Machine Learning Methods for Heavy-Ion Fusion Reaction Cross Sections

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Abstract

This study employs the decision tree-based machine learning algorithm LightGBM (Light Gradient Boosting Machine) to investigate the fusion cross-sections (CS) of heavy-ion reactions in even-even systems. The input features of the machine learning algorithm include physical quantities related to fundamental nuclear properties (such as proton numbers and mass numbers of the projectile and target nuclei, excitation energies of the 2+ and 4+ states, etc.) as well as CS calculated from phenomenological theoretical models, with the fusion cross-section as the output. The results demonstrate that when the phenomenological model-calculated CS is excluded from the input features, the mean absolute error (MAE) between the CS predicted by LightGBM and experimental values on the training set is 0.138, which significantly outperforms the 0.172 obtained from the empirical coupled-channel model (ECC). When the phenomenological model-calculated CS is included in the input features, the MAE decreases to 0.07 due to the incorporation of physical information. Additionally, it is found that the introduction of physical information leads to better agreement between the calculated barrier distribution and experimental data. This indicates that physical information plays a crucial role in machine learning studies of heavy-ion fusion reactions.

Full Text

Preamble

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Machine Learning Methods for Studying Heavy-Ion Fusion Cross Sections

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Abstract

[**Background**]: Heavy-ion fusion reactions represent the exclusive mechanism for synthesizing superheavy elements and novel nuclides, holding paramount significance in nuclear physics. However, conventional physical models exhibit limitations in characterizing the fusion cross sections (CS) of heavy-ion reactions, while experimental measurements for numerous systems remain incomplete or lack sufficient precision. Machine learning (ML), which has been widely applied to scientific research in recent years, can be employed to investigate inherent correlations within large volumes of complex data.

[**Purpose**]: This study establishes the relationship between fusion reaction features and CS by training a dataset using LightGBM (Light Gradient Boosting Machine).

[**Methods**]: Several basic quantities (e.g., proton number, mass number, and excitation energies of the 2^+ and 4^+ states of projectile and target nuclei) along with CS obtained from phenomenological formulas are fed into the LightGBM algorithm to predict CS.

[**Results**]: On the validation set, the mean absolute error (MAE) measuring the average magnitude of absolute difference between $\log_{10}$ of predicted CS and experimental CS is 0.138 when using only basic quantities as input—significantly better than the 0.172 obtained from the empirical coupled-channel model. MAE can be further reduced to 0.07 by including physics-informed input features. The MAE on the test set (consisting of 175 data points from 11 reaction systems not included in the training set) is approximately 0.17 and 0.45 with and without physics-informed features, respectively. By analyzing predicted CS for the systems ^{18}O+^{116}Sn and ^{36}S+^{50}Ti in the test set, fusion barrier distributions were further extracted. The results demonstrate that incorporating physics-informed features significantly enhances agreement between calculated barrier distributions and experimental data. Additionally, the SHAP method was employed to construct a visual correlation map between input feature parameters and CS. Through feature importance ranking, it was revealed that the excitation energies of the 2^+ and 4^+ states of the target nucleus play an important role in predicting CS.

[**Conclusions**]: Physical information plays a crucial role in machine learning studies of heavy-ion fusion reactions.

Keywords: Heavy-ion fusion reactions, Fusion cross section, Machine learning

Introduction

During heavy-ion fusion reactions, two colliding nuclei overcome the fusion barrier to form an excited compound nucleus. This process holds significant importance in both scientific research and practical applications. On one hand, it facilitates deeper understanding of nuclear structure and reaction mechanisms, advancing research on superheavy element synthesis [1,2]. On the other hand, it provides critical references for exploring the origin of elements and energy development applications. Consequently, it has remained a research hotspot in nuclear physics for over six decades [3-7].

Numerous countries have built or are constructing high-energy heavy-ion experimental facilities [8,9], providing essential platforms for studying heavy-ion fusion reactions. Currently operational facilities include China's Cooler Storage Ring (CSR) [10], the U.S. Facility for Rare Isotope Beams (FRIB), France' s Radioactive Ion Beam Production System (SPIRAL2), and Japan' s Radioactive Isotope Beam Factory (RIBF). Meanwhile, several new projects remain under construction, such as China' s High-Intensity Heavy-Ion Accelerator Facility (HIAF) [11,12], Korea' s Rare Isotope Science Project (RAON) [13], and Germany' s Facility for Antiproton and Ion Research (FAIR). Using these facilities, excitation functions for over 1000 different projectile-target combinations have been measured [14], yet many systems remain unmeasured or exhibit large uncertainties.

