Indian J Phys
https://doi.org/10.1007/s12648-021-02099-w

ORIGINAL PAPER

Estimations of first 2^+ energy states of even–even nuclei by using artificial neural networks

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Received: 16 July 2020 / Accepted: 25 March 2021

Abstract: The first excited 2^+ energy states of nuclei give much substantial information related to the nuclear structure. All excited states of nuclei are shown regularities in spin, parity, and energy, including these levels. In the even–even nuclei, the first excited state is generally 2^+, and the energy values of them increase as the closed shells are approached. The nuclei's excited levels can be investigated using theoretical nuclear models, such as the nuclear shell model. In the present study, we have used artificial neural networks to determine the energies of the first 2^+ states in the even–even nuclei in the nuclidic chart as a function of Z and N numbers for the first time. According to the results, the method is convenient for this goal. One can confidently use the method for predicting the first 2^+ state energy values whose experimental values do not exist in the literature.

Keywords: First 2^+ energy; Artificial neural network; Even–even nuclei

1. Introduction

By using a central attractive force, it is found that the ground state is 0^+ and the first excited state is generally 2^+ of even–even nuclei [1]. The first excited state energy value in nuclei regularly depends on the proton and neutron numbers [2]. Some regularities are observed in the first excited state's energy values, and these regularities can be explained in terms of mixtures of excitation states of different neutron and proton pairs [3]. The coupling model and the liquid drop model of the nucleus can explain the regularities in spins and parities of first and second excited states of even–even nuclei [4]. In even–even nuclei, the first excited state includes much information about the nuclear structure, such as the deformation and shape of nuclei, lifetime of nuclear state, and the transitions between levels. Some information about the proton and neutron interactions in partially filled shells might also be obtained from the first excited state. The energy values of these states increase as the closed-shell is approached. Namely, closing a shell causes a sharp increase in the first excited state energy [5]. Therefore, first excited state energy and spin values are sensitive to the shell structure [6]. According to the shell model (SM) of the nucleus, large shell gaps are observed between the shells for stable nuclei. These nuclei have magic proton and neutron numbers whose values are 2, 8, 20, 28, 50, 82, and 126 [7]. Due to these large gaps, large transition energy values are measured between the first 2^+ and ground states in nuclei. Thus, the transition probability from the first excited state to the ground state decreases monotonically. Related to these levels, the second excited state has about twice as much energy [8], and if we excite an odd A nucleus, we would expect to find its first excited state at least as low as that of its even–even core.

Theoretically, the predominance of spin 2 and even parity first excited states of even–even nuclei has been explained using nuclear SM. The first excited state of nuclei is assumed due to the excitation of a single pair of nucleons. If the proton (neutron) shell is closed in nuclei, the first excited state is ascribed to neutron (proton) excitations [6]. Considering the perfect fit with spin and parity values in the experimental data, it is seen that this statement is correct. Some methods, such as conversion coefficient, pair creation, lifetime, E/M ratio, angular

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Published online: 15 April 2021

correlation, and nuclear reactions, can be identified by the first excited state's spin and parity. In this study, the energies of the first 2^+ excited states of even–even nuclei have been estimated by using the artificial neural network (ANN) method [9]. The data have been obtained from the Pritychenko et al. [10] in which adopted values cover the $Z = 2$–104 region, including 636 first 2^+ energy states in the nuclidic chart. The results show that the ANN method is quite a useful method for this type of estimation.

Furthermore, the ANN estimated results are compared with the results from nuclear SM [7] calculations for some *p*, *sd*, *sdpf*, and *pf*-shell nuclei given in Table 4 in the references [10]. According to this comparison, ANN predicts the first 2^+ energy state energy better than SM calculations. In recent years, ANN has been using in many fields in nuclear physics. It has been used successfully for developing nuclear mass systematic [11, 12], obtaining fission barrier heights [13], obtaining nuclear charge radii [14, 15], estimation of beta decay energies [16], and alpha half-lives calculations of super-heavy nuclei [17]. Since this method is successful in understanding the nonlinear relationship between input and output data, layered feed-forward ANN can be used to estimate the first 2^+ excited state energy values in even–even nuclei.

