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USE OF MACHINE LEARNING TECHNIQUES IN THE LEARNING AND PREDICTION OF ALPHA-DECAY HALF-LIVES

COMPUTER SCIENCE NEA 2021/22

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Analysis

Identification of the Problem

Initial Ideas

Over the course of the A-Level, I have taken a deeper interest in the creation of AI using Machine Learning techniques, creating a neural network which feeds forward information into a number of hidden layers, training itself by minimising a cost function using backpropagation. I wished to pair this with my love for Physics and apply ML techniques to a real-world Physics problem. I had a few initial ideas, namely:

1) Analysis of Star Spectra
    - By analysing which wavelengths of light different stars absorb, we are able to see the colour of the star and also which elements are being fused in the core of the star. This allows us to see where the star is in its life cycle and therefore accurately determine its age. The user could manually input the wavelengths absorbed and the AI would be able to determine the elements being fused and provide an estimation of the age of the star.

2) Detection of Gravitationally Lensed Images
    - This was inspired by a bout of research into Special and General Relativity. Captured images of distant galaxies and stars are often warped by a phenomenon called gravitational lensing when very gravitationally dense objects, such as galaxy clusters, in the way, bend the path of the light, resulting in images which would otherwise be unable to be seen to be seen, albeit slightly warped. The proposed project will be able to use ML to detect whether or not an image has been gravitationally lensed and possibly reverse the effects of gravitational lensing to form the original image.

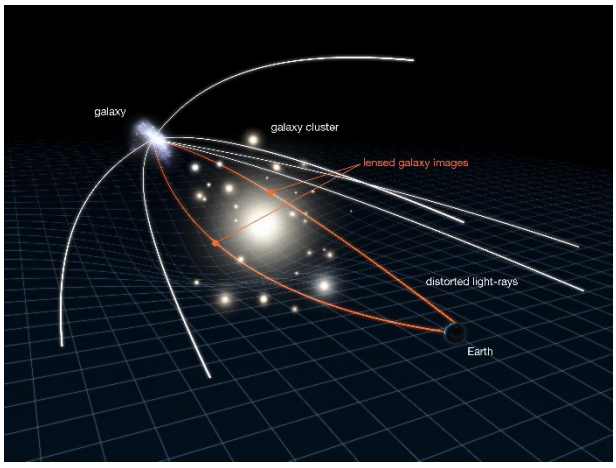

Figure 1: Diagram representing gravitational lensing from (https://esahubble.org/images/heic1106c/)

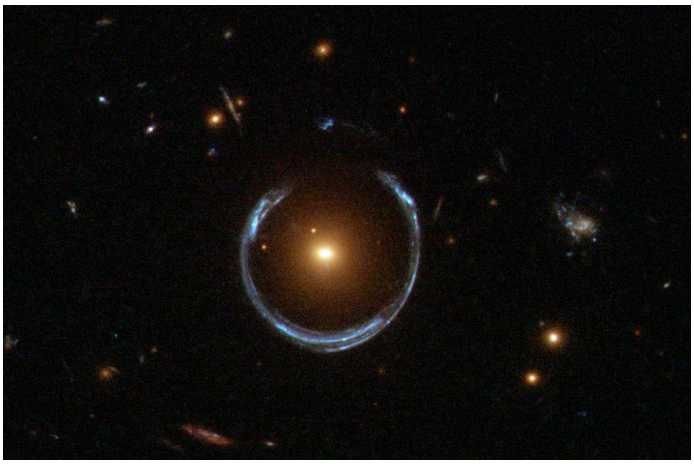

Figure 2: Einstein ring formed due to gravitational lensing (https://en.wikipedia.org/wiki/Gravitational_lens)

3) Prediction of Half-Lives of Radioactive Isotopes
    - This was inspired by recent Physics lessons on Radioactivity in which incredibly long and incredibly short half-lives were discussed. The proposed solution will be able to predict the half-life of a given (radioactive) isotope based on factors such as proton number and neutron number, among other factors.

Preliminary Analysis of Initial Ideas and Selection of Final Idea

1) Analysis of Star Spectra
    - The good thing about this project is that it will involve the AI learning of the link between elements fused and the star spectra of the star. The problem with this project, however, is that this is not an actual problem as all the possible colours and their meanings are already known, meaning there is not much use of an AI which does this. The project can be hard-coded and will perform the same.

2) Detection of Gravitationally Lensed images using ML
    - While there had been research into using ML for this[1], the level of Mathematics and data required for a project like this was much beyond my reach, especially if I wanted to add functionality to reverse the image. This is because it entailed knowing things like when the image was taken, by which telescope, and then the state of all the clusters in the way at that moment, before having to plug it into the field equations for general relativity to be able to reverse the image. The project would have been too data intensive and so I decided against it.

3) Prediction of Half-Lives of Radioactive Isotopes
    - Preliminary research into this showed that using ML for this had been proposed and shown to be effective by a paper in 2014[2] and had since been used for research purposes for both alpha decay[3] and beta decay[4]. The databases were also freely published and available for usage and there is not much to learn in terms of the concept itself. The difficulty in experimentally measuring incredibly long and incredibly short half-lives also justifies the need for a project like this for use in a research setting. For this reason, **I am choosing to continue with this for my final project**.

Stakeholders

For an academic project like this, the main stakeholders include educators and/or researchers. Educators will be able to use this product to show their students the half-lives of specific radioactive nuclei and I could add diagrams to show how half-life changes depending on different factors if I want to make it more specialised to education. For a more academic product, it would be used for predicting half-lives of novel radioactive isotopes which may be discovered or predicted, helping guide their research and expectations.

Why Is It Amenable to a Computational Solution?

Due to the difficulties in measuring very long and very short half-lives, as well as the random nature of radioactive decay, a computational solution may be much more suitable than an analytical one. While there do exist analytical models for alpha decay half-lives, namely the Effective Liquid Drop Models, the Generalised Liquid Drop Models (ELDM and GLDM respectively) and the Viola-Seaborg Model, a paper in 2019[5] showed that an approach based around ML is able to produce more accurate results. Due to the error contained in experimental results as well, an AI which is able to take this into account could potentially be more accurate than experiment. Part of my evaluation process will be to compare my model against the existing analytical models and to see if my model is more accurate.

Another aspect to consider is the fact that the development of neural networks (NN) is very processor heavy, especially in the optimisation and storage of the floating point weights and biases (more on this later) to create an accurate model. For this reason, any approach using a NN requires computationally advanced components, especially a GPU, which is specialised for floating point operations. This is another reason as to why a computational solution is ideal for this project.

Research into Problem

While doing preliminary research, I found that all the papers that did use ML for learning half-lives only focused on predicting half-lives based on 1 mode of decay rather than all of them. I believe the reason this was done was due to the differing complexities of each type of decay; beta decay consisted of many different subtypes while alpha decay has only 1 type. Due to the importance and variety in the types of beta decay, I do not feel that a project which solely focuses on half-lives, like mine, would be a sufficiently good tool to use in education or research. As the complexities

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[1][Pearson, J., Pennock, C. and Robinson, T. (2018). *Auto-detection of strong gravitational lenses using convolutional neural networks.* Emergent Scientist, 2, p.1.] and [arXiv:2104.01014 [astro-ph.IM]]

[2] [Bayram, T., Akkoyun, S. and Kara, S.O. (2014). *α-decay half-life calculations of superheavy nuclei using artificial neural networks.* Journal of Physics: Conference Series, 490, p.012105.]

[3] [Freitas, Paulo & Clark, J.. (2019). *Experiments in machine learning of alpha-decay half-lives*.]

[4] [Niu, Z.M., Liang, H.Z., Sun, B.H., Long, W.H. and Niu, Y.F. (2019). *Predictions of nuclear β -decay half-lives with machine learning and their impact on r -process nucleosynthesis.* Physical Review C, 99(6).]

[5] [Freitas, Paulo & Clark, J.. (2019). *Experiments in machine learning of alpha-decay half-lives*.]

of beta decay are also out of the scope of A-Level syllabus, and I already have a quite advanced project, I do not feel confident in learning all the pre-requisites for a project which focuses on beta decay.

Another reason to focus solely on alpha decay is due to the increasing amounts of research into super-heavy elements (SHEs). More specifically, this includes their production and usage in nuclear fusion. One of the main properties researchers are interested are their half-lives, and as most SHEs decay via alpha decay, my project could go towards research in that field. For this reason, I have decided to focus on alpha decays for my project.

Potential Successes with Selected Problem

Potential successes include being highly accurate in my predictions of alpha decay half-lives and being more accurate than existing models in this regard. A standard way of measuring the efficacy of a model is by measuring the smallness of the standard deviation of the model from experiment[6]:

$\sigma = \frac{1}{n_T}\left(\sum_{n=1}^{n_T}\left(t_n^{exp.} - t_n^{mod.}\right)^2\right)^{\frac{1}{2}}$, where t is the base-10 logarithm of the half-life.

I will include this in my testing to allow myself to compare my model to existing analytical models.

Potential Issues with Selected Problem

The main potential issues occur with not having enough data and therefore not having a very accurate model. To try and combat this I will try and gather data from as many different sources as possible. This may cause me to have duplicate data, however, and so I will have to take care to combat this.

Another issue to consider is the one of predicting a half-life for things which do not have a half-life. This will occur because my training data will not be varied enough to include every single possible isotope and then define which ones will and will not have a half-life with alpha decay, and so, the network will return a half-life for every single input. Because this is to be used in research and education, however, the researchers will know whether or not an isotope will decay via alpha emission, and so it is not too much of an issue. For the sake of completeness, however, I will implement features to allow the dataset to be updated so that in future, these issues can be accounted for.

Analysis of Existing Similar Solutions

While there are similar existing solutions within academia which have used similar techniques, there is no publicly available software employing a NN for this problem. This is understandable as there is not really a need for the public to predict alpha-decay half-lives, however, I still think a tool should be publicly available to researchers and academics who wish to use the tool.

The first paper[7] I looked at used a network with 6 input neurons: atomic number, neutron number, parity, decay energy, distance from (nearest) proton magic number and distance from (nearest) neutron magic number. They then had a hidden layer (of 4 units), a learning rate of 0.001, and the activation function $\tanh(x)$. They also used Nesterov momentum during their gradient descent with the value of the momentum being 0.99, and regularisation with a strength of 0.1.

They used 3000 epochs (passages through the training data) and their cost function was the standard deviation σ. In practice, their results had a standard deviation of 0.4910 from the true values when measured on the test set, which was noticeably better than the standard deviation of the ELDM model, which was 0.5845.

The second source[8] I looked at used only 3 input neurons: atomic number, neutron number and mass number. While it did not go into detail in regard to the structure, it was found that when the network was trained to find the half-life, it was not very successful, however, when the network was trained to find the base-10 logarithm of the half-life, it was found to be very accurate.

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[6] [Freitas, Paulo & Clark, J.. (2019). *Experiments in machine learning of alpha-decay half-lives*.]
[7] Ibid.
[8] [Bayram, T., Akkoyun, S. and Kara, S.O. (2014). *α-decay half-life calculations of superheavy nuclei using artificial neural networks.* Journal of Physics: Conference Series, 490, p.012105.]

Features Adopted and Rejected from the Existing Solutions

Based on the existing solutions, I have decided to follow the following structure for my neural network:

- 6 input neurons: proton number, neutron number, atomic number, decay energy, distance from proton magic number and distance from neutron magic number.
- Learning rate of 0.01
- Minimum of 4 hidden layers of 16 neurons each
- Cost function of σ (standard deviation).
- Output of the base-10 logarithm of the half-life.
- Activation function being the sigmoid function as opposed to the tanh function. More detail on this later.

Interviews/Client Research

For my stakeholders, I chose university researchers and professors in higher education, as they will be the ones that benefit the most from a specialised program such as mine. Because this is not a general half-life predictor, it will not necessarily be of as much value for science-communication or for the general public. Another reason researchers are the ones who will extract the most benefit from a project like this is due to the increasing amount of research into SHEs as was mentioned earlier. Due to this, I got in contact with a researcher from a nearby university who wished to remain anonymous, and after explaining the premise of what I was setting out to do, I asked him the following questions.

Interview Questions

1) How useful are the statistical models for alpha-decay (ELDM, GLDM) in your work?
2) How would you quantify the accuracy of a half-life model?
3) How would a more accurate model benefit your work?
4) How would you like to interact with the software?
5) Would you like the ability to update the dataset which the network is trained from?
6) Would you like the ability to change the structure of the model?
7) How important is the transparency of how the model works?

Interview Results

1) The ELDM and GLDM models are very useful in guiding our assumptions of the behaviour of these isotopes. They act as a useful tool in shaping our expectations and allowing us to build a pretty good model of how things will behave and interact. Obviously, they're not exact but they are close enough to allow us to build a good picture
2) The accuracy is generally quantified by the standard deviation of the logarithm of the model compared to the experimental half-life because it helps get around the different orders of magnitude the half-lives can span.
3) A more accurate model which can predict the half-lives of novel isotopes would be quite useful. We are always trying to develop more and more accurate models based on our increasing understanding of the processes governing radioactive decay, so a modelling method which is more accurate would be very useful. One thing which I may suggest is that, although the model may be very accurate, it should also be clear how it works, as one of the advantages of these models is that they build off of what we understand conceptually to help us build a picture of what is around us.
4) A simple interface would be sufficient in which we can enter the relevant details if we have them and get a prediction. Some software can be very complicated to use, as you have to worry about whether or not you have entered every piece of data etc. so a simple interface would be quite useful.
5) Having the ability to update the dataset would be very useful as it means we will be able to update your model as and when new experimental data comes in. This would help us in keeping as up-to-date as we can with our models.
6) This is not much of a concern as I don't expect us to be fiddling around with the settings of the model, as long as it functions well enough and we can update it based on new experimental data, it should be sufficient.
7) As physicists, we are always trying to increase our understanding of how the world works, however, I understand that with a neural network, it can be difficult to understand the implications of why the model

sets itself up as it does. While it would be nice to understand how the model works, I don't feel that it is necessary in helping us deriving experimental value from it,.

Conclusions from Interview(s)

It is clear from the interviews that the ELDM and GLDM models are very important in research (1) and it was also clear that having a more accurate model would be of great benefit to the researchers (3). For this reason, building a more accurate model than the statistical models will be my aim. I will quantify this using the standard deviation of the logarithm of the half-life compared to the model (2).

The GUI will be very simplistic to allow the researchers to interact quickly with it and not have to worry about whether they have entered the right bits of data in the right places (4). I will also try and allow for the ability to update the dataset as per the stakeholder's wants (5). I may add the ability to update the structure of the network and allow them to retrain it, although, it is clear that this is not something very important to the stakeholder (6).

Requirements

Software Requirements

I am planning to keep the software quite lightweight so that any device is able to run it. Therefore, the software requirements are limited to:

- Python 3.10 (with the appropriate libraries)
- A Python Interpreter

Hardware Requirements

- A PC which is capable of running Python

No specific hardware is required for my program. Any PC capable of running Python should be able to run my program.

Stakeholder Requirements

- A better accuracy than the statistical models for alpha decay
- Simple GUI with easy navigation

These requirements were based on the answers the stakeholders gave to my questions above.

Success Criteria

Essential

Criterion	Type	How to Evidence
Predictions of the neural network must have better accuracy than the statistical model	Functional	Compare standard deviations of both the statistical model and the neural network
The network is able to account for updates to the database of isotopes	Functional	Screenshots of lack of hard-coding
User is able to easily navigate the GUI	Usability	Stakeholder feedback and screenshots of simplistic GUI

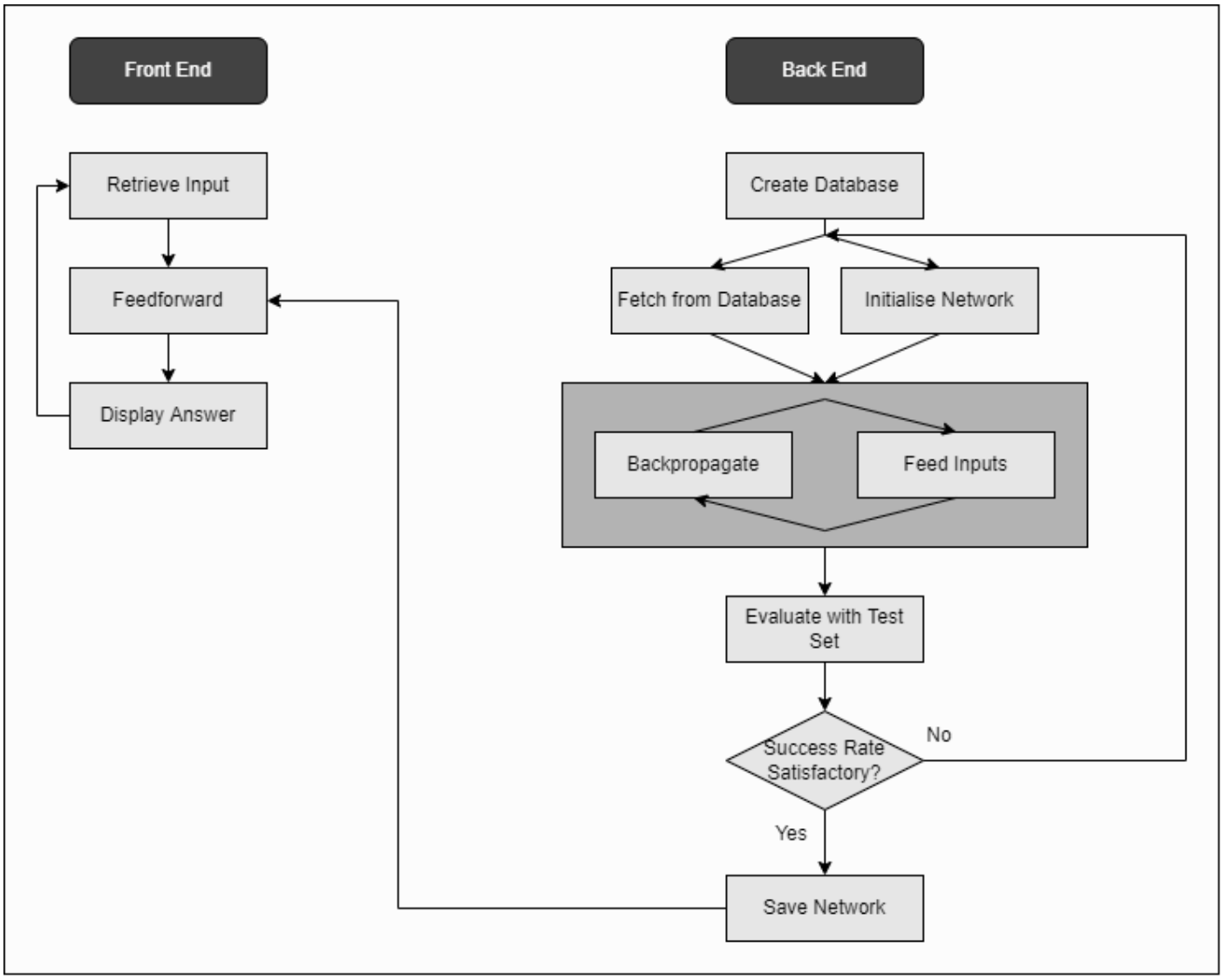
Desirable

Criterion	Type	How to Evidence
User is able to retrain the network with their own structure and settings	Functional and Usability	Screenshots of retraining screen allowing the user to do this
It is easy for the user to make any adjustments to the network	Usability	Stakeholder feedback
User is easily able to update the database	Usability	Screenshots of code allowing the user to do this and stakeholder feedback in regards to the ease

Other desirable criteria include anything which may arise in development, as I have not yet started development and do not know other success criteria may arise.

