Physics Informed Neural Network Approach for Estimating the Coefficients of the Semi-Empirical Mass Formula

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Abstract

Background: The Semi-Empirical Mass Formula (SEMF), also known as the Weizsäcker formula, provides an approximate description of nuclear binding energy by incorporating volume, surface, Coulomb, asymmetry, and pairing effects within the liquid-drop model framework. Conventionally, the coefficients of the SEMF are determined using least-squares regression on experimental nuclear mass data.

Purpose: The purpose of this study is to develop and demonstrate a Physics-Informed Neural Networks (PINNs) framework for estimating the coefficients of the SEMF by embedding the nuclear-physics structure of the model directly into the learning process.

Methods:A physics-informed neural network was developed with the SEMF explicitly embedded in the loss function. Experimental nuclear mass data were used for training, while the SEMF coefficients were treated as trainable parameters. The model was optimized via c^2 minimization, measuring weighted squared deviations between experimental and predicted binding energies, with physically motivated bounds imposed to ensure stability and interpretability.

Results: The PINN framework successfully recovered physically meaningful values of the SEMF coefficients with improved numerical stability compared to conventional regression-based methods. The predicted binding energies exhibited strong agreement with experimental data across a wide range of nuclei. Incorporation of physical constraints significantly reduced overfitting and enhanced the generalization capability of the model.

Conclusion: This study demonstrates that Physics-Informed Neural Networks provide an effective and reliable framework for estimating the coefficients of the Semi-Empirical Mass Formula.

1 Introduction

The atomic nucleus is a complex many-body system governed by the strong nuclear force, and its properties cannot be derived exactly from first principles for most nuclei. To address this challenge, several phenomenological models have been developed to describe nuclear structure and binding energies. One of the earliest and most influential approaches is the Liquid Drop Model (LDM), originally proposed by George Gamow[1] in 1929, in which the nucleus is treated as an incompressible drop of nuclear fluid composed of protons and neutrons. This model successfully captures the collective behavior of nucleons and explains macroscopic nuclear properties such as binding energy, stability, and fission. Gamow also provided a quantum-mechanical explanation of alpha decay, further strengthening the physical foundation of the liquid drop analogy. Building upon the liquid drop picture, the Semi-Empirical Mass Formula (SEMF), also known as the Weizsäcker formula,[2] provides an approximate expression for nuclear binding energy by incorporating five key contributions: volume, surface, Coulomb, asymmetry, and pairing energies. These terms account for both theoretical considerations and empirical observations, allowing the SEMF to reproduce general trends in nuclear masses across the chart of nuclides. The formula represents a mathematical realization of the liquid drop concept, where the total binding energy emerges from the collective contribution of these energy terms, each weighted by a corresponding coefficient.

Traditionally, the coefficients of the SEMF and the Liquid Drop Model are determined by fitting experimental nuclear mass data using least-squares minimization (LSM)[3] techniques. While regression-based approaches are computationally efficient and widely used, they suffer from certain limitations. In least-squares fitting, data points with large deviations can disproportionately influence the optimized parameters, potentially biasing the resulting coefficients. Furthermore, such methods rely heavily on the quality and distribution of the available mass data.

In recent years, stochastic optimization techniques such as Variational Monte Carlo (VMC)[3] have been investigated as alternative methods for determining the coefficients of the Semi-Empirical Mass Formula (SEMF). While VMC provides greater flexibility and avoids strict analytical assumptions, its performance strongly depends on the choice of initial parameter values. The optimization process is sensitive to the initial guess of the coefficients, which can lead to convergence toward different local minima and result in variability across independent runs. These limitations highlight the need for a more robust and stable optimization framework that can reduce dependence on initial conditions and improve reproducibility.

In this work, we determine the coefficients of the Semi-Empirical Mass For-

mula using Physics-Informed Neural Networks (PINNs), treating the PINN framework as an optimization technique. By embedding the underlying physical structure of the SEMF directly into the neural network loss function, the PINN approach enables efficient and stable parameter estimation while maintaining consistency with nuclear physics constraints[4].

2 Methodology

From the LDM,the theoretical binding energy of a nucleus with mass number A_i and proton number Z_i is described using the Semi-Empirical Mass Formula SEMF[3]. The binding energy is expressed as the sum of different energy contributions,

$$B_i^{\text{th}}(A_i, Z_i) = a_v A_i - a_s A_i^{2/3} - a_c \frac{Z_i(Z_i-1)}{A_i^{1/3}} - a_a \frac{(A_i - 2Z_i)^2}{A_i} + \delta_i a_p A_i^{-1/2}, \tag{1}$$

where ,

- a_v : volume energy coefficient,
- a_s : surface energy coefficient,
- a_c : Coulomb energy coefficient,
- a_a : asymmetry energy coefficient,
- a_p : pairing energy coefficient.

