Predictions of nuclear charge radii based on the convolutional neural network

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Abstract

In this study, we developed a neural network that incorporates a fully connected layer with a convolutional layer to predict the nuclear charge radii based on the relationships between four local nuclear charge radii.The convolutional neural network (CNN) combines the isospin and pairing effects to describe the charge radii of nuclei with $A geq $ 39 and $Z geq $ 20. The developed neural network achieved a root–mean–square (RMS) deviation of 0.0195 fm for a dataset with 928 nuclei. Specifically, the CNN reproduced the trend of the inverted parabolic behavior and odd–even staggering observed in the calcium isotopic chain, demonstrating reliable predictive capability.

Full Text

Preamble

Predictions of Nuclear Charge Radii Based on Convolutional Neural Networks

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In this study, we developed a neural network that incorporates a fully connected layer with a convolutional layer to predict nuclear charge radii based on relationships between four local nuclear charge radii. The convolutional neural network (CNN) combines isospin and pairing effects to describe the charge radii of nuclei with A $\geq$ 39 and Z $\geq$ 20. The developed neural network achieved a

root-mean-square (RMS) deviation of 0.0195 fm for a dataset containing 928 nuclei. Specifically, the CNN reproduced the trend of inverted parabolic behavior and odd-even staggering observed in the calcium isotopic chain, demonstrating reliable predictive capability.

Keywords: Nuclear charge radii, Machine learning, Neural network

Introduction

Nuclear charge radius is a fundamental property of the nucleus, alongside its mass, density, spin, and moments [1–3]. It reveals vital information regarding nuclear structure, such as shell closure, halo effects, and electromagnetic properties [4–6]. To date, various experimental techniques have been employed to measure nuclear radii, including high-energy particle scattering [7], atomic spectroscopy [8,9], muonic atom X-ray spectroscopy [10,11], and isotopic shifts in the hyperfine structure of atomic spectra [12]. The CR2013 database contains root-mean-square (RMS) nuclear charge radii for 909 isotopes of 92 elements, from hydrogen to curium [13], with neutron numbers ranging from 0 to 152. More recently, measurements of charge radii have been extended to nuclei far beyond the β-stability line. The latest CR2021 database includes data for 129 charge radii of nuclei with A $\geq$ 21 and Z $\geq$ 14 [14].

Numerous theoretical methods have been developed to describe and predict charge radii, which can be broadly classified into three major categories: macroscopic, microscopic, and macroscopic-microscopic models. Microscopic models employ effective and realistic interactions to study nuclear structure and properties, including the Hartree–Fock–Bogoliubov (HFB) model, relativistic mean-field (RMF) theory, ab initio calculations, and the cluster model [15–19]. For instance, the HFB21 model achieved high accuracy in predicting charge radii, with an RMS deviation of 0.027 fm for 782 measured charge radii [16]. Traditional macroscopic models rely on phenomenological laws to describe charge radii, including the $A^1/^3$ and $Z^1/^3$ laws [21–25], where A represents the mass number and Z denotes the number of protons. Additionally, nuclear charge radii can be accurately predicted using the Garvey–Kelson relationship, which describes nuclear charge radii based on the relative positions of a given nucleus with respect to other known charge radii [26–28]. Although phenomenological models can accurately describe global trends in nuclear charge radii, they often struggle to reveal the underlying physical quantities within individual nuclei.

Machine learning is widely applied in physics owing to the availability of large datasets and powerful computational hardware. It has proven highly effective for processing complex data, uncovering hidden patterns, and solving stochastic processes. In fields such as high-energy physics and astrophysics that require processing enormous amounts of data, machine learning is essential for analyzing galaxy evolution and morphology and extracting information from high-energy reactions [29–36]. In nuclear physics, machine learning techniques such as artificial neural networks (ANNs) [37], Bayesian neural networks (BNNs) [39–44], and radial basis functions (RBFs) have been used to improve predictions of nuclear properties including nuclear mass, charge radius, and β-decay half-lives [45–52]. Furthermore, convolutional neural networks (CNNs) have been employed to solve problems related to density functional theory [54,55]. Currently, fully connected neural networks are generally used to describe nuclear properties in nuclear physics, but these involve numerous weights and high computational complexity. To mitigate this complexity, we consider a CNN with local connections and weight sharing.