Fusion cross sections and fusion barriers serve as core observables in heavy-ion fusion reactions, occupying important positions in both experimental and theoretical research. Accurate prediction of these physical quantities not only holds theoretical value for elucidating reaction mechanisms but also provides theoretical guidance for experimental design, thereby significantly enhancing measurement precision and reliability of physical interpretation. Several theoretical models or empirical formulas have been proposed to study fusion cross sections, representing the most important approach to investigating heavy-ion fusion reactions. Examples include coupled-channel calculations [15,16], time-dependent Hartree-Fock (TDHF) theory [17,18], the empirical coupled-channel (ECC) model [19-25], and the modified Siwek-Wilczyński formula [26]. However, existing methods generally exhibit substantial discrepancies between predictions and experimental data. For instance, below the Coulomb barrier, experimental cross sections show significant enhancement compared to Wong formula predictions [4], while above the barrier, coupled-channel models generally overestimate fusion cross sections [27]. These limitations indicate that current theoretical models remain inadequate in handling complex physical processes such as coupling mechanisms in many-body systems, multi-dimensional barrier tunneling mechanisms, and nuclear structure effects. Particularly in the near-barrier energy region, fusion reactions are influenced by various quantum mechanical mechanisms including dynamical deformation (e.g., inelastic vibrational excitations), shell effects, and kinetic energy dissipation [27]. Purely numerical theoretical calculations struggle to comprehensively capture these microscopic essentials. Therefore, accurately describing these quantum many-body effects remains the core challenge in improving fusion cross-section prediction accuracy. Despite significant advances in experimental techniques and theoretical models in recent years, exploring excitation functions for different projectile-target combinations remains a formidable challenge.

Machine learning (ML), a commonly used method for achieving artificial intelligence, employs various algorithms to "automatically" and "intelligently" identify intrinsic correlations within data to obtain certain rules or mappings, which are then used to make decisions or predictions about new events. As early as the 1990s, pioneering research demonstrated that basic ML algorithms (such as decision trees) could achieve accuracy comparable to traditional theories in predicting nuclear masses and spin-parities [28]. Currently, ML methods have been successfully applied to fundamental nuclear physics research [28-30], including estimating β-decay half-lives and energies [32,33], α-decay [34,35], nuclear masses and charge radii [36-38], nuclear density distributions [39,40], nuclear excitation energies [40], and heavy-ion collisions [42,43]. ML is a rapidly developing field with numerous algorithms continuously being optimized and expanding their adaptability to various data types and tasks.

Recently, a novel artificial intelligence approach combining genetic programming and neural networks was employed to model fusion cross-section data, deriving two empirical formulas for calculating CS [44]. While these formulas can qualitatively describe CS trends, they exhibit certain deviations in accurately predicting absolute values, requiring further improvements in theoretical modeling and ML algorithms to enhance CS theoretical models and reveal deeper physical mechanisms of heavy-ion fusion reactions. In previous work [45], we used the LightGBM algorithm combined with ECC, Wong formula, and E to study heavy-ion fusion reactions, achieving a mean absolute error (MAE) between predicted and experimental CS of approximately 0.08 on the validation set. To further enhance the model' s physical interpretability, we introduced excitation energies of the 2^+ and 4^+ collective excited states of projectile and target nuclei as input features based on [45]. These states are not only easily obtained through Coulomb excitation but also frequently participate in subsequent inelastic scattering processes dominated by nuclear forces, reflecting structural properties closely related to energy dissipation. Reference [27] has indicated that energy dissipation caused by low-lying states during nuclear reactions may play a key role in fusion hindrance mechanisms; therefore, introducing such features helps investigate the relationship between energy dissipation and fusion cross sections in fusion reaction processes.

1 Machine Learning Algorithm and Data Processing

In the present work, predicting heavy-ion fusion reaction cross sections is a supervised task requiring a machine learning algorithm and a labeled dataset with input and output variables. This section briefly introduces these components.

LightGBM represents an innovative architecture of Gradient Boosting Decision Trees (GBDT) [46], with technological breakthroughs mainly reflected in two aspects: 1) It employs a leaf-wise growth strategy with histogram optimization algorithms, significantly improving computational efficiency through dynamic feature splitting, achieving 3-5× speedup over traditional GBDT algorithms when processing high-dimensional heterogeneous nuclear physics data; 2) It possesses unique physical interpretability advantages, enabling analysis of deep correlations between input features and output quantities through feature importance ranking mechanisms and SHAP value analysis.