The pairing factor δ_i accounts for odd–even effects and is defined according to the parity of the proton and neutron numbers[3].

Within the Physics-Informed Neural Network (PINNs) framework, the SEMF coefficients are treated as trainable parameters and collected into a single parameter vector[5],

$$\boldsymbol{a} = \begin{bmatrix} a_v & a_s & a_c & a_a & a_p \end{bmatrix}^{\mathrm{T}}. \tag{2}$$

Here T in superscript is an trainable coefficient vector,each component of $\boldsymbol{a}$ retains a clear physical interpretation and corresponds to a specific contribution to the nuclear binding energy.

2.1 PINN Architecture for SEMF Parameter Estimation

Unlike conventional applications of PINNs, which are typically used to solve partial differential equations [6], in this work we employ the PINNs framework for parameter estimation of the SEMF. The framework for parameter estimation is illustrated in Fig. 1. The network input consists of experimentally measured nuclear properties[7],namely the mass number A_i and proton number Z_i, which are taken from the AME 2020 atomic mass evaluation [8]. The network does not learn the binding energy directly. Instead, the SEMF coefficients $\boldsymbol{a}$ are optimized during training.

During the forward pass, the analytical SEMF expression is evaluated using the current set of coefficients to compute the predicted binding energy B_{i}^{SEMF}. This approach ensures that the physical structure of the SEMF is explicitly preserved throughout the learning process.

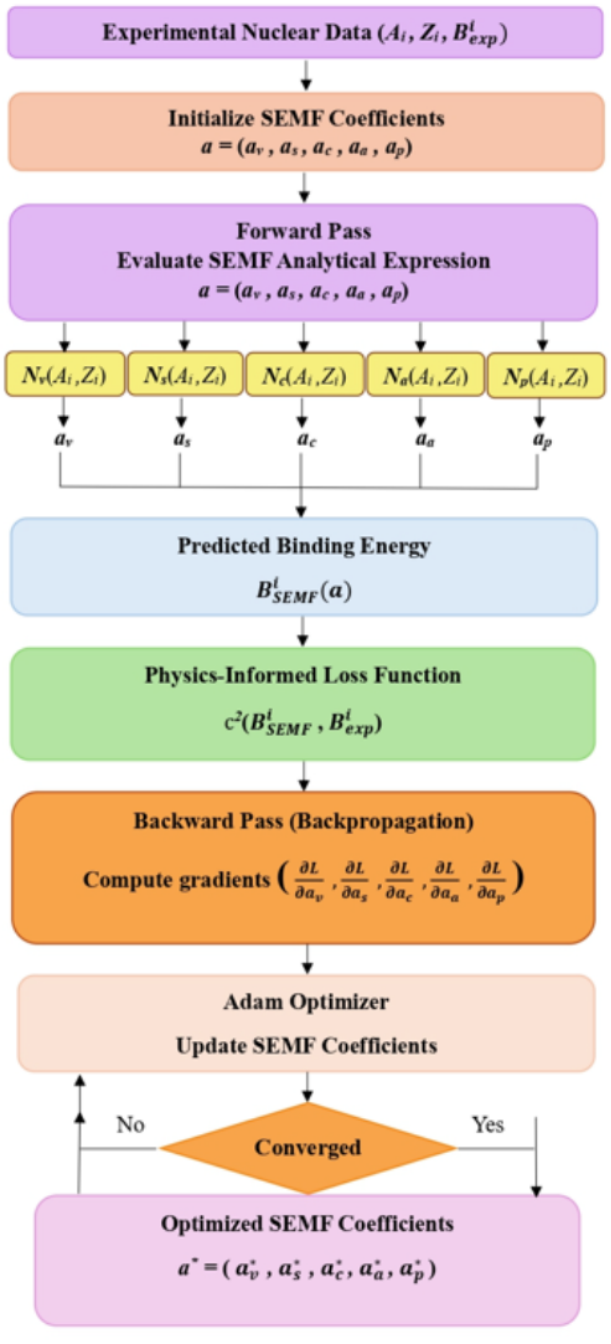


Figure 1: Flowchart for obtaining coefficints of SEMF using PINNs

In the Physics-Informed Neural Network (PINNs) framework adopted in this work.The estimation of the Semi-Empirical Mass Formula (SEMF) coefficients is carried out using a parallel-network architecture. Instead of employing a single neural network to infer all coefficients simultaneously, independent neural networks are assigned to each SEMF coefficient. This design choice preserves the physical interpretability of the parameters and avoids strong coupling between unrelated energy terms.

The SEMF coefficient vector is defined as

$$\boldsymbol{a} = \begin{bmatrix} a_v & a_s & a_c & a_a & a_p \end{bmatrix}^{\mathrm{T}}, \tag{3}$$

where each coefficient corresponds to a distinct physical contribution to the nuclear binding energy.

