Using deep learning to predict the half lives of isotopes given proton and neutron count

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1 Abstract

In this study, we attempt to predict the half-lives of superheavy isotopes through regression models. Superheavy elements usually have very short half-lives, but a few isotopes are predicted to have long enough half-lives for potential applications in nuclear and material science. To calculate these half-lives, we initially used a deep learning regression model with Keras library's dense layers that took proton count and neutron count as inputs and $\log_{10}$ of the half-life as the output. When it was tested on various isotopes of the periodic table, there was an MSE (mean squared error) of 111. Afterwards, more input variables related to proton and neutron count were added to increase complexity, leading to an MSE of 97. This suggests that the model on average falls many orders of magnitude off from the actual half-life, which would make accurate prediction of half-lives difficult. It is possible that more complexity, through different kinds of layers, and different inputs may be needed to accurately predict the half-lives of nuclides (another word for isotopes).

2 Introduction

Superheavy elements are elements of the periodic table with atomic number greater than 103. While almost all isotopes of these elements decay within seconds, there are a few that may have half-lives long enough to hold practical applications. Their location on the periodic table gives them unique physical, chemical, and nuclear properties, which if stable enough, can lead to discoveries in material science or nuclear engineering[1]. Some patterns are known about the half-life of various isotopes - heavier elements are less stable, for example. Some lesser-known factors include whether the proton and neutron counts are odd or even, or whether their amounts are magic numbers, a group of numbers important in nuclear physics[2]. However, it is still not completely known how all these factors influence an atom's stability - for example, magic numbers don't always follow the originally predicted mathematical formula of $2\left(\binom{n}{1}+\binom{n}{2}+\binom{n}{3}\right)$ [2], and empirically observing superheavy elements is difficult due to the costs of synthesizing them.

Instead of trying to find everything that determines a nuclide's half life, we try to find a model that can implicitly learn what trends exist between proton/neutron count and half life. Fortunately, deep learning models are known to be very effective at approximating these trends[3]. They "learn" by inputting training data, then changing parameters until it reaches a local peak accuracy. As a result, we plan to use deep learning models to predict half lives of superheavy isotopes.

3 Background

Periodic table half lives are the result of numerous known effects, but they are not all known or agreed upon. The most obvious noticeable trend is the decreasing stability for heavier elements beyond lead: there are no stable elements beyond lead, and half lives rapidly decrease after Curium, element 96. However, that doesn't explain everything about half-lives - for example, Tc (z (Atomic Number) = 43) and Pm (z = 61), both elements lighter than lead, have no stable isotopes, and between Bi (z = 83) and Th (z = 90), nearly all isotopes decay within days while many isotopes both to the left and right of this region last very long. To explain this, a model known as the nuclear shell model was developed independently by several researchers in the 20th century[4] similar to how energy levels are used to model electrons, they can be used to model protons and neutrons. Protons and neutrons form separate shells, and have "magic numbers" which are numbers at which a shell is filled, leading to a higher binding energy, which is related to a nucleus's stability. For spherical atomic nuclei, some magic numbers are 2, 8, 20, 28, 50, 82, and 126.

Since then, a formula known as the KTUY formula has been developed, which has been used to predict that the half life of the unknown isotope Darmstadtium-290 is around $300 \cdot 10 \pm 3$ years, where 10 ± 3 represents an uncertainty of about 3 orders of magnitude 5[5].

4 Dataset

The training data for this project is a csv file from the international atomic energy agency which lists several characteristics of each known isotope. From this, we extracted the half lives of each isotope in its ground state for the model, and plotted it below.

The data has two axes/features, which are proton and neutron count. Each pixel represents an isotope, and its color represents a half life as shown by the colorbar on the right. Dark purple pixels are stable and white pixels don't correspond to a known isotope. Only two independent input features were chosen, as they were the most defining characteristics of an atom. Some data points were excluded because they lacked half-lives.

