Nuclear charge radius predictions by kernel ridge regression with odd-even effects

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Abstract

The extended kernel ridge regression (EKRR) method with odd-even effects was adopted to improve the charge radius using five commonly used nuclear models. These are: (i) the isospin dependent $A^{1/3}$ formula (ii) relativistic continuum Hartree-Bogoliubov (RCHB) theory (iii) Hartree-Fock-Bogoliubov (HFB) model HFB25 (iv) the Weizsäcker-Skyrme (WS) model WS^{a}st, (v) HFB25^{a}st model. In the last two models, the charge radii were calculated using a five-parameter formula with the nuclear shell corrections and deformations obtained from the WS and HFB25 models, respectively. For each model, the resultant root-mean-square deviation for the 1014 nuclei with proton number $Zgeq8$ can be significantly reduced to 0.009-0.013~fm after considering the modification with the EKRR method. The best among them was the RCHB model, with a root-mean-square deviation of 0.0092~fm. The extrapolation abilities of the KRR and EKRR methods for the neutron-rich region were examined and it was found that after considering the odd-even effects, the extrapolation power was improved compared with that of the original KRR method. The strong odd-even staggering of nuclear charge radii of Ca and Cu isotopes and the abrupt kinks across the neutron $N = 126$ and 82 shell closures were also calculated and could be reproduced quite well by calculations using the EKRR method.

Full Text

Preamble

Nuclear Charge Radius Predictions by Kernel Ridge Regression with Odd-Even Effects

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The extended kernel ridge regression (EKRR) method with odd-even effects was adopted to improve the description of nuclear charge radii using five commonly used nuclear models: (i) the isospin-dependent $A^{1}/^{3}$ formula, (ii) relativistic continuum Hartree-Bogoliubov (RCHB) theory, (iii) the Hartree-Fock-Bogoliubov (HFB) model HFB25, (iv) the Weizsäcker-Skyrme (WS) model WS*, and (v) the HFB25* model. In the last two models, charge radii were calculated using a five-parameter formula with nuclear shell corrections and deformations obtained from the WS and HFB25 models, respectively. For each model, the resultant root-mean-square deviation for the 1014 nuclei with proton number $Z \geq 8$ could be significantly reduced to 0.009–0.013 fm after applying the EKRR modification. The best performance was achieved with the RCHB model, yielding a root-mean-square deviation of 0.0092 fm. The extrapolation abilities of the KRR and EKRR methods for neutron-rich regions were examined, and it was found that incorporating odd-even effects improved the extrapolation power compared to the original KRR method. The strong odd-even staggering of nuclear charge radii in Ca and Cu isotopes and the abrupt kinks across the neutron $N = 126$ and 82 shell closures were also calculated and could be reproduced quite well using the EKRR method.

Keywords: Nuclear charge radius, Machine learning, Kernel ridge regression method

Introduction

The nuclear charge radius, similar to other quantities such as binding energy and half-life, is one of the most fundamental properties reflecting important characteristics of atomic nuclei. Assuming constant saturation density inside the nucleus, the nuclear charge radius is typically described by the $A^{1}/^{3}$ law, where A is the mass number. By studying charge radii, information can be obtained about nuclear shells and subshell structures [**?**, **?**], shape transitions [**?**, **?**], neutron skin and halos \cite{5–7}, and other nuclear phenomena.

With improvements in experimental techniques and measurement methods, various approaches have been adopted for measuring nuclear charge radii [**?**, **?**]. To date, more than 1000 nuclear charge radii have been measured [**?**, **?**]. Recently, the charge radii of several exotic nuclei have attracted particular interest, especially the strong odd-even staggering (OES) observed in some isotope chains and the abrupt kinks across neutron shell closures \cite{2,12–21}, which provide stringent benchmarks for nuclear models.

