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Abstract

This work employs the radial basis function (RBF) method to optimize the accuracy of the Garvey-Kelson local mass relations (GK) and their generalized formulas (GKs and GK+J) in nuclear mass description and prediction. Extensive numerical experiments demonstrate that when reconstructing the prediction deviations of local mass relations, the radial basis function method can achieve high-quality reconstruction of the deviation function and significantly improve the model' s mass prediction capability by utilizing only reference nuclei at a fixed distance around the target nucleus for correction. Based on the known nuclear mass data from AME2003, AME2012, and AME2020, the method in this work can reduce the root-mean-square deviation of the prediction results for the three local mass relations by 17, 16, and 539 keV on average, respectively. The method also exhibits optimization effects for different local mass relations in extrapolation scenarios. This work presents the predicted mass excess values for 19 nuclei most recently measured experimentally after AME2020: 65Cr, 68,69Fe, 74,75Ni, 60Ga, 103Sr, 80Zr, 120Rh, 99,133,134In, 103Sn, 152−154Ce, 150,153Yb, and 251No, among which the prediction accuracy for 12 nuclides is better than that in AME2020.

Full Text

Preamble

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Study on Nuclear Mass by Combining Radial Basis Function Method and Local Mass Relations

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Abstract

This paper employs the radial basis function (RBF) method to optimize the accuracy of the Garvey-Kelson local mass relation (GK) and its generalized formulas (GKs and GK+J) in describing and predicting nuclear masses. Extensive numerical experiments demonstrate that when the RBF method reconstructs the prediction deviations of local mass relations using only reference nuclei at a fixed distance from the target nucleus, it can reconstruct the deviation function with high quality and significantly improve the model' s mass prediction capability. Based on the known nuclear mass data from AME2003, AME2012, and AME2020, our approach reduces the root-mean-square deviation of the predicted results from the three local mass relations by an average of 17 keV, 16 keV, and 539 keV, respectively. The optimization effect is also observed for different local mass relations in extrapolation scenarios. This paper presents mass excess predictions for 19 nuclei measured in experiments after AME2020: ^{65}Cr, ^{68},^{69}Fe, ^{74},^{75}Ni, ^{60}Ga, ^{103}Sr, ^{80}Zr, ^{120}Rh, ^{99},^{133},^{134}In, ^{103}Sn, $^{152-154}$Ce, ^{150},^{153}Yb, and ^{251}No. Among these, the prediction accuracy for 12 nuclides surpasses that of AME2020.

Keywords: nuclear mass; radial basis function method; local mass relation
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1. Introduction

Nuclear mass is a fundamental physical quantity for describing atomic nuclei and plays a crucial role in nuclear physics, astrophysics, and cosmology. Over the past few decades, experimental measurements of nuclear masses have made significant progress. The latest Atomic Mass Evaluation (AME) data table, AME2020, includes approximately 2,500 nuclides with known masses. Research in astrophysics on stellar evolution and nucleosynthesis processes requires calculations of complex nuclear reactions and energy release mechanisms, involving thousands of nuclei far from the β-stability line. However, due to experimental limitations, many of these masses in unstable regions cannot be measured in the short term and must rely on theoretical predictions. Consequently, developing more accurate nuclear mass prediction models remains a key focus in nuclear structure physics.

Current theoretical models for nuclear masses include global mass formulas such as the Finite-Range Droplet Model (FRDM), the Duflo-Zuker (DZ) model, Skyrme-Hartree-Fock-Bogoliubov (HFB) theory, the improved Weizsäcker-Skyrme mass formula (WS), and relativistic density functional theory descriptions. These models are called global mass formulas because their parameters are primarily obtained by fitting mass data and can be applied

across the entire nuclear chart. In contrast, local mass relations consider local interactions and correlations between neighboring nuclear masses, including methods like the Audi-Wapstra extrapolation, the δV mass relation based on proton-neutron (p-n) interactions, the Garvey-Kelson local mass relation (GK) and its generalized form (GKs), the GK+J formula combining Jänecke' s formula with GK, the Isobaric Multiplet Mass Equation (IMME), and mirror nucleus mass formulas. Global and local mass formulas complement each other: global theories reflect systematic variations in nuclear ground-state properties and excel at describing and predicting ground-state physical quantities in regions far from known experimental data, while local formulas emphasize localized features of nuclear ground-state properties based on experimental data and perform well in describing regions with known experimental data.

