Optimized Neural Network Models for Accurate Prediction of Proton Separation Energies in Isotopic Chains

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Date: 2025-07-21T00:00:00+00:00

Abstract

Nuclear masses play a crucial role in nuclear structure and nuclear astrophysics. For exotic nuclei far from the valley of stability, a difference of several hundred keV in separation energy derived from masses can lead to variations in half-life of at least three orders of magnitude. Presently, ^{149}Lu constitutes the shortest-lived proton-emitting nucleus accessible to experimental detection; the separation energies of yet-unobserved nuclides in its vicinity will impact the nucleosynthesis pathway. To address this, we have employed Artificial Neural Networks (ANN) and Bayesian Neural Networks (BNN) to constrain proton separation energies, though empirical evidence indicates that these two approaches suffer from overfitting and precision limitations, respectively. To enhance precision and alleviate overfitting, we have developed the BNN-Beihang (BH) model based on the BNN framework, incorporating both label uncertainty and statistical model errors. The proton separation energy uncertainties predicted by this model for $^{148-151}$Lu and ^{160,161}Re have been reduced below 100 keV for the first time, which will effectively constrain the lifetimes of proton-emitting nuclei along the lutetium and rhenium isotopic chains.

Full Text

Preamble

Nuclear Physics Review
Vol. 32, No. 3
July 2025

Article ID: 1007-4627(2025)03-0001-10

Precise Prediction of Proton Separation Energies for Lu and Re Isotopic Chains via Optimized Neural Network Models

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Abstract

Nuclear mass plays a crucial role in nuclear structure and nuclear astrophysics. For exotic nuclei far from the valley of stability, a difference of a few hundred keV in separation energy derived from nuclear masses can lead to variations in half-life spanning at least three orders of magnitude. To date, ^{149}Lu is the shortest-lived proton-emitting nucleus detected experimentally, and the separation energies of neighboring undiscovered nuclides will influence nucleosynthesis pathways. To address this, we employ Artificial Neural Network (ANN) and Bayesian Neural Network (BNN) models to constrain proton separation energies. Practical applications reveal that these two methods suffer from overfitting and precision issues, respectively. To enhance precision and mitigate overfitting, we have developed the BNN-Beihang (BH) model based on the BNN framework, simultaneously accounting for uncertainties in label values and statistical errors of the model. For the first time, the uncertainties in predicted proton separation energies for $^{148-151}$Lu and ^{160},^{161}Re have reached below 100 keV. These results will effectively constrain the lifetimes of proton-emitting nuclei in the Lu and Re isotopic chains.

Keywords: proton separation energy; neural network model; Lu isotopic chain; Re isotopic chain

1. Introduction

The development of radioactive ion beam physics has enabled investigations of exotic properties of unusual nuclei, such as halo-skin structures [**?**, **?**], islands of inversion [**?**, **?**], and new magic numbers [**?**]. For weakly bound nuclei near the drip lines far from the valley of stability, halo nuclei or nucleon emitters may form [**?**], and the decay modes and lifetimes of these nucleon emitters affect nucleosynthesis pathways in astrophysical evolution [**?**, **?**]. Typically, a difference of a few hundred keV in separation energy can lead to at least three orders of magnitude variation in the lifetimes of nucleon emitters [**?**, **?**]. Therefore, precise theoretical predictions of separation energies are essential for understanding astrophysical nucleosynthesis and nuclear decay processes.

To date, ^{149}Lu is the shortest-lived proton emitter observed experimentally [**?**]. Under the assumption of axial deformation, K. Auranen employed a non-adiabatic quasiparticle model to explore the correlation between deformation and lifetime of ^{149}Lu, initially concluding an oblate shape [**?**]. Subsequently, also under axial deformation, we used the deformed relativistic Hartree-Bogoliubov theory in continuum (DRHBc) [**?**] to definitively rule out prolate deformation for ^{149}Lu, and combined it with semiclassical Wenzel-Kramers-Brillouin (WKB) approximations to calculate proton emission half-lives within experimental error ranges [**?**]. More recently, moving beyond the axial deformation framework,

we employed the triaxial relativistic Hartree-Bogoliubov theory in continuum (TRHBc) [?] to recalculate the ground-state binding energy (E_B) of ^{149}Lu, confirming its triaxially deformed ground state. Further combination with WKB approximation yielded proton emission half-lives still within experimental uncertainties [?]. Notably, the physical quantity $\sqrt{2\mu|E-V(r,\theta,\varphi)|}$ appearing in the exponent' s power, where V is the microscopic potential and decay energy E is determined by nuclear mass, is decisive for lifetime. Clearly, a few hundred keV difference in decay energy E can easily cause orders-of-magnitude variations in emitter lifetimes. Consequently, we must maximize the precision of nuclear mass predictions in this region.