2. Artificial neural network (ANN)

The ANN method is a powerful tool that is used when standard techniques fail [9]. The method mimics the brain functionality of all creatures. Like in the real brain, ANN, which is the base of artificial intelligence, can learn everything through an appropriate algorithm to do what it has learned. Additionally, artificial intelligence can store lots of data in its memory and keep them in mind through the long years. For this task, ANN is composed of mainly three different layers. The data are taken from outside to the input layer as input, and the output data are the desired one, which is exported from output layers. The number of input neurons depends on the problem, and inputs are independent variables. The number of output neurons is the number of output variables that are estimated. Between these two layers, there is one (or more) additional layer in which data are mainly processed in this layer, which is called a hidden layer. In each layer, they have their neurons that are processing units of ANN. Data flow in one direction from input to outputs neurons. Each neuron in the layers is connected to all other neurons in the next layer. Therefore, all neurons in hidden and output layers have at least one own entry. As given in Eq. 1 that all these entries (x_i) are multiplied by the weight values of their connections (w_i) and then summed to get the net entries (n_j) of the neurons.

$$n_j = \sum_{i=1}^{N} w_i \times x_i \tag{1}$$

After this step, the neurons are activated by a chosen function, and the outputs of the neurons are transmitted to the neurons in the next layer.

In the ANN calculations, all data belonging to the given problem have randomly been divided into two separate main sets. The first part of the data (about 80%) was used for the training of ANN to get the relationship between input (independent) and the output (dependent) variables. To determine the method's success, it must be tested over another set of data, which is the rest (about 20%) of all data. The training (learning) process's main task is assigning the values to each weighted connection between neurons. In other words, in the training process, it is aimed to find the best weight values, which give the best estimation of y_i starting from the input x_i. Therefore, the weight values are modified until the acceptable deviation level is between the desired (d_i) and neural network (y_i) outputs. Generally, the mean square error function (MSE) has been used for comparison (Eq. 2). Some parameters are tuned up to reach the best weight values, such as hidden layer number, hidden neuron number, learning algorithm, activation function, and/or neural network in the training stage. In this study, to get the best values, the Levenberg–Marquardt learning algorithm [18, 19], tangent hyperbolic activation function (Eq. 3), and multi-layer feed-forward neural network have been used (Fig. 1).

$$\mathrm{MSE} = \frac{1}{N}\sum_{i=1}^{N}(y_i - d_i)^2 \tag{2}$$

$$G(n_j) = \frac{e^{n_j} - e^{-n_j}}{e^{n_j} + e^{-n_j}} \tag{3}$$

After a successful training step, the constructed ANN is tested over the training data set used in the learning process. Using final weights values, the comparison has been made between neural network outputs and the desired values. However, this result is not sufficient to decide whether the method is good or not. The final weights must also be tested over an unseen data set. The test data set is used for this purpose, and if the ANN outputs are also close to the desired values on this data set, it is safely concluded that the ANN is generalized to the data. Namely, one can confidently use the constructed ANN with its final weights to solve the problem of the same type of data.

In the current study, the inputs were proton (Z) and neutron (N) numbers of the atomic nuclei, and the output was the first 2^+ state energy values of the even–even nuclei. Note that, the range of activation function is ($-$ 1; 1) for the hidden layer's hyperbolic tangent. Therefore, it could be said that it can be difficult to train cases without