In recent years, with advances in numerical algorithms and computational power, machine learning has been widely applied in nuclear physics, particularly in low-energy nuclear physics involving nuclear structure, reactions, and matter properties. Compared to traditional physics research methods, machine learning offers stronger capabilities in complex data analysis, model prediction and fitting, and system modeling. It can discover underlying patterns and trends from known experimental data, providing researchers with an accurate and efficient tool for studying nuclear structure, mass prediction, and reaction simulations, thereby improving efficiency in handling multi-parameter problems and offering support for explaining and predicting complex nuclear physics problems. Bayesian Neural Networks (BNN) have been applied to nuclear masses, charge radii, and β-decay half-lives. Other methods including the Levenberg-Marquardt neural network, Gaussian processes, decision tree algorithms, Multilayer Perceptron (MLP), and Light Gradient Boosting Machine (LightGBM) have also been used to improve global mass models in the nuclear mass domain. Additionally, the radial basis function (RBF) method has been introduced to describe and predict nuclear masses, proving highly effective in improving agreement between theoretical predictions from global mass models and experimental values. An improved RBF method considering systematic odd-even effects has also been proposed.

The purpose of this paper is to improve the description and prediction capabilities of local mass relations using the RBF method. Currently, there is limited work on applying RBF to local mass relations. We focus on investigating the RBF method' s ability to correct predictions from three local mass relations—GK, GKs, and GK+J—and discuss the performance of the RBF-corrected mass prediction models on the latest experimental data. The results demonstrate that RBF provides notable optimization for these three local mass relations.

2. Methods and Numerical Details

The radial basis function method is a machine learning approach that uses the distance between target and sample points as variables, constructing theoretical models through weighted radial basis functions. Its goal is to extrapolate

and fit functions among discrete sample data points—building an approximate function S(x) from numerous discrete sample data points for interpolation or arbitrary approximation. This can be viewed as a curve fitting or function approximation problem in high-dimensional space, where the learning process is equivalent to finding an optimal fitting surface in multidimensional space, and its generalization capability corresponds to using this surface for interpolating input data.

The RBF solution is typically written as:

$$S(x) = \sum_{i=1}^{m} \phi(\|x - x_i\|) w_i,$$

where x represents the position of the target nucleus, x is the reference nucleus position, w corresponds to the weight factor for reference nucleus x , ϕ is the radial basis function, and m is the number of reference nuclei. The "distance" r between target and reference nuclei is defined using the Euclidean norm:

$$r = \|x - x_i\| = \sqrt{(N - N_i)^2 + (Z - Z_i)^2},$$

where N and Z are the neutron and proton numbers of the nucleus, respectively.

Given m reference nuclei (x , d), where d = M - M represents the deviation between experimental mass data and theoretical predictions for reference nucleus i, the RBF solution—a smooth deviation reconstruction function S(x)—should satisfy S(x) = d at reference nucleus positions, expressed as:

$$\begin{pmatrix} \phi_{11} & \phi_{12} & \cdots & \phi_{1m} \\ \phi_{21} & \phi_{22} & \cdots & \phi_{2m} \\ \vdots & \vdots & \ddots & \vdots \\ \phi_{m1} & \phi_{m2} & \cdots & \phi_{mm} \end{pmatrix} \begin{pmatrix} w_1 \\ w_2 \\ \vdots \\ w_m \end{pmatrix} = \begin{pmatrix} d_1 \\ d_2 \\ \vdots \\ d_m \end{pmatrix},$$

where ϕ = ϕ(‖x - x ‖) (i, j = 1, 2, ···, m). From this equation, the weights can be obtained as:

$$\begin{pmatrix} w_1 \\ w_2 \\ \vdots \\ w_m \end{pmatrix} = \begin{pmatrix} \phi_{11} & \phi_{12} & \cdots & \phi_{1m} \\ \phi_{21} & \phi_{22} & \cdots & \phi_{2m} \\ \vdots & \vdots & \ddots & \vdots \\ \phi_{m1} & \phi_{m2} & \cdots & \phi_{mm} \end{pmatrix}^{-1} \begin{pmatrix} d_1 \\ d_2 \\ \vdots \\ d_m \end{pmatrix}.$$

Once the weights w are calculated, the RBF reconstruction of the mass prediction deviation for the target nucleus can be obtained through equation (1). Using this approximate value to replace the target nucleus deviation, i.e., S(N, Z) d(N, Z) = M (N, Z) - M (N, Z), the RBF predicted value is M (N, Z) = M (N, Z) + S(N, Z).

