A study on nuclear binding energy based on neural network

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Introduction

Precise determination of nuclear mass and hence its binding energy has been a longstanding problem. Precision is highly important not only for understanding of the basic nuclear physics but also for the astrophysical interest and investigation of nuclei, especially those far from the stability line. Starting from the earlier works of Bohr, Bethe and Weizsacker [1] to the recent works viz. those involving finite range droplet model (FRDM) of Moller and Nix [2], Hartree-Fock-Bogulibov (HFB) model of Pearson [3], a diverse amount of works have been accomplished to emulate the global trend of nuclear masses. Off late, departing from the conventional way, an artificial neural network (ANN) based model has been developed to predict binding energies of nuclei [4]. The ANN based model depends generally on the existing data whereas the FRDM and the HFB based models rely mostly on theoretical inputs. However, the ANN based model prediction has been found more accurate than the others, as is evident from their observed deviation (root mean square error) of the predicted values from the experimental ones. In an aim to achieve improvement over the earlier predictions, we have initiated another artificial neural network based model, different in structure from the existing one. Though the structure is quite simpler so far as the number of hidden layers is concerned, stress has been given in the incorporation of new input variables. The initial trend of our result is found encouraging, yielding significant accuracy in the N-Z plane used in the present work.

Methods

Nuclear Physics is one of the richest areas of science, with a vast collection of more than 3000 experimentally available nuclear binding energies and masses. Therefore ANN is highly applicable in this domain, providing the so called "data mining" platform.

Our development in the neural network based model deals with multilayer feedforward architecture to estimate binding energy per nucleon. The network consists of one input layer (having five input neurons), two hidden intermediate layers (one with fifteen neurons and another with one neuron) and one output layer giving one set of output (fig. 1). The input layer consists of five inputs: neutron number (N), proton number (Z), beta decay energy, angular momentum and parity (J^{π}). Each neuron in n^{th} hidden layer gets stimulus S_n from the preceding m^{th} layer, such that $S_n = \sum_m (\omega_{mn} I_m) + b_n$, where ω_{mn} is the weight factor and b_n is the bias factor. I_m is the activity of the preceding layer (i.e input from the m^{th} neuron of either input or hidden layer) . *I* and *S* are connected as $I_m = f(S_m)$, where *f* is the nonlinear activation function (in our case this is *tansig* function). The aim is to update the states of all the neurons in a given layer and finally the layers are updated sequentially, starting from the input to output. The neuron number in a layer and the activation function, both have been optimized in terms of minimum root mean square error (RMSE).

We exploited 1470 nuclides, the data concerned being extracted from NUBASE compilation [5]. The training set of data was constructed with 1149 nuclides, chosen randomly starting from N=1 upto N=150. The validation set was consisted of 275 nuclei, while there were three test data sets: test set 1, test set 2 and test set (u) consisting of a total of 46 nuclides. The test set (u) bears nuclides far from stability region, especially in neutron drip line

and superheavy regions. The regions are shown in the N-Z plane (fig. 2).

The training algorithm was taken as backpropagation according to which the calculation was performed in the neural net. The binding energy per nucleon in MeV was intentionally taken as output to reduce the RMSE as small as possible. The result was achieved after 284 epochs.

Results

The difference between experimental binding energy per nucleon and the predicted values from training, validation and test sets are shown in fig3. RMSE was calculated as, $\sqrt{\sum_i (E_i - O_i)^2}$, where E_i and O_i are estimated and observed outputs, respectively. The RMSE for training set is found as 0.81, while for validation set it is 1.1 and it is ranging from 1.1 to 1.5 for the test sets. The RMSE of binding energy for test set (u) i.e for the nuclei far from stability has been the highest (1.5). Ref[4] achieved RMSE of 0.62 to 0.92 for training set, between 1.54 to 1.92 for validation set and 1.88 to 3.1 for test set.

In summary, we have developed a neural network based model to estimate binding energy per nucleon. The present ANN model, though simpler in structure, incorporates beta decay energy and angular momentum as new inputs, achieving RMSE lower than that predicted by the existing model. However, more nuclides have to be exploited for final inference. Detail work is still in progress.

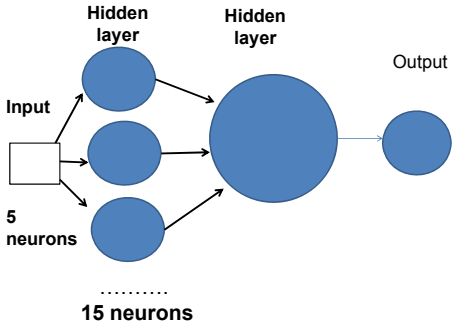

Fig. 1:Neural network structure used in the present work.

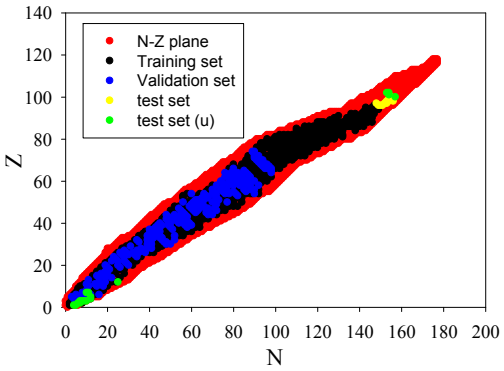

Fig. 2: The N-Z plane showing different nuclides taken in the calculation.

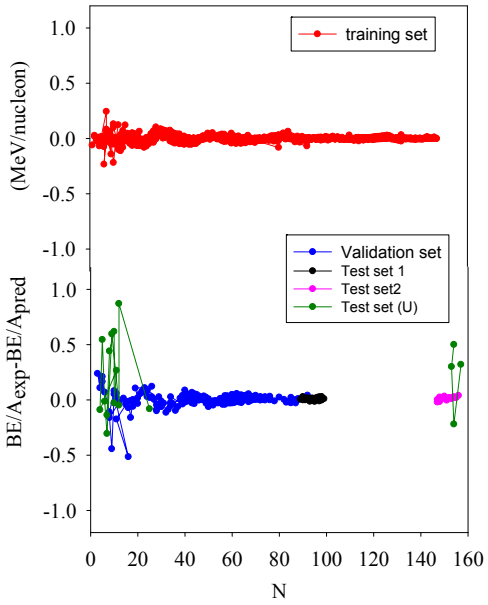

Fig. 3: The difference in binding energy/A from the present calculation.

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