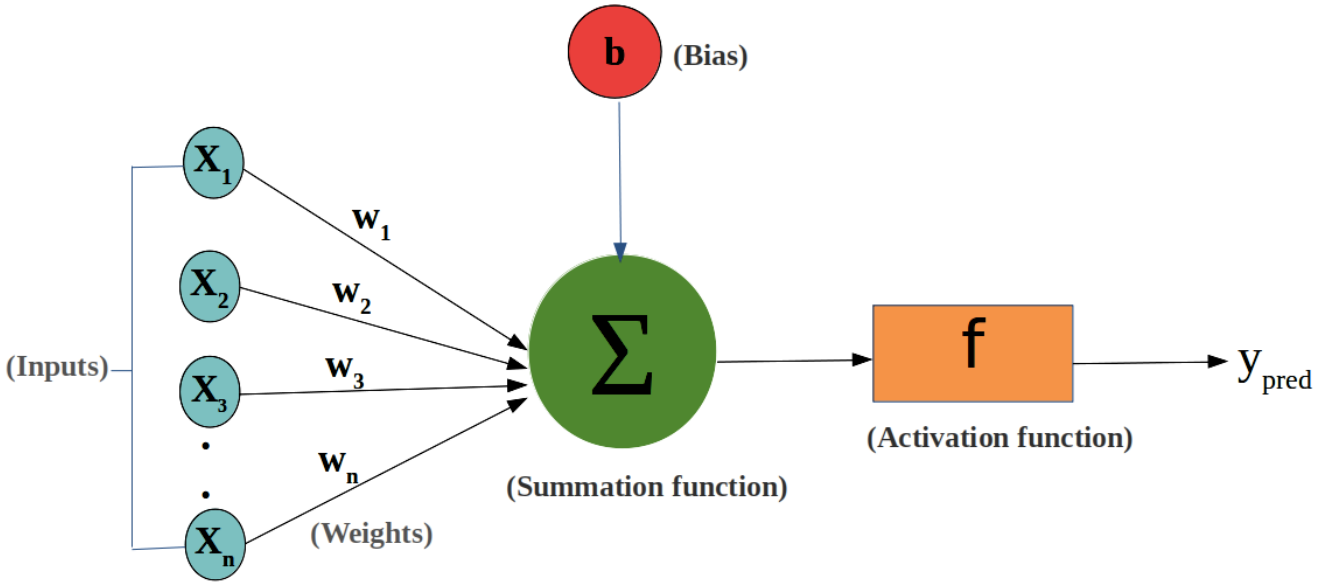
Design

Due to this being a large project, I will have to split it into multiple smaller components to allow it to be manageable. I first split the program into front-end and back-end, to signify which parts of the program the user will and won't interact with. I will update my front-end and back-end development plans once I have done more research into neural networks and machine learning:



Neural Networks and How They Work

Structure and Feeding Forward



2 https://towardsdatascience.com/whats-the-role-of-weights-and-bias-in-a-neural-network-4cf7e9888a0f

Neural networks consist of multiple units of "neurons", structured in layers, with each layer feeding into the next. A neuron can just be thought of as something which stores a number, called its activation. Each neuron has a specific weight which its activation is multiplied by, and a bias which is added to it, which contribute to the activations of each neuron in the next layer. The activation of that next neuron depends on the weighted sum of all the activations in the previous layer, added to their individual biases (pictured above). This sum then put through an activation function, such as the sigmoid activation function or a ReLU (Rectified Linear Unit), to give it its final activation. Every neuron in a layer is linked to every neuron in the next layer, with each of them having their own individual weights and biases. For larger networks, it becomes incredibly complicated to keep track of all the weights and biases, as well as all the indexing of which layer each neuron is in, and so we often use matrix multiplication to represent this more simply:

The activation of neuron 0 is the weighted sum of all the activations of the previous layer (with their own specific weights) + a bias, all plugged through a specific activation function:

$$a = neuron \quad a^{(layer)}_{number} \quad w_{layer,neuron}$$

$$a^{(1)}_0 = \sigma(w_{0,0}\ a^{(0)}_0 + w_{0,1}\ a^{(0)}_1 + \ldots + w_{0,n}\ a^{(0)}_n + b_0)$$

$$\sigma = activation\ function$$

This can be represented more simply using matrices:

$$\sigma\left(\begin{bmatrix} w_{0,0} & w_{0,1} & \cdots & w_{0,n} \\ w_{1,0} & w_{1,1} & \cdots & w_{1,n} \\ \vdots & \vdots & \ddots & \vdots \\ w_{k,0} & w_{k,1} & \cdots & w_{k,n} \end{bmatrix} \begin{bmatrix} a^{(0)}_0 \\ a^{(0)}_1 \\ \vdots \\ a^{(0)}_n \end{bmatrix} + \begin{bmatrix} b_1 \\ b_2 \\ \vdots \\ b_n \end{bmatrix}\right)$$

$$a^{(1)} = \sigma(\mathbf{W}a^{(0)} + \mathbf{b})$$

By using matrices, we can greatly decrease the amount of processing power and data storage we need, as the activations of a whole layer are dependent on only 3 stored quantities. To do this, I will use a library called numpy in Python to define and multiply matrices, as numpy is highly optimised for this, meaning it will greatly decrease the load on the user's PC.

The activation function I am choosing to use is the sigmoid function, which is defined as $y = \frac{1}{1+e^{-x}}$. This is one which is often used in industry because it normalises the value of the sum, giving it a value between 1 and 0, preventing certain factors from influencing the activation a lot more than others. I decided to use this as it is easier to differentiate than something like $y = \tanh(x) = \frac{e^x - e^{-x}}{e^x + e^{-x}}$, and, unlike ReLU, it is non-linear, meaning that its derivative is not a constant. This makes backpropagation work more effectively as the neural network will not be a set of linear transformations.

To ultimately receive an output from the network, a set of inputs has to be multiplied through each layer, before eventually reaching the output layer from which the activations are interpreted to represent the final output of the network.

Backpropagation and Minimising Cost

Gradient Descent

The initial weights and biases of a neural network are initialised randomly, however, due to this, the output from the network will be incredibly inaccurate. I will then need to adjust the weights and biases accordingly to allow a useful output to be reached. This has to be done iteratively, step by step. The reason for this is because it is a practically intractable problem to iterate through every single possible combination of weights and biases in a network before you decide on the one which gives you the outputs you require. For this reason, I will use a technique called gradient descent.

Gradient descent consists of taking the rate of change of the cost (a function of the difference between the desired value and the value given by the network) with respect to each weight and bias. Because we are working with vectors and matrices, the rate of change will give us a gradient vector pointing in the direction of increase. We then negate this to get the vector giving us the direction of the decrease of the cost, and adjust all the weights and biases proportionally. This is similar to finding a local minimum of a graph in a cartesian space. The constant of proportionality is called the learning rate and it can be thought of as the size of the step which the weights and biases take, or the size of the step down the graph. The smaller this is, the less likely the network is to overshoot and miss the local minima, however, it will take longer to train. I have decided to use a learning rate of 0.01 as this is sufficiently small enough to allow for this, but not so small that the network won't converge in a reasonable amount of time.

Backpropagation

Backpropagation is a technique which allows you to compute this gradient vector. By taking the error of the output layer, we know how much we need to adjust the output value by, however, because each neuron in the previous layer contributes a different amount to the overall value, we need to propagate the error backwards using the weights and biases to see how much we need to adjust each activation in the previous layer. As these next activations are dependent on the activations of the layer before that, we propagate the error back etc. and continue doing this until we have the adjustments that need to be made to each weight and bias. To propagate the error backwards, we have to use the transpose of the weight matrix to undo the transformation the weight matrix makes on the activations.

To compute the change of the cost with respect to each weight and bias, we first need to compute an intermediary quantity called the error. If our activation is defined as $a^1 = \sigma\left(\boldsymbol{W}a^{(0)} + \boldsymbol{b}\right)$, (activation in layer 1 is the weighted sum of the activations in layer 0 + the biases, all in the sigmoid function) we can define $z = \boldsymbol{W}a + \boldsymbol{b}$. If we nudge this "presigmoid" value by a small change $\boldsymbol{\Delta}z$, the overall change to the cost is $\frac{\partial C}{\partial z}\boldsymbol{\Delta}z$. If $\frac{\partial C}{\partial z}$ is small, then that means the small change in z will not have much of an effect, meaning that the neuron is already quite optimal. If it is large, then that means a small adjustment has a large effect on the cost. Because of this, $\frac{\partial C}{\partial z}$ can be thought of as the error δ.

By the chain rule:

$$\delta = \frac{\partial C}{\partial z} = \frac{\partial C}{\partial a}\frac{\partial a}{\partial z} = \frac{\partial C}{\partial a}\sigma'(z)$$

In matrix form, this can be represented as:

$$\delta = \nabla_a C \odot \sigma'(z)$$

where $\odot$ is the Hadamard product (element-wise product), and $\nabla_a C$ is the gradient vector of the cost with respect to the activations. My cost function for a single training example is $(a - t^{exp.})^2$. The derivative of this (without the constants) is simply $(a - t^{exp.})$. I can disregard the constants as the result will be multiplied by the learning rate anyway. The derivative of the sigmoid function $\sigma(x)$ can be shown to be $\sigma'(x) = \sigma(x)(1 - \sigma(x))$. In this way, we now have a formula for finding the error of a particular layer of neurons.

Backpropagation works because δ can be written in terms of the layer in front using the idea of propagating the error backwards, giving us a recursive relationship between the error of each layer. If L represents the current layer:

$$\delta^L = ((w^{L+1})^T \delta^{L+1}) \odot \sigma'(z^L)$$

It can then be shown that:

$$\frac{\partial C}{\partial b_j^L} = \delta_j^L$$

That is, the derivative of the cost with respect to a bias is just the error of that particular neuron. For the weights, the derivative of each weight is the activation of the neuron from previous layer multiplied by the error of the neuron (each connection has a weight):

$$\frac{\partial C}{\partial w_{jk}^L} = a_k^{L-1}\delta_j^L$$

When applied iteratively backwards through a network, these relationships then give us the gradient vector of the cost function with respect to each of the weights and biases, which is exactly what we want.

I will apply backpropagation to adjust the weights and biases feeding a training example through the network and measuring the error. When this is applied and averaged over all the training examples multiple times, the weights should hopefully be in a good enough state to make accurate predictions over all training examples. To avoid the need for the user to constantly have to train the network, I will then save the states of the weights and just feed forward the user inputs.

Turning Classification into Regression

One of the things I have to consider is that I am not trying to get an output between 0 and 1. For this reason, I will not apply the sigmoid function to the output layer neuron, meaning the output will just be a linear combination of the activations of the previous neurons. This will mean my σ' or the derivative of my activation function will be 1. This is something I will have to account for in my code.

Development Plan

My development plan will involve me first extracting and storing the data in a convenient way so that it can be read and written to easily. I will then develop the network in a class. I have chosen to develop it in a class as this will allow me to encapsulate all the methods and attributes I need under one structure. It will also take away the need to rewrite code as I can just call all the relevant functions I need. I will then finally develop a user interface to allow the network to be interacted with and predictions to be made.

Extracting Data

Based on a paper[9] which did something similar to my project, I decided to take my data from 2 main sources:

- Cui, J.P., Zhang, Y.L., Zhang, S. and Wang, Y.Z. (2018). *α -decay half-lives of superheavy nuclei.* Physical Review C, 97(1).
- Cui, J.P., Xiao, Y., Gao, Y.H. and Wang, Y.Z. (2019). *α-decay half-lives of neutron-deficient nuclei.* Nuclear Physics A, [online] 987, pp.99–111.

This gives me a total of 213 isotopes which I can use to train and evaluate my data. I will write all the information about these, including the half-life predicted by the ELDM model, into a text file which I will convert into a csv file. I will do it like this as it is simpler to write to text files than it is to csv files in Python. As the papers storing the data are pdfs, I will first copy and paste the data into a text file to read from, before rewriting it in a useful format.

Database
Data Array
Get Proton Number Array
Get Neutron Number Array
Get Nucleon Number Array
Get Proton MN Distance Array
Get Neutron MN Distance Array
Get Energy Release Array

I will then develop a database class in which I can encapsulate all the methods I need to fetch whichever data I need from the database. This will greatly improve readability and also mean I do not have to worry about where each relevant piece of data is stored.

To allow for any future additions to the database, I will not hard-code the database or the feature retrieval, improving the longevity of the code and conforming to the stakeholder's wants.

Usability Features

This part of the project will not be interacted with by the user so I do not need to consider any usability features in this section.

Developing the Network

Network	
Attributes	**Datatype**
Weights	Array of Numpy Matrices
Biases	Array of Numpy Matrices
Activations	Array of Numpy Matrices
Pre-Activations	Array of Numpy Matrices
Learning Rate	Float
Methods	**Explanation**
Feed Forward	Feed an input through and make a prediction
Backpropagate	Backpropagate for a given input
Train	Iterate through a training set, feeding forward and backpropagating for a given number of epochs
Evaluate	Evaluate the performance on a testing set

As was mentioned earlier, the network will be developed in a class to allow me to easily encapsulate all the methods and variables I need. I drew a class diagram on the left to help me visualise what needs to be done. In terms of developing the algorithms themselves, it will be a case of transferring the above mathematical formulas into code. As I don't want to hard-code the structure of the program, I will be coding the backpropagation and feedforward algorithms iteratively, letting the user define the structure of the network, however, I will first hard-code each step to make sure I understand the whole process. This will make it easier to first spot any errors but also prevent me getting confused with indexing in the loops as I anticipate this will be something that trips me up. To help with this, I decided to write some pseudocode to make sure I understood all the maths above:

[9] [Freitas, Paulo & Clark, J.. (2019). *Experiments in machine learning of alpha-decay half-lives*.]

Pseudocode for Network

```
class Network ():

    def __init__ (self, structure):
        self.weights = []
        self.biases = []

        for x in range (len(structure) - 1):
            self.weights.append (random numpy matrix of size specified by structure) # initialise weights randomly
            self.biases.append (random numpy matrix of size specified by structure) # initialise biases randomly

        self.activations = []
        self.preactivations = []

        for x in range (len(structure))
            self.activations.append(numpy matrix of 0) # initialise activations as being 0
            self.preactivations.append (numpy matrix of 0) # initialise preactivations as being 0

        self.learningrate = 0.01 # default value for learning rate

    def feedforward (Z,N,Q,A,ZDist,NDist):
        self.activations[0] = [Z,N,Q,A,ZDist,NDist] # first layer activations are fed in

        for x in range (len(structure)-1): # from the first layer to the penultimate layer
            activation = self.activations[x]
            weighted = np.matmul (self.weights[x], a) # multiply weights with activations
            sum = weighted + biases [x] # calculate weighted sum + biases to get a final sum
            self.preactivations.append (sum) # append non-activated sum to preactivations
            self.activations.append (sigmoid (sum) # append sigmoid-ed sum to activation

        aFinal = np.array([]) # calculate last layer activations manually to avoid sigmoid
        weighted = np.matmul(self.weights[len(structure)-1])
        sum = weighted + biases [len(structure)-1]
        self.preactivations.append(sum)
        self.activations.append(sum) # append non-activated sum to activations

    def backpropagate (activation, target):
        deltaWeights = [] # declare change in weights array
        deltaBiases = [] # declare change in biases array

        # error in last layer
        errorL = target - activation # last layer error
        deltaBiases.insert (0, errorL) # change in biases = error
        ''' change in weights = error multiplied with previous layer activations (no hadamard as last layer
        activation is linear) '''
        deltaWeights.insert (0, np.matmul (errorL, self.activations[len(structure)-2].transpose()))

        # error in second-last layer
        # propagate previous layer error backwards using transpose of weight matrix
        propagated = np.matmul (self.weights(size-2).transpose(), errorL)
        error2L = np.multiply (propagated, sigmoid_prime (preactivations[size-3]))
        deltaBiases.insert (0, error2L) # inserting at start so I can iterate through normally
        deltaWeights.insert (0, np.matmul(error2L, self.activations[len(structure)-3].transpose()))

        .
        .
        .

        # do for each layer (in loop in final version)
        for x in range (0, len(structure - 1)):
            self.weights [x] = weights [x] + deltaWeights [x]
            self.biases [x] = biases [x] + deltaBiases [x]

    def train (trainSet, targets, epochs):
        for x in range (epochs):
            for y in range (len(trainSet)):
                activation = self.feedforward(trainSet[y])
                self.backpropagate (activation, targets[y])

    def evaluate (testSet, targets):
        errors = []
        for x in range (len(testSet)):
            error = self.feedforward (testSet[x]) - targets[x]
            errors.append (error**2)
        stddev = sum (errors) ** (1/2) / (len(testSet))
        return stddev
```

Once I have trained the network to a suitable standard, I will save the states of the weights and biases using a joblib dump which will convert the matrices into a bitstream which can be read from later. I am using joblib as it is specialised for storing numpy matrices, which is what all the weights and biases in my program will be stored as. I can then load these wherever I need to use the neural network.

