Revisiting the Semi-Empirical Liquid Drop Model

Robert (Rob) Netzke
B.A. Applied Mathematics, B.A. Data Science

August 24, 2022

1 Abstract

The semi-empirical liquid drop model is used to approximate the binding energy of a particular nucleus. The formula includes 5 terms, each of which is derived from a property of physics or geometry. The "empirical" nature of the formula is the result of the method in which the coefficients of this formula are derived. The formula estimates the binding energy, in MeV, of a nucleus, but many isotopes have a binding energy that can be directly computed, as the mass of the nucleus is measurable. These nuclides and their binding energies can be used to fit the formula's parameters to an optimum using a least squares fit. Hence, the actual parameters are the model are derived from the observations and serve as an approximation of the binding energy for unobserved nuclides. The purpose of this short report is to explore the potential for better estimates using a nonlinear estimation function. The topics discussed are highly interdisciplinary, so the reader should feel free to skip around sections and skim to their discretion.

2 Formula

Mentioned in the abstract, the conventional formula includes 5 terms. In combination, the binding energy of a nucleus E_B may be approximated by the following:

$$E_B(N,Z) = a_V A - a_S A^{2/3} - a_C \frac{Z(Z-1)}{A^{1/3}} - a_A \frac{(N-Z)^2}{A} + \delta(N,Z)\,. \tag{1}$$

The first term with coefficient a_v is known as the volume term. The basis for this term is in the strong nuclear force. Estimating the nucleus as a Fermi ball of A nucleons yields an expected value of a_V near $17MeV$, which is quite close to the empirical estimates in previous studies. The second term with coefficient a_S is a correction to the volume term. Nucleons on the outside the center of the nucleus will have fewer neighbors, and this term accounts for this relationship. The third term is known as the Coulomb term, and has the appropriate coefficient subscript C. This term is a rough estimation from the electrostatic repulsion between protons and assumes the nucleus can be considered a sphere of uniform charge density. The fourth term with coefficient a_A is known as the aysmmetry term. This term has a complicated theoretical basis, one which is over my head. It is based in the Pauli exclusion principle and may be researched by an expert physicist. The fifth term is a pairing term. This term is yet another complicated term on a theoretical basis, but it attempts to capture the effect of spin-coupling. Empirically, this term depends on the mass of the nucleus and has changed as

data has become more available. It is given by the following piece-wise function:

$$\begin{cases} +\delta_0 & Z, N \text{ even} \\ 0 & A \text{ odd} \\ -\delta_0 & Z, N \text{ odd} \end{cases} \tag{2}$$

$$\delta_0 = a_p A^{k_p} \tag{3}$$

The most recent experiments estimate k_p as $-1/2$, which will be used in the following model.

3 Data

The data used for this project comes from an ambiguous source. A Google search of "binding energy table" yields some databases, but, at first glance, none have a tabular format. One PDF table shows up in the search results that contains the nuclear binding energies in MeV for all isotopes up to $Z = 44$ or Ruthenium. There is no clear citation, so model predictions are to be taken with a grain of salt. The purpose of this exercise is to show that a non-linear function estimator may be used to approximate the binding energy of an arbitrary nucleus. With proper data and citation, any resulting models can be used for actual estimations.

An example of a record in the formatted table is as follows. The proton number and neutron number are simply associated with a measurement of the binding energy. The table is 1036 records long, representing the stable isotopes up to $Z = 44$.

Z	N	$Element$	$BE(MeV)$
12	20	Mg	134.4703

(4)

4 Model

4.1 Motivation

Neural networks have powerful implications for a variety of fields. When a functional form is unknown, but data is available, neural networks act as universal function estimators. Given an input vector X and an expected output vector y, a neural network is a function f that that approximates $f(X) = y$. This function f is not limited to be linear, and complex functional forms can be estimated using this function. Even groups can be estimated, such as the space of modulo 5. The power of these networks are attributed to the power of matrix multiplication. For instance, a simple matrix can represent the arbitrary rotation of a point around an axis by angle θ.

Given the context of the efficacy of neural networks to solve complex problems, the implications for the semi-empirical liquid drop model become more plausible. As mentioned in the section on the formula, the a_S term acts as a correction to the volume term. This correction is limited by the conventional model to be a simple linear relationship between terms. A neural network can approximate a non-linear relationship between terms to better fit to the data available. Furthermore, complex relationships may be formed between an arbitrary number of the terms. As estimates improve with the allowance of non-linear relationships between terms, insight towards the projected valley of stability may be cross-validated and improved – a topic discussed at the end of this report.