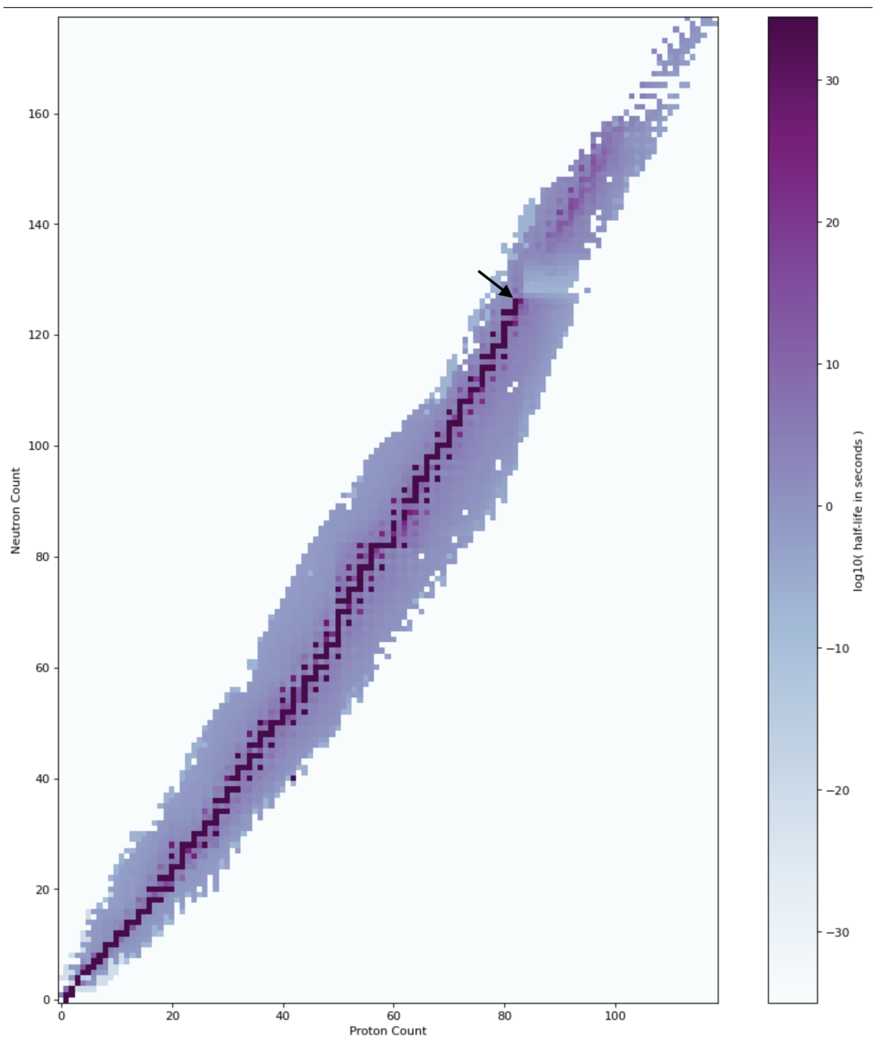

Figure 1: Each known nuclide is plotted based on its proton count on the x-axis and neutron count on the y-axis, and is colored based on its half-life in the legend. The long purple line represents stable isotopes. Lead-208, with 82 protons and 126 neutrons, is one of the last stable isotopes, and is is indicated by the arrow pointing to it.

5 Methodology and Models

5.1 1st Model

The model originally had two input variables, proton and neutron count, and outputted: a the predicted $\log_{10}$ of the half life. Several activation functions (relu, arctanh), were tested. The diagram below represents roughly how the model works:

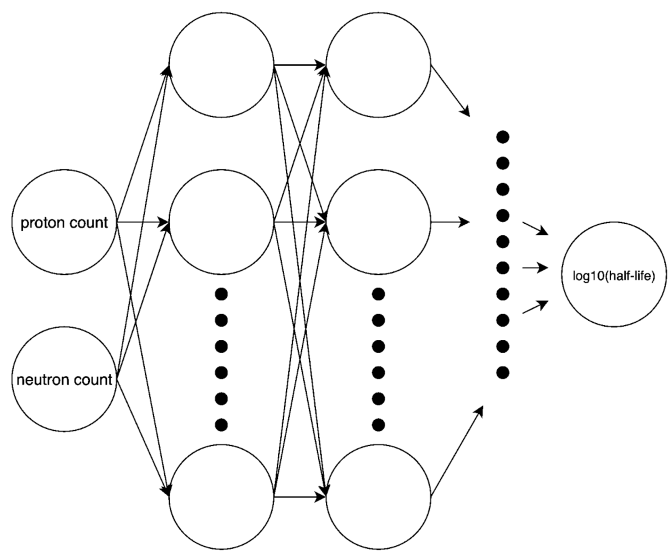

Figure 2: Neural networks set multipliers to each arrow and a bias/constant to each neuron. An algorithm then changes the neurons using the output results until the model reaches minimum error.

The first model only included two features, which were proton count and neutron count, followed by several dense layers which eventually fed into a single output, $\log_{10}$(half-life). The initial model was trained with 10 epochs and a train/test ratio of 0.7.

5.2 2nd Model

Several more features were added based on their relevance to physics[6], but they still depended entirely on the amounts of protons and neutrons. This new model was trained with more layers as well as convolution layers, with the same train/test ratio of 0.7 as before and 100 epochs.

Feature Name	Variable Type	Definition
a	int	$z + n$
n-z	int	$n - z$
a2/3	float	$a^{\frac{2}{3}}$
a-1/3	float	$a^{-\frac{1}{3}}$
z_{magic}	boolean	z in $\{2, 8, 20, 28, 50, 82, 114\}$
n_{magic}	boolean	n in $\{2, 8, 20, 28, 50, 82, 126, 184\}$

Table 1: These additional features were chosen based on their relevance to physics. a is short for atomic mass, while the magic subscript refers to magic numbers referenced in the background of this paper. These features were selected from Li et al[6].

6 Results and Discussion

The original model had a mean squared error of 111 in $\log_{10}$(half-life), while the new model above had a mean squared error of 97. This suggests that increasing the complexity of the model improves the accuracy of the model. In the past, models have been developed with much higher complexity; there were 64 native features and 517 word vector-related inputs led to a mean absolute error of 0.392 on test data[6]. While this is not the exact same unit of measurement, it is almost certainly much more accurate than the model.

The reasons for why simpler deep learning models may not work could be attributed to the relatively small dataset size with only proton count, neutron count, and half life. While there are 3000-4000 known isotopes, many decay within seconds, so they may not add any information besides the location of the line that contains the relatively stable isotopes in the dataset further above. Furthermore, nearly all stable isotopes are expected to decay after very large amounts of time, and while this information would significantly help predict regions of stability and how half life trends across the beta-stability line (purple line in figure 1), that is not known for most isotopes, and as a result it would be hard for the model to identify isotopes with long half lives compared to others with similar proton and neutron counts.

7 Conclusion

Through mean squared errors of 111 and 97, it is implied that the application of deep learning to half lives of periodic table isotopes requires more complexity, as older literature has succeeded, but only with large amounts of features. However, it is possible that a completely different type of model may produce more meaningful results. If good models are created and applied on superheavy isotopes, they could help identify unknown isotopes with large enough half lives to be used outside of just nuclear research.

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9 References

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