Harnessing Deep Neural Network (DNN) for Predicting Binding Energy Across the Nuclear Chart

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1. Introduction

Binding energy is the energy required to hold a nucleus together, making it a key factor in understanding nuclear stability, fission, fusion, and energy production in stars. Traditional methods, such as semi-empirical mass formulas and quantum mechanical models, often struggle with accuracy and computational efficiency. Deep learning, with its ability to detect complex, non-linear patterns in data, offers a promising alternative [1]. This paper presents a novel approach utilizing Deep Neural Networks (DNN) to predict the binding energy per nucleon across the entire nuclear chart, encompassing even exotic nuclei near the drip line.

2. Data Prepossessing

The dataset used in this study was obtained from the National Nuclear Data Center (NNDC), NuDat database [2]. The dataset contained the proton number (Z), neutron number (N), and the experimentally measured binding energy per nucleon (BE/A).

A. Feature Engineering

Feature engineering involved adding derived features, including the mass number ($A = Z + N$) and the neutron-to-proton ratio (N/Z), as additional input parameters.

B. Data Optimization and Cleaning

The features were normalized to bring them to a similar scale, aiding in improved convergence during training. Additionally, missing or anomalous data points were removed to enhance model accuracy.

C. Data Splitting

The dataset was shuffled and split using the Scikit-learn library into training, validation, and test sets in the ratio [80 : 15 : 5], ensuring a balanced representation of light and heavy nuclei.

3. Neural Network Architecture

The DNN model, developed using TensorFlow [3] with several fully connected layers, was optimized through a trial-and-error process by fine-tuning the hyper-parameters.

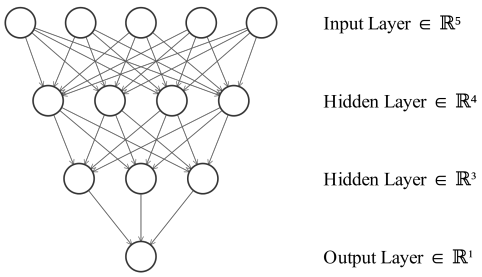

FIG. 1: A schematic of a DNN consisting of an input layer, hidden layers and an output layer.

A. Structural Overview

The DNN consists of an input layer receiving input features like Z and N, as well as A and N/Z. It is followed by seven fully connected hidden layers that ultimately lead to an output layer predicting BE/A.

B. Heterogeneous Activation Functions

The Hyperbolic Tangent (Tanh) activation function was applied in the first four hidden layers, followed by the Rectified Linear Unit (ReLU) in the subsequent three layers as shown in Table I. Tanh, with its zero-centered outputs, helps stabilizes learning and accelerates convergence, while ReLU addresses the

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vanishing gradient issue and encourages sparsity by outputting zero for negative inputs. This combination allows the network to benefit from improved gradient flow of Tanh in the initial layers and efficient training performance of ReLU in the deeper layers.

Layer (type)	Output Shape	Activation
Dense (128)	(None, 128)	tanh
Dense (64)	(None, 64)	tanh
Dense (32)	(None, 32)	tanh
Dense (16)	(None, 16)	tanh
Dense (16)	(None, 16)	relu
Dense (8)	(None, 8)	relu
Dense (4)	(None, 4)	relu
Dense (1)	(None, 1)	-

TABLE I: DNN model with 7 hidden layers utilizing a combination of tanh and ReLU activation.

C. Training Process

The model was trained using the "Adaptive Moment Estimation" (Adam) optimizer with mean squared error (MSE) as the loss function. It underwent 250 epochs of training with a batch size of 50, while the validation set was continuously monitored to assess performance.

4. Validating Model Performance

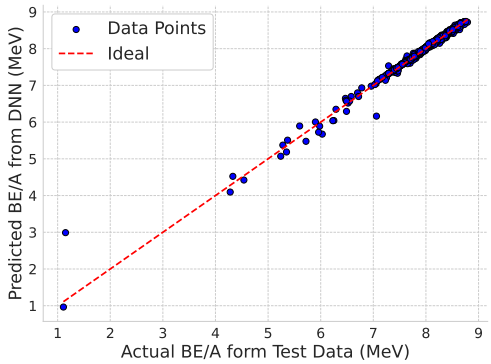

FIG. 2: (Colour Online) Scatter plot of predicted vs. actual binding energy for the test set, showing a close match between predicted and actual values with minimal deviations.

The performance of the model was assessed using the test set, where its predictions were compared to the actual binding energy values. It achieved a remarkable accuracy of **99.46%**. Figure 2 presents a scatter plot of DNN prediction vs. actual binding energy from the test set, showing an excellent agreement between them.

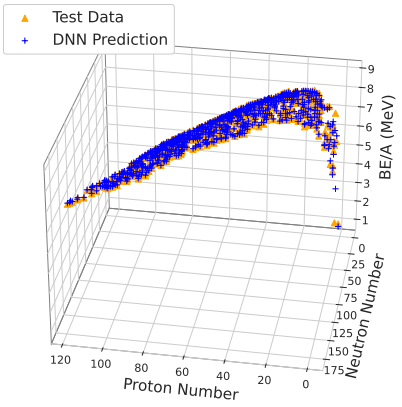

FIG. 3: (Colour Online) Binding energy per nucleon w.r.t. proton and neutron numbers. The triangular-orange and plus-blue markers correspond to the test data and DNN prediction.

Figure 3 demonstrates the reliability of the DNN in predicting BE/A across the proton and neutron numbers. For instance, the model can predict the BE/A for an exotic nucleus such as ^{132}Sn with an accuracy of **99.09%**.

Conclusion

The DNN effectively captured subtle nonlinear relationships between nucleon properties and binding energies with outstanding accuracy. It showed strong performance even for exotic nuclei, where semi-empirical formulas typically exhibit larger prediction errors.

References

[1] A. Boehnlein et al., Rev. Mod. Phys. 94, 031003 (2021).

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[3] M. Abadi et al., OSDI 16, 265-283 (2016).