4.2 Architecture

Figure 1 displays the neural network architecture chosen for the model. The wideness of the hidden layers was chosen with the intent for the number of parameters to be sufficient in representing an

arbitrary function. One might notice that the input vector is of size 5. The inputs to this model are the surface term, volume term, Coulomb term, asymmetry term, and pairing term for a number of protons Z and number of neutrons N. The output of the model is one real number value, the binding energy of the nucleus in MeV. The activation function at each layer is ReLU.

With some thought, the diagram shows that the traditional linear model can be encapsulated by a small fraction of the network. With a fully connected model of this size, the representation for many non-linear relationships may be captured after fitting to the data.

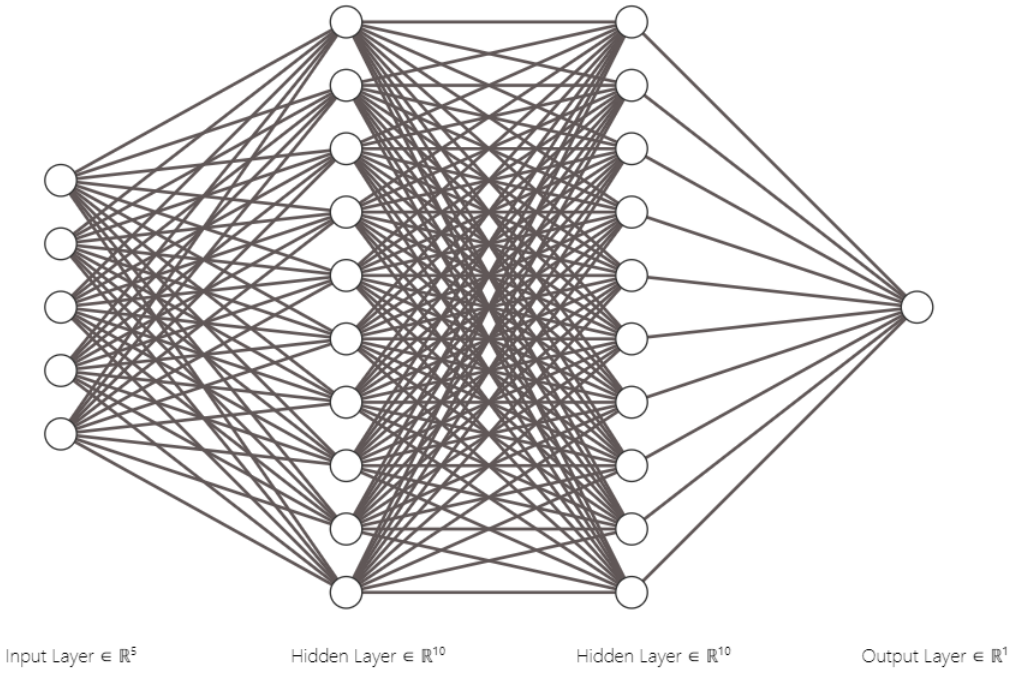

Figure 1: Fully Connected Model

4.3 Training

The model was trained on all available data over 1000 epochs. $ADAM$ was chosen as the optimizer for the model and the mean squared error as the loss function. The learning rate for $ADAM$ was chosen as 0.001. Shown in Figure 2 (found on page 4), there is a convergence in the loss function around the 400th epoch, indicating that an optima of the loss function was found. Therefore, the model parameters have reached an optima.

5 Results

Figure 3 (found on page 5) displays the actual and predicted binding energies for different values of A. The model encapsulates the macro-trends in the binding energies for the isotopes it was trained on, and, with more data, an improvement in these results may occur.