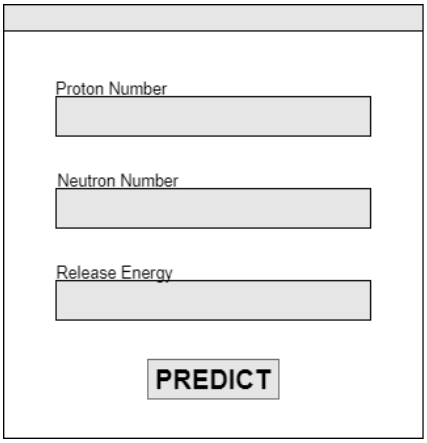
Usability Features

This part of the project will not be interacted with by the user so I do not need to consider any usability features in this section.

User Interface

This will be the last part of the project which I code and should be the simplest. There will be a basic UI which will allow the user to enter the data they need. For this, I will only need 3 text boxes to allow the user to enter value for the number of protons, neutrons, and the release energy. The distance from magic numbers and the nucleon numbers can be calculated from these. I will then feed them through my (trained) network which I will load from the joblib dump. The prediction will then pop up in a new window to make it clear which number on screen is the half-life.

The UI will be coded in tkinter as it is simple to design and add interactive elements onto. I mocked up a simple diagram on the right to illustrate how the interface may look.



Usability Features

This is the main part, if not the only part of the program which the user interacts with. For this reason, I need to make sure the UI is intuitive to understand and use. I also need to cater for all the incorrect inputs which a user may give, such as typing a letter when the program wants numbers. This will be done by creating try, catch statements in Python to catch any of the errors which may occur when I try to parse the user input. I will then need to clearly prompt the user for correct input. Overall, the UI is quite simple, so it should not be too difficult to both implement or use.

Testing Plan

Back-End Testing

Num.	Test	Success Criteria	Purpose
(1)	Feed forward a 3 neuron input through a small network manually	The network successfully outputs a 1x1 array	This will determine whether or not the matrix multiplication is correct and whether I can move forward with creating a more complicated network.
(2)	Feed forward a 6 neuron input with varying dimensions iteratively	The network successfully outputs a 1x1 array	This will determine whether or not my iterative feed-forward algorithm works.
(3)	Backpropagate a 3 layer network	The network successfully updates both sets of weights	This will determine whether or not my backpropagation is dimensionally correct
(4)	Check the error of my procedural backpropagation algorithm	Tends towards 0	This will determine whether or not the backpropagation is training the network to predict the half-life more and more accurately or not
(5)	Check the error of my iterative backpropagation with varying dimensions	Tends towards 0	This will determine whether or not the backpropagation is training the network to predict the half-life more and more accurately or not
(6)	Upload and load a small joblib array	Uploaded and downloaded are the same	If successful, I can use joblib to upload weights and biases to download and use them in my front end

Front-End Testing

Num.	Test	Success Criteria	Purpose
(i)	Enter incorrect data	The software catches incorrect data and prints out that incorrect data has been entered	This allows me to catch incorrect inputs and prompt the user for correct inputs
(ii)	Enter correct data	UI stores correct data and calculates extra data it needs	Allows me to determine whether my input system works as it should
(iii)	Feedforward an input	UI successfully computes half-life	Determines whether my feedforward and joblib loading is functional
(iv)	Try and create window	Window is created	Allows me to prompt the user for re-entry of data and to show them the results of the prediction
(v)	Enter correct data	Prediction is outputted correctly in new window	Determines whether the UI is functional in terms of feeding forward and showing data

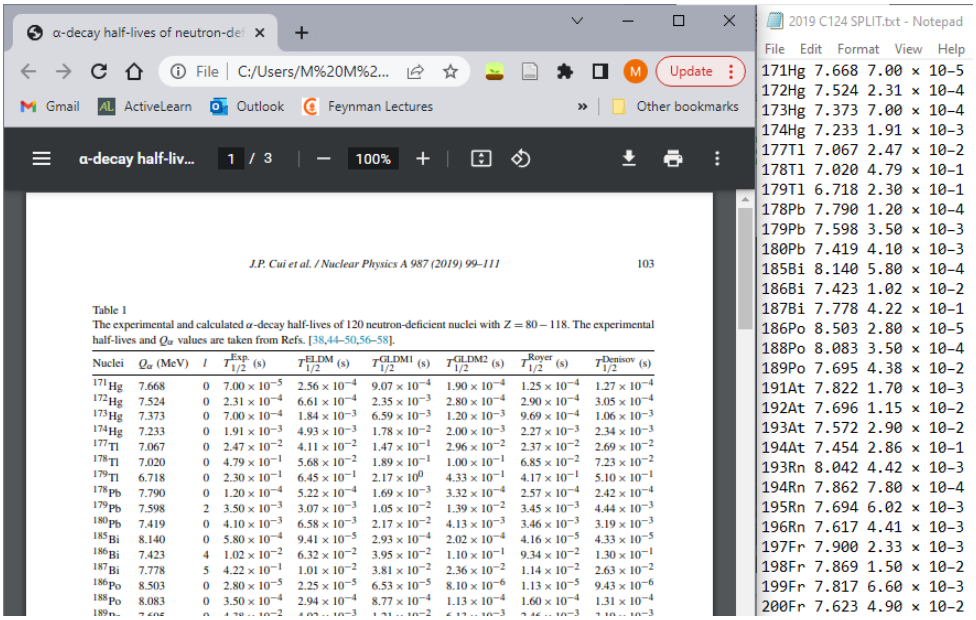
Development and Implementation

Extracting Data

I first started on my data extraction. The data which I will use comes from 2 main academic papers, mentioned above, however, the main problem I initially had was that they were pdfs, and reading from tables in pdfs is very difficult in Python. For this reason, I decided to copy and paste the data into text files and read from them. The 2 sources were formatted differently, however, and so I had to read from them separately. I decided to use the ELDM model to test against as this was common to both sources.

Retrieving the Data

I first copied the data into a text file because of the reasons mentioned above:



I then read from the text file into an array using this simple program:

```python
for line in file:
  N  = file.read(3)
  name = file.read(2)
  spaces = file.read(1)
  Q = file.read(5)
  spaces = file.read(1)
  t12 = file.read(11)
  spaces = file.read()
  eldm = file.read(11)
  data.append(name,N,Q,t12,eldm)
data.pop()
#python sees end of document as a \n so there was an extra
empty cell in the array
for x in range(0,len(data)):
  for y in range (0,len(elements)):
    if elements[y][0] == data[x][0]:
      data[x].insert(1, elements[y][1])
```

```
215U
216U
217U
218U
219Np
```

This works because the values under each of the columns were each of the same length. This made it easy to specify a number. One of the outliers, however, was Uranium, as its chemical symbol is U. For this reason, I made sure to add an extra space after the U in my text file (above right) This was feasible as there were only 4 Uranium isotopes.

The second code block is one where I was adding all the proton numbers. This source didn't use isotope numbers and instead listed all the elements according to their name. For this reason, I looked for an easy way to convert all these elements into their proton numbers. I found a csv file[10] online which contained this information, and after stripping it of what I didn't need, I compared the name of the element given in the database to the elements in the csv file and inserted the appropriate proton numbers in.

I then wrote the data into a text file. The code was not very readable, however, I knew that I would only have to do this once and never come back to it, so I didn't take the time to overly neaten it. This was when I encountered another issue: although the bases of the exponents were of the same length, the exponents weren't. This meant that I had to read different lengths for different exponents, and so the one size fits all approach which I was implementing didn't work. You can see I had artefacts of following data in my ELDM data (last column in screenshot on left) due to the different exponent lengths (below).

```
Fm, 100, 243, 8.690, 2.54 × 10-1, 7.52 × 10-1
Md, 101, 246, 8.890, 9.20 × 10-1, 3.95 × 10-1
Md, 101, 247, 8.764, 1.20 × 100, 1.05 × 100 1.
No, 102, 251, 8.752, 9.64 × 10-1, 2.06 × 100 3
Lr, 103, 253, 8.918, 7.02 × 10-1, 1.40 × 100 2
Lr, 103, 254, 8.816, 2.38 × 101, 2.79 × 100 3.
Rf, 104, 255, 9.055, 3.46 × 100, 1.35 × 100 1.
Rf, 104, 256, 8.923, 2.08 × 100, 2.87 × 100 3.
Md, 101, 247, 8.764, 1.20 × 100, 1.05 × 100 1.
No, 102, 251, 8.752, 9.64 × 10-1, 2.06 × 100 3
Lr, 103, 253, 8.918, 7.02 × 10-1, 1.40 × 100 2
Lr, 103, 254, 8.816, 2.38 × 101, 2.79 × 100 3.
Rf, 104, 255, 9.055, 3.46 × 100, 1.35 × 100 1.
Rf, 104, 256, 8.923, 2.08 × 100, 2.87 × 100 3.
Db, 105, 256, 9.340, 2.84 × 100, 3.82 × 10-1 5
Db, 105, 257, 9.206, 2.45 × 100, 9.08 × 10-1 1
Db, 105, 258, 9.500, 5.58 × 100, 1.24 × 10-1 1
Sg, 106, 259, 9.804, 3.11 × 10-1, 3.90 × 10-2
Sg, 106, 260, 9.901, 1.24 × 10-2, 2.07 × 10-2
Sg, 106, 261, 9.714, 1.87 × 10-1, 6.38 × 10-2
```

```
243Fm 8.690 2.54 × 10-1   7.52 × 10-1
246Md 8.890 9.20 × 10-1   3.95 × 10-1
247Md 8.764 1.20 × 100   1.05 × 100
251No 8.752 9.64 × 10-1   2.06 × 100
253Lr 8.918 7.02 × 10-1   1.40 × 100
254Lr 8.816 2.38 × 101   2.79 × 100
255Rf 9.055 3.46 × 100   1.35 × 100
256Rf 8.923 2.08 × 100   2.87 × 100
256Db 9.340 2.84 × 100   3.82 × 10-1
257Db 9.206 2.45 × 100   9.08 × 10-1
```

I thought about coding an elegant solution which takes into account the '–' signs but in the end, I decided to instead, introduce a gap of 3 whitespaces between all the data which may cause an issue. Then, I can read a fixed number of digits and stripped them of the whitespaces with the Python strip function. It did take some time to go through adding all the spaces but it was easier and quicker than reading and accounting for '–' signs. My function became:

[10] [https://gist.github.com/GoodmanSciences/c2dd862cd38f21b0ad36b8f96b4bf1ee]

```python
for line in file:
    N = file.read(3)
    name = (file.read(2)).strip()
    Q = (file.read(7)).strip()
    t12 = (file.read(12)).strip()
    eldm = (file.read(14)).strip()
    data.append([name,N, Q, t12, eldm])
data.pop()
```

```
237Cf 8.220 1.14 × 100    4.96 × 100    8.57 × 100
240Cf 7.719 9.76 × 101    2.41 × 102    4.35 × 102
242Es 8.160 3.12 × 101    1.52 × 101    2.90 × 101
243Es 8.072 3.29 × 102    3.11 × 101    5.51 × 101
243Fm 8.690 2.54 × 10-1    7.52 × 10-1    1.25 × 10
246Md 8.890 9.20 × 10-1    3.95 × 10-1    5.98 × 10
247Md 8.764 1.20 × 100    1.05 × 100    1.42 × 100
251No 8.752 9.64 × 10-1    2.06 × 100    3.14 × 100
253Lr 8.918 7.02 × 10-1    1.40 × 100    2.09 × 100
```

This worked very well, and I no longer had any of the artefacts as you can see below. The stripping also got rid of the space after the U for Uranium which I forgot to account for, also pictured below.

```
Cm, 96, 234, 7.365, 1.28 × 102, 9.07 × 102
Cm, 96, 236, 7.067, 2.27 × 103, 1.27 × 104
Cf, 98, 237, 8.220, 1.14 × 100, 4.96 × 100
Cf, 98, 240, 7.719, 9.76 × 101, 2.41 × 102
Np, 93, 223, 9.650, 2.15 × 10-6, 1.13 × 10-5
Np, 93, 225, 8.790, 3.60 × 10-3, 1.77 × 10-3
Np, 93, 226, 8.200, 3.50 × 10-2, 9.42 × 10-2
```

```
U , 92, 215, 8.588,
U , 92, 216, 8.542,
U , 92, 217, 8.169,
U , 92, 218, 8.775,
```

The next thing to get rid of was the exponent, as the" x 10" cannot be read or used by Python. Instead of converting out of standard form, I decided to convert the exponent to "e" which means the same thing as " x 10" and is understood by Python. This was an easy fix:

```python
for x in range(0,len(data)):
    data[x][5] = data[x][5].replace(" × 10", "e")
    data[x][4] = data[x][4].replace(" × 10", "e")
    # note: x=/=×
```

This did not work the first time when I typed in " x 10" by myself. To fix this, I decided to copy and paste what the text file had and realised that the multiply sign was not the letter x but the actual Unicode multiplication sign, which is why it did not work. I fixed this but didn't screenshot the difference because the code looked virtually the same. This gave me the format I wanted:

```
Cm,96,138,234,7.365,1.28e2,9.07e2
Cm,96,140,236,7.067,2.27e3,1.27e4
Cf,98,139,237,8.220,1.14e0,4.96e0
Cf,98,142,240,7.719,9.76e1,2.41e2
```

Source 2

I then repeated the same processes above for the second source. When I wrote the database, I formatted it as if it was a csv file. This was because I was planning to convert it to a csv file anyway (by changing the file extension) as they are very easy to read data from. I wrote to the text file using the following code:

```python
Database = open('Database.txt','w')

Database.write("Element, Z (Protons), N (Neutrons), Nucleons, Energy, Half-Life, ELDM\n")

for x in range(0,len(data)):
  for y in range(0,7):
    Database.write(str(data[x][y]))
    if y==6:
      Database.write("\n")
    else:
      Database.write(",")

#Database.write("Source 2 -----------------\n") # Debugging

for x in range(0,len(data2)):
  for y in range(0,7):
    Database.write(str(data2[x][y]))
    if y==6:
      Database.write("\n")
    else:
      Database.write(",")

print("Databasing Done!")
Database.close()
pTable.close()
file.close()
source2.close()
```

In the end, I had a database of 213 elements which I could use to train and test my neural network. I decided to use the traditional 80-20 split, where 80% of my data will be used to train the network and the remaining 20% will be used to test it. The whole databasing was done using an online IDE and is available here: https://replit.com/@MAmjad/Read-Data-Test#main.py.

Reading from Database and Encapsulation

The next step was reading from the database. I used the class diagram I made earlier and read from the database into a master data array. Whenever a function is called to retrieve a particular feature/data item, I read from this master array to a smaller array and returned that smaller array:

```python
import csv as csv
import numpy as np

class Data ():

    def __init__ (self):
        self.data = []
        with open("Database.csv") as database:
            csvreader = csv.reader (database)
            for row in csvreader:
                self.data.append([row[0],int(row[1]),int(row[2]),int(row[3]),float(row[4]),float(row[5]),float(row[6])])

        # Format: Element, Z, N, A, Q, T12, ELDM
        for isotope in self.data:

            Zdist = min([abs(isotope[1]-2), abs(isotope[1]-8), abs(isotope[1]-20),
                abs(isotope[1]-28), abs(isotope[1]-50), abs(isotope[1]-82), abs(isotope[1]-126)])
            isotope.insert (2, Zdist)

            Ndist = min([abs(isotope[3]-2), abs(isotope[3]-8), abs(isotope[3]-20),
                abs(isotope[3]-28), abs(isotope[3]-50), abs(isotope[3]-82), abs(isotope[3]-84), abs(isotope[3]-126)])
            isotope.insert (4, Ndist)

        # Format: Element, Z, ZDist, N, NDist, A, Q, T12, ELDM
```

I also added the Zdist and Ndist data items. These are the distances from the nearest proton magic numbers and neutron magic numbers respectively (2, 8, 20, 28, 50, 82, 126 for protons and neutrons as well as 84 for neutrons). This was one of the inputs of a solution I looked at which had better results than the statistical model.

```python
def getZ (self):
    Z = []
    for x in self.data:
        Z.append(x[1])
    return Z

def getZDist (self):
    ZDist = []
    for x in self.data:
        ZDist.append(x[2])
    return ZDist
```

```python
def getN (self):
    N = []
    for x in self.data:
        N.append (x[3])
    return N

def getNDist (self):
    NDist = []
    for x in self.data:
        NDist.append(x[4])
    return NDist
```

```python
def getA (self):
    A = []
    for x in self.data:
        A.append (x[5])
    return A

def getQ (self):
    Q = []
    for x in self.data:
        Q.append (x[6])
    return Q
```

```python
def getHL (self):
    HL = []
    for x in self.data:
        HL.append (x[7])
    return HL

def getModel (self):
    Model = []
    for x in self.data:
        Model.append (x[8])
    return Model
```

I then defined all the above subroutines to read from the data array and allow me to retrieve any of the data whenever I wanted. This was relatively straightforward, and so there weren't any bugs to fix in this part of the project. This did make my life easier later on when retrieving data to train the model. I then went onto the model next.