Theoretically, various methods have been used to systematically investigate nuclear charge radii, including phenomenological formulae \cite{22–29}, local-relationship-based models \cite{30–35}, macroscopic-microscopic models \cite{36–39}, nonrelativistic \cite{40–43} and relativistic mean-field models \cite{44–52}. In addition, the ab initio no-core shell model has been adopted for this topic [?, ?]. While each model provides fairly good descriptions of nuclear charge radii across the nuclear chart, with the exception of models based on local relationships, all these methods have root-mean-square (RMS) deviations larger than 0.02 fm. It should be noted that few of these models can reproduce the strong OES and abrupt kinks across neutron shell closures. To understand these nuclear phenomena, a more accurate description of nuclear charge radii is required.

Recently, due to the development of high-performance computing, machine learning methods have been widely adopted for investigating various aspects of nuclear physics \cite{55–59}. Several machine learning methods have been used to improve the description of nuclear charge radii, such as artificial neural networks \cite{60–63}, Bayesian neural networks \cite{64–68}, the radial basis function approach [?], and kernel ridge regression (KRR) [?]. By training a machine learning network using radius residuals—that is, the deviations between experimental and calculated nuclear charge radii—these methods can reduce the corresponding RMS deviations to 0.01–0.02 fm.

The KRR method is one of the most popular machine learning approaches, representing an extension of ridge regression for nonlinear problems [?, ?]. It has been improved by including odd-even effects and gradient kernel functions and has provided successful descriptions of various aspects of nuclear physics, including nuclear masses \cite{73–77}, nuclear energy density functionals [?], and neutron-capture reaction cross sections [?]. In the present study, the extended KRR (EKRR) method with odd-even effects included through remodulation of the KRR kernel function [?] is used to improve the description of nuclear charge radii. Importantly, compared with the KRR method, the number of weight parameters does not increase in the EKRR method.

The remainder of this paper is organized as follows. A brief introduction to the EKRR method is presented in Sec. II. The numerical details of the study are presented in Sec. III. The results obtained using the KRR and EKRR methods are presented in Sec. IV, including a discussion of the extrapolation power of the EKRR method and investigations of the strong OES of nuclear charge radii in Ca and Cu isotopes and abrupt kinks across the neutron N = 126 and 82 shell closures. Finally, a summary is presented in Sec. V.

Theoretical Framework

The KRR method was successfully applied to improve descriptions of nuclear charge radii obtained using several widely used phenomenological formulae [?]. To include odd-even effects, the KRR function $S(\mathbf{x}) = \sum_{i=1}^{m} K(\mathbf{x}_j; \mathbf{x}_i)\alpha_i$ is extended to the EKRR function [?]:

$$S(\mathbf{x}_j) = \sum_{i=1}^{m} K(\mathbf{x}_j; \mathbf{x}_i)\alpha_i + \sum_{i=1}^{m} K_{oe}(\mathbf{x}_j; \mathbf{x}_i)\beta_i$$

where $\mathbf{x}_i$ are the locations of nuclei in the nuclear chart, with $\mathbf{x}_i = (Z_i, N_i)$. Here m is the number of training data points, α_i and β_i are the weights, and $K(\mathbf{x}_j; \mathbf{x}_i)$ and $K_{oe}(\mathbf{x}_j; \mathbf{x}_i)$ are kernel functions that characterize the similarity between data points. In this study, a Gaussian kernel was adopted, expressed as:

$$K(\mathbf{x}_j; \mathbf{x}_i) = \exp\left(-\frac{\|\mathbf{x}_i - \mathbf{x}_j\|^2}{2\sigma^2}\right)$$

where $\|\mathbf{x}_i - \mathbf{x}_j\| = \sqrt{(Z_i - Z_j)^2 + (N_i - N_j)^2}$ is the distance between two nuclei. $K_{oe}(\mathbf{x}_j; \mathbf{x}_i)$ was introduced to enhance correlations between nuclei with the same parity of neutron and proton numbers, which can be written as:

$$K_{oe}(\mathbf{x}_j; \mathbf{x}_i) = \epsilon_{oe}(\mathbf{x}_j; \mathbf{x}_i) \exp\left(-\frac{\|\mathbf{x}_i - \mathbf{x}_j\|^2}{2\sigma_{oe}^2}\right)$$

where $\epsilon_{oe}(\mathbf{x}_j; \mathbf{x}_i) = 1$ (0) if the two nuclei have the same (different) parity of proton and neutron numbers. The parameters σ and σ_{oe} are hyperparameters that define the range affected by the kernel.