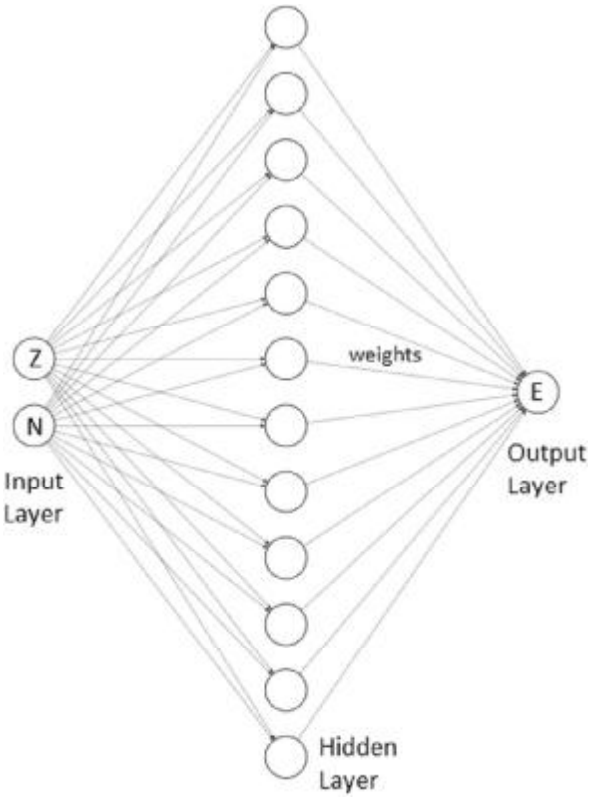

Fig. 1 Used 2-12-1 ANN architecture to estimate the first 2^+ excited state energies of even–even nuclei

normalizing or softening the data. The data are normalized or smoothed to speed up the learning process and increase the learning rate. In the case of the data are always positive, and their scales vary drastically, one simple way is to use the data's logarithm transformation. Thus, we have taken the logarithm of the output values (first 2^+ state energies) into consideration in the calculations.

3. Results and discussion

Two different ANN approaches have been developed to estimate the first 2^+ state energies. In the first approach, a model has been developed which covers all even–even nuclei in the range of nuclei whose atomic numbers are between 2 and 104. Since it was observed that the ANN performance changes in regions where the atomic number is less than 40 and greater than 40, as a second approach, two separate ANN models also have been developed for the regions with $Z < 40$ and $Z \geq 40$. The total number of nuclei samples was 646 in the whole data set, as shown in Fig. 2. Nevertheless, 15 extremum points exceeding the energy value of 2500 keV were not included in the calculations. These higher energy values are very few in all data and are considered unusual points. Therefore, the total number of samples for ANN calculations (indicated as data points in the figures) is 631. The adopted literature data (which the recommended values based on all the available experimental data) have been taken from a previous compilation [10]. Due to the different behavior of the regions according to the atomic masses, the estimations have also been performed upon two separated parts of the nuclidic chart (Fig. 2). The first part includes the nuclei whose atomic mass smaller than 40, and the second one includes greater than or equal 40. As shown in Fig. 2, the first part includes many more nuclei whose first 2^+ excited states are higher in energy. The average value of this region is 1393 keV. The second part's average value is just 479 keV, and only for two nuclei, the first 2^+ excited states have energy values, which are greater than 2000 keV. These nuclei are ^{132}Sn, and ^{208}Pb which are doubly magic nuclei, and the first 2^+ excited state energy values are 4041.20 keV and 4085.52 keV, respectively. Also, for the heavy elements after atomic number, which is 90, the first excited state energies are lower than the order of 40 keV. In each calculation for different regions, the data in the range has been portioned into two separate parts for training and test of the ANN. To assess the estimation performance of ANN, two error performance indexes were used. Mean absolute error (MAE) is calculated by using;

$$\mathrm{MAE} = \frac{1}{n}\sum_{i=1}^{n}|y_i - d_i| \tag{4}$$

Root mean square error (RMSE) is calculated by using;

$$\mathrm{RMSE} = \left[\frac{1}{n}\sum_{i=1}^{n}|y_i - d_i|^2\right]^{\frac{1}{2}} \tag{5}$$

where d_i is the actual desired value, y_i is the predicted value for n instants.