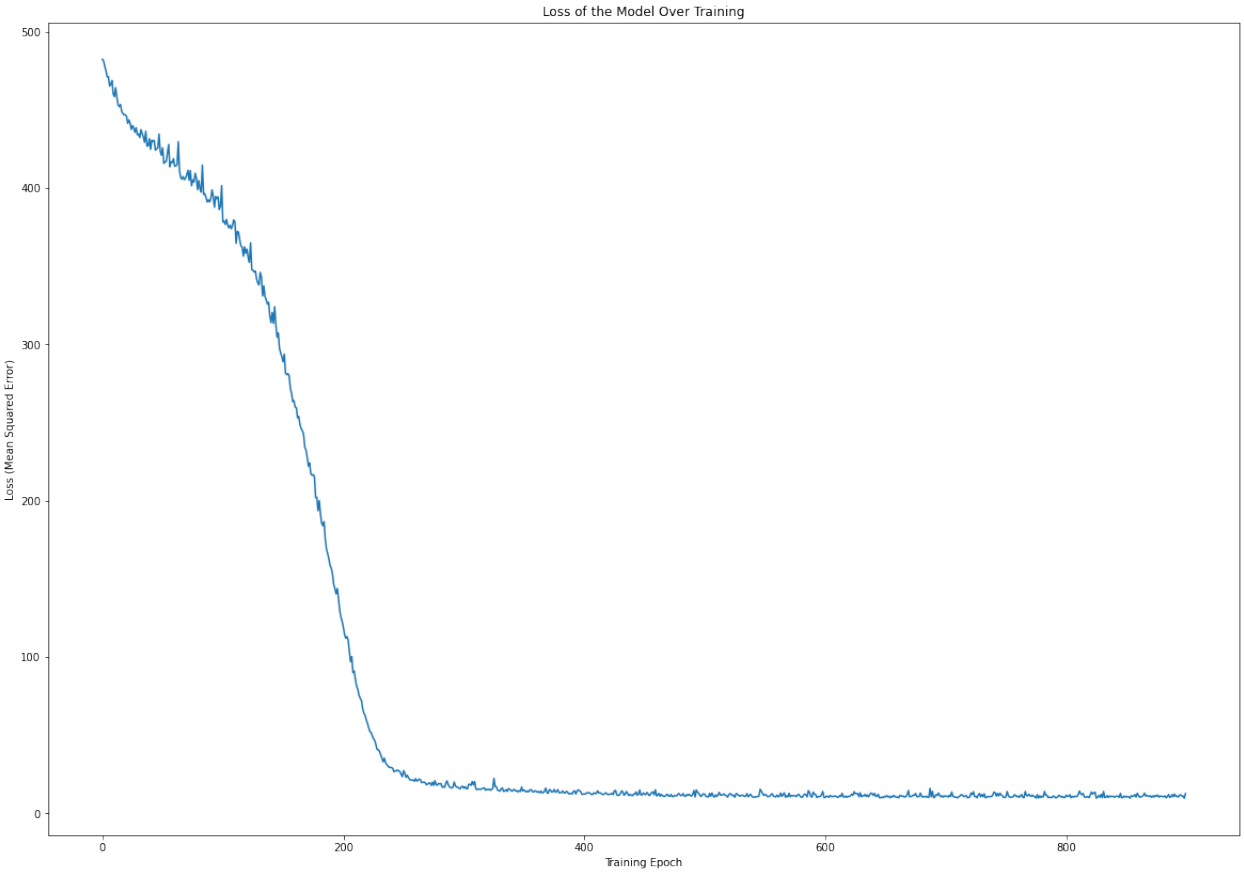

Figure 2: Training Losses

Turning to the residual errors shown in Figure 4 (found on page 6), the model prediction rarely deviated by more than 15 MeV from the actual binding energy of the nucleus. These problematic predictions for the model occurred at $4He$, which is an exceptional Helium isotope that has 4 times stronger binding energy than $3He$, and at $23Si$, which has a relatively low binding energy compared to its other isotopes.

Considering previous models, previous studies consider the binding energy per nucleon whereas my study only analyzed the predictions for the total binding energy of the nucleus. The binding energy per nucleon is as it sounds: it is found by dividing the binding energy by A. Considering this metric, the neural network outperforms the conventional model for larger sized nuclei that the model trained on, but further data is necessary to train an effective model that scales to projections for super-heavy elements. Furthermore, the results have not been extended past $Z = 44$.