The kernel weights α_i and β_i are determined by minimizing the following loss function:

$$\mathcal{L}(\alpha, \beta) = \sum_{i=1}^{m} [S(\mathbf{x}_i) - y(\mathbf{x}_i)]^2 + \lambda \alpha^T \mathbf{K} \alpha + \lambda_{oe} \beta^T \mathbf{K}_{oe} \beta$$

The first term is the variance between the training data $y(\mathbf{x}_i)$ and the EKRR prediction $S(\mathbf{x}_i)$. The second and third terms are regularizers, where the hyperparameters λ and λ_{oe} determine the regularization strength and are adopted to reduce the risk of overfitting.

By minimizing the loss function [Eq. (4)], we obtain:

$$\beta = \frac{\lambda}{\lambda_{oe}} \alpha$$

$$\alpha = \left(\mathbf{K} + \frac{\lambda}{\lambda_{oe}} \mathbf{K}_{oe} + \lambda \mathbf{I}\right)^{-1} \mathbf{y}$$

According to Eq. (5), the EKRR function [Eq. (1)] can be written as a standard KRR function:

$$S(\mathbf{x}_j) = \sum_{i=1}^{m} K'(\mathbf{x}_j; \mathbf{x}_i)\alpha_i$$

where $K'(\mathbf{x}_j; \mathbf{x}_i)$ is the remodulated kernel:

$$K'(\mathbf{x}_j; \mathbf{x}_i) = K(\mathbf{x}_j; \mathbf{x}_i) + \frac{\lambda}{\lambda_{oe}} K_{oe}(\mathbf{x}_j; \mathbf{x}_i)$$

According to Eq. (5), the number of weight parameters in the EKRR method is identical to that in the original KRR method.

Numerical Details

In this study, 1014 experimental data points with $Z \geq 8$ were considered, obtained from Refs. [**?**, **?**]. The EKRR function (7) was trained to reconstruct the residual radius—that is, the deviations $\Delta R(N,Z) = R_{\text{exp}}(N,Z) - R_{\text{th}}(N,Z)$ between experimental data $R_{\text{exp}}(N,Z)$ and theoretical predictions $R_{\text{th}}(N,Z)$ for the following five nuclear models:

(i) The widely used phenomenological formula $R_c = r_A[1 - b(N-Z)/A]A^{1/3}$ [**?**] with parameters $r_A = 1.282$ fm and $b = 0.342$ fitted to experimental data (denoted as A1/3).

(ii) The relativistic continuum Hartree-Bogoliubov (RCHB) theory [**?**].

(iii) The Hartree-Fock-Bogoliubov (HFB) model HFB25 [**?**].

(iv) The Weizsäcker-Skyrme (WS) model WS* [**?**].

(v) The HFB25* model [**?**].

Note that by considering nuclear shell corrections and deformations obtained from the WS and HFB25 models, a five-parameter nuclear charge radii formula was proposed in [**?**]. In this study, these methods are denoted as WS* and HFB25*, respectively. The parameters in the formulae of these two models were obtained from Ref. [**?**]. The RMS deviations between experimental data and the five models (Δ_{rms}) are listed in Table 1 . Once the weights α_i were obtained, the EKRR function $S(N,Z)$ was determined for each nucleus. Therefore, the predicted charge radius for a nucleus with neutron number N and proton number Z is given by $R_{\text{EKRR}} = R_{\text{th}}(N,Z) + S(N,Z)$.