In the first approach, 126 of all data were used in the test stage and 505 of them in the training stage which data splitting was performed randomly. In Figs. 3 and 4, the training results and the test stages are given, respectively. The root minimum square error (RMSE) and correlation coefficient (r) values of the predictions were obtained as 137.6 keV and 0.96 for the training data, respectively. The RMSE and r values on the test data were obtained as 172.1 keV and 0.95, respectively. One hidden layer ANN structure with varying numbers of neurons from 8 to 36 has been tested, and the best result has been obtained with 30 hidden layer neurons. Training and test performances for 30 hidden neuron numbers have been shown in Figs. 3 and 4. After 30 neuron numbers, the test data set results have started to get worse again, and the result before 12 neuron numbers was unacceptably bad. For 30 neurons in hidden layer architecture, the total number of weighted

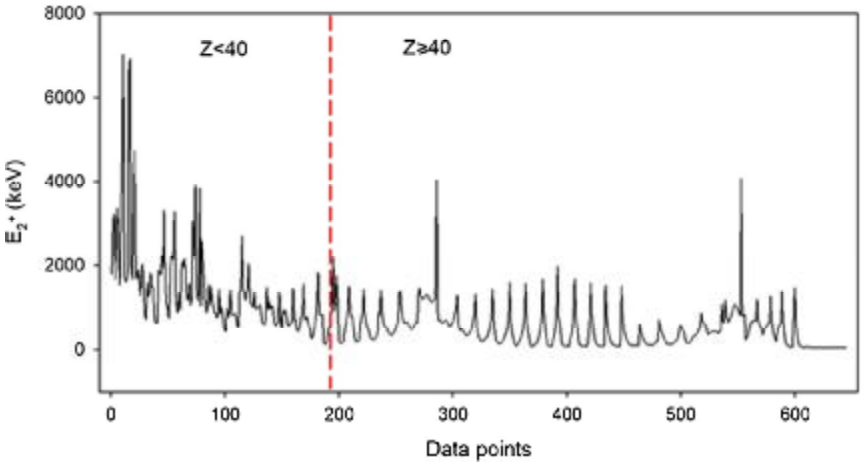

Fig. 2 First 2^+ excited energy values of nuclei for $Z < 40$ (left) and $Z \geq 40$ (right) regions

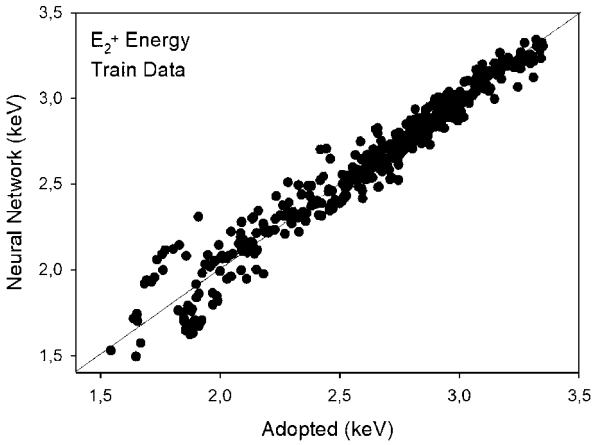

Fig. 3 Adopted [10] versus ANN estimated first 2^+ excited state energies (log) for even–even nuclei in train data

connections is 90 whose 60 of them are from the input to the hidden layer, and the rest of them are from the hidden layer to the output layer. For the ANN training, the RMSE values are 263.7, 220.1, 218.6, 158.8, 145.8, 142.3 keV for hidden neuron numbers 8, 12, 16, 20, 24, and 36, respectively. The corresponding values for the test data are 292.1, 230.4, 219.2, 179.5, 175.8, and 183.7 keV for hidden neuron numbers 8, 12, 16, 20, 24, and 36, respectively.

In the second approach, the first model has been constructed for the $Z < 40$ regions, which covers 175 samples. The data are divided randomly as 142 samples for the ANN training, which corresponds to 80% of the total data. Similarly, one hidden layer ANN structure with a varying number of neurons from 8 to 36 has been tested, and the best result has been obtained with 12 hidden layer neurons. Training and test performances for 12 hidden neuron numbers are shown in Figs. 5 and 6. The total number of weighted connections is 36, whose 24 of them are from the input to the hidden layer, and the rest of them are from the