Developing the Network

Feed-Forward Method

Step-By-Step

When doing the feed-forward method, I decided to first code a smaller version of my final network so I could get my head round the matrix multiplication. For this, I chose a 3 layer network with 3 input neurons, 1 hidden layer of 20 neurons and 1 output neuron which I defined as an array called `structure`, where `structure = [3, 20, 1]`.

I then defined and randomly initialised the weight matrix `w1` as being the weights going into layer 1. This was a 20x3 matrix which would be multiplied by the 3x1 activations matrix (for the first layer neurons), giving me a 20x1 matrix, which signify the 20 neurons in layer 2. I then defined the bias randomly as well. I was originally going to define and initialise these manually with Python's random library to randomly make up values, but then I discovered numpy's `np.random.rand(shape)` which automatically defines a matrix with the given shape with random float values between 0 and 1:

```
import numpy as np
'''
This will be a 3 layer structure, 3 input neurons, 20 neurons in 1 hidden layer
and then 1 output neuron
'''
structure = [3,20,1]

# sigmoid ##########################################################################
def sigmoid(x):
    return 1.0/(1.0+np.exp(-x))

# define matrix for first sets of weights to second layer using a 2d array ####################

'''w1noob = []
for x in range (structure[1]):
    w1noob.append([0,0,0])
w1 = np.array(w1noob)'''

# or:

w1 = np.asarray(np.random.rand(structure[1],structure[0]))
'''
print("Initial Weights -------------------------")
print(w1)
print(w1.shape)
'''

# define biases ####################################################################
b1 = np.asarray(np.random.rand(structure[1],1))
'''
print("Initial Biases -------------------------")
print(b1)
print(b1.shape)
'''
```

```
# store given activations for first layer ##############################

Z = 92
N = 126
Q = 8.775

'''
Z = int(input("Protons: "))
N = int(input("Neutrons: "))
Q = float(input("Energy Release: "))
'''

print("Initial Layer 2 Activations ----------------------")
a0 = np.array([[Z],[N],[Q]])
'''
print(a0)
print(a0.shape)
'''
```

I then went to compute the second layer's activations by multiplying the weight and activation matrices and adding the biases on. When I printed the shape of the matrix to check it was correct however, it gave me an unexpected result:

```
# compute activations of second layer
a1 = np.array([])
mult = np.array([np.matmul(w1,a0)])
print (mult.shape)
a1 = sigmoid (mult+b1)
print (a1)
```

```
(1, 20, 1)
```

It was saying that the `mult` array was a 3D matrix of size 1x20x1. This could cause errors further down the line if I didn't sort it so to be on the safe side, I used numpy's `reshape` function which lets you reshape arrays without losing any of the data (if it is possible to do so).

```
# compute activations of second layer
a1 = np.array([])

mult = np.array([np.matmul(w1,a0)])
mult = np.reshape(mult, (20,1))

a1 = sigmoid((mult+b1))
print(a1)
#print(a1.shape)
```

I then printed `a1` thinking that the sigmoid function would give me a range of values between 0 and 1, as was its job. When I printed the result, however, I got the following (left):

```
Initial Layer 2 Activations -------
[[1.]
 [1.]
 [1.]
 [1.]
 [1.]
 [1.]
 [1.]
 [1.]
 [1.]
 [1.]
 [1.]
 [1.]
 [1.]
 [1.]
 [1.]
 [1.]
 [1.]
 [1.]
 [1.]
 [1.]]
[Finished in 852ms]
```

This was clearly not what I wanted. The sigmoid function only outputs values close to 1 for very high inputs. The fact that they were all 1 indicated to me that my weights may not be doing what they should be in weakening or strengthening the activations as appropriate.

To check this, I printed out my weighted sum to see what the matrix going into the sigmoid function was:

```
presigmoid = mult + b1
print(presigmoid)
```

This outputted the following:

```
Initial Layer 2 Activations ----------------------
[[ 74.27588157]
 [ 95.75869071]
 [220.0405366 ]
 [102.66039312]
 [ 90.52561058]
 [140.31741174]
 [200.58701259]
 [ 46.79606826]
 [138.84777331]
 [109.0972436 ]
 [108.98609931]
 [ 79.92519062]
 [135.35501945]
 [115.42719549]
 [ 32.33742461]
 [ 78.98760372]
 [131.86221612]
 [204.4874777 ]
 [ 56.39202016]
 [164.09997967]]
[Finished in 873ms]
```

From this, it is clear what went wrong. Although the weights and biases had been initialised randomly and were small (between 0 and 1), this did not account for the massive discrepancies in the sizes of my input data. My release energy was below 10 while my proton and neutron numbers were in or near the hundreds. This made me realise that I needed to **normalise** the data.

Normalisation

Normalisation is the taking of a value and transforming it in some way to be between 0 and 1. An article by Tensorflow[11] stated that it is good practice to normalise features that use different scales and ranges. You are unlikely to converge to a solution without normalisation.

After researching normalisation, I determined that min-max normalisation would be the easiest form to use in this context. The formula for min-max normalisation is as follows:

$$x = \frac{x - x_{min}}{x_{max} - x_{min}}$$

This guarantees a value between 0 and 1, and because the minimum and maximum values were easily found due to my database class having all the arrays I needed along with the python `min()` and `max()` functions, I decided to use this. I imported my Data class and initialised an object called gd (getData) and added the following:

```
Z = 92
N = 126
Q = 8.775

# min max normalisation

Qmin = min(gd.getQArray())
Qmax = max(gd.getQArray())

Z = (Z-80)/(118-80)
N = (N-92)/(177-92)
Q = (Q-Qmin)/(Qmax-Qmin)
```

I knew the minimum and maximum values for the protons and neutrons so I decided to just use them rather than retrieving the array to save time. This had the desired effect:

```
# compute activations of second layer
a1 = np.array([])
mult = np.array([np.matmul(w1,a0)])
mult = np.reshape(mult, (20,1))
presigmoid = mult + b1
print(presigmoid)
```

```
[[[1.4976883 ]
  [1.47894352]
  [1.37529387]
  [0.57983906]
  [1.34072499]
  [1.42724619]
  [1.0644913 ]
  [0.47814135]
  [1.10725799]
  [0.79080841]
  [0.87429872]
  [1.21127459]
  [1.33845756]
  [0.65039746]
  [1.58987488]
  [1.28279449]
  [0.88129606]
  [1.36796447]
```

[11] [https://www.tensorflow.org/tutorials/keras/regression#the_normalization_layer]

I then put this through the sigmoid function:

```
# compute activations of second layer
a1 = np.array([])
mult = np.array([np.matmul(w1,a0)])
mult = np.reshape(mult, (20,1))
presigmoid = mult + b1
#print(presigmoid)
a1 = sigmoid(presigmoid)
print(a1)
```

```
[[0.68779067]
 [0.78360365]
 [0.75375648]
 [0.71434007]
 [0.63102291]
 [0.66414528]
 [0.6519257 ]
 [0.77343133]
 [0.73042665]
 [0.80363014]
 [0.78391699]
 [0.71545361]
 [0.72994329]
 [0.65117453]
 [0.79762319]
 [0.64716551]
 [0.77420752]
 [0.71269508]
 [0.7934463 ]
 [0.78701092]]
```

These activations looked much better. I then moved on, calculating the final layer activation and this time, not plugging it into the sigmoid function because I wanted a regression network rather than a classification network:

```
# define matrix for second set of weights to 3rd layer using 2d array (which will be 1d anyway)
w2 = np.asarray(np.random.rand(structure[2],structure[1]))
b2 = np.asarray(np.random.rand(structure[2],1))
mult = np.matmul(w2,a1)
result = mult + b2
print("Final Half-Life: ", result)
```

```
Final Half-Life:  [[7.48140465]]
```

[Evidence for Test 1]

This worked. The final output is a 1x1 numpy matrix, showing all my matrix multiplication was consistent. This meant I was ready to code a more sophisticated network which would be able to perform the feed forward iteratively for a given structure.

```
# compute activations of second layer ################################
a1 = np.array([])

mult = np.array([np.matmul(w1,a0)])
mult = np.reshape(mult, (20,1))

presigmoid = mult + b1

print(presigmoid)
print ("-----------------")

a1 = sigmoid(presigmoid)
print(a1)
print(a1.shape)

# define matrix for second set of weights to 3rd layer using 2d array (which will be 1d anyway)
print("--------------------------------------------------")
w2 = np.asarray(np.random.rand(structure[2],structure[1]))
print (w2)
result = np.matmul(w2,a1)
print(result.shape)
print("Final Half-Life: ", result)
```

Iterative Feed Forward

I then decided to code my iterative feed-forward which had all six inputs:

- Proton Number
- Neutron Number
- Nucleon Number
- Release Energy
- Distance from Proton Magic Number
- Distance from Neutron Magic Number

I first used my Data library to import all the arrays I needed and defined my structure with 4 hidden layers of 16 neurons each:

```
Zdist = gd.getZdist()
Ndist = gd.getNdist()
ZArr = gd.getZ()
NArr = gd.getN()
AArr = gd.getA()
QArr = gd.getQ()
```

```
structure = [6,16,16,16,16,1]
```

I then used my procedural code from above to create an iterative feed method, manually adding and normalising the first layer activations and manually applying the last layer activations:

Defining and initialising `weights` and `biases`: ------->

Normalising input values using min-max normalisation: ------>

Setting normalised values to be initial activations: ---------->

Defined an array ah for hidden activation and tried to compute activations: --------->

Manually apply last layer activations ---------->

```
weights = []
biases = []
for x in range (0,(len(structure)-1)):
    weights.append(np.asarray(np.random.rand(structure[x+1],structure[x])))
    biases.append(np.asarray(np.random.rand(structure[x+1],1)))
print (len(weights))
print (len(biases))

def iterfeed(Z, N, A, Q, Zd, Nd, structure):
    # min-max scaling
    Z = (Z-min(ZArr))/(max(ZArr)-min(ZArr))
    N = (N-min(NArr))/(max(NArr)-min(NArr))
    A = (A-min(AArr))/(max(AArr)-min(AArr))
    Q = (Q-min(QArr))/(max(QArr)-min(QArr))
    Zd = (Zd-min(Zdist))/(max(Zdist)-min(Zdist))
    Nd = (Nd-min(Ndist))/(max(Ndist)-min(Ndist))

    a0 = np.array([[Z], [N], [A], [Q], [Zd], [Nd]]) # use scaled inputs as initial activations

    ah = np.array([])
    for x in range (0, len(structure) - 2):
        mult = np.array([np.matmul(weights[x], ah)])
        mult = np.reshape(mult, (structure[x],1))
        ah = sigmoid(mult + biases[x])

    af = np.array([])

    mult = np.array([np.matmul(weights[len(structure)-1],ah)])
    mult = np.reshape (mult, (structure[len(structure)-1],1))
    af = mult + biases[len(structure)]

    return af
```

When I ran this, however, I got an error:

```
  File "C:\Users\M M Amjad\Documents\[=] A Level\Sixth Form\CS Project\Code\NetworkPrototype2.py", line 53, in iterfeed
    mult = np.array([np.matmul(weights[x], ah)])
ValueError: matmul: Input operand 1 has a mismatch in its core dimension 0, with gufunc signature (n?,k),(k,m?)->(n?,m?) (size 0 is different from 6)
```

It was saying that it could not multiply a matrix of size 0 with the weights matrix. I realised that the reason this threw the error was because I had defined ah as being empty, and then tried to use the values in ah to compute the next values in ah. For the second layer activations, I had to multiply by the first layer activations but I was multiplying by ah. I did not want to use if statements as that would have been inefficient and difficult to scale, so I decided to change the strategy with which I stored the activations and brought in an `activations` array. I was planning to do this later on when I introduced backpropagation, but this made me realise that I needed it now. I then added this in:

```
weights = []
biases = []
activations = []

for x in range (0,(len(structure) - 1)):
    weights.append(np.asarray(np.random.rand(structure[x+1],structure[x])))
    biases.append(np.asarray(np.random.rand(structure[x+1],1)))

for x in range (0, len(structure)):
    activations.append(np.zeros((structure[x],1)))

size = len(structure)

print (len(weights))
print (len(biases))
print (len(activations))
```

The reason `activations` is longer than the `weights` and `biases` arrays is because the weights act between layers, and so there are only `l-1` weights (1->2, 2->3, …, n-1->n), and the biases don't change the activations of the first layer, meaning there will be `l-1` biases. Every layer, however, has an activation, so there needs to be as many activations as layers. I initialised the activations with 0s rather than random numbers as then it would be clear when an activation has been computed or not. (It was around this point I experimented with different IDE themes so I apologise for the inconsistencies in the colours).

I updated my feed method accordingly:

Apply `weights[x]` to `activations [x]` and add the biases to get `activations [x+1]` (the next activation):

```
def iterfeed(Z, N, A, Q, Zd, Nd, structure):
    # min-max scaling
    Z = (Z-min(ZArr))/(max(ZArr)-min(ZArr))
    N = (N-min(NArr))/(max(NArr)-min(NArr))
    A = (A-min(AArr))/(max(AArr)-min(AArr))
    Q = (Q-min(QArr))/(max(QArr)-min(QArr))
    Zd = (Zd-min(Zdist))/(max(Zdist)-min(Zdist))
    Nd = (Nd-min(Ndist))/(max(Ndist)-min(Ndist))

    activations [0] = np.array([[Z], [N], [A], [Q], [Zd], [Nd]]) # use scaled inputs

    for x in range (0, size - 2):
        a = activations [x]
        mult = np.array([np.matmul(weights[x], a)])
        mult = np.reshape(mult, (structure[x+1],1))
        activations [x+1] = sigmoid(mult + biases[x])

    af = np.array([])
    mult = np.array([np.matmul(weights[size - 2],activations [size - 2])])
    mult = np.reshape (mult, (structure[size - 1],1))
    af = mult + biases[size - 2]
    activations.append ([af])
    return af
```

This worked:

```
i=0

t12 = iterfeed (ZArr[i], NArr[i], AArr[i], QArr[i], Zdist[i], Ndist[i], structure)
print ("Half-Life I: "+ str(t12[0][0]) + "s")
```

```
Half-Life I: 8.108464016701873s
[Finished in 880ms]
```

In order to test whether it was doing what I thought, however, I decided to recode my iterative feed-forward quickly and see what outputs it gave when I initialised the weights and biases the same:

```
weights[0], weights[1], weights[2], weights[3], weights[4] = w01, w12, w23, w34, w45
biases[0], biases[1], biases[2], biases[3], biases[4]= b01,b12,b23,b34,b45
```

```
    a0 = np.array([[Z], [N], [A], [Q], [Zd], [Nd]]) # use scaled inputs as initial activations

    a1 = np.array([]) # declaring array
    mult = np.array([np.matmul(w01,a0)]) # multiply weights with activations
    mult = np.reshape(mult, (structure[1],1)) # reshape to make 20x1 matrix
    a1 = sigmoid(mult+b01) # add biases and plug into sigmoid # fix subtract 1 to allow for neg activations

    a2 = np.array([])
    mult = np.array([np.matmul(w12,a1)])
    mult = np.reshape (mult, (structure[2],1))
    a2 = sigmoid (mult + b12)

    a3 = np.array([])
    mult = np.array([np.matmul(w23,a2)])
    mult = np.reshape (mult, (structure[3],1))
    a3 = sigmoid (mult + b23)

    a4 = np.array([])
    mult = np.array([np.matmul(w34,a3)])
    mult = np.reshape (mult, (structure[4],1))
    a4 = sigmoid (mult + b34)

    a5 = np.array([])
    mult = np.array([np.matmul(w45,a4)])
    mult = np.reshape (mult, (structure[5],1))
    a5 = mult + b45

    return a5
```

When I did this, I got the following outputs:

```
Half-Life V: 8.053886135524223s
Half-Life I: 8.053886135524223s
```

(I = Iterative, V = Original) This showed that they had the exact same outputs and therefore were doing the same things. However, to truly test whether this worked, I needed to change the structure and see if it still gave me an output.

When I changed the structure to the following: I received the following output:

```
structure = [6,25,30,30,25,1]
```

```
Half-Life: 13.679712681562432s
```

I then changed the length of structure to the following, and received the following output:

```
structure = [6,10,25,30,25,10,1]
t12 = iterfeed (ZArr[i], NArr[i], AArr[i], QArr[i], Zdist[i], Ndist[i], structure)
print ("Half-Life I: "+ str(t12[0][0]) + "s")
```

```
Half-Life I: 5.834881078276307s
[Finished in 1.4s]
```

[Evidence for Test 2]

This showed that my iterative feedforward method did in fact work for varying lengths and sizes of hidden layers. I was ready to move on to the next step.