In this study, the KRR method was also adopted for predicting charge radii for comparison. Leave-one-out cross-validation was used to determine the two hyperparameters (σ and λ) in the KRR method and the four hyperparameters (σ, λ, σ_{oe}, and λ_{oe}) in the EKRR method. The predicted radius for each of the 1014 nuclei was given by the KRR/EKRR method trained on the remaining 1013 nuclei with a given set of hyperparameters. The optimized hyperparameters (see Table 1) were obtained when the RMS deviation between experimental and calculated radii reached a minimum value.

Results and Discussion

Table 1 lists the hyperparameters (σ, λ, σ_{oe}, and λ_{oe}) for both KRR and EKRR methods, along with the RMS deviations between experimental data and predictions from the five models. The RMS deviations with (without) KRR and EKRR corrections are denoted by $\Delta_{\mathrm{rms}}^{\mathrm{KRR}}$ and $\Delta_{\mathrm{rms}}^{\mathrm{EKRR}}$ (Δ_{rms}). With the exception of the phenomenological A1/3 formula, all other models provided good global descriptions of nuclear charge radii, particularly WS*. It should be noted that a spherical shape is considered in the RCHB theory when investigating the entire nuclear landscape [**?**], which results in a slightly larger RMS deviation compared to the nonrelativistic HFB25 model. To date, only even-even nuclei have been calculated in the deformed relativistic Hartree-Bogoliubov theory in continuum (DRHBc) [**?**, **?**], and the description of nuclear charge radii could be further improved when all nuclei in the nuclear chart are calculated using this model.

It can also be observed that HFB25 and HFB25* yield similar RMS deviations when describing nuclear charge radii. After applying the KRR method, all RMS deviations for these five models could be significantly reduced to approximately 0.015–0.018 fm, particularly for the A1/3 formula. Interestingly, while the RMS deviations of HFB25 and HFB25* were smaller than those of the A1/3 formula and RCHB model without KRR corrections, this situation was reversed after applying the KRR method. After considering odd-even effects, the predictive power of the five models was further improved by the EKRR method compared to the KRR method. The RMS deviation was reduced by approximately 0.006 fm for all five models, with the exception of HFB25, for which it was reduced by less than 0.005 fm. The RMS deviations of three models (A1/3 formula, RCHB, and WS*) were reduced to less than 0.01 fm, with the smallest value being 0.0092 fm for the RCHB model. This represents the best result for nuclear charge radius predictions using machine learning approaches, to the best of our knowledge. For comparison, typical RMS deviations from other popular machine learning approaches are: (i) artificial neural network: 0.028 fm [**?**]; (ii) Bayesian neural network: 0.014 fm [**?**]; (iii) radial basis function approach: 0.017 fm [**?**]. Note that if the full nuclear landscape is calculated using the DRHBc theory, the description of nuclear charge radii can still be improved using the EKRR method. For visual comparison, these five models are illustrated in Fig. 1 [Figure 1: see original paper].

Figure 2 [Figure 2: see original paper] shows the differences between experimental data and calculations from the RCHB model (grey solid circles), KRR method (red triangles), and EKRR method (blue crosses). Since the improvements achieved by KRR and EKRR methods were similar across the five models, we consider only the RCHB model as an example. To study the odd-even effects included in the EKRR method, the data were divided into four groups characterized by even or odd proton numbers Z and neutron numbers N: even-even, even-odd, odd-even, and odd-odd. Clearly, the predictive power of the RCHB model could be further improved using the EKRR method compared to the original KRR method. The significant improvement of the EKRR method is mainly due to the consideration of odd-even effects, which eliminates the staggering behavior of radius deviations arising from odd and even numbers of nucleons present in the KRR method. When the mass number is $A \sim 150$, the predictions of the KRR method exhibit significant deviations from the data, which can be substantially improved using the EKRR method. This provides clear evidence of the importance of considering odd-even effects in predictions of nuclear charge radius.

