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Theoretical Study on the Calculation of the Mass of the Nucleus ^{103}Sn

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Abstract

The mass of an atomic nucleus holds significant importance in the fields of nuclear structure and nuclear astrophysics. Accurate mass predictions of radionuclides, which are often challenging to measure experimentally, are crucial for advancing research in these areas. Machine learning, with its ability to process and analyze large datasets effectively, is particularly suited for this task. This study integrates insights from nuclear physics and computer science, employing various machine learning algorithms to predict the mass of the nucleus ^{103}Sn. These algorithms utilize inputs such as the number of protons, neutrons, and other experimental measurements. The objective is to optimize the algorithm for the best-fitting residuals and predictive accuracy. Additionally, the performance of these machine learning models is compared with traditional theoretical nuclear models to highlight differences and potential improvements. This comparative analysis helps in understanding the advantages of using machine learning techniques over conventional methods in nuclear mass predictions.

Keywords

Machine learning, nuclear physics, theoretical calculation

1. Background and Significance

The atomic nucleus is the core material that makes up all visible matter in the universe (including stars, planets, and ourselves), accounting for 99.9% of the mass. The nucleus is a quantum many-body system composed of protons and neutrons (collectively known as nucleons) [1-3]. The mass of a nucleus is the sum of the masses of its constituent nucleons and their interactions (i.e., the binding energy of the nucleus). Since the masses of protons and neutrons have been measured very precisely, accurately measuring or calculating the mass of the nucleus is equivalent to quantitatively studying the binding energy of the nucleus. Among the various properties of the nucleus, mass or binding energy plays an important role in all fields of nuclear physics [4, 5]. Firstly, in fundamental physics, the total binding energy of a nucleus results from the combined effects of the three fundamental forces in nature—strong interaction, electromagnetic interaction, and weak interaction. Therefore, the nucleus serves as an ideal "experimental site" for studying the complex interactions among these three fundamental forces [6]. Secondly, in nuclear structure research, the binding energy difference between neighboring nuclei can be viewed as different-order derivatives of the binding energy with respect to the number of protons or neutrons, providing an effective way to explore various issues such as testing different nuclear mass models [7-9], the disappearance of traditional magic numbers, the emergence of new magic numbers, nucleon pairing condensation, the positions of proton and neutron drip lines, and the Q values involved in various nuclear reactions. Thirdly, in nuclear astrophysics research, the Q values of reactions and nucleon separation energies derived from the binding energy differences of nuclei are essential input quantities for theoretical models calculating β-decay reactions, neutron and proton capture reactions, and equilibrium state nucleosynthesis abundance distributions [10-12].

2. Related Research

Artificial intelligence is currently a hot research direction in statistics, computer science, and data science. Like the steam engine in the steam age, the generator in the electrical age, and the computer and the internet in the information age, artificial intelligence is becoming a decisive force driving humanity into the intelligent age [13-15]. Machine learning, the mainstream method for solving many artificial intelligence problems, is the essence of modern artificial intelligence. Besides its applications in daily life, such as speech recognition, facial recognition, and virtual assistants, artificial intelligence has greatly promoted research in other disciplines. One of the most exciting achievements in advancing scientific progress has occurred in biology: DeepMind's AlphaFold2 artificial intelligence program can accurately predict the three-dimensional folded structure of proteins from their amino acid sequences, far surpassing traditional computer programs in accuracy [16]. Recently, it even predicted 98.5% of human protein structures at once. In 2020, the U.S. Department of Energy released a report titled "A.I. for Science", systematically elaborating on the application prospects of artificial intelligence in various fields of natural science research, with Chapter Five specifically explaining the current applications, challenges, and opportunities of machine learning in nuclear physics experiments and theory [17]. The same year, the U.S. nuclear physics community held the A.I. for Nuclear Physics workshop and published a related review report, further detailing the application prospects of machine learning in the overall tuning of accelerators and detection systems [18], experimental data processing, and theoretical calculations in nuclear physics experiments. Last year, Longgang Pang and others in China published a review article titled "Applications of Deep Learning in Nuclear Physics," introducing the applications of deep learning (currently the most prominent area in machine learning algorithms) in the equation of state of nuclear matter, nuclear structure, nuclear mass, decay, and fission, and demonstrating how to train neural networks to predict nuclear mass [19].

