

The study of Nuclear Mass Model by Sequential Least Squares Programming

Authors: Yang, Mr. Hang, Cunyu Chen, Xu, Xiao Yu, Jalili, Dr. Amir, Wang, Dr. Han Kui, Wang, You-Bao, Yang, Hang, Chen, Cunyu, Ms. Xiao Yu Xu, Jalili, Dr. Amir, Wang You-Bao

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Abstract

Nuclear mass is an important property in both nuclear and astrophysics. Some algorithms are applied to improve the accuracy of the nuclear mass model. The algorithm of Sequential Least Squares Programming significantly enhances the precision of multinomial mass models by reducing the error from 1.863 MeV to 1.631 MeV. We further test these algorithms by 200 samples of mass formulas selecting from the δE term of $E_{isospin}$ mass model. Among these algorithms, the Sequential Least Squares Programming has the best performance in both root mean square errors and computational efficiency. This algorithm is suitable to deal with large-scale, multi-parameter optimization tasks in nuclear physics.

Full Text

Preamble

Nuclear mass represents a critical property in both nuclear physics and astrophysics. Various algorithms have been applied to enhance the accuracy of nuclear mass models, among which Sequential Least Squares Programming (SLSQP) demonstrates particular promise. This algorithm improves the precision of multinomial mass models by reducing the root-mean-square error from 1.863 MeV to 1.631 MeV. To further validate its performance, we conducted tests on 200 sample mass formulas derived from the δE term of the Eispin mass model. Across all evaluated algorithms, SLSQP exhibits the best performance in terms of both root-mean-square error and computational efficiency, making it highly suitable for large-scale, multi-parameter optimization tasks in nuclear physics.

Keywords: Nuclear mass model, binding energy, magic nuclei, sequential least squares algorithm

Introduction

An atomic nucleus contains fundamental information about atomic structure and represents a basic physical property [1]. Variations in atomic mass directly influence nuclear stability and the energy released during nuclear reactions [2]. The mass of neutron-rich nuclei plays a crucial role in rapid neutron capture (r-process) during stellar nucleosynthesis, making the study of nuclear mass essential for understanding the formation and evolution of elements in the universe [3–5]. Recent advances in radioactive ion beam facilities have enabled experimental measurements of over 3000 ground-state atomic masses [6, 7], with research continuously extending to both sides of the β -stability line. However, astrophysical applications require extensive data on neutron-rich or neutron-deficient nuclei far from the valley of stability—regions that remain difficult to access with current experimental techniques. Consequently, numerous theoretical mass models have been developed.

In 1935, Bethe and Weizsäcker proposed the semi-empirical BW2 mass formula [8–10], which predicts nuclear masses with an accuracy of approximately 3 MeV. Reference [11] divided nuclear binding energy into two components: a large, smooth term and a small, fluctuating term. While the classical liquid-drop model accounts for the smooth trend, it fails to reproduce the rapid fluctuations in binding energy near shell gaps as functions of proton and neutron numbers, indicating that important physical effects are missing from the classical formulation [12, 13]. To address this limitation, physicists developed macroscopic-microscopic mass models that incorporate shell correction terms, such as the Finite-Range Droplet Model (FRDM) [14], Koura-Tachibana-Uno-Yamada (KTUY) [15], Lublin-Strasbourg Drop (LSD) [16], and microscopic models including the Hartree-Fock-Bogoliubov (HFB) approach [17, 18] and relativistic mean-field theory (RMF) [19]. These approaches are primarily based on density functional theory (DFT) [20], which, despite its greater complexity, exhibits superior extrapolation capabilities.