In this paper, we present a novel approach for improving predictions of nuclear charge radii within local charge radius (CR) relations by utilizing a CNN. In Section 2, we provide a brief overview of the theoretical background of local CR relations and the principles of CNNs. In Section 3, we describe the proposed methodology for training a CNN using existing experimental data on nuclear radii. We present the results of our analysis, including the global RMS deviation obtained by the proposed model, and provide relevant discussions and predictions based on the findings. Finally, we summarize the present findings and conclusions of this study, highlighting the potential of CNNs as powerful tools for improving predictions of nuclear charge radii.

II. Theoretical Formalism

The Garvey–Kelson relationship was introduced in 1966 as a method for predicting nuclear masses. Owing to the complexity of the Hamiltonian for a many-body system, the mass of a nucleus cannot be directly calculated from first principles. Instead, the mass of a given nucleus can be accurately inferred from the masses of its neighboring nuclei [57,58]. Similarly, four local CR relations were proposed [27]:

$$\delta R_{in-jp} = 0, \quad i, j = 1, 2,$$

which are based on the charge radii of four neighboring nuclei and are referred to as the 1n−1p, 1n−2p, 2n−1p, and 2n−2p CR relations, respectively, where

$$\delta R_{in-jp} = R(N, Z) + R(N-i, Z-j) - R(N-i, Z) - R(N, Z-j).$$

As reported in Ref. [27], the RMS deviation was 0.0078 fm for all nuclei with N, Z $\geq$ 2. However, the Garvey–Kelson relationships are expressed as local formulas, meaning the radii of neighboring nuclei must be known to obtain the radius of a specific nucleus. Inspired by Refs. [27,28], we aimed to utilize local CR relationships to characterize the global nuclear radius.

When i = 1 and j = 1, $\delta R_{1\ \ 1}$ represents the charge radius relationship between the four nearest neighbor nuclei, and the following four subrelations can be derived:

$$\delta R_{1n-1p} = R(N,Z) + R(N-1,Z-1) - R(N-1,Z) - R(N,Z-1),$$
$$\delta R_{1n-1p} = R(N+1,Z+1) + R(N,Z) - R(N,Z+1) - R(N+1,Z),$$
$$\delta R_{1n-1p} = R(N+1,Z) + R(N,Z-1) - R(N,Z) - R(N+1,Z-1),$$
$$\delta R_{1n-1p} = R(N,Z+1) + R(N-1,Z) - R(N-1,Z+1) - R(N,Z).$$

Therefore, for i, j = 1, 2, we can utilize 16 subrelations to calculate R(N, Z). Subsequently, these 16 subrelations are summed to obtain a radius relation for 25 nuclei, and the 25 nuclear charge radii were reshaped into a 5$×$5 matrix with corresponding coefficients. This local relationship is displayed in Fig. 1 Figure 1: see original paper. Similarly, we considered the local relation of nine nuclear charge radii, as depicted in Fig. 1(b).

CNNs are commonly applied in computer vision [59]. They can identify local features in images using fewer parameters and effectively reduce overfitting. By arranging the charge radii from CR2013 for nuclei with Z $\geq$ 18 (Fig. 1), a 79 $\times$ 153 nuclear charge radius matrix was formed. The coefficient matrix in Fig. 1 is treated as a convolutional kernel in CNNs. The sliding of the convolutional kernel across the matrix forms a convolution process that is crucial for CNNs. The two-dimensional convolution formula is stated as follows:

$$O(u,v) = \sum\sum g(i,j)h(u-i,v-j),$$

where O(u, v) denotes the value of the element at coordinates (u, v) in the output matrix, g(i, j) denotes the value of the element at coordinates (i, j) in the input matrix, and h(u—i, v—j) represents the value of the element at coordinates (u—i, v—j) in the convolution kernel.

The empirical formula developed by Nerlo–Pomorska and Pomorski [23] is:

$$R_c(Z,N,A) = r_0\left[1 - a\frac{N-Z}{A}\right]A^{1/3},$$

where r_0 = 0.9561 fm, a = 0.1426. This three-parameter formula improves the description of the radius of even–even nuclei, with an RMS deviation of 0.0385 fm for nuclei with A $\geq$ 39 and Z $\geq$ 20, which were used as the training set. Since odd-even staggering crucially affects several isotopes, we introduced a δ term into Eq. (7) to obtain:

$$R_c(Z,N,A) = r_0\left[1 - a\frac{N-Z}{A} + b\frac{\delta}{A}\right]A^{1/3},$$

where r_0 = 0.9562 fm, a = 0.1429, b = 2.0825, and c = 0.0694. The parameters were obtained by fitting the training set and the RMS deviation was 0.0385 fm.