For known nuclei (where the target nucleus has experimentally measured mass data), the distance from itself is r = 0, so the remaining reference nuclei must be used to calculate weights. Let the k-th nucleus be the target nucleus, define $d^{(\ )} = (d_1, d_2, \cdots, d_{\ 1}, d_{\ 1}, \cdots, d\ )$ and $w^{(\ )} = (w_1, w_2, \cdots, w_{\ 1}, w_{\ 1}, \cdots, w\ )$, which removes the target nucleus element from the m mass-known reference nuclei. Similarly, the radial basis function matrix is:

$$\phi^{(k)} = \begin{pmatrix} \phi_{11} & \cdots & \phi_{1,k-1} & \phi_{1,k+1} & \cdots & \phi_{1m} \\ \phi_{21} & \cdots & \phi_{2,k-1} & \phi_{2,k+1} & \cdots & \phi_{2m} \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ \phi_{k-1,1} & \cdots & \phi_{k-1,k-1} & \phi_{k-1,k+1} & \cdots & \phi_{k-1,m} \\ \phi_{k+1,1} & \cdots & \phi_{k+1,k-1} & \phi_{k+1,k+1} & \cdots & \phi_{k+1,m} \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ \phi_{m1} & \cdots & \phi_{m,k-1} & \phi_{m,k+1} & \cdots & \phi_{mm} \end{pmatrix},$$

which removes the k-th row and k-th column from the original m×m ϕ matrix. The reconstructed deviation for the target nucleus mass is obtained through $S(x\ ) =\ _1, \neq\ \phi(\|x\ -\ x\ \|)w^{(\ )}$, yielding $M\ \ (x\ ) = M\ \ (x\ ) + S(x\ )$.

The RBF results typically depend only on the selection of reference nuclei, distance, and basis function definition, exhibiting certain local characteristics. This paper includes all experimentally known nuclear mass data in the reference nucleus selection. If only reference nuclei with experimental errors less than 100 keV are considered, the number of nuclei that can be predicted through extrapolation would decrease significantly (by approximately 13%–52%), but the prediction accuracy would not improve noticeably. Furthermore, since $\phi(r) =$ r better reconstructs mass deviations compared to other basis functions, it is adopted in this work.

3. Results and Analysis

This section describes and predicts nuclear masses based on the AME2003, AME2012, and AME2020 datasets combined with the RBF method and local mass relations GK, GKs, and GK+J.

We first investigated the RBF optimization capability on nuclei with known masses. By controlling distance r to adjust reference nucleus positions, we examined three cases: $1 \leq r \leq R\ $, $R\ \ \leq r$ (with no limit on $R\ $), and $r = R$. Through extensive numerical experiments, we found that using r = R (i.e., utilizing only reference nuclei at a fixed distance from the target nucleus during the process) yields optimal RBF correction for each local mass relation at a specific distance R, as shown in [Figure 1: see original paper] and . The results in [Figure 1: see original paper] and are based on nuclear mass data with $A \geq 16$ from the three AME datasets. σ_0 represents the root-mean-square deviation of local mass relation predictions, while σ denotes the root-mean-square deviation after RBF correction at fixed distance R, defined as:

$$\sigma_0 = \sqrt{\frac{1}{\mathcal{N}}\sum_{i=1}^{\mathcal{N}}(M_i^{\mathrm{expt}} - M_i^{\mathrm{th}})^2},$$

$$\sigma_R = \sqrt{\frac{1}{\mathcal{N}}\sum_{i=1}^{\mathcal{N}}(M_i^{\mathrm{expt}} - M_i^{\mathrm{RBF}})^2},$$

where is the total number of nuclei for which local mass relations can provide mass predictions. The ratio σ /σ_0 reflects the overall optimization capability of the RBF method on mass prediction models; when σ $<$ 1, the RBF method provides clear overall improvement. $\Delta = \sigma_0$ - σ represents the change in root-mean-square deviation after RBF correction, and a positive Δ indicates significant improvement in prediction capability.

As shown, at r = $\sqrt{5}$, RBF correction reduces the root-mean-square deviation of GK on known nuclei by 23 keV, 13 keV, and 16 keV (averaging 17 keV) across the three AME datasets, demonstrating stable optimization capability. At r = 2$\sqrt{2}$, RBF correction reduces the GKs root-mean-square deviation by 16 keV, 19 keV, and 14 keV (averaging 16 keV). At r = 1, GK+J with RBF correction achieves optimal mass prediction, with root-mean-square deviations decreasing by 481 keV, 531 keV, and 605 keV (averaging 539 keV). Notably, the RBF correction effect is more pronounced in the light nuclear region with 16 $\leq$ A $\leq$ 60, where root-mean-square deviations decrease by averages of 35 keV, 57 keV, and 1558 keV, respectively.