Kirson et al. introduced six physical terms as multiple constraints to the mass model [21–27], yielding an improved BW2 formulation that partially resolved issues of missing physics and overfitting present in early semi-empirical approaches, thereby reducing the root-mean-square deviation (RMSD) [28] to 1.92 MeV. Machine learning has found important applications in nuclear physics due to its ability to handle complex problems, such as predicting half-lives, charge radii, and charge densities [29–32]. By incorporating α -decay energies and Garvey-Kelson relations (GKs) and applying multi-objective optimization (MOO) methods [13, 33, 34], Qian and collaborators significantly improved the theoretical accuracy of the BW2 model. Considering isospin dependence, Bhagwat enhanced the liquid-drop model to include isospin-related terms and added fluctuation terms [35], which successfully explained nucleon binding energies. Sequential Least Squares Programming (SLSQP) [36] is particularly suitable for solving constrained nonlinear optimization problems, as it can efficiently handle multiple constraints and nonlinear objective functions. Initially applied to an-

tenna array layout optimization, SLSQP has since demonstrated its feasibility and applicability to nuclear mass models.

In this study, we employ an improved BW3 mass model that incorporates higher-order symmetry energy terms to describe nucleon binding energies [37]. We systematically test and analyze a set of model coefficients using multiple algorithms to enhance both the theoretical accuracy and extrapolation capability of the model. To verify the universality of the SLSQP algorithm, we apply it to 200 sample mass formulas. The results demonstrate that SLSQP not only provides stable performance with small root-mean-square errors but also maintains high computational efficiency.

Section 2 introduces the BW3 and Eisospin mass models along with the SLSQP algorithm. Section 3 presents the performance of SLSQP in improving the mass model. Section 4 provides a summary.

II. Semi-Empirical Mass Formula

A. BW3 Mass Model

The BW3 mass model derives from the droplet model and improves upon the semi-empirical mass formula [8-10] by incorporating additional physical constraints [37]:

$$BBW_3 = \alpha_V A + \alpha_S A^{2/3} + \alpha_C \frac{|N - Z|}{A} + \alpha_p \delta(N, Z) A^{-1/2} + \alpha_R A^{1/3} + \alpha_m P + \beta_m P^2 \frac{(N - Z)^2}{A} + \alpha_{st} \frac{(Z - N)^2}{A^{4/3}} + \alpha_x \frac{(N - Z)^4}{A^2}$$

Equation (1) involves 12 parameters, with $\delta(N, Z)$ defined as $\delta(N, Z) = [(-1)^N + (-1)^Z]/2$, where $\delta = 1$ denotes even-even nuclei, $\delta = -1$ odd-odd nuclei, and $\delta = 0$ odd-A nuclei. The pairing term P can be expressed as:

$$P = \frac{v_p + v_n}{A^{1/3}}$$

where v_p (v_n) represents the difference between the proton number Z (neutron number N) and the nearest magic number. The shell correction parameter α_{pm} is given by:

$$\alpha_{pm} = \left(\frac{9\pi}{4} \right)^{2/3}$$

These physical terms derive from applying the Fermi gas model to account for nucleon binding energies. Subject to Pauli's exclusion principle, nucleons (protons, neutrons, and nuclei) are assumed to move freely within the nuclear volume, with each nucleon experiencing a potential formed by the superposition of potentials from other nucleons. Such a fermionic system is treated as a

degenerate gas at temperatures below the Fermi temperature. The Fermi energy at 0 K is expressed as:

$$\langle E(Z, N) \rangle = \left(\frac{9\pi}{4} \right)^{2/3} \left[\frac{N^{5/3} + Z^{5/3}}{A^{2/3}} + \frac{(N - Z)^2}{A^{4/3}} + \dots \right]$$

The first term contributes to the volume term in the mass formula, while the second term corrects for $N \neq Z$. The third term represents the higher-order addition to the symmetry energy used to enhance the mass model.

B. Eisospin Mass Model

The Eisospin mass formula can be expressed through Strutinsky' s theorem [35]:

$$E_{isospin}(Z, N) = -(E_{LDM} + \delta E)$$

where E_{LDM} represents the macroscopic component and δE accounts for fluctuations in binding energy. The macroscopic component includes the volume term related to isospin, the Coulomb term, the surface term, the surface-diffusion-related Coulomb energy correction term, and the pairing term:

$$E_{LDM} = \alpha_V \left[1 - \frac{4k_V T_z (T_z + 1)}{A} \right] A - \alpha_S \left[1 - \frac{4k_S T_z (T_z + 1)}{A} \right] A^{2/3} - \alpha_C \frac{Z^2}{A^{1/3}} - \frac{3Z^2 e^2}{5r_0 A^{1/3}} + E_p$$