Within the PINN architecture, five parallel feedforward neural networks are employed:

$$a_v = \mathcal{N}_v(A_i, Z_i), \tag{4}$$
$$a_s = \mathcal{N}_s(A_i, Z_i), \tag{5}$$
$$a_c = \mathcal{N}_c(A_i, Z_i), \tag{6}$$
$$a_a = \mathcal{N}_a(A_i, Z_i), \tag{7}$$
$$a_p = \mathcal{N}_p(A_i, Z_i), \tag{8}$$

where $\mathcal{N}_v$, $\mathcal{N}_s$, $\mathcal{N}_c$, $\mathcal{N}_a$, and $\mathcal{N}_p$ denote five independent neural networks with identical architectures but separate trainable parameters.

Each network receives the same physical inputs, namely the mass number A_i and proton number Z_i, and outputs a single scalar corresponding to one SEMF co-

efficient. The outputs of these parallel networks are then embedded directly into the analytical SEMF expression to compute the predicted binding energy:

$$B_i^{\mathrm{SEMF}} = \mathcal{N}_v A_i - \mathcal{N}_s A_i^{2/3} - \mathcal{N}_c \frac{Z_i(Z_i-1)}{A_i^{1/3}} - \mathcal{N}_a \frac{(A_i-2Z_i)^2}{A_i} + \delta_i \mathcal{N}_p A_i^{-1/2}. \tag{9}$$

The parallel-network structure ensures that each SEMF coefficient is optimized independently while remaining constrained by the governing physical model. During training, a single physics-informed loss function is minimized, and gradient-based optimization[9] updates the parameters of all five networks simultaneously.

2.2 Working Principle of the Physics-Informed Neural Network

The PINNs operates through a physics-guided optimization strategy. For each nucleus characterized by (A_i, Z_i), the SEMF-based binding energy is computed using the current parameter vector $\boldsymbol{a}$. The difference between the predicted and experimentally measured binding energies is then quantified using a physics-informed loss function.

Unlike conventional neural networks that employ hidden layers to learn implicit representations, the present architecture performs optimization directly on physically meaningful parameters. Gradient-based optimization algorithms such as adam optimizer[10] are employed to iteratively update the SEMF coefficients until convergence is achieved.

This formulation ensures that the learned parameters remain consistent with nuclear-physics principles and avoids the emergence of unphysical solutions. The loss function is constructed by comparing the SEMF-based predictions with experimental binding energy data. A c^2 - square loss is defined as

$$\mathcal{L} = \frac{1}{N} \sum_{i=1}^{N} \frac{\left(B_i^{\mathrm{SEMF}} - B_i^{\mathrm{exp}}\right)^2}{B_i^{\mathrm{exp}}}, \tag{10}$$

where N denotes the total number of nuclei in the training data set, and B_i^{exp} represents the experimentally measured binding energy.

In analogy with the residual loss used in PDE-based PINNs, this loss function enforces consistency between the physical model and experimental observations. The present framework therefore addresses an inverse problem in which the physics-informed constraint is algebraic rather than differential.

Within the PINNs framework, the optimization of the Semi-Empirical Mass Formula (SEMF) coefficients is carried out using backpropagation[11]. Unlike conventional neural networks, backpropagation does not propagate errors through an arbitrary mapping between inputs and outputs. Instead, the gradients are propagated through the analytical SEMF expression itself.

During training, the gradients of the loss function with respect to each SEMF coefficient are computed using backpropaga-

tion,

$$\frac{\partial \mathcal{L}}{\partial \boldsymbol{a}} = \left(\frac{\partial \mathcal{L}}{\partial a_v}, \frac{\partial \mathcal{L}}{\partial a_s}, \frac{\partial \mathcal{L}}{\partial a_c}, \frac{\partial \mathcal{L}}{\partial a_a}, \frac{\partial \mathcal{L}}{\partial a_p} \right). \quad (11)$$

These gradients propagate through the SEMF analytical structure, ensuring that updates to the coefficients are consistent with the underlying nuclear-physics model. Gradient-based optimization algorithms, such as stochastic gradient descent or adaptive optimizers, use these gradients to update the parameters iteratively[5],

$$\boldsymbol{a}^{(k+1)} = \boldsymbol{a}^{(k)} - \eta \frac{\partial \mathcal{L}}{\partial \boldsymbol{a}}, \quad (12)$$

where η denotes the learning rate and k represents the iteration index.

By embedding backpropagation directly within the SEMF formulation, the PINN ensures that learning is guided simultaneously by experimental data and established nuclear-physics constraints. As a result, the optimized coefficients remain physically interpretable while achieving optimal agreement with experimental binding energies.