Numerous theoretical models describe nuclear masses, including phenomenological models like the Liquid Drop Model (LDM), Duflo-Zuker (DZ) model [?], and microscopic mean-field theories. P. Möller' s Finite-Range Droplet Model (FRDM) achieves a precision of 570 keV [?]. In 1995, Duflo and Zuker used a 28-parameter DZ model to achieve 375 keV precision for 1751 nuclei [?]. Within the non-relativistic density functional theory framework, S. Goriely employed the Skyrme-Hartree-Fock-Bogoliubov (SHFB) method in 2016 to achieve 561 keV precision for 2353 nuclei [?]. In 2010, Zhao Pengwei used covariant density functional theory (CDFT) to achieve 1330 keV precision for 60 nuclei [?]. Currently, the most accurate phenomenological model is the Weizsäcker-Skyrme 4 (WS4) model [?], which achieves 298 keV precision for experimentally measured masses in the Atomic Mass Evaluation 2012 (AME2012) [?] and 474 keV prediction error for all nuclei in AME2020 [?]. However, proton emission problems require mass or separation energy prediction deviations within 100 keV to constrain lifetime uncertainties to 1-2 orders of magnitude. Therefore, to improve model precision, we apply machine learning methods to constrain proton separation energy (S_p).

In recent years, machine learning methods have been widely applied across various dimensions of nuclear physics research due to their powerful fitting capabilities. Neural network models were first used to distinguish nuclear stability [?]. Subsequently, machine learning models predicted other nuclear properties: neural networks for proton separation energies [?]; Support Vector Machines (SVM) for multiple properties (mass, β-decay lifetimes, ground-state spin/parity) [?]; Bayesian Neural Networks (BNN) [?] and Convolutional Neural Networks (CNN) [?] for charge radii; reduced-basis methods to decrease computational cost in few-body systems [?]; Variational Autoencoders (VAE) [?] and Ensemble Learning [?] for neutron star equation of state inference; VAE for constructing collective variables in many-fermion systems [?]. Interpretable machine learning models like SHapley Additive exPlanation (SHAP) [?] have been used to assess input feature importance [?, ?].

Recently, machine learning models have been extensively applied to predict high-precision nuclear masses. Decision trees [?] and Light Gradient Boosting Machine (LightGBM) [?] based on decision trees offer good fitting performance without easy overfitting. Kernel Ridge Regression (KRR) mitigates overfitting

in nonlinear problems [**?**, **?**] but is computationally expensive for small datasets. Symbolic Regression (SR) provides analytical expressions for predictions with better interpretability [**?**]. Multi-layer Perceptron [**?**, **?**], Artificial Neural Networks (ANN) [**?**, **?**], Kolmogorov-Arnold Networks (KAN) [**?**], and Radial Basis Functions (RBF) [**?**] demonstrate strong fitting and generalization capabilities.

However, these models only provide single predictions without uncertainty estimates. In contrast, Gaussian Process (GP) [**?**, **?**], BNN [**?**], and Mixture Density Network (MDN) [**?**, **?**] offer strong fitting capabilities with predictive distributions. MDN still suffers from overfitting, while GP' s high time complexity makes it unsuitable for large datasets. Therefore, we adopt BNN models to predict proton separation energies.

Machine learning approaches can be categorized by prediction target: fitting experimental values (or traditional theoretical predictions) versus fitting residuals (differences between theoretical predictions and experimental values). Fitting experimental values requires no assumptions but yields lower precision, while residual-fitting models achieve higher precision but depend on physical models. Among experimental-value fitting models, the ANN model achieves 260 keV test-set precision with appropriate features and Garvey-Kelson (GK) relation constraints [**?**, **?**], effectively mitigating overfitting and representing the current best practice [**?**]. Among residual-fitting models, Bayesian Machine Learning (BML) achieves 84 keV precision [**?**], and CNN models reach 70 keV [**?**]. Although these residual-fitting models are precise, they still exhibit overfitting issues.

In reality, existing models face a trade-off between precision and overfitting. Overfitting means models fit training data well but extrapolate poorly. For instance, BML models show significantly larger uncertainties for nuclei far from the β-stability line compared to those near it. The optimal phenomenological WS4 model achieves ~468 keV precision for all nuclei in AME2016 [**?**] but only ~1295 keV for newly introduced nuclei in AME2020—a nearly threefold difference. Therefore, we need a machine learning model balancing precision and overfitting.