One thing I saw which was quite clunky was the way in which I entered the data, as I had to enter each data item individually. For this reason, I decided to amend this and instead have it so the network takes in an array of data items. One issue which may arise is that the data may be entered in the wrong order, however, as the user does not interact with this directly, I do not have to worry about this. I then created a `getIsotope()` method in my data class which returns an array `[Z, N, A, Q, ZDist, NDist]`:

```
def getIsotope (self):
    Isotope = []
    for x in self.data:
        Isotope.append ([x[1], x[3], x[5], x[6], x[2], x[4]])
    return Isotope
```

This then cleaned up my feedforward call:

```
def feedforward (self, data):

    # min-max normalise all values
    Z = (data[0]-min(d.getZ()))/(max(d.getZ())-min(d.getZ()))
    N = (data[1]-min(d.getN()))/(max(d.getN())-min(d.getN()))
    A = (data[2]-min(d.getA()))/(max(d.getA())-min(d.getA()))
    Q = (data[3]-min(d.getQ()))/(max(d.getQ())-min(d.getQ()))
    Zd = (data[4]-min(d.getZDist()))/(max(d.getZDist())-min(d.getZDist()))
    Nd = (data[5]-min(d.getNDist()))/(max(d.getNDist())-min(d.getNDist()))
```

This also means there is less chance for error when entering the data as I won't swap 2 data items around in the call. I was now quite happy with my feedforward method and so I decided to begin the Network class and placing everything I needed into the class.

Object-Oriented Encapsulation

I put my constructor and feedforward method into a Network class which initialises all the weights, biases, activations etc. based on the structure of NN specified by the user:

```
class Network ():

    def __init__ (self, structure, learningrate = 0.01):
        d = Data ()
        self.size = len(structure) # set size equal to number of layers
        self.structure = structure # set structure (n of neurons) to match input

        self.weights = [] # declare weight array
        self.biases = [] # declare bias array
        for x in range (0, (self.size - 1)):
            # initialise weights and biases with random values
            self.weights.append(np.asarray(np.random.rand(structure[x+1],structure[x])))
            self.biases.append(np.asarray(np.random.rand(structure[x+1],1)))

        self.preactive = []

        self.activations = [] # declare activations
        for x in range (0, self.size):
            # initialise activations with zeros
            self.activations.append(np.zeros((structure[x],1)))

        self.learningrate = learningrate
```

```
# iterate through hidden layers using weights and biases (except for last)
for x in range (0, self.size - 1):
    a = self.activations [x]
    mult = np.array([np.matmul(self.weights[x], a)])
    mult = np.reshape(mult, (self.structure[x+1],1))
    presig = mult + self.biases [x]
    self.preactive.append(presig)
    self.activations [x+1] = sigmoid(mult + self.biases[x])

#manually apply last layer weights and biases to avoid sigmoid

af = np.array([])
mult = np.array([np.matmul(self.weights[self.size - 2], self.activations [self.size - 2])])
mult = np.reshape (mult, (self.structure[self.size - 1],1))
af = mult + self.biases[self.size - 2]

self.activations.append ([af])
self.preactive.append ([af])

return af
```

After confirming it was still working at this point[12], that I started on my backpropagation method.

Backpropagation Method

I coded my backpropagation method in a similar way to how I coded my feed-forward method, first doing each thing step-by-step on a 3-layer network before then coding it iteratively.

Step-By-Step

The first step of the backpropagation algorithm is to compute the error in the last layer, which is the (derivative of the cost function with respect to the activation) multiplied by (the derivative of the activation function with respect to z). The last layer activations, however, were not fed through an activation function, and instead were a linear combination of the previous layer activations. Because of this, the derivative of the activation function was 1. The derivative of the cost with respect to the activation is the `activation-target`, which is easy to compute. I added this in:

```
def backprop (target):
    outputError = target - result
    grad = learningrate * outputError
    hidden_T = np.transpose(weights[1])
    weights[1] += np.matmul(hidden_T, grad)  ✕ File "C:\Users\M M Amjad

    hiddenError = np.matmul (outputError, np.transpose(w2))
    grad = learningrate * hiddenError * sigmoid (a1) * (1-sigmoid(a1))
    w1 += np.matmul (grad, np.transpose (a0))
```

I then defined the hidden error according to the maths above and shifted the weights in the last line accordingly. As you can see, I got an error:

```
ValueError: matmul: Input operand 1 does not have enough dimensions (has 0, gufunc core with signature (n?,k),(k,m?)->(n?,m?) requires 1)
```

It was saying that my `grad` vector had a dimensionality of 0. I was curious as to why so I tried to print `grad.shape`:

```
    print (grad.shape)
AttributeError: 'float' object has no attribute 'shape'
```

It was saying, in essence, that grad was not a vector, it was a scalar. I fixed this by adding a line after grad saying `grad = np.array (grad)` which converted grad to an array, and when I ran it, there were no errors, and the weights were shifted from the original. This means my backpropagation was dimensionally correct and so I decided to try this on the 6 layer network I was planning to use.

[12] Note: While looking over the project once I had finished, I noticed a logic error with my activations. I initialised all the activations I needed with 0s, however, my feedforward appended a new activation layer onto the end meaning I had an extra layer. For this reason, I changed the following line:
self.activations.append([af]) → self.activations[-1] = [af] (see end for code block). This does not affect the weights and biases, however, as the activations before this are 0s and it they do not affect the last, additional layer and so the rest of the project does not need to be changed.

6 Layer Step-By-Step Backpropagation

For my backpropagation algorithm I am taking advantage of a Python feature in which you can use negative indexing to iterate through an array backwards (-1 refers to the final item, -2 to the second last etc). To make my life easier, I also defined a sigmoid prime function (derivative of the sigmoid) using lambda functions as follows:

```
sigmoid = lambda x : 1.0/(1.0+np.exp(-x))

sigmoid_prime = lambda z : sigmoid(z)*(1-sigmoid(z))
```

```
# remember, last weight = weights[size-2], last bias = biases [size-2]
# do last weight linearly, do the rest with inverse sigmoid

def backpropagation (activation, target, learningrate):

    global activations
    global biases
    global weights

    error_1 = activations [-1] - target
    error_1 = np.reshape (error_1, (1, structure[-1]))
    deltab = []
    deltab.insert (0, error_1)
    deltaw = []
    deltaw.insert (0, np.matmul(activations[-2], error_1))

    # second last layer

    #print (weights[-1].shape)
    #print (error_1.shape)
    foo = np.matmul (weights[-1].transpose(), error_1)
    error_21 = np.multiply (foo, sigmoid_prime (preactive[-2]))
    error_21 = np.reshape (error_21, (1,structure[-2]))

    deltab.insert (0, error_21)
    deltaw.insert (0, np.matmul(activations[-3], error_21))


    # third last layer
    #print (weights[-2].transpose().shape)
    #print (error_21.shape)
    foo = np.matmul (weights[-2].transpose(), error_21.transpose())
    error_31 = np.multiply (foo, sigmoid_prime (preactive[-3]))
    error_31 = np.reshape (error_31, (1, structure[-3]))
    deltab.insert (0, error_31)
    deltaw.insert (0, np.matmul(activations[-4], error_31))

    # fourth last layer
    foo = np.matmul (weights[-3].transpose(), error_31.transpose())
    error_41 = np.multiply (foo, sigmoid_prime (preactive[-4]))
    error_41 = np.reshape (error_41, (1,structure[-4]))
    deltab.insert (0, error_41)
    deltaw.insert (0, np.matmul(activations[-5], error_41))
```

I then coded my backpropagation algorithm following the above maths and pseudocode. The target was the base 10 logarithm of the half-life.

I frequently kept printing the sizes and shapes of each of the vectors I was multiplying in order to avoid errors in my matrix multiplication being inconsistent. It was also done to check for numpy "quirks" such as the following:

```
# second last layer
foo = np.matmul (weights[-1].transpose(), error_1)
error_21 = np.multiply (foo, sigmoid_prime (preactive[-2]))
print (error_21.shape)
error_21 = np.reshape (error_21, (1,16))
print (error_21.shape)
print (activations [-3].shape)
```

```
(1, 16, 1)
(1, 16)
(16, 1)
```

I continued the algorithm on the left until I had a delta for each of the weights and biases, and then adjusted them using the following loop. I checked the shape and resized due it throwing a similar error to the above:

```
for x in range (0,5):
    print(f"Original Shape: {weights[x].shape}")
    weights[x] = weights[x] + learningrate * deltaw [x]
    weights[x] = np.reshape (weights[x], (structure[x+1], structure[x]))
    print(f"New Shape: {weights[x].shape}")

for b,db in zip (biases, deltab):
    b = b+learningrate*db
```

I then ran my backpropagation algorithm, printing out the original error when feeding forward an isotope and then the error after running the backpropagation a few times. I received the following results:

```
error = feedforward (isotope[i], structure) - np.log10 (d.getHL()[i])
print (f"Error: {error}")

for z in range (0, 3):
    activation = feedforward (isotope[i], structure)
    backpropagation (feedforward (isotope[i], structure), np.log10 (d.getHL()[i]))
    #print (f"{z+1} iterations done")
    error = feedforward (isotope[i], structure) - np.log10 (d.getHL()[i])
print (error)
```

```
Error: [[13.58972631]]
1 iterations done
2 iterations done
3 iterations done
Error: [[552.78375256]]
```

This seemed strange as it indicated that my error was actually increasing. I had a look over my algorithm and realised the reason for this was that I was increasing my weights and biases by the delta rather than decreasing them (see above). For this reason, I simply changed the + sign to a – sign and reprinted the errors which gave me the following:

```
for x in range (0,5):
    #print(f"Original Shape: {weights[x].shape}")
    weights[x] = weights[x] - learningrate * deltaw [x]
    weights[x] = np.reshape (weights[x], (structure[x+1], structure[x]))
    #print(f"New Shape: {weights[x].shape}")

for b,db in zip (biases, deltab):
    b = b-learningrate*db
```

```
Error: [[11.69336131]]
1 iterations done
2 iterations done
3 iterations done
Error: [[2.07139489]]
[Finished in 1.3s]
```

This was a good sign, as my error was decreasing. I then decided to run the backpropagation for just a few more iterations and see how low I could get my error for a particular training example. I did this with a different isotope:

```
143    for z in range (0, 2000):
Error: [[11.87025293]]
Error: [[3.63638802]]
[Finished in 4.7s]
```

```
143    for z in range (0, 3000):
Error: [[9.98561257]]
Error: [[3.63638802]]
[Finished in 9.4s]
```

This showed that my error was converging to a particular value, which it should not have done. Backpropagation should theoretically reduce the error to 0, and this was not. I initially thought to look at my weights, as I thought the reason this could be happening may be because the weights don't budge past a particular value. When I did this, I realised I did not initialise my weights with negative values as `numpy.random.rand(shape)` initialises with float values between 0 and 1. I thought about just subtracting 1 from the weights and biases but then I came across the `nump.random.uniform` function in which it initialises a matrix with values in a uniform distribution between 2 values. I changed my weights and biases lines to the following:

```
for x in range (0, (size - 1)):
    weights.append(np.asarray(np.random.uniform(-1,1, (structure[x+1],structure[x]))))
    biases.append(np.asarray(np.random.uniform(-1,1, (structure[x+1],1))))
```

This gives me initial values distributed randomly with a uniform distribution between -1 and 1. I then rechecked the error:

```
Error: [[1.7460133]]
Error: [[3.63638356]]
[Finished in 4.4s]
```

All this did was decrease the initial error. I then thought it might be an issue with the algorithm itself, so I tried to find in which iteration/how quickly the error converges by appending the error to an array at each iteration and finding the index of the error:

```
errors = []

for z in range (0, 2000):
    #activation = feedforward (isotope[i], structure)
    backpropagation (feedforward (isotope[i], structure), np.log10 (d.getHL()[i]), 0.01)
    #print (f"{z+1} iterations done")
    error = feedforward (isotope[i], structure) - np.log10 (d.getHL()[i])
    errors.append (error)

print (f"Index of Converged Value: {errors.index(3.63632997)}")  x File "C:\Users\M M Amjad\Documents\[=

Error: [[0.69515337]]
Traceback (most recent call last):
  File "C:\Users\M M Amjad\Documents\[=] A Level\Sixth Form\CS Project\Code\BackpropPrototype.py", line 150, in <module>
    print (f"Index of Converged Value: {errors.index(3.63632997)}")
ValueError: 3.63632997 is not in list
[Finished in 6.7s]
```

This said that the exact error which it converged to was not in the list. I then decided to just print the error array to see if anything else was happening:

```
Error: [[5.52755923]]
[array([[4.58913909]]), array([[4.19554979]]), array([[3.98373609]]), array([[3.8585255]]), array([[3.78084367]]), array([[3.73129043]]), array([[3.69913864]]), array([[3.67805211]]),
array([[3.6641264]]), array([[3.65488799]]), array([[3.64874083]]), array([[3.64464246]]), array([[3.64190645]]), array([[3.64007832]]), array([[3.6388561]]), array([[3.63803865]]),
array([[3.63749178]]), array([[3.63712586]]), array([[3.63688099]]), array([[3.63671711]]), array([[3.63660743]]), array([[3.63653402]]), array([[3.63648489]]), array([[3.636452]]),
array([[3.63642999]]), array([[3.63641525]]), array([[3.63640539]]), array([[3.63639879]]), array([[3.63639437]]), array([[3.63639142]]), array([[3.63638944]]), array([[3.63638811]]),
array([[3.63638723]]), array([[3.63638664]]), array([[3.63638624]]), array([[3.63638597]]), array([[3.6363858]]), array([[3.63638568]]), array([[3.6363856]]), array([[3.63638555]]),
array([[3.63638551]]), array([[3.63638549]]), array([[3.63638547]]), array([[3.63638546]]), array([[3.63638546]]), array([[3.63638545]]), array([[3.63638545]]), array([[3.63638545]]),
array([[3.63638545]]), array([[3.63638545]]), array([[3.63638545]]), array([[3.63638545]]), array([[3.63638545]]), array([[3.63638545]]), array([[3.63638545]]), array([[3.63638545]]),
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array([[3.63638547]]), array([[3.63638547]]), array([[3.63638547]]), array([[3.63638547]]), array([[3.63638547]]), array([[3.63638547]]), array([[3.63638548]]), array([[3.63638548]]),
array([[3.63638548]]), array([[3.63638548]]), array([[3.63638548]]), array([[3.63638548]]), array([[3.63638548]]), array([[3.63638548]]), array([[3.63638548]]), array([[3.63638548]]),
array([[3.63638548]]), array([[3.63638548]]), array([[3.63638548]]), array([[3.63638549]]), array([[3.63638549]]), array([[3.63638549]]), array([[3.63638549]]), array([[3.63638549]]),
array([[3.63638549]]), array([[3.63638549]]), array([[3.63638549]]), array([[3.63638549]]), array([[3.63638549]]), array([[3.63638549]]), array([[3.63638549]]), array([[3.63638549]]),
```

This showed me that it converged incredibly quickly to a value very close to 3.6368549 before slowly eventually reaching that value. At this point I had run out of things to check so I decided to check my backpropagation algorithm against the maths.