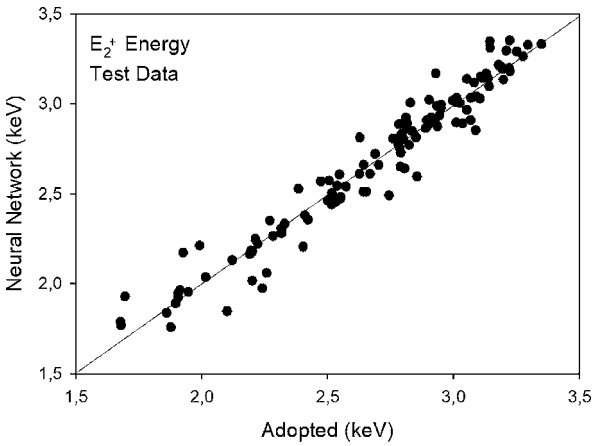

Fig. 4 Adopted [10] versus ANN estimated first 2^+ excited state energies (log) for even–even nuclei in test data

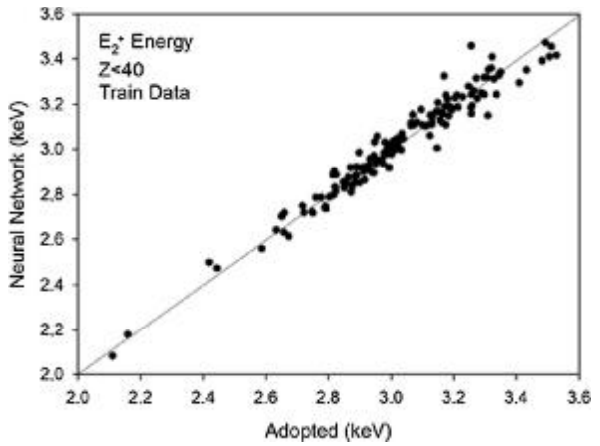

Fig. 5 Adopted [10] versus ANN estimated first 2^+ excited state energies (log) for $Z < 40$ even–even nuclei in train data

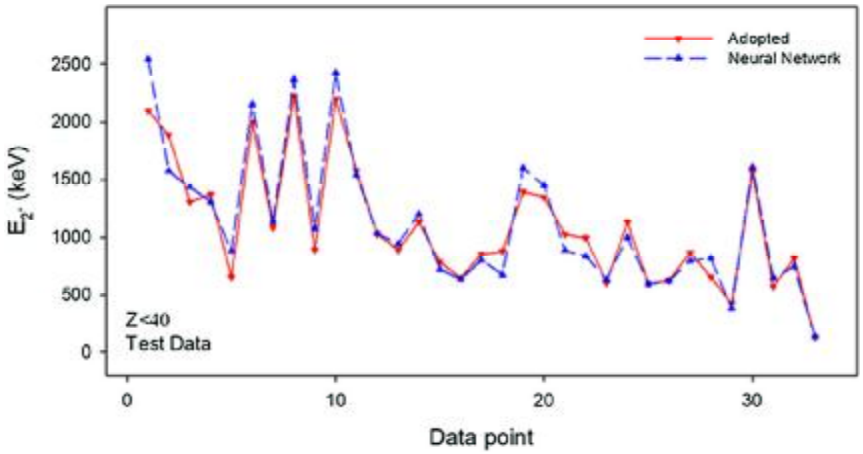

Fig. 6 Adopted [10] and ANN estimated first 2^+ excited state energies for $Z < 40$ even–even nuclei in test data

hidden layer to the output layer. After applying the ANN method, the results are converted to normal values from their logarithms. The root minimum square error (RMSE) and correlation coefficient (r) values have been obtained as 125.1 keV and 0.96, respectively. The correlation coefficient indicates that the method helps determine the first excited 2^+ state energy values for the atomic nuclei. The RMSE values for the other neuron number structures of ANN are between 140 and 250 keV. In Fig. 5, we have shown the adopted versus neural network predicted values of even–even nuclei in the $Z < 40$ regions. It is clear in the figure that the neural network estimation is in agreement with the adopted values. The data in the figure are concentrated in the (adopted = neural network) line.