The data in this study are divided into three parts: training set, validation set, and test set. The training and validation sets are collectively referred to as training data. The training set is used to adjust parameters in the LightGBM algorithm, while the validation set—typically a portion partitioned from training data—aims to find the minimal loss function through gradient descent methods. Additionally, the validation set monitors model performance and prevents overfitting. The test set evaluates LightGBM' s predictive capability on unseen data. Training data are sourced from reference [19], comprising 2610 experimental data points from 146 even-even reaction systems collected before 2016. The training and validation sets are randomly partitioned from these data at a certain ratio. For research accuracy, systems with specific PTZ representations (where Z denotes proton numbers of projectile and target nuclei, and A denotes mass number of the compound nucleus) are selected, avoiding overly heavy or light systems where fusion-fission and quasi-fission may dominate in heavy systems, or breakup and transfer reactions may complicate analysis in light systems. The test set contains 175 data points from 11 even-even reaction systems derived from recent experiments [47-53]. Notably, reaction systems in the test set never appeared in the training set. Table 1 details the relevant reaction systems in the test set, data point counts per system, and energy ranges.

Since CS typically varies by orders of magnitude across different energy ranges, such large data differences may affect ML algorithm prediction performance. Therefore, this study selects the logarithm of CS as the output variable for the LightGBM model. Building upon reference [44], this study adds additional basic features including differences between neutron numbers and nearest magic numbers, differences between proton numbers and nearest magic numbers, Casten factors, and excitation energies of 2^+ and 4^+ states for even-even nuclei. These input features are listed in Table 2 . These quantities represent basic nuclear features (BF) expected to be closely related to fusion processes in even-even systems. Generally, adding features strongly correlated with CS can improve model prediction accuracy. To better obtain mapping relationships between input features and CS, physics information related to heavy-ion fusion processes must be introduced to guide ML algorithms in finding correlations between BF and CS. This work uses CS calculated from Wong formula and the gp1 formula obtained through genetic programming as input features. The specific forms of Wong formula and gp1 formula are as follows:

$$\text{Wong} = \ln\left(1 + \exp\left(\frac{E - V_B}{\omega}\right)\right)$$

$$\text{gp1} = 1103 \exp\left(-\frac{(E - E_0)^2}{2\sigma^2}\right)$$

Detailed information about Wong formula and gp1 formula can be found in references [19,45]. These two input features are termed physics-guided features or physics-informed features, listed in Table 3 . The primary objective of this work is to establish relationships between fusion reaction features and fusion cross sections through LightGBM learning on the training set. During training, three different input feature combinations are used, as shown in Table 4 . In Mode_{BF}, input features consist of 30 basic features from Table 2. In Mode_W and Mode_{gp1}, CS calculated from Wong formula and gp1 formula are included in addition to the 30 basic features. ML algorithm capability in predicting fusion cross sections can be quantitatively evaluated through Mean Absolute Error (MAE):

$$\text{MAE} = \frac{1}{N}\sum_{i=1}^{N}\left|\log_{10}(\sigma_{\text{pred}}) - \log_{10}(\sigma_{\text{exp}})\right|$$

The main hyperparameters of LightGBM algorithm include: num_{leaves} (maximum leaves per tree), max_{depth} (maximum depth per tree), and num_{iterations} (boosting iterations). Their values are set to 30, -1 (indicating no limit), and 10000, respectively. This study incorporates over thirty input features. Adding more features significantly increases parameter numbers while enhancing predictive capability. With these hyperparameters, LightGBM algorithm parameter count (including all root, internal, and leaf nodes) is approximately 800,000. Modern ML or deep learning algorithms like deep convolutional neural networks (CNN) and CatBoost typically involve millions of parameters. Given limited data points, one might question the appropriateness of using modern ML algorithms. In fact, by employing LightGBM, our purpose is to evaluate its effectiveness on unseen data and explore complex correlations between outputs and inputs, rather than merely obtaining minimal MAE on the training set.