According to the latest Atomic Mass Evaluation (AME) 2020, there are currently 2550 nuclides with precisely measurable masses experimentally [20]. As of 2021, more than 3310 nuclides have been discovered in experiments, and theoretically, the number of existing nuclides exceeds 7000. Figure 1 shows the distribution of nuclear masses and unknown nuclear masses on the nuclide chart in different periods included in the AME. The main reason why the masses of unknown nuclides cannot be directly measured experimentally at present is that the current experimental devices cannot produce them [21]. Accurately predicting the masses of these unmeasured nuclides is of great significance for nuclear structure research and nuclear astrophysics research. Traditionally, theoretical models for predicting nuclear masses can be divided into three categories: macroscopic models mainly represented by the Weizsäcker-Bethe mass formula, macroscopic-microscopic models mainly represented by the finite-range droplet model (FRDM) and the Weizsäcker-Skyrme (WS) model, and microscopic models mainly represented by the Skyrme-Hartree-Fock-Bogoliubov (Skyrme-HFB) mass formula and the relativistic mean-field model. The mass residuals (differences between calculated values and experimental values) obtained from these mass models range from 300 keV to 3 MeV, which is still insufficient for studying issues related to nuclear structure and nuclear astrophysics, especially for neutron-rich nuclides far from the stability line without experimental mass data, where the differences between the predicted values extrapolated from these mass models can reach tens of MeV. Therefore, new theoretical calculation models need to be developed to improve mass prediction accuracy [22].

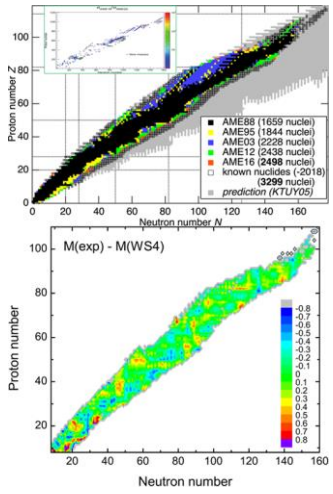

Figure 1. Upper panel: Nuclear masses included in different periods of the AME; the inset in the upper left corner is the update of the latest AME2020. Lower panel: Residuals of nuclear masses fitted by the most accurate WS theoretical model.

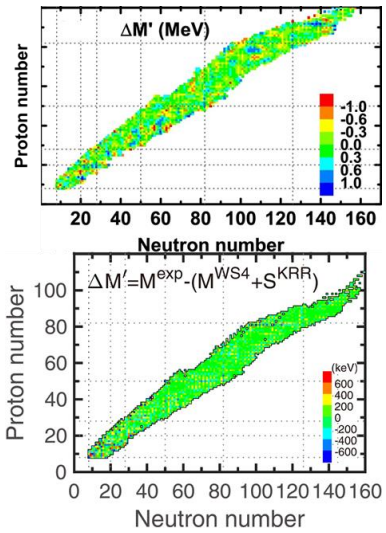

Figure 2. Residuals of nuclear masses fitted by two machine learning algorithms. The upper panel is the result of the BNN algorithm, and the lower panel is the result of the KRR algorithm.

Using machine learning algorithms to predict nuclear masses has rapidly developed in recent years. The main algorithms used are the Bayesian neural network (BNN) method and the kernel ridge regression (KRR) method. The mass residuals obtained by these methods can be reduced to 200 keV, with accuracy superior to that of any traditional theoretical model and better extrapolation capability for unknown nuclide masses. The input variables of these machine learning algorithms are usually the proton number Z and neutron number N (and some other physical quantities constructed through theoretical models), and the output variable is the nuclide mass. The machine learning framework is trained using the experimental mass data evaluated by AME to minimize the mass residuals (without overfitting).

3. Theoretical Calculation

3.1 Introduction to Mixture Density Networks

In a standard feed-forward neural network (NN), the goal is to optimize the complex non-linear mapping between the input feature space x and the output space y, typically represented as $y = f(x)$. This mapping is usually deterministic, not accounting for stochasticity, which makes these networks often struggle to accurately reproduce probabilistic training sets. To address these challenges, especially to account for uncertainties in the training set, we employ a probabilistic machine learning technique called the Mixture Density Network (MDN). MDN describes the output as a mixture of Gaussian functions rather than directly mapping the input to the output.

In MDN, the output $y(x)$ is represented as a weighted sum of multiple Gaussian distributions:

$$y(x) = \sum_{i=1}^{m} \alpha_i(x) \cdot \mathcal{N}\left(\mu_i(x), \sigma_i(x)\right)$$

where $\alpha_i(x), \mu_i(x), \text{and } \sigma_i(x)$ are the weights, means, and standard deviations of each Gaussian distribution, learned by the standard feed-forward neural network. The loss function changes from a simple mean squared error (MSE) estimate to a log-likelihood loss:

$$L = -\ln\left(\sum_{i=1}^{m} \frac{\alpha_i(x)}{(2\pi)^{k/2}\sigma_i(x)} \exp\left(-\frac{\| t - \mu_i(x) \|^2}{2\sigma_i(x)^2}\right)\right)$$

where t is the training output vector, and m is the total number of Gaussian mixtures. This loss function minimizes the difference between the true distribution of the training set and the predicted posterior distribution.