When checking against the maths, I realised I had been doing my matrix multiplication the wrong way round the whole time. One of the reasons I didn't spot this earlier was because all 4 of my hidden layers had the same dimensions, so no matter which way you multiplied them, they gave a correctly shaped output. It was my inept multiplication that also caused me to add transposes where I did not need transposes to make everything consistent. I amended the backpropagation to match the maths exactly and ended up with the following:

```
    # error in last layer
    error_l = activation - target # getting error
    error_l = error_l = np.reshape (error_l, (1, structure[-1])) # reshaping error to be array
    deltab.insert (0, error_l)
    deltaw.insert (0, np.matmul(error_l, activations[-2].transpose()))

    # error in second last layer
    foo = np.matmul (weights[-1].transpose(), error_l)
    error_2l = np.multiply (foo, sigmoid_prime (preactive[-2]))
    error_2l = np.reshape (error_2l, (structure[-2], 1))
    deltab.insert (0, error_2l)
    deltaw.insert (0, np.matmul(error_2l, activations[-3].transpose()))

    # error in third last layer
    foo = np.matmul (weights[-2].transpose(), error_2l)
    error_3l = np.reshape (error_2l, (structure[-3], 1))
    deltab.insert (0, error_3l)
    deltaw.insert (0, np.matmul(error_3l, activations[-4].transpose()))

    # error in fourth last layer
    foo = np.matmul (weights[-3].transpose(), error_3l)
    error_4l = np.reshape (error_3l, (structure[-4], 1))
    deltab.insert (0, error_4l)
    deltaw.insert (0, np.matmul(error_4l, activations[-5].transpose()))

    # error in 5th last layer
    foo = np.matmul (weights[-4].transpose(), error_4l)
    error_5l = np.reshape (error_4l, (structure[-5], 1))
    deltab.insert (0, error_5l)
    deltaw.insert (0, np.matmul(error_5l, activations[-6].transpose()))

[Finished in 1.1s]
```

I updated the weights in the same way I did before and rechecked the error:

```
i = 100
isotope = d.getIsotope()

error = feedforward (isotope[i], structure) - np.log10 (d.getHL()[i])
print (f"Error Before: {error}")

for z in range (0, 100):
    activation = feedforward (isotope[i], structure)
    backpropagation (activation, np.log10 (d.getHL()[i]), 0.01)

error = feedforward (isotope[i], structure) - np.log10 (d.getHL()[i])
print (f"Error After: {error}")

Error Before: [[1.49498189]]
Error After: [[0.00197646]]
[Finished in 1.6s]
```

This was promising as my error was much lower than it was previously. I then ran it again for more iterations to see whether or not it still tended towards a particular value:

```
i = 100
isotope = d.getIsotope()

error = feedforward (isotope[i], structure) - np.log10 (d.getHL()[i])
print (f"Error Before: {error}")

for z in range (0, 1000):
    activation = feedforward (isotope[i], structure)
    backpropagation (activation, np.log10 (d.getHL()[i]), 0.01)

error = feedforward (isotope[i], structure) - np.log10 (d.getHL()[i])
print (f"Error After: {error}")

Error Before: [[4.06367428]]
Error After: [[8.8817842e-16]]
[Finished in 2.7s]
```

[Evidence for Test 4]

The error was tending towards 0. This was exactly what I wanted, as the NN is being trained to predict the value of the training example more and more accurately, tending the error closer and closer to 0. My final non-iterative backpropagation algorithm is as follows:

```
def backpropagation (activation, target, learningrate):
    global weights
    global biases

    deltaw = []
    deltab = []

    # error in last layer
    error_1 = activation - target # getting error
    error_1 = error_1 = np.reshape (error_1, (structure[-1], 1)) # reshaping error to be array
    deltab.insert (0, error_1) # error = delta biases
    deltaw.insert (0, np.matmul(error_1, activations[4].transpose())) # weight delta is error propagated backwards

    # error in second last layer
    foo = np.matmul (weights[-1].transpose(), error_1)
    error_2l = np.multiply (foo, sigmoid_prime (preactive[-3]))
    error_2l = np.reshape (error_2l, (structure[-2], 1))
    deltab.insert (0, error_2l)
    deltaw.insert (0, np.matmul(error_2l, activations[3].transpose()))

    # error in third last layer
    foo = np.matmul (weights[-2].transpose(), error_2l)
    error_3l = np.multiply (foo, sigmoid_prime (preactive[-4]))
    error_3l = np.reshape (error_3l, (structure[-3], 1))
    deltab.insert (0, error_3l)
    deltaw.insert (0, np.matmul(error_3l, activations[2].transpose()))

    # error in fourth last layer
    foo = np.matmul (weights[-3].transpose(), error_3l)
    error_4l = np.multiply (foo, sigmoid_prime (preactive[-5]))
    error_4l = np.reshape (error_4l, (structure[-4], 1))
    deltab.insert (0, error_4l)
    deltaw.insert (0, np.matmul(error_4l, activations[1].transpose()))

    # error in 5th last layer
    foo = np.matmul (weights[-4].transpose(), error_4l)
    error_5l = np.multiply (foo, sigmoid_prime (preactive[-6]))
    error_5l = np.reshape (error_5l, (structure[-5], 1))
    deltab.insert (0, error_5l)
    deltaw.insert (0, np.matmul(error_5l, activations[0].transpose()))


    for x in range (0,5):
        weights [x] = weights [x] - (learningrate * deltaw[x])
    for x in range (0,5):
        biases[x] = biases [x] - (learningrate * deltab[x])
```

I then decided that I was ready to start coding it iteratively.

Iterative Backpropagation

I then followed the procedural algorithm above and copied it into my iterative algorithm:

```python
def iterbackprop (activation, target, learningrate):
    global weights
    global biases

    deltaw = []
    deltab = []

    # error in last layer
    error_l = activation - target # getting error
    error_l = error_l = np.reshape (error_l, (structure[-1], 1)) # reshaping error to be array
    deltab.insert (0, error_l) # error = delta biases
    deltaw.insert (0, np.matmul(error_l, activations[4].transpose())) # weight delta is error propagated backwards

    for x in range (0, size - 2): # iterating from 0 to 4
        prop = np.matmul (weights[-(x+1)].transpose(), error_l)
        error_l = np.multiply (prop, sigmoid_prime (preactive[-(x+3)]))
        error_l = np.reshape (error_l, (structure[-(x+2)] , 1))
        deltab.insert (0, error_l)
        print (f"x={x}")
        deltaw.insert (0, np.matmul(error_l, activations[(x-3)].transpose()))  x File "C:\Users\M M Amjad\Docume

    for x in range (0,5):
        weights [x] = weights [x] - (learningrate * deltaw[x])
    for x in range (0,5):
        biases[x] = biases [x] - (learningrate * deltab[x])
```

```
Error Before: [[-0.84655192]]
x=0
x=1
Traceback (most recent call last):
  File "C:\Users\M M Amjad\Documents\[=] A Level\Sixth Form\CS Project\Code\BackpropPrototype2.py", line 150, in <module>
    iterbackprop (activation, np.log10 (d.getHL()[i]), 0.01)
  File "C:\Users\M M Amjad\Documents\[=] A Level\Sixth Form\CS Project\Code\BackpropPrototype2.py", line 127, in iterbackprop
    deltaw.insert (0, np.matmul(error_l, activations[(x-3)].transpose()))
AttributeError: 'list' object has no attribute 'transpose'
[Finished in 1.5s]
```

As you can see, this gave me an error. I printed out the index values to see which iteration caused the issue. It was when x=3, and it only affected the `deltaw` line. The only thing which depended on x in that line was the activation which it used to multiply the error by. After following the logic through, I realised that I was iterating through the activations the wrong way, going forwards rather than backwards, meaning I reached the end before I should have. I then amended this line by multiplying x-3 by -1 to get 3-x which fixed the program and gave me no errors:

```python
    for x in range (0, size - 2): # iterating from 0 to 4
        prop = np.matmul (weights[-(x+1)].transpose(), error_l)
        error_l = np.multiply (prop, sigmoid_prime (preactive[-(x+3)]))
        error_l = np.reshape (error_l, (structure[-(x+2)] , 1))
        deltab.insert (0, error_l)
        deltaw.insert (0, np.matmul(error_l, activations[(3-x)].transpose()))

    for x in range (0,5):
        weights [x] = weights [x] - (learningrate * deltaw[x])
    for x in range (0,5):
        biases[x] = biases [x] - (learningrate * deltab[x])
```

```
Error Before: [[-0.37588114]]
Error After: [[-4.02455846e-16]]
[Finished in 2.8s]
```

I decided to run it again but for more iterations to see if the error value suddenly changed, but instead I got the following:

```python
for z in range (0, 5000):
    activation = feedforward (isotope[i], structure)
    iterbackprop (activation, np.log10 (d.getHL()[i]), 0.01)

error = feedforward (isotope[i], structure) - np.log10 (d.getHL()[i])
print (f"Error After: {error}")
```

```
Error Before: [[2.18834266]]
Error After: [[0.]]
[Finished in 7.9s]
```

This meant my algorithm was predicting the half-life with perfect accuracy. I then changed the structure to the following and checked again:

```
            deltaw.insert (0, np.matmul(error_l, activations[(3-x)].transpose()))

        for x in range (0,5):
            weights [x] = weights [x] - (learningrate * deltaw[x])
        for x in range (0,5):
            biases[x] = biases [x] - (learningrate * deltab[x])

    structure = [6,16,16,16,16,16,1]
```

```
Error Before: [[0.04354551]]
Traceback (most recent call last):
  File "C:\Users\M M Amjad\Documents\[=] A Level\Sixth Form\CS Project\Code\BackpropPrototype2.py", line 149, in <module>
    iterbackprop (activation, np.log10 (d.getHL()[i]), 0.01)
  File "C:\Users\M M Amjad\Documents\[=] A Level\Sixth Form\CS Project\Code\BackpropPrototype2.py", line 126, in iterbackprop
    deltaw.insert (0, np.matmul(error_l, activations[(3-x)].transpose()))
AttributeError: 'list' object has no attribute 'transpose'
[Finished in 1.3s]
```

This threw an error for the same line. I rechecked why I started at layer 3 and realised that this was hardcoded to match my 6 layer structure. I changed 3 to size-3 and this fixed the error:

```
        for x in range (0, size - 2):
            prop = np.matmul (weights[-(x+1)].transpose(), error_l)
            error_l = np.multiply (prop, sigmoid_prime (preactive[-(x+3)]))
            error_l = np.reshape (error_l, (structure[-(x+2)] , 1))
            deltab.insert (0, error_l)
            deltaw.insert (0, np.matmul(error_l, activations[((size-3)-x)].transpose()))

        for x in range (0,5):
            weights [x] = weights [x] - (learningrate * deltaw[x])
        for x in range (0,5):
            biases[x] = biases [x] - (learningrate * deltab[x])

    structure = [6,16,16,16,16,16,1]
```

```
Error Before: [[1.77903619]]
Error After: [[5.66213743e-15]]
[Finished in 8.2s]
```

I also realised that me starting at activations[4] for my first layer error was hardcoded and so amended that line as well later on to the following:

```
deltaw.insert (0, np.matmul(error_l, self.activations[self.size-2].transpose()))
```

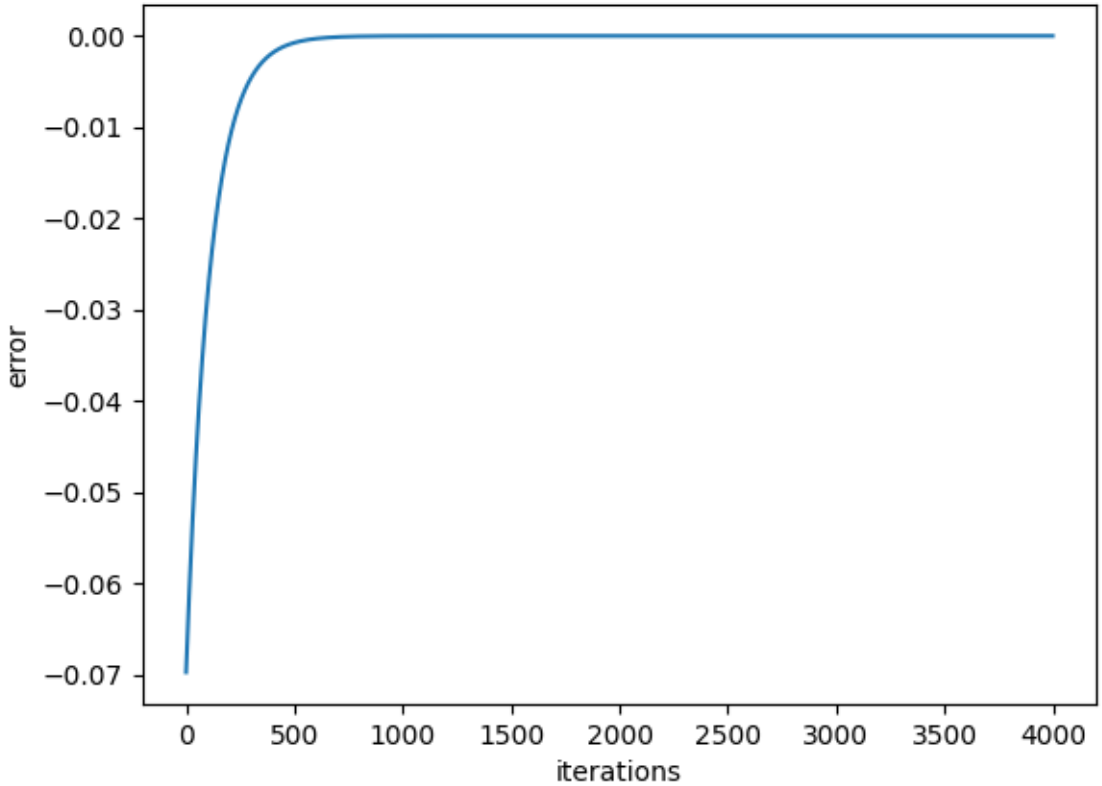
When I then ran my backpropagation iteratively, however, I ran into a similar issue I had earlier. The error was converging:

```
    print (f"Error Before Backpropagation: {net.feedforward (isotope[i]) - np.log10 (d.getHL()[i])}")
    for x in range (0, 4000):
        activation = net.feedforward (isotope[i]) - np.log10 (d.getHL()[i])
        net.backpropagation (activation, np.log10 (d.getHL()[i]), 0.01)

    error = net.feedforward (isotope[i]) - np.log10 (d.getHL()[i])
    print (f"Error After: {error}")
```

```
Error Before Backpropagation: [[2.72776958]]
Error After: [[-0.7212464]]
[Finished in 11.2s]
```

I decided to use the same strategy as before of appending to an errors array and seeing where it starts converging, but this time I decided to plot it to make it easier to see. I added the following:

This gave me the following output:



This showed me that my error was in fact tending towards 0. This was contrary to what the error value I calculated suggested. I decided to then print the final error value and received the following output:

```
print (f"Error Before Backpropagation: {net.feedforward (isotope[i]) - np.log10 (d.getHL()[i])}")
for x in range (0, 4000):
    activation = net.feedforward (isotope[i]) - np.log10 (d.getHL()[i])
    net.backpropagation (activation, np.log10 (d.getHL()[i]), 0.01)
    error = activation - np.log10 (d.getHL()[i])
    errors.append(float(error))
    if x == 3999:
        print (f"Final Error in BackProp: {error}")

error = net.feedforward (isotope[i]) - np.log10 (d.getHL()[i])
print (f"Error After: {error}")
```

```
Error Before Backpropagation: [[-0.61139538]]
Final Error in BackProp: [[1.48769885e-14]]
Error After: [[-0.7212464]]
[Finished in 11.3s]
```

This showed the error was actually going towards 0, but the error after was something completely different.

I decided to check the actual values of my predictions and target by printing them and received the following:

```python
errors = []

print (f"Error Before Backpropagation: {net.feedforward (isotope[i]) - np.log10 (d.getHL()[i])}")
for x in range (0, 4000):
    activation = net.feedforward (isotope[i]) - np.log10 (d.getHL()[i])
    net.backpropagation (activation, np.log10 (d.getHL()[i]), 0.01)
    error = activation - np.log10 (d.getHL()[i])
    errors.append(float(error))
    if x == 3999:
        print (f"Final Error in BackProp: {error}")
        print (f"Log 10 of Predicted Half Life = {activation}")
        print (f"Log 10 of Actual Half Life = {np.log10 (d.getHL()[i])}")

error = (net.feedforward (isotope[i]) - np.log10 (d.getHL()[i]))
print (f"Error After: {error}")
```

```
Error Before Backpropagation: [[0.94118985]]
Final Error in BackProp: [[7.10542736e-15]]
Log 10 of Predicted Half Life = [[-0.7212464]]
Log 10 of Actual Half Life = -0.721246399047171
Error After: [[-0.7212464]]
[Finished in 17.4s]
```

This showed me that instead of printing the error, Python was printing the actual half-life predictions (it was negative as I am training to find the base 10 log of the half-life). This was why the error seemed to converge. This didn't matter, however, as my backpropagation itself was working. This meant that I had all the tools I needed to train and test my network. It was ready to implement.

Appending to Class

```python
def backpropagation (self, activation, target):

    deltaBiases = [] # define arrays for change in biases
    deltaWeights = [] # define arrays for change in weights

    learningrate = self.learningrate

    # error in last layer
    error_l = activation - target # getting error
    error_l = np.reshape (error_l, (self.structure[-1], 1)) # reshaping error to be array
    deltaBiases.insert (0, error_l) # error = delta biases
    deltaWeights.insert (0, np.matmul(error_l, self.activations[self.size-2].transpose())) # weight delta is error propagated backwards

    for x in range (0, self.size - 2):
        prop = np.matmul (self.weights[-(x+1)].transpose(), error_l) # propagate error backwards
        error_l = np.multiply (prop, sigmoid_prime (self.preactive[-(x+3)])) # hadamard product with preactivationss
        error_l = np.reshape (error_l, (self.structure[-(x+2)] , 1)) # reshape because numpy is peculiar
        deltaBiases.insert (0, error_l) # error = delta bias so add to start
        deltaWeights.insert (0, np.matmul(error_l, self.activations[((self.size-3)-x)].transpose())) # add delta weights

    for x in range (0,self.size-1):
        self.weights [x] = self.weights [x] - (learningrate * deltaWeights[x]) # adjust each weight by delta weight
        self.biases[x] = self.biases [x] - (learningrate * deltaBiases[x]) # adjust each bias by delta bias
```

Training and Testing the Network

I defined a simple subroutine to generate all the test and training sets I would need and added this to my network.py document but not my network class:

```python
def getSets ():

    isotopes = d.getIsotope()
    halflives = d.getHL()

    numTrain = len(isotopes)*8//10 # number of training isotopes = len(dataset) * 0.8
    numTest = len(isotopes)-numTrain # number of testing is what remains

    totalNums = np.arange(len(isotopes)) # all the possible indices I can use for isotopes

    randomNums = np.random.choice (len(isotopes), numTrain, replace = False) # replace: whether or not a sample is returned to the sample pool
    testingNums = np.delete(totalNums, randomNums) # define testing indices to be whatever is left after getting rid of training

    trainSet = []
    trainLabels = []

    for x in range (numTrain):
        trainSet.append (isotopes[randomNums[x]])
        trainLabels.append (np.log10(halflives[randomNums[x]]))

    testSet = []
    testLabels = []

    for x in range (numTest):
        testSet.append (isotopes[testingNums[x]])
        testLabels.append (np.log10(halflives[testingNums[x]]))

    model = d.getModel()
    errors = []

    for x in range (numTest):
        actual = np.log10(halflives[testingNums[x]])
        models = np.log10(model[testingNums[x]])
        error = models - actual
        errors.append(error**2)

    sigma =  (np.sum(errors)**(1/2)) / (numTest)
    print (f"Statistical Model Error: {sigma}")

    return trainSet, trainLabels, testSet, testLabels
```