Similarly, we constructed a pairing term for δ local relations to describe the odd–even staggering effect of the charge radius for the nuclei portrayed in Fig. 1(c). Considering the characteristics of nuclei near the β-stability line, we added the isospin dependence T, which is also referred to as the NP relation [44]. δ and T are defined as follows:

$$\delta = \frac{(-1)^Z + (-1)^N}{2}, \quad T = \frac{N-Z}{A}.$$

The structure of the neural network is depicted in Fig. 2 [Figure 2: see original paper]. The neural network comprises an input layer, a fully connected layer, a convolutional layer, and two output layers. The input data are the proton number Z, neutron number N, and mass number A of 928 nuclei. The activation function from the input layer to the fully connected layer is Mish(x), expressed as:

$$\mathrm{Mish}(x) = x \cdot \tanh(\ln(1+e^x)).$$

The fully connected layer processes these inputs to generate numerous nuclear charge radii, which are then reshaped into a 79×153 matrix. This matrix serves as input to the convolutional layer. As depicted in Fig. 2, the convolutional layer comprises four components: convolution of the nuclear radius matrix with 5\$$\times 5 CRrelations, 3\times 3 CRrelations, 5\times 5 isospindependence(NPrelations), and 5\times$\$5 delta relations. Thereafter, we assigned each component a weight w and added it to the final output of the neural network. The calculation process for the convolutional layer can be expressed as:

$$f(O) = \sum R(\omega_i O_i) + b,$$

where R(x) represents the activation function, O represents the convolutional result as depicted in Eq. (6), and b denotes the bias. ω and b are the training parameters of the neural network. Finally, we obtain the output of the convolutional neural network. The loss function is consistent with the RMS deviation (σ):

$$\mathrm{Loss} = \sqrt{\frac{1}{m}\sum_{i=1}^{m}(R_{\mathrm{Exp.}} - R_{\mathrm{Cal.}})^2},$$

where R_{Cal.} denotes the neural network predictions and R_{Exp.} denotes the experimental values of the dataset, and m indicates the number of data points.

Table 1 . RMS deviation of training set, validation set, and entire set for Eq. (8) and the proposed neural network (CNN).

Dataset	σEq.(8)	σCNN	Improvement
Training set	[value]	[value]	σEq.(8)$-\sigma$CNN
Validation set	[value]	[value]	σEq.(8)$-\sigma$CNN
Entire set	[value]	[value]	σEq.(8)$-\sigma$CNN

III. Results and Discussions

Based on local CR relations, we propose a neural network containing convolutional layers to study nuclear charge radii. We aimed to explore whether local CR relations could describe global nuclear charge radii and their ability to predict charge radii of unknown nuclei.

In this study, datasets were obtained from CR2013 and CR2021 [13,14]. To test the predictive ability of the neural networks, we selected 814 charge radii data points with $Z \geq 20$ from CR2013 as the training set and 114 charge radii data points from CR2021 as the validation set. The entire set included both training and validation sets, containing 928 nuclear charge radii.

Similar to alternative neural networks [37,38,44], we considered the proton number Z, neutron number N, and mass number A as inputs for the neural network. Owing to the local connection property of the convolutional layer, we must generate nuclear charge radius data through the fully connected layer and arrange them into a matrix of 79 rows and 153 columns. Here, 79 represents the number of protons, ranging from 18 to 96, and 153 represents the number of neutrons, ranging from 0 to 152. When the loss value of the validation set diminishes to a minimum, the generalization of the neural network is optimal. Therefore, we compute the RMS deviation of the entire set for the CNN. The root-mean-square (RMS) deviations for Eq. (8) and the CNN for the training, validation, and entire sets are presented in Table 1. The CNN yielded an RMS deviation of 0.0195 fm for the entire dataset and 0.0156 fm for the validation dataset. Compared to Eq. (8), the entire set is improved by 48% and the accuracy of the validation set significantly improved by 53%.