2.1 Validation Set Performance

This study first examines ML method effectiveness and investigates how training-to-validation set ratios affect LightGBM performance. To this end, 2610 data points in the training data are randomly partitioned into training and validation sets. Figures 1 Figure 1: see original paper show model performance on validation and total datasets under different training set proportions. As expected, MAE gradually decreases with increasing training set proportion. However, due to reduced validation set size, uncertainty in validation results increases (see Figures 1(a-b)). LightGBM' s strong fitting capability on training samples typically yields MAE on training sets smaller than on validation sets. Figures 1(c-d) display learning curves for Mode_{gp1} and Mode_W models when training-to-validation ratio is 4:1. Learning curves reflect loss function evolution with decision tree numbers. During training, loss gradually decreases with increasing decision trees and saturates at a specific value, indicating training should stop at this point. Additionally, observing differences between training and validation curves provides another important training benchmark. For reasonable training, training and validation curves should be close; significant differences may indicate overfitting or underfitting. Figures 1(c-d) show that for both models, loss on validation and training sets gradually decreases with increasing tree numbers, saturating at approximately 500 trees. Meanwhile, validation and training loss curves nearly coincide, indicating no overfitting occurs. Consequently, very low MAE values can be obtained on training sets while achieving reasonable MAE on validation sets. Even with a 1:1 training-to-validation ratio, MAE values remain significantly lower than many traditional physical models like the empirical coupled-channel model. In this work, to avoid excessively large MAE values or uncertainties, a 4:1 ratio is selected for subsequent discussions.

To investigate the impact of physics-informed features on LightGBM prediction accuracy, Figure 2 [Figure 2: see original paper] shows MAE density distributions for Mode_{gp1}, Mode_W, and Mode_{BF}, along with ECC model MAE. Table 5 lists corresponding mean values and standard deviations. As shown in Table 5, Mode_{gp1} and Mode_W containing physics-informed features exhibit optimal MAE values, with average prediction errors of approximately 0.07—about 46% lower than Mode_{BF}. This result demonstrates that physics-informed features are particularly crucial for building stable ML models [54]. Notably, although the ECC model provides reasonable fits to fusion excitation functions near the Coulomb barrier by comprehensively considering complex physical mechanisms such as neutron transfer channels, coupling between relative motion and intrinsic degrees of freedom, and nuclear deformation, Mode_{BF} based on LightGBM achieves MAE of 0.138, lower than ECC' s 0.172. This indicates that ML methods demonstrate powerful advantages in CS prediction tasks through appropriate selection of reaction system basic features. The study also reveals limitations of empirical formulas: Wong formula' s MAE in predicting CS is approximately 2.59, indicating large deviations from experimental measurements with error ranges reaching two orders of magnitude. This deviation primarily stems from the training dataset containing numerous data points far below Coulomb barrier energies, where Wong formula exhibits significant limitations and cannot provide accurate predictions. Table 5 results demonstrate that selecting appropriate physics-informed features is crucial for improving model accuracy in predicting nuclear fusion cross sections, while also highlighting limitations of traditional theoretical models in specific energy regions.

Experimental data accuracy and theoretical model limitations significantly impact ML model prediction performance. Theoretical model prediction effects and experimental data uncertainties or systematic biases substantially limit ML model learning capability and generalization performance. ML models demonstrate better performance when experimental data errors are small and theoretical models are superior. Future work will further explore effective incorporation of experimental data uncertainties or systematic biases into ML models to enhance their adaptability to data noise. Simultaneously, we will select more suitable theoretical models for ML model construction.

To verify the rationality of selecting 2^+ and 4^+ state excitation energies as input features, comparative studies were conducted on training data (146 systems containing 2610 data points). Specifically, two feature combinations were constructed: F6 without excitation energy information (ZP, AP, ZT, AT, Ec.m., and sig_W) and F10 containing projectile and target 2^+, 4^+ state excitation energies (ZP, AP, ZT, AT, Ec.m., sig_W, 2^+P, 4^+P, 2^+T, 4^+T). The 2610 data points were partitioned into training and validation sets at a 4:1 ratio, with 500 independent training runs for each feature combination. Results show that introducing 2^+, 4^+ state excitation energies reduces average validation set MAE from 0.092 ± 0.007 to 0.078 ± 0.006—approximately 15% improvement. This demonstrates that low-lying state energies as input features effectively enhance model performance, validating their physical significance in predicting fusion cross sections.

2.2 Test Set Performance

This study further validated LightGBM performance using a test set (175 data points from 11 reaction systems). Figure 3 [Figure 3: see original paper] compares CS predicted by Mode_{BF}, Mode_{gp1}, and Mode_W models with latest experimental data. Results show that CS obtained from Wong formula are similar to experimental data in high-energy regions but significantly lower in low-energy regions. This difference primarily arises because parabolic approximations fail at energies far below the Coulomb barrier, a phenomenon widely discussed in literature [4,55]. Among feature combinations containing physics information, Mode_{gp1} and Mode_W predictions show better agreement with experimental data in energy dependence, while Mode_{BF} exhibits larger discrepancies in energy-dependent behavior for certain reaction systems. MAE values on the test set are 0.171 ± 0.006 and 0.174 ± 0.006 for Mode_{gp1} and Mode_W, respectively—both superior to Mode_{BF}' s 0.446 ± 0.016. These results demonstrate that introducing physics-informed features is crucial for ML algorithms to accurately capture energy dependence, effectively improving model performance. Test set MAE values are higher than validation set MAE values, as expected, because test set reaction systems were not included in the training set.

