Machine learning predictions of nuclear level density parameters

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Artificial Intelligence (AI) and Machine Learning (ML) refers to methods for the next generation of algorithms which are self learning in nature [1–4]. ML is an application of AI which provides the machine to learn from *'experience'* without actually being programmed. This *'experience'* is gained by making models based purely on data.

This is done by training on a known data set to generate a model and then test it. Consider a set of data where the input variables $x_{i,j}$ (*features*) give a resultant output observable y_i through some process. The aim is to find a model M, such that, $M(x_{i,j}) = y_i$, where $i, j = 1, 2, \ldots$.

For this, first a randomly selected subset of data known as *training* set is considered. The algorithm generates models which may be based on trees, minimising loss functions, neural networks, etc. Once the model is generated, its performance is measured by the *test* set, which is the remaining subset of the data. If the model performs well on the test set, it can be used to predict data for which these observables are unknown. A very standard way to measure the performance of such predictions is standard deviation (σ), which is defined as the root mean square of difference between predicted values by the model and values given by the test data.

Nuclear data are well documented in data libraries [5–7]. These data are derived and collected from various experiments or phenomenological models obtained by rigorous computation. The data in these libraries are a standard in nuclear physics for both, experimental and theoretical calculations. By using appropriate ML algorithms we can obtain a model for the observable values which can be used for predictions for nuclei beyond the experimentally known one.

In this work, we train the ML algorithm of Gradient boosted trees (GBT) on the nuclear level density parameter. Level density parameter (LDP) is the most important extracted quantity to understand nuclear observables like neutron resonances and reaction cross sections [8]. Recent semiclassical trace formula (STF) [9] evaluates the temperature-dependent LDP within 10%-15% of the experimental values for magic and semi magic nuclei. This trace formula models nucleus using Harmonic oscillator [10] with spin-orbit interactions [11]. This formalism also incorporates the shell effects in the nuclei [12]. The Gilbert-Cameron (GC) model fits the Fermi gas model with the neutron resonances to obtain asymptotic LDP. These LDP are tabulated in [7] for 289 nuclei from $Z = 11$ to 98.

We train the ML model using the data generated from both the GC model and the STF. The features of the problem are taken to be the number of neutrons and protons and the energy terms from the liquid drop model. We use GBT[13] which works on minimising the loss function. The loss function, $L(y_i, y_i^p)$, defined here is the mean square of error in prediction. For an i^{th} data point y_i and its predicted value y_i^p,

$$L(y_i, y_i^p) = \sum_i (y_i - y_i^p)^2 \tag{1}$$

The algorithm begins with an assumed model and reads the training data and calculates the loss function. The model changes the parameters of the model to minimise the loss function with every iteration of each data point. GBT is based on prediction trees.

The figures are plots of the data versus predicted value, for the predictions on the test set. The closer the values are to the $y = x$ line, the better is the predicted value and nearer to the value given by the data set.

The results from GC show (Fig. 1) a standard deviation of 0.73 and a good agreement with the asymptotic level densities.

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The STF is an exact formula with no adjustable parameters and this formalism also gives LDP as a function of temperature. We train the algorithm for temperature dependent LDP for 32 nuclei for various temperatures. We have 3000 data points. Temperature is added as a feature in this case along with the liquid drop energies and number of neutrons and protons. The ML generated model shows a standard deviation of 0.3 and the predicted values show a good agreement with the data values (Fig. 2).

The validity of using ML algorithms in nuclear data for calculation of LDP is shown in this work. The generated ML models show good agreement with the accepted values. We show predictions by the phenomenological GC model and from the exact STF. We find that the STF is modelled better using GBT algorithm. GBT has not been used before in the context of nuclear physics. The low standard deviations show that these algorithms can be used for understanding nuclear data and possibly show trends which may open a window to new physics.

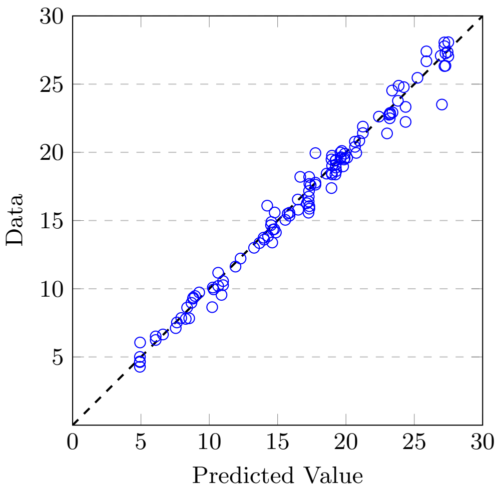

FIG. 1: By training and testing Level Density Parameter (MeV^{-1}) by the GC model for 289 nuclei, we get the standard deviation of 0.73.

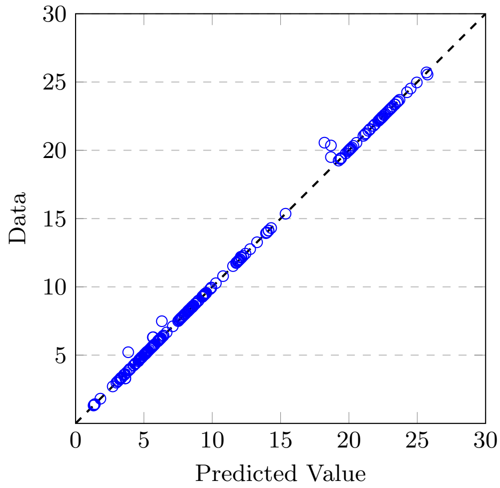

FIG. 2: Training and testing on the temperature dependent LDP (MeV^{-1}) by STF for 32 nuclei at various temperatures (3000 data points) gives the standard deviation of 0.3.

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