Here, a_V , k_V , a_S , k_S , a_C , and r_0 represent the volume energy, isospin dependence of volume energy, surface energy, isospin dependence of surface energy, Coulomb energy, and Coulomb radius, respectively. T_z is the third component of isospin, and e is the electron charge. The smooth pairing energy is given by [38]:

$$E_p = \begin{cases} -\lambda_n N^{-1/3}, & Z \text{ even}, N \text{ odd} \\ -\lambda_p Z^{-1/3}, & Z \text{ odd}, N \text{ even} \\ -\lambda_{np} N^{-1/3} - \lambda_{np} Z^{-1/3}, & Z, N \text{ odd} \\ 0, & N, Z \text{ even} \end{cases}$$

where λ_n , λ_p , and λ_{np} are free parameters.

The fluctuation term δE can be expressed as:

$$\delta E(\vec{x}) = \sum_{\vec{k} \neq \vec{0}} \left[a_{\vec{k}} \cos(2\pi \vec{x} \cdot \vec{k}) + b_{\vec{k}} \sin(2\pi \vec{x} \cdot \vec{k}) \right]$$

where $\vec{k} \equiv (k_1, k_2, k_3, k_4)$ with $0 \leq k_i \leq M$ for $i = 1, 2, 3, 4$, and $\vec{x} \equiv (x_1, x_2, x_3, x_4)$:

$$x_1 = \beta_1 |N - N_0|, \quad x_2 = \beta_2 |Z - Z_0|, \quad x_3 = \beta_3 N^{1/3}, \quad x_4 = \beta_4 Z^{1/3}$$

In this formula, $N_0(Z_0)$ represents the nearest magic number. The parameters $\beta_1, \beta_2, \beta_3$, and β_4 are free parameters, where β_1 and β_2 describe the proximity to shell closure for protons and neutrons, respectively, while β_3 and β_4 are proportional to the Fermi momentum. The total number of parameters becomes quite large ($2M^4 + 4$), though not all terms require expansion to M . Therefore, the expression can be simplified as:

$$\delta E(\vec{x}) = \sum_{k_1=0}^M \sum_{k_2=0}^{M-k_1} \sum_{k_3=0}^{M-k_1-k_2} \sum_{k_4=0}^{M-k_1-k_2-k_3} [a_{\vec{k}} \cos(2\pi\vec{x} \cdot \vec{k}) + b_{\vec{k}} \sin(2\pi\vec{x} \cdot \vec{k})]$$

This reduces the number of parameters to $\frac{1}{12}(M+4)!/M! + 4$. Since the mean of δE is approximately zero, the number of free parameters can be further reduced to $\frac{1}{12}(M+4)!/M! + 2$.

C. Algorithm Principles

This work investigates more than ten algorithms, including Ordinary Least Squares (OLS) [39], SLSQP [36], Constrained Optimization by Linear Approximation (COBYLA) [40], Broyden-Fletcher-Goldfarb-Shanno (BFGS) [41], Conjugate Gradient (CG) [42], and others. Among these, SLSQP, COBYLA, and Trust-Constr [43] proved most effective for solving constrained optimization problems (COPs). For solving the COP in Eq. (9), SLSQP was selected because it fully utilizes gradient and Hessian matrix information [44], enabling faster convergence to the optimal solution.

The general constrained optimization problem is formulated as:

$$\begin{aligned} & \text{minimize} && f(\vec{x}) \\ & \text{subject to} && g(\vec{x}) = 0, \quad h(\vec{x}) \geq 0 \\ & \text{where} && \vec{x} = (x_1, x_2, x_3, \dots, x_{k-2}, x_{k-1}, x_k) \in X \\ & && X = \{\vec{x} \mid \vec{l} \leq \vec{x} \leq \vec{u}\} \\ & && \vec{l} = (l_1, l_2, l_3, \dots, l_{i-2}, l_{i-1}, l_i) \\ & && \vec{u} = (u_1, u_2, u_3, \dots, u_{j-2}, u_{j-1}, u_j) \end{aligned}$$

In this formulation, $\vec{x}$ is the solution vector, X is the solution space, $\vec{l}$ and $\vec{u}$ are the lower and upper bounds of the solution space, $g(\vec{x})$ represents equality

constraints, $h(\vec{x})$ represents inequality constraints, and $f(\vec{x})$ is the objective optimization function [45].