6 Conclusions

This report has shown the potential for improvements in the semi-empirical liquid drop model by bringing modern computing techniques to the physics that has developed over the last century. With less than half of the known stable isotopes, an effective model can be trained to predict a nuclear binding energy given just the proton and neutron number of said nucleus. Such predictions may be

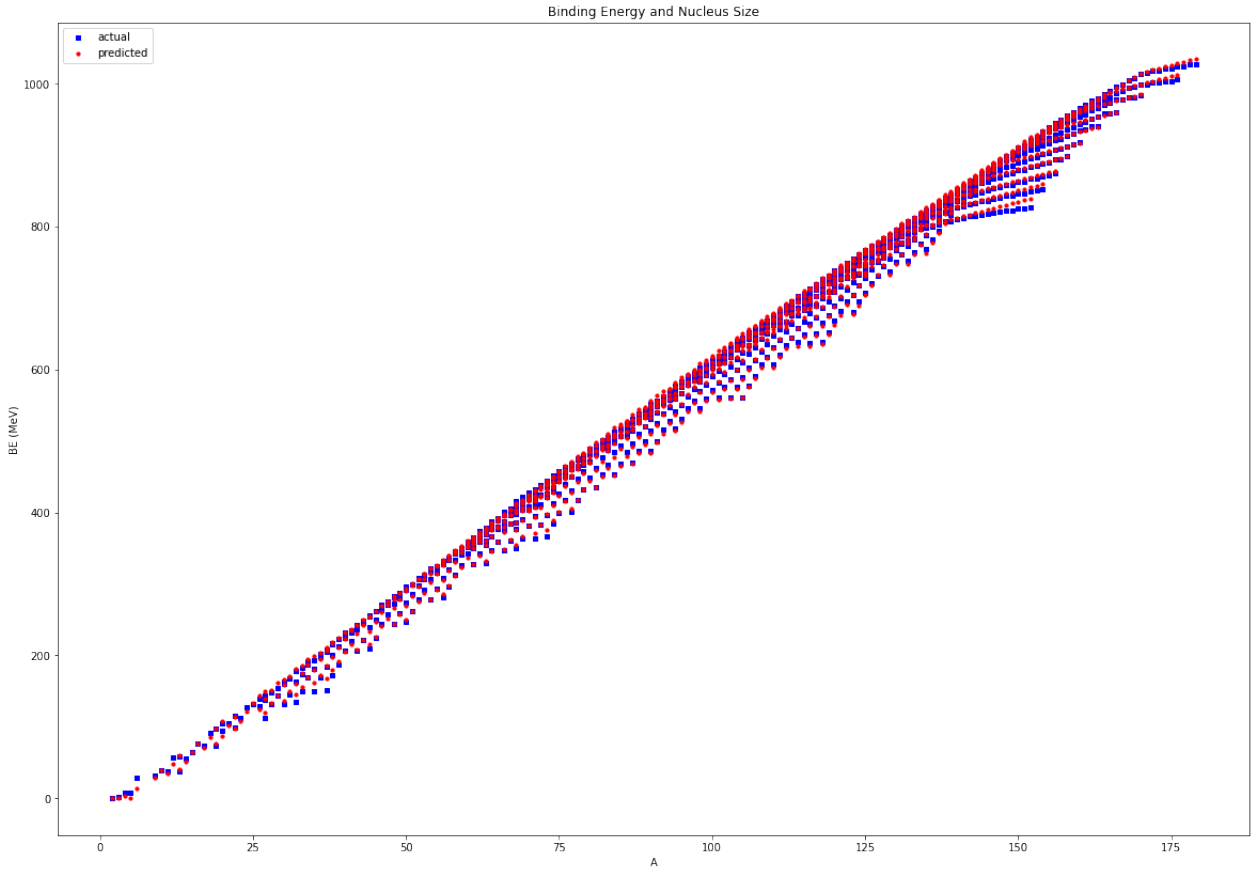

Figure 3: Binding Energy with respect to A

used to cross-validate existing theory.

The island of stability is a hypothesis in nuclear science that projects a locale of stable nuclei beyond the known stable isotopes. This hypothesis arises from the nuclear shell model of the nucleus, which predicts there are some "magic numbers" for stable nuclei. In other words, theory implies that there are optimal numbers of protons and neutrons in a spherical nucleus that locally maximize the binding energy of the nucleus. Lead-208, as the strongest bound nucleus for measurable isotopes, aligns directly with this theory. A strong statistical model, in the form of a neural network, could cross validate theory with predictions driven by strong data. Furthermore, in essence, an effectively trained neural network may have the potential learn a modern physics model without having touched a physics or mathematics textbook.