In principle, all fusion dynamics information is contained in excitation functions, but extracting fusion barrier distributions (BD) through high-precision measurements is crucial for resolving coupling mechanisms underlying cross-section enhancement [15,56-58]. Fusion cross-section excitation functions are typically presented on linear or logarithmic scales; however, logarithmic scale steep variations make identifying structural features or theoretical deviations particularly difficult. Therefore, this study extracted BD from ML-predicted fusion cross sections and compared them with experimental data to assess whether ML methods can properly reproduce BD behavior. Detailed BD extraction methods are described in reference [5]. Considering that extracting BD from CS excitation functions requires sufficient data points, the $^{18}O+^{116}Sn$ and $^{36}S+^{50}Ti$ systems were selected for investigation. Figure 4 [Figure 4: see original paper] compares BD predicted by Mode_{gp1} and Mode_W with latest experimental data for these systems. Although all three models can well describe CS in the $^{18}O+^{116}Sn$ system in Figure 3, Figure 4 shows that Mode_{gp1} and Mode_W better reproduce BD variation with Ec.m., indicating stronger predictive capability. This conclusion is further supported by test set MAE results. Note that because absolute errors above-barrier CS are larger and corresponding energies are higher, BD errors are larger above the barrier and smaller below it. In summary, both Mode_{gp1} and Mode_W can reproduce fusion barrier distribution variation curves with Ec.m. within error ranges, proving that physics information plays an important role in ML studies of heavy-ion fusion reactions.

2.3 Model Interpretability Analysis

As previously mentioned, LightGBM offers high interpretability, which holds important value for studying physical problems [60]. To deeply understand the mechanism by which LightGBM generates specific results and its learning patterns, we employed the SHAP method [61-63]. SHAP is a widely used feature attribution method that effectively identifies features contributing most to predictions. Figure 6 [Figure 6: see original paper] shows feature importance ranking, where top-ranked features are most important for fusion cross-section prediction while lower-ranked features have minimal impact. In Mode_{gp1} and Mode_W, physics-informed features (sig_{gp1} and sig_W) occupy top positions with SHAP values significantly higher than other features. Furthermore, features were categorized into projectile (ZP, AP, vP, PP, BP, 2^+P, 4^+P), target (ZT, AT, vT, PT, BT, 2^+T, 4^+T), compound nucleus (Z, A, vn, vp, P, B, I, β), reaction conditions (Ec.m. and Q), and physics information (sig_W and sig_{gp1}). Contribution proportion plots for each category are shown in Figure 6. Notably, in Mode_{BF}, the system category contributes up to 60.8%; when physics-informed features are included, the physics information category becomes the highest contributor. Moreover, regardless of mode, 2^+ and 4^+ excitation energies related to even-even systems rank among the top positions. This indicates that projectile and target 2^+ and 4^+ state excitation energies play an important role in CS prediction, helping further improve ML credibility and interpretability.

Conclusion

Building upon previous work, this study investigated heavy-ion fusion reactions in even-even systems by further considering characteristics such as projectile and target 2^+ and 4^+ state excitation energies. Physics-informed features used include fusion cross sections calculated by gp1 and Wong formulas. Results show that on the validation set, LightGBM can predict experimental fusion cross-section data within a factor of 10^0.138 = 1.37 using only basic physical quantities—superior to the 10^0.172 = 1.47 factor obtained from the empirical coupled-channel model. When physics-informed features are included in input, the discrepancy between LightGBM predictions and experimental data reduces to a factor of 10^0.07 = 1.17. Using only basic physical features, test set MAE (175 data points from 11 reaction systems) is approximately 0.44; this value decreases to about 0.17 when physics-informed features are included. To further verify LightGBM reliability, fusion barrier distributions for the $^{18}O+^{116}Sn$ and $^{36}S+^{50}Ti$ systems were extracted from predicted CS on the test set, revealing that modes containing physics-informed features better reproduce barrier distribution variation with Ec.m. Additionally, SHAP analysis constructed visual correlation maps between input features and CS, with feature importance ranking revealing that projectile and target 2^+ and 4^+ state excitation energies play an important role in CS prediction. Our study demonstrates that physics information plays a crucial role in ML research on heavy-ion fusion reactions.

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