The SLSQP algorithm iteratively minimizes the objective function under constraints through linear approximation, transforming the nonlinear constrained problem into an unconstrained least-squares problem. In each iteration, the gradient and Hessian matrix [44] are calculated to update the solution using Lagrange multipliers for the constraints:

$$L(\vec{x}, \vec{\lambda}, \vec{\mu}) = f(\vec{x}) + \vec{\lambda}^T \cdot g(\vec{x}) + \vec{\mu}^T \cdot h(\vec{x})$$

where the superscript T denotes the vector transpose, and $\vec{\lambda}$ and $\vec{\mu}$ represent the penalty terms associated with equality and inequality constraints, respectively [46].

By solving the unconstrained least-squares problem, an update rule is obtained for each iteration that satisfies both equality and inequality constraints as well as the first-order necessary conditions:

$$\nabla L(\vec{x}, \vec{\lambda}, \vec{\mu}) = \nabla f(\vec{x}) + J_g^T \cdot \vec{\lambda} + J_h^T \cdot \vec{\mu} = 0$$

where J_g and J_h denote the Jacobian matrices of the equality and inequality constraints, respectively [47].

According to this update rule, an initial value $\vec{x}_1$ is chosen and a stopping criterion ε is set. The gradient vector $\nabla f_k(\vec{x}_k)$ is computed at each iteration k . If $\|\nabla f_k(\vec{x}_k)\| < \varepsilon$, the algorithm terminates and returns the approximate solution $\vec{x}^*$. This process constructs a sequential programming model:

$$\begin{aligned} \text{minimize} \quad & q(\vec{x}) = f_k(\vec{x}) + g_k^T(\vec{x} - \vec{x}_k) + \frac{1}{2}(\vec{x} - \vec{x}_k)^T B_k(\vec{x} - \vec{x}_k) \\ \text{subject to} \quad & A_{eq}(\vec{x} - \vec{x}_0) = 0 \\ & g_k(\vec{x}) \geq 0, \quad k = 1, 2, \dots, k \end{aligned}$$

where B_k is a positive-definite symmetric matrix approximating the inverse Hessian matrix, and A_{eq} is the Jacobian matrix of the equality constraints.

This model is solved to obtain the search direction $\Delta\vec{x}$, and the step size α is computed to ensure sufficient decrease of the objective function along this direction:

$$\alpha = \min(1, r), \quad r = \max(\beta_s, r_t)$$

where s and t are positive scale factors. Finally, the estimated points are updated as $\vec{x}_{k+1} = \vec{x}_k + \alpha\Delta\vec{x}$. Through this iterative process, the objective function is gradually optimized to determine the optimal solution satisfying all constraints.

III. Discussion

The coefficients of the BW3 model are optimized using the SLSQP algorithm [36] to reduce discrepancies between theoretical calculations and experimental data. To ensure physical feasibility, the following constraints are imposed:

1. After satisfying Condition 1, the specific binding energy of the remaining nuclides, $B_{Th}/(N + Z)$, is distributed in the range of 5-9 MeV.

Model performance is evaluated using RMSD [28], defined as:

$$\text{RMSD} = \sqrt{\frac{\sum_{i=1}^n (BE_{xi} - BE_{thi})^2}{n}}$$

where n represents the total number of nuclides in the calculation, and BE_{xi} and BE_{thi} are the experimental and theoretical binding energies, respectively.

The optimized coefficients for several algorithms are listed in Table I. Different algorithms modify the weights of various terms in the model, as shown in the table. These weights indicate the extent to which each term influences the model, with signs indicating positive or negative corrections. The volume, surface, symmetry, Wigner, surface symmetry, pairing, higher-order correction, and curvature terms carry high weights due to their significant influence on the mass model, whereas the Coulomb, Coulomb exchange, and shell effect terms [21-27] have low weights because of their minor impact.