Subsequently, we provide the radius residuals δR between the experimental values R_{Exp.} and the CNN predictions R_{Cal.}, i.e., δR = R_{Exp.} $-$ R_{Cal.}. The radius residuals δR of 928 nuclei with proton number Z are shown in Fig. 3 [Figure 3: see original paper]. As observed, $|\delta R| \leq 0.04$ fm for the validation set. $|\delta R| \geq 0.06$ fm for certain heavy nuclei in the training set, especially near isotopes of Z = 65 and 80. In Ref. [61], Figure 1 displays significant radius differences for isotopes near N = 60, 90, and Z = 80. Near the N = 60 and 90 regions, the enlarged amplitudes of the radius differences are attributed to heavy nuclei with strong static deformation [62–64]. The abnormal radius difference in the Z = 80 region is due to shape staggering, indicating that the shape of heavy nuclei changes from prolate to oblate, and thereafter back to prolate [61,65,66].

The RMS radii for calcium isotopes from the CNN, Eq. (7), Eq. (8), and experimental data are comparatively presented in Fig. 4 Figure 4: see original paper. The experimental data revealed significant odd–even staggering in the charge radius of calcium isotopes between N = 20 and N = 28, with a pronounced shell effect at N = 28. Although Eq. (8) contains the δ term, it fails to provide a satisfactory description of the experimental data. In addition, the amplitudes of the odd–even staggering calculated by the CNN were smaller than those of the experimental data. Furthermore, CNN calculations indicate an inverted parabolic trend between N = 20 and N = 28 along the calcium isotopic chain [5,67,68]. The current predictions for the radii of ^{38,49,51}Ca isotopes yielded results aligned with available experimental data. The results indicate that the CNN is reliable and provides predictive ability. However, the shell kinks at N = 20 and N = 28, as demonstrated by the CNN, were insignificant. Certain studies have employed the macroscopic-microscopic method, incorporating shell corrections and quadrupole and hexadecapole deformations to achieve shell kinks of calcium isotopic chains [5,67].

As depicted in Fig. 4(b), the CNN fails to accurately reproduce the prominent shell kinks of zirconium isotopes at N = 50, suggesting that accounting for the shell effect may improve the description of nuclear charge radii.

In Ref. [25], a five-parameter formula was proposed that included many physical features such as the shell effect and odd–even staggering, achieving an RMS deviation of 0.023 fm for nuclei with A $\geq$ 40. Recently, Ref. [44] combined pairing and shell effects using a three-parameter formula and BNN to describe nuclear charge radius, achieving an RMS deviation of 0.015 fm for the entire set. In Ref. [53], BNN inputs included four engineered features: the pairing effect, shell effect, isospin effect, and "abnormal" shape staggering effect. The proposed method obtained an RMS deviation of 0.014 fm for the training and validation datasets. The BNN outperformed the CNN for describing the trend of nuclear charge radius, indicating that shell and shape staggering effects can considerably describe the trend of nuclear charge radius [5,60].

The difference between the theoretical results of the CNN and the experimental data for all nuclei in the entire set is shown in Fig. 5 [Figure 5: see original paper]. As observed, the residual of the charge radius of nuclei located near closed shells is less than 0.04 fm, implying that the neural network combined with local CR relations can accurately describe nuclear charge radii.

Fig. 4 [Figure 4: see original paper]. (Color online) Charge radii of (a) calcium and (b) zirconium isotopes predicted by Eq. (7), Eq. (8), and CNN, compared with experimental data.

Fig. 5 [Figure 5: see original paper]. (Color online) Differences between predicted and experimental values of charge radii for 928 nuclei.

IV. Summary

We developed a neural network with a convolutional layer to analyze the nuclear charge radii of 928 nuclei. We incorporated the isospin-dependence T and pairing relations δ into the convolutional layer to account for the physical factors that influence nuclear charge radius. The network model achieved an RMS deviation of 0.0201 fm for nuclei with A $\geq$ 39 and Z $\geq$ 20 in the CR2013 database, and 0.0156 fm for CR2021 as the validation set. The proposed neural network reproduced the trend of nuclear charge radius, especially the shell effect and odd–even staggering in calcium isotopes.

There are limitations to the application of convolutional neural networks for nuclear charge radii. Existing experimental data on nuclear charge radius are limited and scattered. Therefore, we generated data in fully connected layers, such that the regular convolutional kernel in the convolutional layer could act on the data. Presently, graph neural networks and deformable convolutional kernels have offered significant advantages in processing irregular data. Perhaps graph convolutional neural networks (GCNs) could be used to overcome the limitations of nuclear charge radius data.

V. References

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Note: Figure translations are in progress. See original paper for figures.