After the ANN training, the constructed ANN with final weight values has been used to determine the method's generalization ability. In this test stage, the rest of all data (33 data points) have been used for this purpose. The RMSE and r values have been obtained as 140.1 keV and 0.94, respectively. The correlation coefficient again indicates that the method is still useful for determining the first excited states' energies in the nuclei. The RMSE values for the other neuron number structures of ANN are between 165 and 290 keV. In Fig. 6, the comparison between the adopted value of the first 2^+ energies of even–even nuclei in $Z < 40$ regions and the predicted value of it by using a neural network have been given.

In the second approach, the second model is constructed for the $Z \geq 40$ region, covering 456 samples. The data are divided randomly as 364 samples for the training, and 92 of them are for the test, which corresponds to 80% and 20% of total data. Similarly, one hidden layer ANN structure with varying numbers of neurons from 8 to 36 has been tested, and the best result has been obtained with 12 hidden layer neurons. The results are again presented as real energy values after converting ANN results from logarithmic values. The RMSE and r values have been obtained as 82.4 keV and 0.97, respectively. The r has taken almost its maximum value, which indicates that the method is still useful for determining the first excited 2^+ state energy values for the atomic nuclei. The RMSE values for the other neuron number structures of ANN are between 95 and 150 keV. In Fig. 7, we have given the adopted versus neural network predicted energy values of even–even nuclei in the $Z \geq 40$ region. The figure's data are concentrated in the (adopted = neural network) line, indicating the neural network estimations agree with the adopted values in the literature.

After the nuclei's training stage in the $Z \geq 40$ region, the constructed ANN with final weight values has been tested on the test data set. The rest of all data (92 data points) have been taken into account for this purpose. The RMSE and r values have been obtained as 91.4 keV and 0.94, respectively. The correlation coefficients for both stages indicate that the method is quite useful for determining the atomic nuclei's first excited states. The RMSE

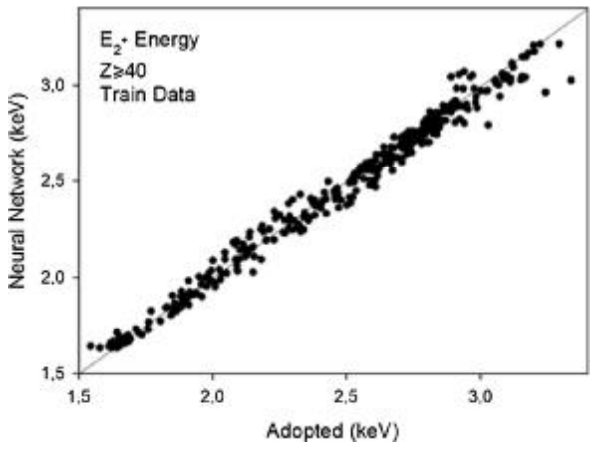

Fig. 7 Adopted [10] versus ANN estimated first 2^+ excited state energies (log) for $Z \geq 40$ even–even nuclei in train data

values for the other neuron number structures of ANN are between 95 and 165 keV. The log values of adopted and neural network predicted energies of even–even nuclei in the $Z \geq 40$ region in comparison with each other have been presented in Fig. 8. The fact that ANN results do not have the same values as the adopted data indicates that ANN performs well and does not memorize. All RMSE and r values in the training and test data for both regions also support this.

At the end of the study, both of the ANN estimations for the first 2^+ excited state energies from the present study and the nuclear shell model (SM) results have been compared with some nuclei's adopted values in Table 4 of the reference [10]. SM is one of the most common and the best theoretical models for the calculations of nuclear excited states. However, due to some reasons, such as the limitation of the model space used in the SM calculations and not the exact values of two-body interaction matrix elements and single-particle energies, the theoretical results cannot be the same as the experimental ones. As it is seen in Table 1 that the mean absolute error (MAE) values from the adopted values are 139.6 keV and 178.2 keV for ANN estimations and SM results, respectively. Since the data have been split for the test and training phase was performed as random, the comparison data belong to both the test and train data set. An asterisk sign was used to indicate the data samples involved in the test data set. For the training data set, the MAE values are 124.2 keV and 158.7 keV for ANN estimations and SM results, respectively. These values are 176.9 keV for ANN results and 227.3 keV for SM results on the test data set. For 28 of the total 49 data points, the ANN gives closer results than the SM calculations. Maximum and minimum deviations of ANN estimations from adopted values are 869 keV and 2 keV, respectively, whereas for SM calculations, these values are 1217 keV and 3 keV. According to the ANN and SM results, the ANN predictions outperform SM for 57% of the test nuclei and lead to an overall reduction of 22% of the test error with 36 ANN structure parameters. Of course, different results can be obtained by using SM calculations using different effective interactions. However, the used present effective interactions are usually those that work the best for the respective nuclei. Therefore, the values given in this reference are considered to be the closest results to the adopted results.