The horizontal axis in the plots represents neutron number N , while the vertical axis shows the percentage of relative error [12], defined as $\delta B/B(\%) = (BE_x - BE_{th})/BE_x \times 100\%$. The errors exhibit distinct trends across different nuclide regions for different algorithms. Figures 1-a, 1-b, and 1-c demonstrate overall error reduction and narrowed fluctuation ranges in light and medium-mass regions. In Figures 1-e and 1-f, while the fluctuation amplitude in heavy nuclide regions improves, the fluctuation amplitude in light nuclide regions increases, resulting in no net improvement or even deterioration of the total RMSD. When comparing performance metrics such as $\delta B/B(\%)$ [12] and RMSD [28] for mass models obtained with different algorithms, SLSQP [36] shows greater advantages in reducing model errors. This is attributed to SLSQP's reduction of surface and curvature term weights and its increase of Wigner, surface symmetry, pairing, and higher-order correction term weights.

The results also reveal that in AME2020, the influence of surface and curvature terms on binding energy decreases, while the influence of Wigner, surface symmetry, pairing, and higher-order correction terms increases. This indicates that the impact of surface and curvature terms is diminished, whereas the Wigner term's contribution to the overall effect becomes more significant. The mass model thereby improves its extrapolation capability [17, 18] under SLSQP and more accurately reflects the contributions of different physical terms to binding energy.

Figure 2 [Figure 2: see original paper] shows the relative error between theoretical and experimental values for the BW3 mass model using both SLSQP and OLS algorithms, with the x-axis representing neutron number, y-axis representing atomic number, and z-axis representing relative error percentage $\delta B/B(\%)$. The figure reveals more pronounced fluctuations for magic nuclei, particularly around doubly magic nuclei, indicating different interaction mechanisms between magic and non-magic nuclei. SLSQP improves the errors near doubly magic nuclei, captures special interaction effects around magic nuclei more accurately, and enhances the precision of the theoretical model.

The Eisospin mass model consists of two components: the liquid-drop-model-based E_{LDM} with 5 terms and 9 free parameters, and the fluctuation term δE . Setting the degree of freedom M to 4 yields 153 parameters. Using the latest nuclear mass dataset AME2020, these parameters are optimized via Ordinary Least Squares (OLS), achieving a minimum root-mean-square deviation of 1.268 MeV. By analyzing parameter significance, 62 influential parameters were selected as a sample set. Ten parameters were randomly chosen from this set to form a sample mass formula with the E_{LDM} term, and this random process was repeated to generate 200 sample mass formulas. Subsequently, SLSQP, Trust-Constr, BFGS, and L-BFGS-B algorithms were applied to optimize these formulas.

Figure 3 [Figure 3: see original paper] illustrates SLSQP performance on even-even, odd-odd, and odd-A nuclei. The optimization effects show significant differences across nucleus types, with the most substantial improvement for even-even nuclei and noticeable improvements for odd-A and odd-odd nuclei as well. Figure 3-a demonstrates that for even-even nuclei [48] (both Z and N even), SLSQP reduces RMSD [28] by 0.29 MeV, corresponding to a performance improvement of approximately 15.18% compared to the BW3 model with OLS coefficients. In Figure 3-b, for odd- Z and even- N nuclei, SLSQP optimization reduces model RMSD by 0.19 MeV (9.79% improvement). Similarly, Figure 3-c shows that for even- Z and odd- N nuclei, RMSD decreases by 0.23 MeV (12.23% improvement), with optimization results in the medium-mass region closely approaching experimental values. For odd-odd nuclei (both Z and N odd), Figure 3-d shows that SLSQP optimization reduces RMSD by 0.22 MeV, yielding a 12.02% performance improvement, particularly in heavy-mass regions where results converge toward experimental values. These findings further validate SLSQP's effectiveness in mass model optimization.