I also made it print the error of the statistical model so that I could make an easy comparison between my model and the test model. I defined training and testing methods in my class as follows:

```python
    def train (self, dataset, targets, epochs):
        for x in range (epochs): # for the specified amount of epochs
            #print (f"Epoch {x+1}")
            for y in range (0, len(dataset)): # for each value in the dataset
                activation = self.feedforward (dataset[y]) # feed it forward
                self.backpropagation (activation, targets[y]) # backpropagate against the target

    def evaluate (self, dataset, targets):
        predictions = [] # define array for predictions
        errors = [] # define array for errors
        for isotope in dataset:
            prediction = self.feedforward (isotope)
            predictions.append(prediction) # add predictions to array of predictions
        for x in range (len(predictions)):
            error = predictions[x] - targets[x] # calculate errors
            errors.append (error**2) # append error^2 to array
        stddev =  (np.sum(errors)**(1/2)) / len(dataset) # sigma = (1/n)*(sum of (errors)^2)^(1/2)
        return float(stddev)
```

I then made sure it worked by running the following code:

```python
trainSet, trainLabels, testSet, testLabels = getSets ()

print ("Training...")
net.train(trainSet, trainLabels, epochs = 100)
print ("Training Complete")
stddev = net.evaluate(testSet, testLabels)
print (f"Standard Deviation: {stddev}")
```

I received the following output:

```
Statistical Model Error: 0.08317506780411073
Training...
Training Complete
Standard Deviation: 0.074377018577843
[Finished in 23.1s]
```

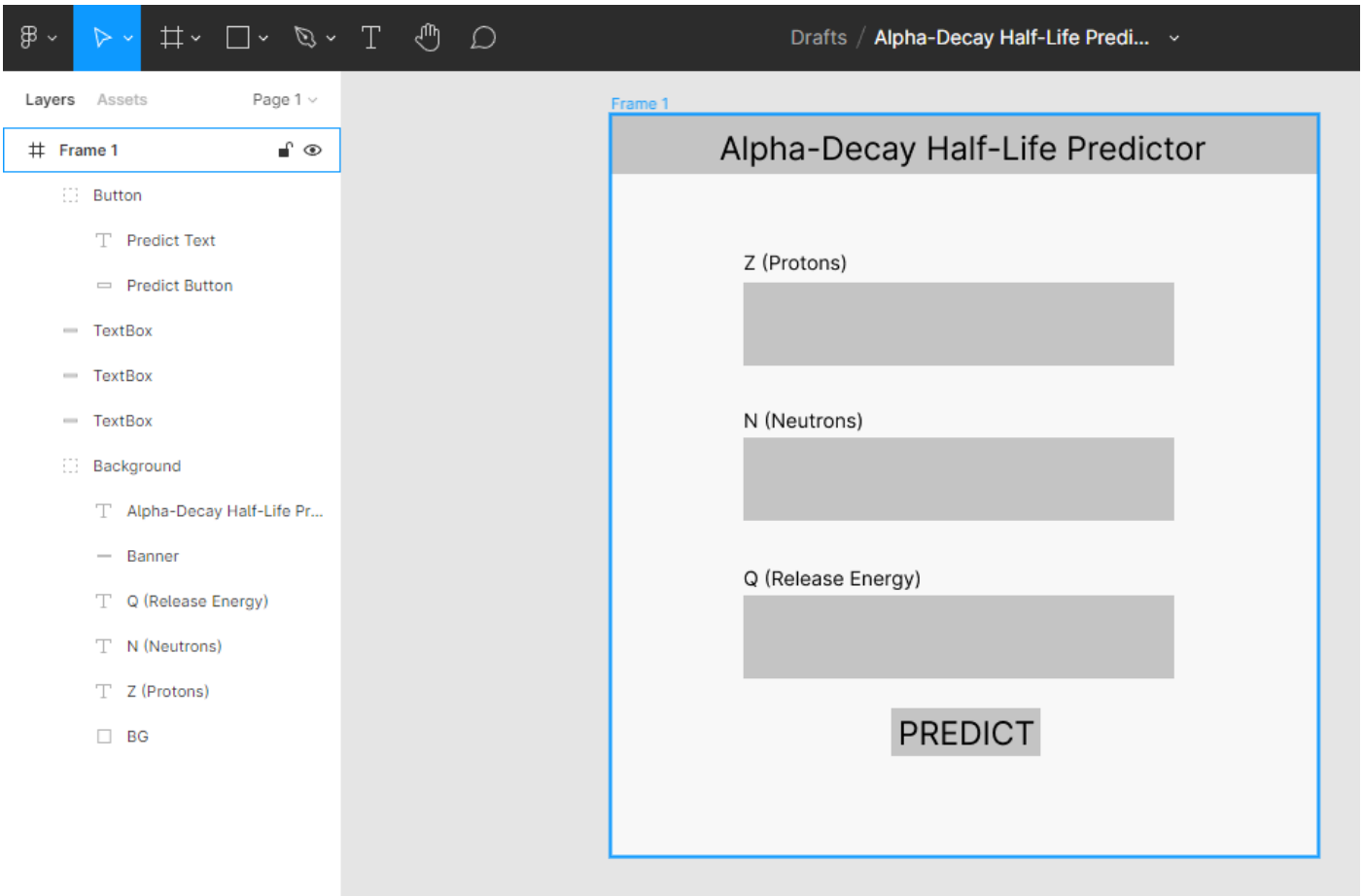
This indicated that my model worked and it achieved a better score than the statistical model! This was also only with 100 epochs. This indicated that my network was completely up and running so at this point, I decided to work on my UI, as the main back-end of my project was done.

User Interface

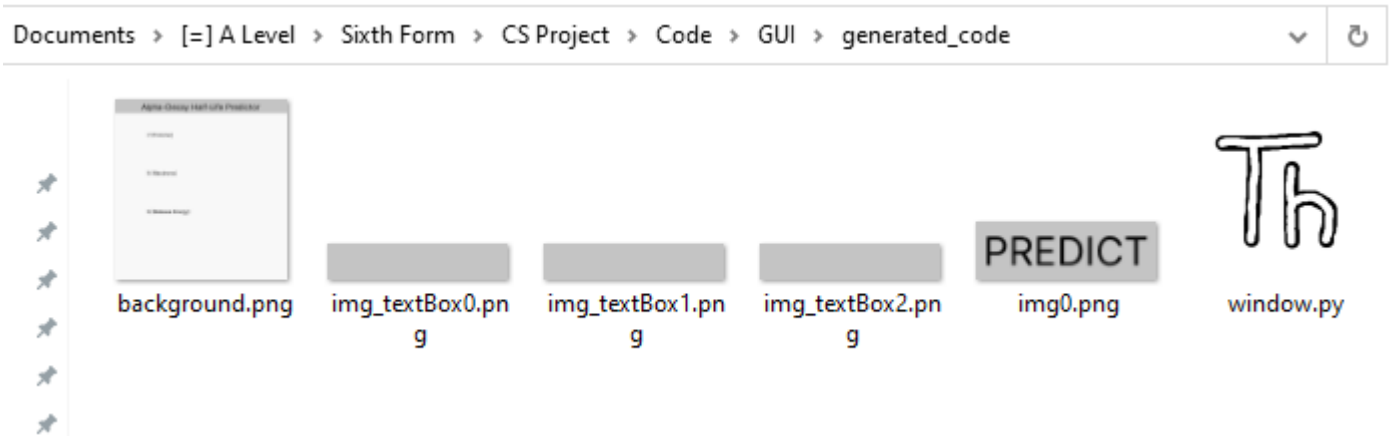
I created my user interface using a tool called figma[13], which allows you to create templates for UIs and feed them into other programs. I did this because I also found on GitHub[14], a tool which takes figma templates and renders them in tkinter. I decided this would be a valid way of creating my UI as my UI is very simple, and this also saves time.

Input Space

I created my template on figma as follows:



I defined the buttons and text boxes on the left. I then fed this into the GUI-Designer software I found on GitHub, which generated for me the following folder containing all the back-end I needed for the UI:



I then went into the window.py file and added all the functionality I needed, as this was not added by the GUI designer.

[13] [https://www.figma.com/]
[14] [https://github.com/TestTest4253/GUI-Designer]

Adding Functionality

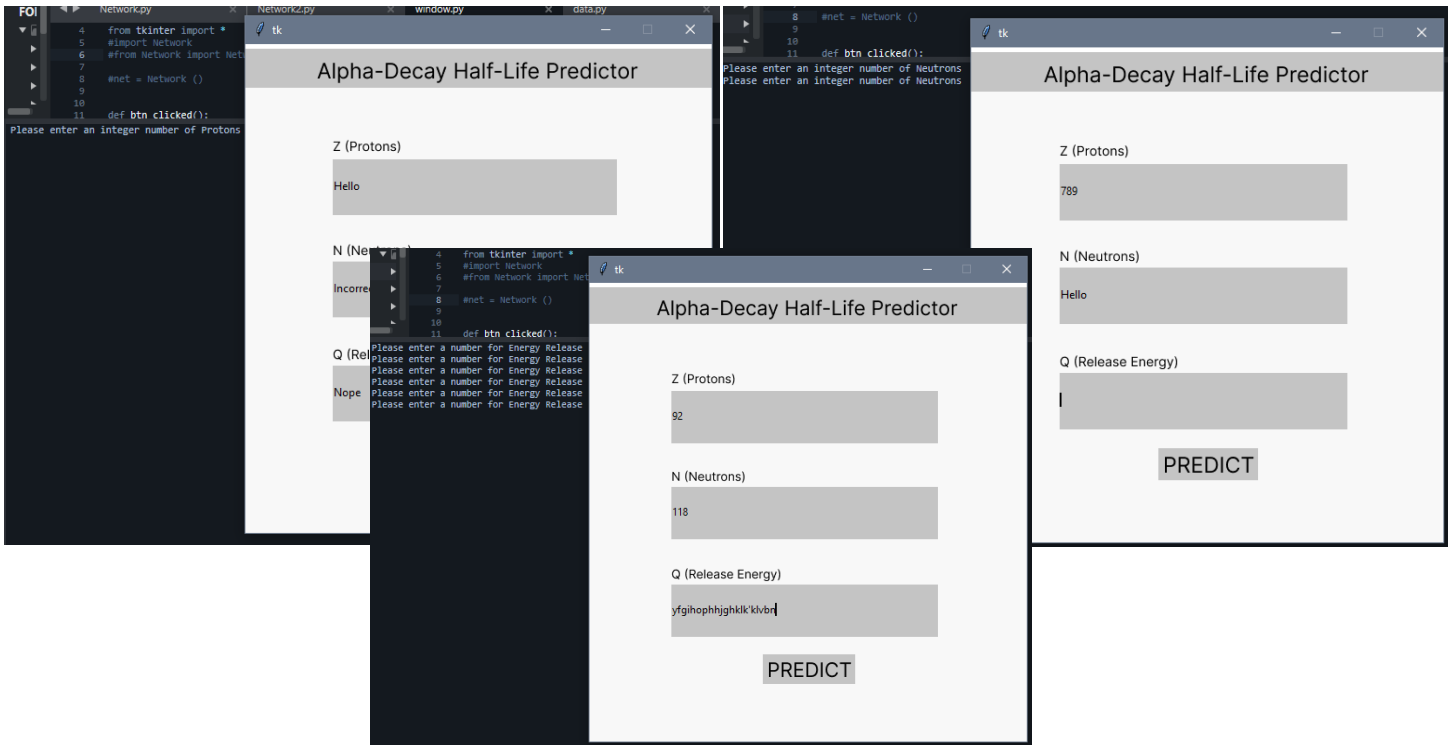
The main functionality of my UI rests in what happens when the user presses the PREDICT button. When this is pressed, the software needs to read the content of each of the boxes and feed them into my neural network. This also needs to account for the user inputting incorrect data. I decided that try, except statements would be the best way to implement this. The button was defined as follows:

```
b0 = Button(
    image = img0,
    borderwidth = 0,
    highlightthickness = 0,
    command = btn_clicked,
    relief = "flat")
```

This called the btn_clicked function on click. I then defined the btn_clicked function as follows:

```
def btn_clicked():
    data = []

    try:
        Z = int (entry0.get())
    except ValueError:
        print ("Please enter an integer number of Protons")
        return

    try:
        N = int (entry1.get())
    except ValueError:
        print ("Please enter an integer number of Neutrons")
        return

    try:
        Q = float (entry2.get())
    except ValueError:
        print ("Please enter a number for Energy Release")
        return

    A = Z+N
    Zdist = min ([abs(Z-28), abs(Z-50), abs(Z-82), abs(Z-126)])
    Ndist = min ([abs(N-28), abs(N-50), abs(N-82), abs(N-84), abs(N-126)])
    data.append(Z)
    data.append(N)
    data.append(A)
    data.append(Q)
    data.append(Zdist)
    data.append(Ndist)

    print (data)
```

This does the following:



[Evidence for Test i]

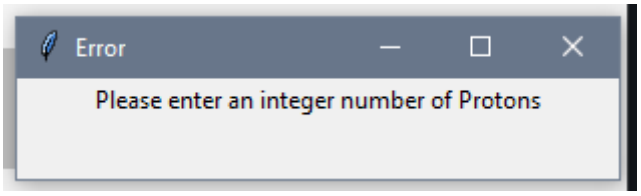
The software printed to the console for every incorrect input, meaning that the software can correctly recognise them. I now need a way of displaying the prompts to the user. For this, I decided to open a new window which had the prompt on. For this, I defined a new window class[15] which took in string as a parameter that defined the error text:

```
class NewWindow(Toplevel):

    def __init__(self, master = None, texts = "Error"):

        super().__init__(master = master)
        self.title("Error")
        self.geometry("300x50")
        label = Label(self, text = texts)
        label.pack()
```

I then called this class in each of my except statements with the text defined for each of them:

```
def btn_clicked():
    data = []

    try:
        Z = int (entry0.get())
    except ValueError:
        print ("Please enter an integer number of Protons")
        entry0.delete (0,END)
        NewWindow (window, "Please enter an integer number of Protons")
        return

    try:
        N = int (entry1.get())
    except ValueError:
        print ("Please enter an integer number of Neutrons")
        entry1.delete(0,END)
        NewWindow (window, "Please enter an integer number of Neutrons")
        return

    try:
        Q = float (entry2.get())
    except ValueError:
        print ("Please enter a number for Energy Release")
        entry2.delete(0,END)
        NewWindow (window, "Please enter a number for Energy Release")
        return
```

I also used a feature called entry.delete(0,END) which deletes the contents of the entry box whenever the user enters something incorrect so that they do not have to do this manually:

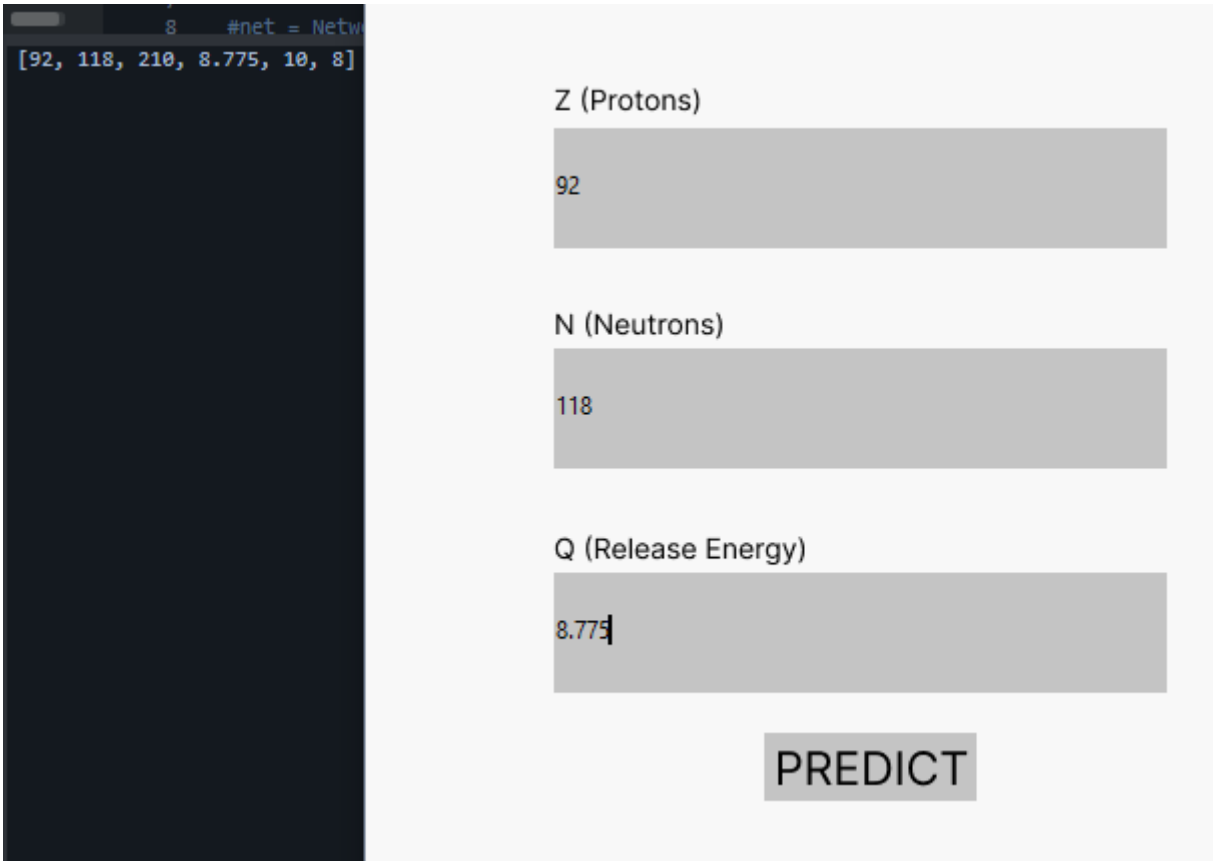


A video of this working is at the end of the project. Once the user entered completely correct data, I defined the rest of the variables based on their input (nucleon number, ZDist and NDist) and stored them in an array:

```
A = Z+N
Zdist = min ([abs(Z-2), abs(Z-8), abs(Z-20), abs(Z-28), abs(Z-50), abs(Z-82), abs(Z-126)])
Ndist = min ([abs(N-2), abs(N-8), abs(N-20), abs(N-28), abs(N-50), abs(N-82), abs(N-84), abs(N-126)])
data.append(Z)
data.append(N)
data.append(A)
data.append(Q)
data.append(Zdist)
data.append(Ndist)
```

This gave the following output when I printed `data`:

[15] [https://www.geeksforgeeks.org/open-a-new-window-with-a-button-in-python-tkinter/]



[Evidence for Test ii]

I now had to calculate the half-life and then finally make a window to display the half-life, which I will add when I amalgamate the front-end and back-end.