MDN not only represents probabilistic data sets better than traditional deterministic neural networks but also predicts the complete posterior distribution of each value rather than just the mean and standard deviation. The Gaussian mixture model allows us to provide a joint distribution that considers discrepancies in the training set rather than simply averaging

them. This is particularly useful for handling multimodal data.

3.2 Mathematical Formulations and Model Details

The goal of MDN is to optimize the model parameters by minimizing the log-likelihood loss function. Specifically, given a training dataset (x_i, t_i) and model parameters θ, the MDN is trained by minimizing the following loss function:

$$L(\theta) = -\sum_{i=1}^{N} \ln\left(\sum_{j=1}^{m} \alpha_j(x_i;\theta) \cdot \mathcal{N}\left(t_i \mid \mu_j(x_i;\theta), \sigma_j(x_i;\theta)\right)\right)$$

where N is the number of training samples, and $\mathcal{N}$ represents the Gaussian distribution. For each sample $\mathrm{X_i}$, the MDN outputs the parameters of m Gaussian distributions: weights $\alpha_j(x_i;\theta)$, means $\mu_j(x_i;\theta)$, and standard deviations $\sigma_j(x_i;\theta)$.

To ensure that the weights $\alpha_j(x_i;\theta)$ sum to 1, we use the softmax function:

$$\alpha_j(x_i;\theta) = \frac{\exp\left(z_j(x_i;\theta)\right)}{\sum_{k=1}^{m} \exp\left(z_k(x_i;\theta)\right)}$$

where $z_j(x_i;\theta)$ are the unnormalized scores output by the network. The means and standard deviations of the Gaussian distributions are computed through the network's linear layers and nonlinear activation functions:

$$\mu_j(x_i;\theta) = W_{\mu,j} \cdot h(x_i) + b_{\mu_j}$$

$$\sigma_j(x_i;\theta) = \exp\left(W_{\sigma,j} \cdot h(x_i) + b_{\sigma_j}\right)$$

where $W_{\mu,j}$ and $W_{\sigma,j}$ are weight matrices, $b_{\mu,j}$ and $b_{\sigma,j}$ are bias terms, and $h(x_i)$ is the output of the network's hidden layers.

Additionally, to prevent overfitting and improve the model's generalization, we incorporate regularization techniques such as L2 regularization and dropout. L2 regularization is achieved by adding the sum of the squared weight parameters to the loss function:

$$L_{reg}(\theta) = \lambda \sum_{k=1}^{K} \| \theta_k \|^2$$

where λ is the regularization coefficient, and θ_k is the k-th parameter of the model.

3.3 Implementation and Optimization

Our MDN implementation is based on PyTorch and can run on both CPU and GPU. We use the Adam optimizer with a learning rate of 0.001, and the activation function is the hyperbolic tangent (tanh). The weights of the neural network are initialized randomly, and the MDN converges after training for 100,000 epochs.

$$\sigma_{RMS} = \sqrt{\frac{1}{K}\sum_{i=1}^{K}(y_i - \hat{y}_i)^2}$$

To evaluate the model's performance, we use the root mean square error (RMSE): where y_i is the actual value, $\hat{y}_i$ is the predicted value, and K is the number of samples in the test set. Through the aforementioned methods, our MDN model effectively handles the problem of nuclear mass prediction and provides reliable uncertainty quantification.

3.4 Calculating the Mass of ^{103}Sn Using MDN

To calculate the mass of the ^{103}Sn nucleus, we employ the trained MDN model with the feature inputs corresponding to the number of protons (50) and neutrons (53). By feeding these inputs into the MDN, the model outputs the parameters of the Gaussian mixture representing the mass distribution of ^{103}Sn:

Input features for ^{103}Sn:$(Z, N) = (50,53)$

The MDN processes these inputs through its layers to compute the means μ_j, standard deviations σ_j, and weights α_j

of the Gaussian mixtures. The resulting mass prediction $M_{103\mathrm{Sn}}$ is given by the weighted sum of these Gaussians:

$$M_{103\mathrm{Sn}} = \sum_{j=1}^{m} \alpha_j (Z,N) \cdot \mathcal{N}\left(\mu_j(Z,N), \sigma_j(Z,N)\right)$$

This calculation provides not only the predicted mass of ^{103}Sn but also the associated uncertainty, enabling a comprehensive understanding of the prediction's reliability. By leveraging the probabilistic nature of MDN, we achieve a robust and well-quantified prediction for the mass of ^{103}Sn.

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