The hope for the iteration of this model is that, with extensive data, the model predictions align with existing theory. There are "magic number" projections that predict the most stable of the super heavy elements, and these elements would represent a local increase in existing binding energy trends (which is why it is known as the "island of stability"). It may be difficult for the model to predict a reversion in the binding energy trends as the size of the nucleus increases, but a predictive model that does in fact predict this local uptrend in binding energy would be quite promising for estimations outside the scope of the known stable isotopes.

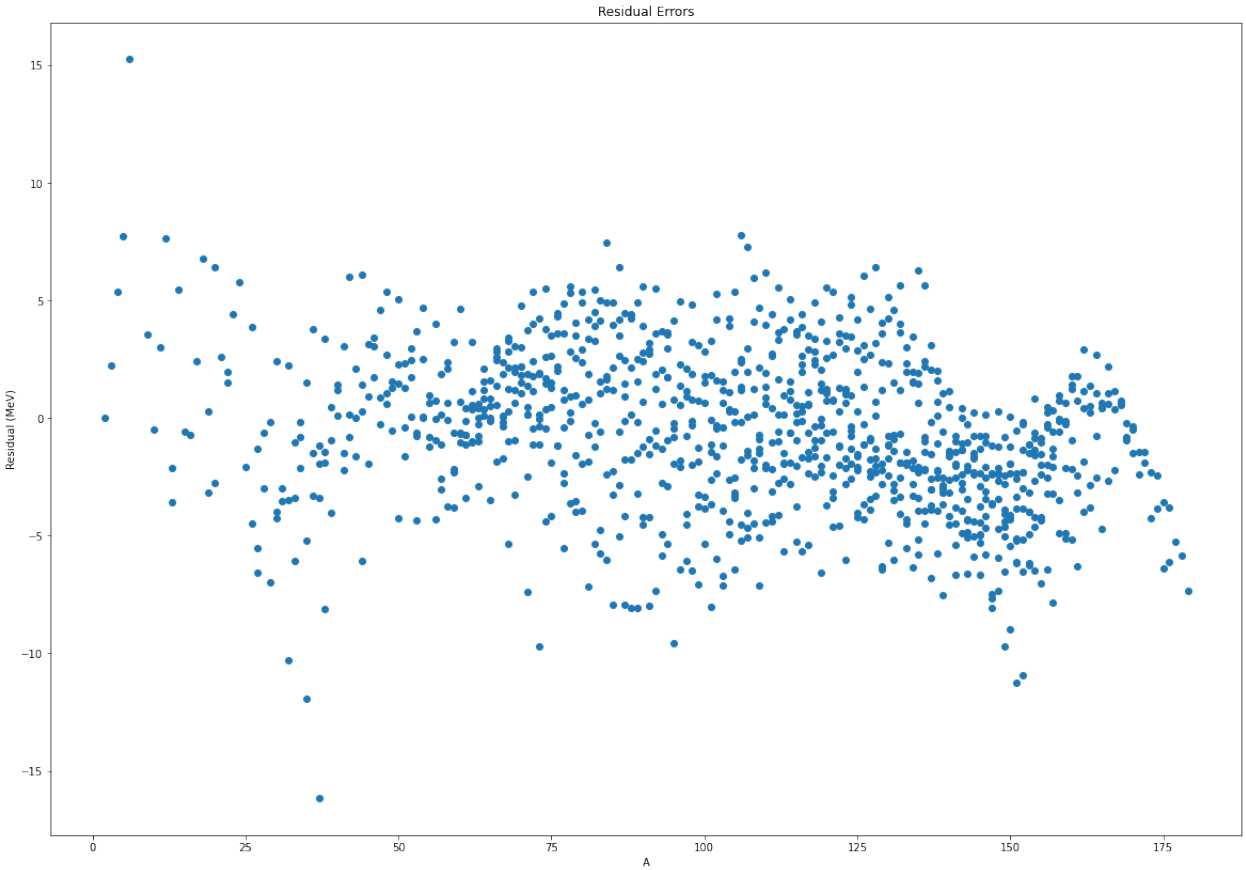

Figure 4: Residual Errors with respect to A

6.1 Assistance and Collaboration

I have found my search for credible and easy-to-use data on nuclear binding energies to be far more arduous than I thought it would be at the start of this project. If a reader knows of someone I may talk to or a site I may visit to find more data on nuclear binding energies, I would be grateful for the referral! + If the reader has taken interest and would like to discuss, I may be reached at rob.netzke@gmail.com!