This work aims to construct a machine learning model with high prediction precision and minimal overfitting for Lu and Re isotopic chains. The paper comprises three parts: Section 1 introduces the theoretical frameworks of ANN and BNN models; Section 2 presents computational details and results, analyzing issues with ANN and BNN models, combining their advantages to propose an improved BNN-Beihang (BH) model, and evaluating its predictive performance for Lu and Re isotopic chains; Section 3 provides summary and outlook.

1.1 Artificial Neural Network (ANN)

As shown in Figure 1 [Figure 1: see original paper], the ANN model consists of an input layer, several hidden layers, and an output layer. Adjacent layers L1 and L2 are connected via parameter matrix W and bias vector b: $L2 = f(W \times L1 + b)$. The nonlinear activation function f enhances fitting capability. Here, we select

Gaussian Error Linear Unit (GELU) [**?**] as the activation function.

Model precision is evaluated using root mean square deviation (RMSD): $\sigma_{\text{rms}} = \sqrt{\frac{\sum_i (O_i - L_i)^2}{N}}$, where O represents model predictions, L represents label values, and N is the dataset size. Overfitting is assessed using the ratio $r_{\text{set}} = \sigma_{\text{rms}}^{\text{test}} / \sigma_{\text{rms}}^{\text{train}}$ between test-set and training-set RMSD. We consider $r_{\text{set}} < 1.1$ as slight overfitting, > 1.1 as obvious overfitting, > 1.5 as severe overfitting, and > 2 as very severe overfitting.

The loss function measures differences between predictions and labels. For input vector I, the model produces output vector O. The loss function $LOSS(O, L)$ is determined by O and label L, with parameters updated via the backpropagation algorithm (BP) [**?**]. Model training iterates this process from input to parameter update. The Adam optimization algorithm [**?**] ensures good convergence speed.

Parameter update magnitude is characterized by the learning rate. Excessively large learning rates cause oscillation and poor convergence, while overly small rates slow convergence. Thus, learning rate selection must balance speed and precision. If pre-update parameters are w, backpropagation yields gradient δw, then updated parameters become $w' = w - \delta w \times l_r$, where l_r is the learning rate.

To ensure parameter updates in deep networks, Xavier initialization [**?**] sets initial ANN parameters before training. Different random seeds for Xavier initialization lead to different random number selections, resulting in different model parameters and prediction variations.

1.2 Bayesian Neural Network (BNN)

Unlike ANN, BNN represents each parameter as a probability distribution, making outputs probabilistic distributions. Typically, Gaussian distributions $N(\mu, \sigma)$ represent model parameters, doubling the parameter count compared to ANN.

In BNN training and prediction, multiple random samplings from each parameter' s Gaussian distribution $N(\mu, \sigma)$ yield predictions O_1, O_2, etc., enabling calculation of mean $\bar{O}$ and uncertainty σ_O. To ensure reproducibility, random sampling requires seed setting. While seeds affect both ANN and BNN predictions, the difference lies in: for ANN, seeds determine initial parameters via Xavier initialization; for BNN, seeds cause output variations through random parameter sampling.

The loss function incorporates Kullback-Leibler (KL) divergence: $LOSS_{\text{BNN}} = Loss(\bar{O}, L) + 0.01 D_{KL}$, where $Loss(\bar{O}, L)$ measures loss between prediction mean $\bar{O}$ and label L, and $D_{KL}(p||q) = \int p(x) \log[p(x)/q(x)]dx$ evaluates divergence between predictive distribution q and prior distribution p. Training proceeds identically to ANN.

2. Computational Details and Results

2.1 ANN7 Model Fitting Residuals

The ANN7 model' s training labels are residuals, defined as differences between theoretical predictions and experimental values: $\Delta S_p = S_p^{\text{Theory}} - S_p^{\text{Exp}}$, where S_p^{Theory} uses WS4 model predictions and S_p^{Exp} are experimental values from the National Nuclear Data Center (NNDC) [**?**].

Data selection matches the WS4 model scope ($Z, N \geq 8$), totaling 3287 nuclei. Randomly selecting 70% as training set and 30% as test set is denoted sub70. The neural network architecture is (7,32,16,1) (input layer $L1$ with 7 nodes, hidden layers $L2$ and $L3$ with 32 and 16 nodes, output layer $L4$ with 1 node). The ANN7 model uses $L1$ loss function defined as $\sum_i |O_i - L_i|$. The learning rate is 0.001.