While the above methods apply to a single nuclear mass formula, we conducted a general investigation to verify universality by applying the approach to another multi-term nuclear mass formula. The results demonstrate that SLSQP performs better when optimizing multi-term formulas, achieving smaller errors and faster convergence.

Figure 4 [Figure 4: see original paper] shows the process of identifying 62 important parameters from the δE term of the Eisospin mass model, randomly selecting 10 parameters as a sample formula with E_{LDM} , and generating 200 sample

mass formulas. The quantity ΔRMSD is defined as $(\text{RMSD} - \text{RMSD}_{\min}) \times 100$, where $\text{RMSD}_{\min}$ is the minimum root-mean-square deviation achieved by the algorithm across 200 samples.

As shown in Figure 4, the SLSQP algorithm significantly outperforms BFGS and L-BFGS algorithms. For example, at the 48th sample point, SLSQP's ΔRMSD is 4 MeV, while BFGS and L-BFGS yield 23.9 MeV and 23.0 MeV, respectively. At the 67th sample point, SLSQP's ΔRMSD is 2.7 MeV, compared to 22.7 MeV and 21.8 MeV for BFGS and L-BFGS. The Trust-Constr algorithm exhibits large error amplitudes, indicating poor stability in parameter optimization. In terms of computational efficiency relative to SLSQP, BFGS requires approximately 2.44 times longer, L-BFGS-B requires 2.78 times longer, and the Trust-Constr algorithm requires 8.44 times longer. Thus, SLSQP demonstrates both excellent stability with small root-mean-square errors and high computational efficiency.

To verify SLSQP's effectiveness, Figure 5 [Figure 5: see original paper] compares experimental and theoretical values. Experimental binding energies (BE) are taken from AME2020, while theoretical values are predicted by the SLSQP-optimized BW3 mass model. For oxygen isotopes, the maximum BE is currently measured at $^{24}\text{O}_{16}$ with $BE = 168.95$ MeV; beyond this point, BE decreases with increasing N . The SLSQP-optimized theoretical model predicts the maximum at $^{26}\text{O}_{18}$ with $BE = 168.95$ MeV, followed by a similar decrease. For other isotope chains, experimental BE values show an overall increasing trend without reaching a maximum. Optimization of the BW3 model with SLSQP predicts the following BE maxima: $^{64}\text{Ca}_{44} = 464.33$ MeV, $^{88}\text{Ni}_{60} = 656.72$ MeV, $^{123}\text{Nb}_{82} = 950.29$ MeV, $^{141}\text{Rh}_{96} = 1035.66$ MeV, $^{100}\text{Ge}_{68} = 745.77$ MeV, $^{156}\text{Sn}_{106} = 1148.31$ MeV, $^{184}\text{Ce}_{126} = 1311.84$ MeV, $^{206}\text{Dy}_{140} = 1463.63$ MeV, $^{230}\text{W}_{156} = 1613.36$ MeV, and $^{252}\text{Pb}_{170} = 1761.89$ MeV.

IV. Conclusions

This work applies several algorithms to improve the accuracy of the BW3 mass model. The SLSQP algorithm demonstrates the best performance in both root-mean-square error and computational efficiency, reducing the global RMSD from 1.863 MeV to 1.631 MeV (a 12.45% reduction) and thereby enhancing the precision of multinomial mass models. We examined nuclei with odd and even proton and neutron numbers, finding that SLSQP reduces the local RMSD from 1.91 MeV to 1.62 MeV (15.18% optimization) for nuclei with even numbers of both protons and neutrons. For nuclei with odd numbers of both protons and neutrons, the local RMSD decreases from 1.83 MeV to 1.61 MeV. With odd proton and even neutron numbers, the local RMSD is reduced from 1.94 MeV to 1.75 MeV (9.79% optimization). For even proton and odd neutron numbers, the local RMSD decreases from 1.88 MeV to 1.65 MeV (12.23% optimization). We further tested these algorithms on 200 sample mass formulas selected from the δE term of the Eisospin mass model. Compared to other algorithms, SLSQP shows small errors and fast convergence, confirming its superiority for nuclear mass model optimization.

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