To investigate the extrapolation abilities of the KRR and EKRR methods for neutron-rich regions, the 1014 nuclei with known charge radii were redivided into one training set and six test sets as follows: For each isotopic chain with more than nine nuclei, the six most neutron-rich nuclei were selected and classified into six test sets based on their distance from the previous nucleus. Test set 1 (6) had the shortest (longest) extrapolation distance. This classification scheme is the same as that used in our previous study [**?**]. The hyperparameters obtained by leave-one-out cross-validation in the KRR/EKRR method remained unchanged in subsequent calculations.

The RMS deviations of the KRR and EKRR methods for different extrapolation steps for the five models are shown in Figs. 3(a)–(e). A clearer comparison of the RMS deviations, scaled to the corresponding RMS deviations of the five models without KRR/EKRR corrections, is shown in Figs. 3(f)–(j). Regardless of whether the KRR or EKRR method is considered, the RMS deviation increased with extrapolation distance. For the A1/3 formula and RCHB model, the KRR/EKRR method could improve the radius description for all extrapolation distances. For the other three models, the KRR method only improved the radius description for extrapolation distances of one or two steps, which could be further improved after considering odd-even effects with the EKRR method. This indicates that the KRR/EKRR method loses its extrapolation power at distances larger than three for these three models, likely because the charge radii calculated using these models were already quite accurate with sufficiently small RMS deviations. The KRR/EKRR method automatically identifies the extrapolation distance limit through optimization of the hyperparameters σ and σ_{oe} using the training data. Refs. [**?**, **?**] demonstrated that KRR and EKRR methods lose predictive power at larger extrapolation distances (approximately six steps) when predicting nuclear masses using the WS4 mass model [**?**]. This may be due to the existence of much more mass data than charge radius data, allowing the KRR/EKRR networks to be better trained with more data. In general, the EKRR method has better predictive power than the KRR method for extrapolation distances less than three. For distances greater than three, the results of KRR and EKRR methods were similar in most cases. Almost none of these extrapolations exhibited overfitting, except for WS* at an extrapolation distance of three, where the overfitting was quite small. This indicates that both KRR and EKRR methods have good extrapolation power and can largely avoid the risk of overfitting.

The observation of strong OES of charge radii throughout the nuclear landscape provides a particularly stringent test for nuclear theory. To examine the predictive power of the EKRR method, which is improved by considering odd-even effects compared to the original KRR method, we investigate the recently observed OES of radii in calcium and copper isotopes \cite{14–16}. Similar to the gap parameter, the OES parameter for charge radii is defined as:

$$\Delta^{(3)}r(Z,N)=\frac{1}{2}[r(Z,N-1)-2r(Z,N)+r(Z,N+1)]$$

where $r(Z,N)$ is the RMS charge radius of a nucleus with proton number Z and neutron number N.

Figure 4 [Figure 4: see original paper] compares experimental and calculated OES results for radii ($\Delta^{(3)}r$) of calcium (left panels) and copper (right panels) isotopes. Experimental data show that for calcium isotopes [Figs. 4(a)–(e)], strong OES exists between $N = 20$ and 28, with a reduction in OES appearing for $N \geq 28$. Only RCHB theory could reproduce the trend of experimental OES without KRR/EKRR corrections, though the amplitude of calculated OES was significantly less pronounced than experimental data. Interestingly, after applying KRR corrections, the calculated OES worsened for $N < 28$, particularly when the phase of OES was opposite to that of the data. The A1/3 formula showed no OES over the entire isotopic chain, and the WS* model exhibited weak OES except at the $N = 20$ and 28 shell closures. The OES in HFB25 and HFB25* models was slightly stronger but still weak compared to data. Although OES could be obtained in WS*, HFB25, and HFB25* models, the phases of calculated OES were opposite to those of experimental data. With the KRR method, OES in these four models increased, particularly for WS* and HFB25* models where calculated OES became stronger than data. However, the OES phases remained opposite to experimental data. Therefore, although the KRR method improves charge radius description substantially, it cannot reproduce the observed OES. After applying the EKRR method, experimental OES values could be reproduced quite well, especially for the A1/3 formula and RCHB theory for copper isotopes [Figs. 4(f)–(j)]. This situation is similar for calcium isotopes, though the description of Cu isotopes is less accurate than that of Ca isotopes when considering EKRR corrections. OES is overestimated in all calculations for $N < 33$ and $N > 46$, and the OES phases between $N = 38-40$ are not well reproduced. Nevertheless, the EKRR approach significantly improves OES description compared to original theory, indicating that after considering odd-even effects, shell structures and many-body correlations important for OES can be well learned using an EKRR network.

