately predict the BE values of super heavy elements, the values in the island of stability region and the extreme limits of both the proton drip line and neutron drip lines.

It is possible to emit either a positron or an electron during β-decay. For spontaneous β-decay to occur, the Q value must be positive. Fig. 4 illustrates that nuclei close to the neutron drip line have a positive Q value (indicated by the red region), making the spontaneous emission of β-decay energy highly favourable. However, nuclei at the proton drip line's limit (blue region) has a negative Q value, indicating that β-decay cannot occur without external energy. Our model can predict if β-decay

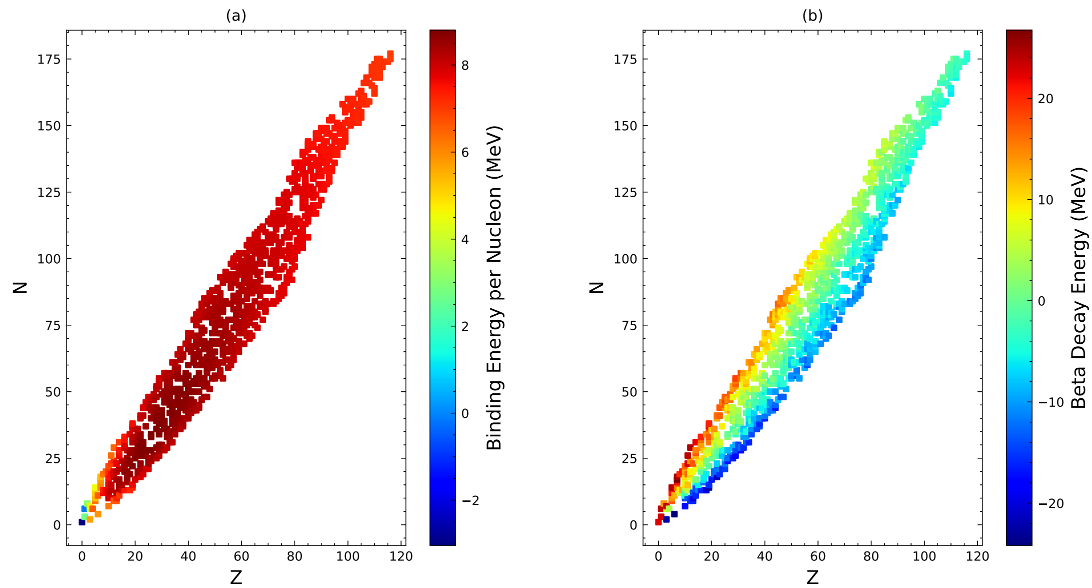

Fig. 4. Predicted binding energy (a) and beta decay energy (b) values on the entire nuclear landscape.

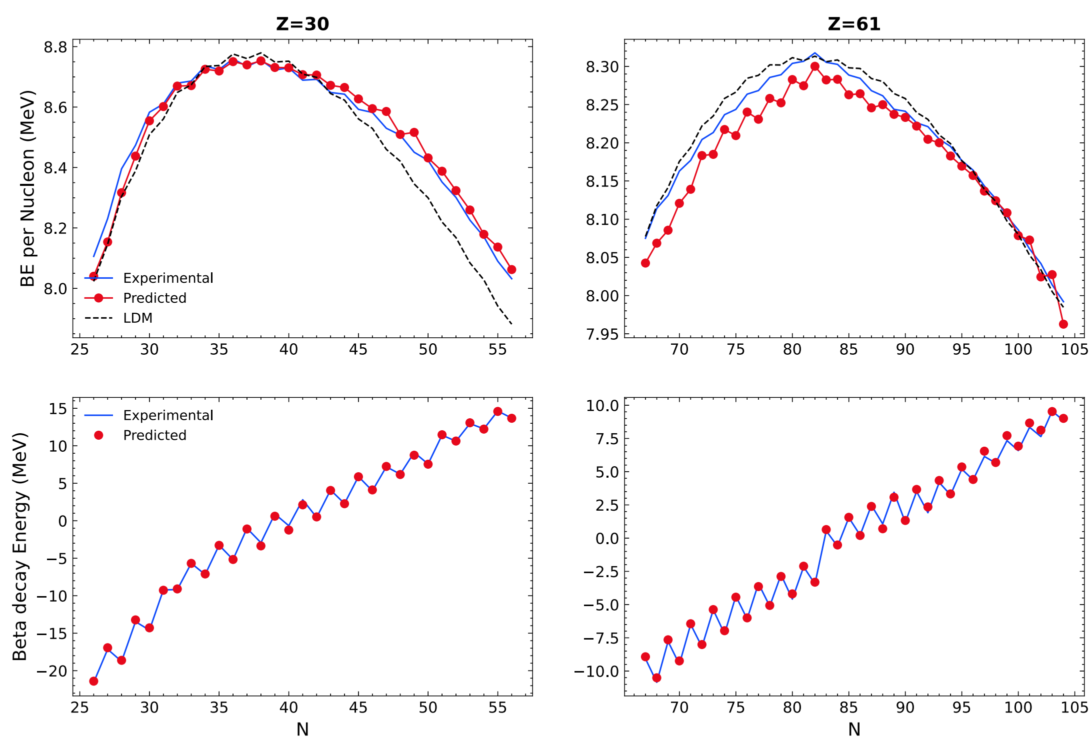

Fig. 5. Binding energy (top row) and beta decay energy (bottom row) for different isotopes of some selected elements.

is possible for specific nuclei, providing valuable insights into the decay process.

In Fig. 5, the top row displays the BE while the bottom row shows the β-DE of randomly selected Zinc and Promethium isotopes. These isotopes were chosen randomly to test the accuracy of our DNN model. The BE/A and β-DE for Zinc isotopes were determined for neutron numbers ranging from 25 to 60, while for Promethium isotopes, neutron numbers ranged from 60 to 100. We have calculated the total BE for all nuclei using a semi-empirical mass formula and compared it with our model's predictions, which are shown in the top row of Fig. 5. Analysis of the β-DE graph in Fig. 5 reveals a strong correlation between the magic number dependence of our DNN model and experimental results. Specifically, a significant jump in β-DE is observed at neutron number 82 (which is a magic number) for Promethium isotopes. This indicates that our DNN model accurately captures the magic number dependence of nuclear properties, including β-DE.

4. Summary

This study presents the application of the DNN for predicting the total ground state BE and β-DE of atomic nuclei. We used a training data set of 3560 nuclear data to train the DNN model and found that the model's predictive power depends on the number of inputs, hidden layers, and neurons. The predicted values of the BE and β-DE using the DNN model are comparable with the experimental results, with a MAE of 0.093 MeV for BE and 0.608 MeV for β-DE.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

The data that has been used is confidential.

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