3 Results and Discussion

The Physics-Informed Neural Network (PINNs) framework successfully converged to a stable and well-defined set of coefficients for the Semi-Empirical Mass Formula (SEMF). The optimized coefficients were found to be physically reasonable and consistent with the expected orders of magnitude reported in the literature. Moreover, the robustness of these coefficients across multiple independent training runs demonstrates that the incorporation of physical constraints within the loss function[9] effectively regularizes the learning process and mitigates overfitting.

To quantitatively access the accuracy of the obtained coefficients, the deviation between theoretical and experimental nuclear binding energies was evaluated using the c-square minimization criteria. This metric penalizes large discrepancies between predicted and observed values while preserving the original physical units (MeV), thereby providing a meaningful measure of model performance.

The c^2-square error is defined as

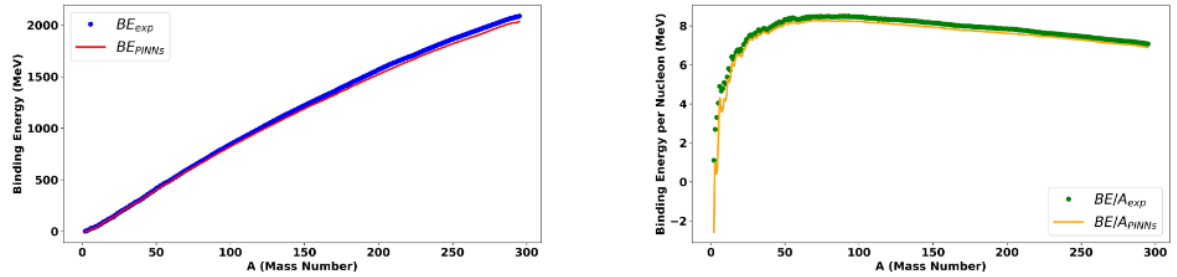
$$c^2 = \frac{1}{n} \sum_{i=1}^{n} \frac{\left(B_i^T - B_i^E\right)^2}{B_i^E}, \quad (13)$$

where B_i^T and B_i^E represent the theoretical and experimental binding energies of the i-th nucleus, respectively, and n denotes the total number of nuclei included in the dataset.

The optimized SEMF coefficients are recovered after embedding the physical constraints into the PINN architecture are given by

$$\begin{aligned} a_v &= 15.072 MeV, \\ a_s &= 16.597 MeV, \\ a_c &= 0.690 MeV, \\ a_a &= 20.907 MeV, \\ a_p &= 12.605 MeV. \end{aligned} \quad (14)$$

The comparison between experimental nuclear binding energies and those pre-



(a) (b)

Figure 2: (a) Comparison of experimental nuclear binding energies with those predicted by the Semi-Empirical Mass Formula using PINN-optimized coefficients. (b) Comparison of experimental nuclear binding energies per nucleon with those predicted by the Semi-Empirical Mass Formula using PINN-optimized coefficients, both as a function of mass number A.

dicted by the Semi-Empirical Mass Formula (SEMF) using PINN-optimized coefficients is shown in Fig. 2b. Similarly, Fig. 2b presents the comparison of experimental binding energy per nucleon with the values predicted by the SEMF, both plotted as a function of mass number A. The PINNs predictions closely follow the experimental trends across a wide range of mass numbers A, indicating that this framework effectively captures the dominant physical contributions governing nuclear binding.

Since the SEMF is explicitly embedded within the model architecture, the learned parameters retain clear physical interpretations, in contrast to purely data-driven neural network approaches where model parameters often lack physical meaning. By combining experimental data with established nuclear-physics principles, the PINNs approach yields improved numerical stability, enhanced predictive capability, and greater physical consistency, highlighting its effectiveness for inverse problems in nuclear physics[9].

4 Conclusion

In this work, the PINNs methodology was applied to the Semi-Empirical Mass Formula to estimate its phenomenological coefficients while preserving the analytical structure and physical foundations of the model. By treating the SEMF coefficients as trainable parameters constrained by the functional form of the mass formula, the PINNs approach ensures that the learned parameters remain physically interpretable and consistent with nuclear theory.During the forward pass, the analytical SEMF expression was evaluated to compute the predicted binding energy, ensuring that the physical form of the model was maintained throughout the learning process. The

backward pass propagated loss gradients through the SEMF formulation itself, allowing gradient-based optimization to update the coefficients in a manner consistent with nuclear-physics constraints[5].The use of parallel neural networks for individual SEMF coefficients enabled independent optimization of each energy term while retaining clear physical interpret-ability. The physics-informed loss function, based on chi-square minimization, ensured consistency between theoretical predictions and experimental observations.The advantage of using PINNS to obatin the SEMF coefficients is that the physical laws of SEMF embedded directly into the optimization process resulting in stable parameter estimates with reduced senstivity to initial conditions compared to purely regression based methods(LSM)[3].

Acknowledgments

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