Similar to OES, abrupt kinks across neutron shell closures provide a particularly stringent test for nuclear theory. In this study, Pb and Sn isotopes were considered as examples for investigating kinks across neutron $N = 126$ and 82 shell closures. Figure 5 [Figure 5: see original paper] compares experimental and calculated differential mean-square charge radii $\Delta\langle r^2\rangle_{N',N} = \langle r^2\rangle_N - \langle r^2\rangle_{N'}$ for some even-even Pb [Figs. 5(a)–(e)] (relative to ^{208}Pb, $N' = 126$) and Sn [Figs. 5(f)–(j)] (relative to ^{132}Sn, $N' = 82$) isotopes. For Pb isotopes, RCHB theory can perfectly reproduce the kink at $N = 126$ [Fig. 5(b)]. The A1/3 formula and HFB25 model show no kink [Figs. 5(a) and (c)]. The kink could be reproduced using WS* and HFB25* models but with slight overestimation [Figs. 5(d) and (e)]. Results obtained with KRR and EKRR methods were similar. Several interpretations of kinks exist \cite{50,82–85}, and our results indicate that kinks may not be connected to odd-even effects such as pairing correlations. The well-reproduced kinks also provide a test of the proposed KRR/EKRR method. Kinks at $N = 126$ in all five models could be reproduced quite well, though the calculated differential mean-square charge radius at $N = 132$ was too large compared to data.

For Sn isotopes, only WS* and HFB25* models reproduced the kink at $N = 82$. However, the absolute values of calculated $\Delta\langle r^2\rangle$ from $N = 74 - 78$ were small compared to data, especially for the WS* model. After applying the KRR/EKRR method, results reproduced data quite well. KRR/EKRR corrections to the A1/3 formula and HFB25 model were inconspicuous, so the kink at $N = 82$ cannot be reproduced using the KRR/EKRR method. For the RCHB model, differential mean-square charge radii calculated from $N = 74$ to 80 were improved, and a kink appeared, though it remained slightly weaker than data.

Summary

In summary, the extended kernel ridge regression method with odd-even effects was adopted to improve the description of nuclear charge radii using five commonly used nuclear models. The hyperparameters of KRR and EKRR methods for each model were determined using leave-one-out cross-validation. For each model, the resultant root-mean-square deviations for the 1014 nuclei with proton number $Z \geq 8$ could be significantly reduced to 0.009–0.013 fm after applying EKRR modifications. The best performance was achieved with the RCHB model, yielding a root-mean-square deviation of 0.0092 fm, which represents the best result for nuclear charge radius predictions using machine learning approaches to our knowledge. The extrapolation abilities of KRR and EKRR methods for neutron-rich regions were examined, and it was found that incorporating odd-even effects improved extrapolation power compared to the original KRR method. Strong odd-even staggering of nuclear charge radii in Ca and Cu isotopes was investigated and reproduced quite well using the EKRR method, indicating that after considering odd-even effects, shell structures and many-body correlations can be learned effectively using an EKRR network. Abrupt kinks across neutron $N = 126$ and 82 shell closures were also investigated and reproduced well by the EKRR method.

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