To assess ANN7 overfitting, we select the training result with minimum test-set RMSD as final, shown in Table 1 . Training-set RMSD ranges between 180-200 keV, test-set RMSD between 210-220 keV, with $r_{\text{set}} \geq 1.14$ indicating obvious overfitting. Predicted RMSD for Lu isotopic chain distributes mainly between 100-150 keV. The model with seed=30 describes the Lu chain best. Unless specified otherwise, subsequent discussions use seed=30 ANN7 results. Attempts to fit E_B yielded $r_{\text{set}} \approx 2$, indicating more severe overfitting.

To examine seed effects, we predict Lu isotopic chain S_p deviations using residual-fitting ANN7 models, as shown in Figure 2 [Figure 2: see original paper]. Different seed initializations produce considerable prediction fluctuations for the same nuclide, exceeding 100 keV for some nuclei, indicating significant statistical errors.

2.2 BNN Model Fitting Experimental Values

Since experimental error information may be overlearned by ANN models, causing overfitting, we introduce BNN models fitting experimental values (using NNDC S_p data as labels). BNN' s advantage lies in providing probability distributions for each prediction, effectively mitigating overfitting.

We evaluate BNN models from precision and overfitting perspectives, calculating training-set, test-set, and Lu chain RMSD values, shown in Table 2 . Although these BNN models' RMSD precision is inferior to ANN7, the <32-32> architecture reduces r_{set} below 1.14, less than residual-fitting ANN7, effectively mitigating overfitting. Two hidden layers perform better than one hidden layer and better than residual-fitting ANN7 in overfitting mitigation. However, the Lu chain S_p description precision of ~300 keV remains below expectations.

2.3 Improved BNN-BH Model

While BNN models effectively mitigate overfitting, their precision fitting experimental values is insufficient. Below, we improve precision by fitting residuals

based on BNN models, seeking solutions to overfitting. First, since label uncertainties are an overfitting source, we incorporate them into the BNN model to mitigate overfitting. Second, by examining multiple physical quantities, the model can learn more information—we adopt simultaneous fitting of E_B and S_p. Third, considering that BNN uncertainties represent only part of the total error, we incorporate additional error sources. Thus, besides BNN uncertainty, we also consider statistical errors, yielding the improved BNN-BH model.

For the first point, we incorporate label uncertainties as weights into the loss function. Specifically, we multiply prediction-label differences by the inverse of experimental uncertainties $1/\sigma_{\mathrm{Exp}}$ to increase high-precision labels' influence during training, thereby mitigating overfitting. To avoid the pitfall of excessively small uncertainties preventing the model from learning all samples, we set uncertainties below 20 keV to 20 keV.

For the second point, besides simultaneously fitting E_B and S_p, we expand residual sources to five mass models. We train residuals for E_B and S_p from five mass models (WS4, BW2 [**?**], FRDM2012 [**?**], KTUY05 [**?**], and RMF [**?**]), with experimental values from AME2020 and NNDC. This reduces the total dataset to 3056 nuclei covered by all five models and experimental values. BNN-BH model integrates predictions and uncertainties from all five models into a unified weighted average:

$$O(Z,N) = \frac{\sum_{i=1}^{n_{\mathrm{model}}} O_i(Z,N)/\sigma_i^2(Z,N)}{\sum_{i=1}^{n_{\mathrm{model}}} 1/\sigma_i^2(Z,N)}$$

where O_i and σ_i are BNN-BH predictions and uncertainties for the i-th mass model' s label L_i, with $n_{\mathrm{model}} = 5$.

For the third point, error sources are not unique. Besides BNN model uncertainty σ_{BNN}, we must consider statistical error σ_{stat}. Total uncertainty σ_{total} combines both:

$$\sigma_{\mathrm{total}} = \chi_\nu \sqrt{\sigma_{\mathrm{BNN}}^2 + \sigma_{\mathrm{stat}}^2}$$

where χ_ν is an uncertainty scaling factor:

$$\chi_\nu = \sqrt{\frac{\sum_i (O_i - L_i)^2}{\sum_i \sigma_{\mathrm{mix},i}^2}}$$

The summation only traverses isotopic chains requiring prediction. Here, σ_{mix} is mixed error defined as $\sigma_{\mathrm{mix}}^2 = \sigma_{\mathrm{stat}}^2 + \sigma_{\mathrm{BNN}}^2$.