[Figure 2: see original paper] illustrates the reconstruction of prediction deviations for the three local mass relations using the RBF method at the distances discussed above. Blue solid circles represent the reconstruction function S(N, Z) obtained through RBF, while gray squares show deviations between local mass relation predictions and experimental data. According to the methodology, the closer the RBF correction value S is to the deviation d, the closer the RBF prediction is to the true experimental mass. The degree of overlap between different colored blocks demonstrates that the RBF method can reconstruct mass prediction deviations of local relations with high quality. In the light mass region (16 $\leq$ A $\leq$ 60), there is modest fitting between RBF corrections and deviations for some nuclides, but the model' s prediction deviations are generally larger in this region, resulting in more significant reduction of root-mean-square deviation (correspondingly larger Δ). In the heavy nuclear region, the fitting between RBF corrections and deviations is excellent, though the model' s mass predictions are already quite accurate, yielding less dramatic optimization.

Beyond studying known nuclear data, we further investigated the extrapolation capability of local mass relations in unknown regions using the RBF method, specifically examining extrapolation from AME2003 to AME2012 and from AME2012 to AME2020. The AME2003 to AME2012 period added 225 new experimental mass data points, while AME2012 to AME2020 added 129. The

detailed results are presented in and [Figure 3: see original paper]. The definitions of σ , σ_0, and in are consistent with , and calculations involve only nuclei with mass number A $\geq$ 16. [Figure 3: see original paper] shows the reconstruction of prediction deviations during extrapolation for the three local mass relations, similar to [Figure 2: see original paper].

As shown in , the RBF method provides overall optimization for the extrapolation capability of the three local mass relations. The optimization is most effective for GK+J, with the root-mean-square deviation decreasing by an average of 1196 keV after RBF correction, and the reconstruction in [FIGURE:3(c)] shows the highest fitting degree. The overlap in [FIGURE:3(a)] and [FIGURE:3(b)] is comparable, but RBF provides positive optimization for GK, reducing the root-mean-square deviation by an average of 44 keV. The optimization effect for GKs+RBF is less pronounced, performing poorly in the AME2012 to AME2020 extrapolation because, although the overlap in [FIGURE:3(b)] is high, there are cases where reconstructed values have opposite signs to actual deviations, causing the root-mean-square deviation to increase by 39 keV after RBF correction. This indicates that the systematic deviation of the GKs model differs from that of GK and GK+J, warranting further investigation.

After AME2020, experimental mass excess data for over one hundred nuclei were measured. Three local mass relations can predict 19 of these through single-step extrapolation from AME2020 known data: ^{65}Cr, ^{68},^{69}Fe, ^{74},^{75}Ni, ^{60}Ga, ^{103}Sr, ^{80}Zr, ^{120}Rh, ^{99},^{133},^{134}In, ^{103}Sn, $^{152-154}$Ce, ^{150},^{153}Yb, and ^{251}No. Using the RBF method to correct GK, GKs, and GK+J, we obtained RBF predictions for the three local mass relations, presented in [Figure 4: see original paper] and . The vertical axis in the figure shows deviations between predicted mass excess values and experimental data. Predictions from the three local mass relations are represented by circles, diamonds, and triangles, respectively, while theoretical predictions adopted in the AME2020 evaluation are marked with asterisks, and experimental values are shown as red stars. If a particular local mass relation cannot provide a mass excess prediction for a given nucleus, no corresponding symbol appears in that subplot. The values with smallest deviation from experimental mass among the three RBF predictions are designated as "best predicted values" and compiled in column 2 of .

The results show that among the 19 newly measured nuclides, 12 have prediction accuracy better than the reference data provided in AME2020: ^{68}Fe, ^{69}Fe, ^{74}Ni, ^{75}Ni, ^{60}Ga, ^{99}In, ^{103}Sn, ^{152}Ce, ^{153}Ce, ^{154}Ce, ^{150}Yb, and ^{153}Yb (marked in bold in). Notably, the mass excess predictions for ^{99}In, ^{103}Sn, and ^{153}Yb fall within the error limits given in the latest experimental literature. The overall root-mean-square deviation of our results relative to the latest experimental data for all 19 nuclei is 197 keV, while for the 12 well-predicted nuclei it is only 116 keV, representing a 93 keV improvement over the reference values given in AME2020.

4. Summary and Discussion

This paper primarily investigates the optimization of local mass relations using the radial basis function method and the predictive capability of the corrected models. Through extensive numerical experiments, we find that the RBF method can significantly improve the prediction ability of local mass relations at specific distances. The optimization for describing known nuclei is stable and effective, reducing the root-mean-square deviations of the three local mass relations by averages of 17 keV, 16 keV, and 539 keV, respectively. Validation results under extrapolation conditions further demonstrate the effectiveness of the RBF method, which also proves competitive in predicting the latest experimental data, reducing the root-mean-square deviation by 93 keV for 12 nuclei compared to AME2020.

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