4. Conclusions

In this work, the first 2^+ excited state energies of even–even nuclei in the nuclidic chart have been predicted the first time by using the ANN method. The inputs of the ANN are atomic and neutron numbers of the nuclei. One hidden layer with 12 neurons that gives better results for the problem has been used after several trials. According to the estimation performance obtained from correlation coefficients, the method can be useful for predicting the first excited 2^+ energy states of nuclei. The method has been applied with two approaches. The first approach uses an ANN model covering all even–even nuclei whose Z is between 2 and 104, while the second approach uses two different ANN models for $Z < 40$ and the $Z \geq 40$ region. It has been observed that the second approach was more successful for the current problem. The RMSE values of ANN estimations in the second approach on the test data set are 140.1 keV and 91.4 keV for $Z < 40$ and $Z \geq 40$, respectively. The obtained correlation coefficients of $Z < 40$ regions are 0.96 and 0.94 for the training and test phases. For $Z \geq 40$ regions, correlation coefficients are almost the same as 0.97 and 0.94 for the training and test phase, respectively. Also, the ANN method results have been compared with the results from nuclear SM calculations to determine the method's success. The ANN results give better results than the theoretical SM calculations.

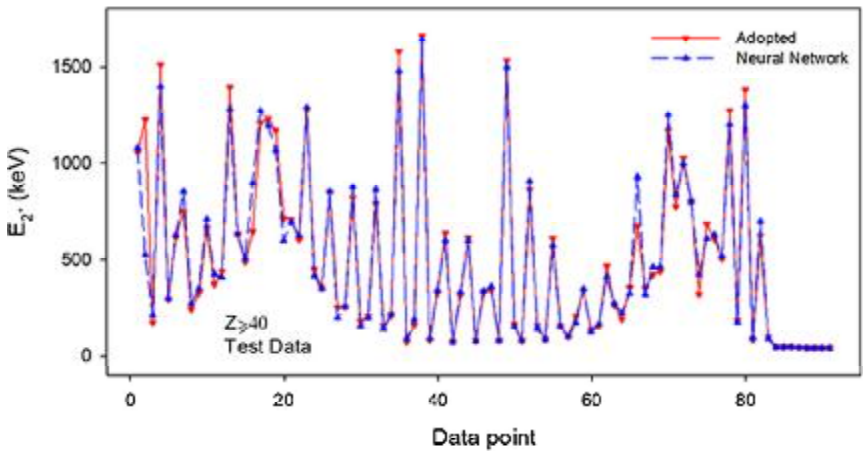

Fig. 8 Adopted [10] and ANN estimated first 2^+ excited state energies for $Z \geq 40$ even–even nuclei in test data

Table 1 Comparison of first 2^+ excited state energies from SM calculations [10] and ANN estimations (ANN results with "*" belongs to the test data set)