To obtain model prediction uncertainty σ_{BNN}, we construct 20 BNN models with (7,32,16,10) architecture, initialize sampling with 20 different seeds, and train them. For each nucleus, these models yield 20 different mean values S_p^{seed}

and uncertainties σ_{seed}. Using equations (1) and (2), we integrate the 20 predictions and uncertainties into weighted average S_p^{BNN} and uncertainty σ_{BNN}. We further consider statistical error σ_{stat}, which includes only differences in model predictions caused by different seed initializations:

$$\sigma_{\text{stat}} = \sqrt{\frac{\sum_{\text{seed}}(S_p^{\text{seed}} - S_p^{\text{BNN}})^2}{N_{\text{seed}} - 1}}$$

This improved BNN-BH model offers two advantages: first, it accounts for more comprehensive error sources, including both model prediction uncertainty σ_{BNN} and statistical error σ_{stat}; second, by restricting χ_ν calculation to local nuclei, it achieves more accurate uncertainty predictions for S_p in that region.

Given the importance of recently discovered ^{149}Lu in nuclear structure and astrophysics, and that neighboring ^{148}Lu will be the next proton emission candidate, we predict S_p for $^{148-151}$Lu using the newly developed BNN-BH model, as shown in Table 3 . The BNN-BH predictions agree well with experimental values for ^{149}Lu and ^{151}Lu. While the deviation for ^{150}Lu is larger, it shows significant improvement over BML model deviations (Figure 3 [Figure 3: see original paper]). Moreover, the predicted uncertainties for the four nuclei from ^{148}Lu to ^{151}Lu are similar, without dramatic increase due to extrapolation distance, indicating stable extrapolation capability of BNN-BH for Lu isotopes near the proton drip line.

The best current model providing uncertainties is the BML model, which serves as a reference for evaluating BNN-BH effectiveness. Figure 3 [Figure 3: see original paper] shows deviations of BNN-BH and BML predictions for Lu chain S_p. Among 38 Lu isotopes, 10 have BNN-BH predictions deviating between 1σ and 2σ, demonstrating credible uncertainty estimation (orange shaded region in Figure 3). For undiscovered ^{148}Lu, BNN-BH predicts S_p uncertainty of 98.44 keV, below 100 keV. Furthermore, BNN-BH' s S_p predictions for Lu chain yield $\sigma_{\text{rms}} = 97.65$ keV, similar to the uncertainty for undiscovered ^{148}Lu, indicating stable extrapolation. Thus, BNN-BH achieves high precision for Lu chain with stable extrapolation to unknown ^{148}Lu, outperforming BML model (blue shaded region in Figure 3) in extrapolation stability.

Since experimental-value fitting BNN models are less precise than residual-fitting ANN7 models, we compare improved BNN-BH with ANN7 using Lu chain, as shown in Table 4 . While RMSD differences on training and test sets are small, BNN-BH' s smaller r_{set} indicates more effective overfitting mitigation. ANN7 RMSD exceeds 100 keV, whereas BNN-BH RMSD falls below 100 keV. Thus, BNN-BH outperforms ANN7 in both overfitting mitigation and precision improvement.

To demonstrate BNN-BH feasibility, we systematically analyze Lu chain and neighboring nuclei, using Re isotopic chain ($Z = 75$) as an example. Figure 4 [Figure 4: see original paper] shows S_p deviations for Re chain. Near the

proton drip line, for proton-emitting nuclei ^{160},^{161}Re, BML uncertainties expand to nearly 400 keV, while BNN-BH uncertainties are 86.9 keV and 81.2 keV, respectively—both below 100 keV—and well cover experimental values. This demonstrates BNN-BH's capability to accurately predict proton-emitting nuclei in the Re isotopic chain.

3. Summary and Outlook

Residual-fitting ANN7 models and experimental-value fitting BNN models suffer from overfitting and precision issues, respectively. To address both, we developed the improved BNN-BH model by comprehensively considering label uncertainties and model statistical errors. Practical applications demonstrate these improvements are effective. For the first time, this model achieves prediction uncertainties below 100 keV for undiscovered ^{148}Lu and measured proton-emitting nuclei ^{160},^{161}Re (98.44 keV, 86.9 keV, and 81.2 keV), significantly lower than BML model. This provides effective theoretical support for subsequent lifetime estimates of proton-emitting nuclei in Lu and Re isotopic chains and nearby regions.

Acknowledgments: We thank Prof. Geng Lisheng for discussions on statistical errors and Prof. Niu Zhongming for discussions on BNN model error analysis.

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