A	*Z*	*N*	Energy (keV)				
			Adopted	ANN	SM	ANN Dev.	SM Dev.
6	2	4	1797	1801	1894	4	97
10	4	6	3368	3262	3704	106	336
12	4	8	2102	2338*	3319	236	1217
18	8	10	1982	2050	1999	68	17
20	8	12	1674	2541*	1746	867	72
22	8	14	3199	2767	3158	432	41
18	10	8	1887	1576*	1999	311	112
20	10	10	1634	1529	1747	105	113
22	10	12	1275	1636	1363	361	88
24	10	14	1982	1848	2111	134	129
26	10	16	2018	1879	2063	139	45
28	10	18	1304	1433*	1623	129	319
20	12	8	1598	1601	1746	3	148
22	12	10	1247	1276	1363	29	116
24	12	12	1369	1306*	1502	63	133
26	12	14	1809	1544	1897	265	88
28	12	16	1474	1681	1518	207	44
30	12	18	1483	1434	1591	49	108
24	14	10	1879	1794	2111	85	232
26	14	12	1796	1874	1897	78	101
28	14	14	1779	2159*	1932	380	153
30	14	16	2235	2331	2266	96	31
32	14	18	1941	2084	2053	143	112
36	14	22	1399	1168	1723	231	324
38	14	24	1084	1132*	1395	48	311
40	14	26	986	1095	1217	109	231
30	16	14	2211	2076	2266	135	55
32	16	16	2231	2368*	2160	137	71
34	16	18	2128	2251	2131	123	3
38	16	22	1292	1156	1459	136	167
40	16	24	904	1019	942	115	38
42	16	26	890	1077*	999	187	109
32	18	14	1867	1816	2053	51	186
34	18	16	2091	2312	2131	221	40
58	28	30	1454	1485*	1478	31	24
60	28	32	1333	1310	1474	23	141
62	28	34	1173	1193*	1149	20	24
66	28	38	1425	1647	1265	222	160
68	28	40	2034	1727	1963	307	71
70	28	42	1260	1401	1599	141	339
72	28	44	1096	1036	1505	60	409
76	28	48	992	994	1374	2	382
62	30	32	954	947*	1013	7	59
66	30	36	1039	1018	950	21	89
68	30	38	1077	1070	879	7	198
70	30	40	885	909*	1109	24	224
72	30	42	653	690*	1007	37	354
76	30	46	599	601	976	2	377
78	30	48	730	718	1045	12	315
Overall MAE						139.6	178.2
MAE for training data						124.2	158.7
MAE for test data						176.9	227.3

More accurate nuclear structure properties might be obtained by getting better information about the first 2^+ state energy values. Therefore, to predict the nuclei's excited state energy values, the ANN method can be a good alternative with many advantages, such as quick calculation, no need for any complex formulation, and easy applicability.

Declarations

Conflict of interest The authors declare that they have no conflict of interest.

References

[1] M Goldhaber and A W Sunyar *Phys. Rev.* **83** 906 (1951)
[2] P Stahelin and P Preiswerk *Phys. Acta* **24** 623 (1951)
[3] A De-Shalit and M Goldhaber *Phys. Rev.* **92** 1211 (1953)
[4] G Scharfi-Goldhaber *Phys. Rev.* **90** 587 (1953)
[5] K W Ford *Phys. Rev.* **90** 29 (1953)
[6] P Preiswerk and P Stahelin *Physica* **18** 1118 (1952)
[7] M G Mayer *Phys. Rev.* **74** 235 (1948)
[8] S T Balyaev *J. Exp. Theor. Phys.* **12** 968 (1961)
[9] S Haykin *Neural Networks: A Comprehensive Foundation*. (Englewood Clifis: Prentice-Hall In.) (1999)
[10] B Pritychenko et al *Atomic Data Nucl. Data Tables* **107** 1 (2016)
[11] T Bayram et al *Ann. Nucl. Energy* **63** 172 (2014)
[12] R Utama, J Piekarewicz and H B Prosper *Phys. Rev. C* **93** 014311 (2016)
[13] S Akkoyun and T Bayram *Int. J. Mod. Phys. E* **23** 1450064 (2014)
[14] S Akkoyun et al *J. Phys. G* **40** 055106 (2013)
[15] R Utama et al *J. Phys. G* **43** 114002 (2016)
[16] S Akkoyun et al *Radiat. Phys. Chem.* **96** 186 (2014)
[17] U B Rodriguez et al *J. Phys. G* **46** 115109 (2019)
[18] K Levenberg *Quart. Appl. Math.* **2** 164 (1944)
[19] D Marquardt *SIAM J. Appl. Math.* **11** 431 (1963)