Amalgamating Front-End and Back-End

The last part was to combine the front-end and back-end. As all the network has to do to make a prediction is feedforward an input through the specified weights and biases, I determined the best way to implement this would be to store the states of my trained weights and biases and feed them forward locally. I would first have to train the network to a suitable standard, and then store the weights and biases using a joblib dump. I can then load this dump locally and define my weights and biases from it.

To implement this, I first tested to see how the joblib dump would work. I did this by generating a small ordered array using `numpy.arange()` and dumping that using joblib to a file called test1:

```
import numpy as np
import joblib

numbers = np.arange (15)
joblib.dump(numbers, "test1")
```

test1	15/04/2022 11:15	File	1 KB

I then loaded this and printed the 2 arrays:

```
import numpy as np
import joblib

numbers = np.arange (15)
joblib.dump(numbers, "test1")
numbers2 = joblib.load ("test1")

print (numbers)
print(numbers2)
```

```
[ 0  1  2  3  4  5  6  7  8  9 10 11 12 13 14]
[ 0  1  2  3  4  5  6  7  8  9 10 11 12 13 14]
[Finished in 1.2s]
```

[Evidence for Test 6]

The 2 arrays were the same. This means I could use joblib for my weights and biases and it would return the same arrays. I then defined a Network.save() method as follows:

```
def save (self):
    joblib.dump(self.weights, "weights")
    joblib.dump(self.biases, "biases")
```

This will allow me to save the weights and biases with filenames “weights” and “biases” respectively if I found them suitable. I then had to train the network to a suitable standard. I defined a suitable standard as being better than the statistical model on 3 separate randomly generated test sets. To determine this, I set up the following routine:

```
trainSet, trainLabels, testSet, testLabels, stddevModel = getSets ()

net = Network ([6,16,20,20,16,1])

print ("Training...")
net.train(trainSet, trainLabels, epochs = 500) # train network
print ("Training Complete")

print ("Round 1")
stddevNetwork = net.evaluate(testSet, testLabels) # evaluate network on given test set
print (f"Network Deviation: {stddevNetwork}") # print net score
print (f"Stat Model Deviation: {stddevModel}") # print model score

if stddevNetwork < stddevModel: # if net is better than model
    print("Round 2") # round 2
    trainSet, trainLabels, testSet, testLabels, stddevModel = getSets () # fresh sets
    stddevNetwork = net.evaluate(testSet, testLabels) # evaluate using already trained weights and biases
    print (f"Network Deviation: {stddevNetwork}") # print net score
    print (f"Stat Model Deviation: {stddevModel}") # print model score

    if stddevNetwork < stddevModel:
        print("Round 3")
        trainSet, trainLabels, testSet, testLabels, stddevModel = getSets () # repeat above
        stddevNetwork = net.evaluate(testSet, testLabels)
        print (f"Network Deviation: {stddevNetwork}")
        print (f"Stat Model Deviation: {stddevModel}")

        if stddevNetwork < stddevModel: # if net better than model 3 times
            print ("Saving")
            net.save() # save weights and biases
```

I also modified the structure to have more neurons in the central 2 hidden layers as this would hopefully also increase the accuracy. I upped the epoch number to 500 to better train the network. I then set this running, however, it was not very successful. It rarely got to Round 3 and when it did it rarely saved. Due to this, after around 10 attempts, I upped the epoch number to 1000. On my 2nd attempt, I got the following:

```
Training...
Training Complete
Round 1
Network Deviation: 0.07139960162705565
Stat Model Deviation: 0.08820546738830637
Round 2
Network Deviation: 0.0768375723413901
Stat Model Deviation: 0.09222547068959369
Round 3
Network Deviation: 0.06477328713484788
Stat Model Deviation: 0.08070372707862815
Saving
[Finished in 60.3s]
```

This was, looking at the results, a very good network. It had a difference of nearly 0.02 on each round compared to the statistical mode, meaning the network was outperforming it by a fair way on each test. Because of this, I decided to stop here and take these weights and biases. The reason I did not want to go for many more epochs was because I did not want to run the risk of overfitting the network to the current dataset. This is when the network has been

trained so much that it starts to spot patterns in the random noise of the training set. It then overly fits its weights and biases to the training set, such that it performs less effectively when being used on the testing set. For fun, I ran the training algorithm for 10,000 epochs and got the following results:

```
Training...
Training Complete
Round 1
Network Deviation: 0.0660569986370034
Stat Model Deviation: 0.08288146937820234
Round 2
Network Deviation: 0.05556136776135095
Stat Model Deviation: 0.08279958484413724
Round 3
Network Deviation: 0.05161126429918567
Stat Model Deviation: 0.09256688260351674
Saving
[Finished in 587.5s]
```

Although this has an even lower standard deviation from the test set than my current model, I have decided not to use these weights and biases to avoid running the risk of overfitting the network.

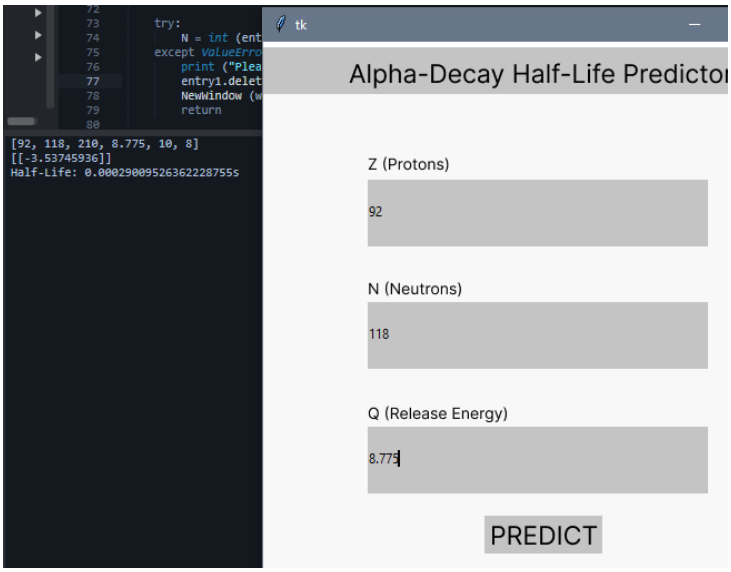
The net.save did its job and the weights and biases were saved in the local directory of my GUI. I then added the following code to my GUI:

```
weights = joblib.load("weights")
biases = joblib.load ("biases")
activations = []

structure = [6,16,20,20,16,1]
size = len(structure)
for x in range (size):
    activations.append(np.zeros((structure[x],1)))

def feedforward (data):
    # min-max normalise all values
    Z = (data[0]-min(d.getZ()))/(max(d.getZ())-min(d.getZ()))
    N = (data[1]-min(d.getN()))/(max(d.getN())-min(d.getN()))
    A = (data[2]-min(d.getA()))/(max(d.getA())-min(d.getA()))
    Q = (data[3]-min(d.getQ()))/(max(d.getQ())-min(d.getQ()))
    Zd = (data[4]-min(d.getZDist()))/(max(d.getZDist())-min(d.getZDist()))
    Nd = (data[5]-min(d.getNDist()))/(max(d.getNDist())-min(d.getNDist()))

    activations [0] = np.array([[Z], [N], [A], [Q], [Zd], [Nd]])


    # iterate through hidden layers using weights and biases (except for last)
    for x in range (0, size - 1):
        a = activations [x]
        mult = np.array([np.matmul(weights[x], a)])
        mult = np.reshape(mult, (structure[x+1],1))
        presig = mult + biases [x]
        activations [x+1] = sigmoid(mult + biases[x])

    #manually apply last layer weights and biases to avoid sigmoid
    af = np.array([])
    mult = np.array([np.matmul(weights[size - 2], activations [size - 2])])
    mult = np.reshape (mult, (structure[size - 1],1))
    af = mult + biases[size - 2]
    activations.append ([af])
    return af
```

In my btn_clicked routine, I added the following at the end:

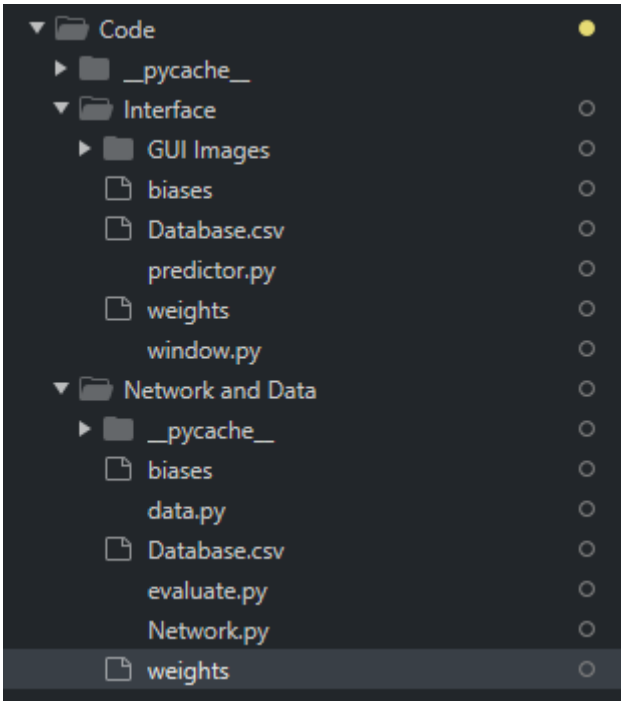
```
A = Z+N
Zdist = min ([abs(Z-2), abs(Z-8), abs(Z-20), abs(Z-28), abs(Z-50), abs(Z-82), abs(Z-126)])
Ndist = min ([abs(N-2), abs(N-8), abs(N-20), abs(N-28), abs(N-50), abs(N-82), abs(N-84), abs(N-126)])
data.append(Z)
data.append(N)
data.append(A)
data.append(Q)
data.append(Zdist)
data.append(Ndist)

print (data)
loghalflife = feedforward (data)
print (loghalflife)
halflife = np.float_power (10, loghalflife)
print (f"Half-Life: {float(halflife)}s")
```

When I then ran the code, I received the following output for this input:



[Evidence for Test iii]

This showed me that my predictor was working. The last thing I had to do was just display this on the user's screen, however, before this, I decided to clean up my code directories. Until this point, things like my network class and database were in a folder with old prototypes and many different things were amalgamated into single files. As my project was nearing completion, I thought that now would be a good time to organise my source code files. I organised them into the following tree:



The plan is to have my window.py call the predictor.py which will hold the feedforward method. This feedforward method will import the data it needs from data.py and return a value back to window.py which will display it. To do this, I have to play with the directories. I have to be careful, however, not to hardcode this to only work with my file paths. I added the following to my predictor.py to allow it to import data.py:

```
import os
import sys

data_dir = os.path.abspath (os.path.join("..","Network and Data"))
# find directory to current file
# go to parent directory ("..")
# from parent, add "Network and Data" to the path
sys.path.insert(1, data_dir) # add this path to system path

from data import Data
d = Data()
```

I then placed the feedforward into my predictor.py:

```python
sigmoid = lambda x : 1.0/(1.0+np.exp(-x))

weights = joblib.load("weights")
biases = joblib.load ("biases")
activations = []

structure = [6,16,20,20,16,1]
size = len(structure)
for x in range (size):
    activations.append(np.zeros((structure[x],1)))

def feedforward (data):
    # min-max normalise all values
    Z = (data[0]-min(d.getZ()))/(max(d.getZ())-min(d.getZ()))
    N = (data[1]-min(d.getN()))/(max(d.getN())-min(d.getN()))
    A = (data[2]-min(d.getA()))/(max(d.getA())-min(d.getA()))
    Q = (data[3]-min(d.getQ()))/(max(d.getQ())-min(d.getQ()))
    Zd = (data[4]-min(d.getZDist()))/(max(d.getZDist())-min(d.getZDist()))
    Nd = (data[5]-min(d.getNDist()))/(max(d.getNDist())-min(d.getNDist()))

    activations [0] = np.array([[Z], [N], [A], [Q], [Zd], [Nd]])


    # iterate through hidden layers using weights and biases (except for last)
    for x in range (0, size - 1):
        a = activations [x]
        mult = np.array([np.matmul(weights[x], a)])
        mult = np.reshape(mult, (structure[x+1],1))
        presig = mult + biases [x]
        activations [x+1] = sigmoid(mult + biases[x])

    #manually apply last layer weights and biases to avoid sigmoid
    af = np.array([])
    mult = np.array([np.matmul(weights[size - 2], activations [size - 2])])
    mult = np.reshape (mult, (structure[size - 1],1))
    af = mult + biases[size - 2]
    activations.append ([af])
    return af
```

I then imported this as ff for feedforward in my window.py:

```python
from pathlib import Path
designPath = Path ("GUI Images/")
import predictor as ff
from tkinter import *
import numpy as np
```

I then called this in my btn_click method:

```python
loghalflife = ff.feedforward (data)
halflife = np.float_power (10, loghalflife)
```

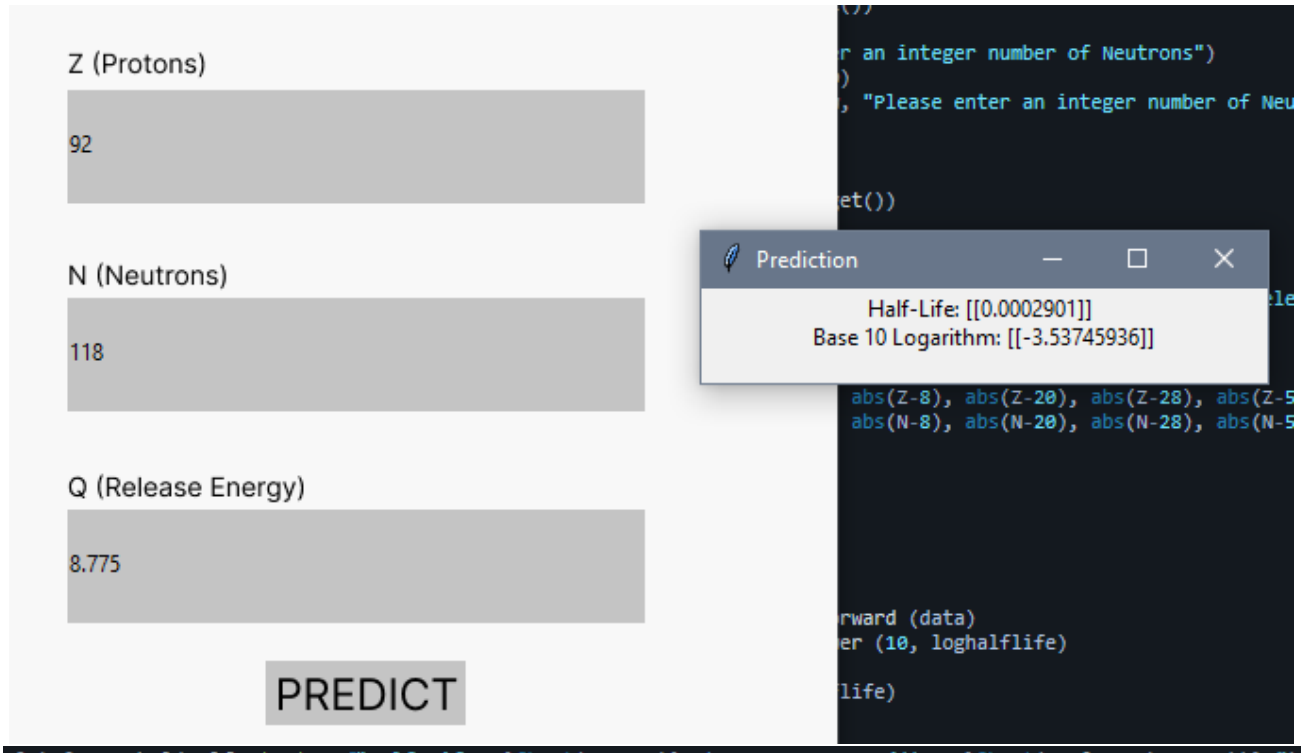
I then also defined a new class for my answer window, which will display the answer of the half-life to the user:

```python
class answindow (Toplevel):

    def __init__ (self, master = None, answer = "Error"):
        super().__init__(master = master)
        self.title("Prediction")
        self.geometry("300x50")
        label = Label(self, text = f"Half-Life: {answer} \nBase 10 Logarithm: {np.log10(answer)}")
        label.pack()
```

I set the default answer to Error as I wanted to know if I hadn't passed an answer to the box. I then created an answer window with my predicted half-life:

```python
answindow (window, halflife)
```

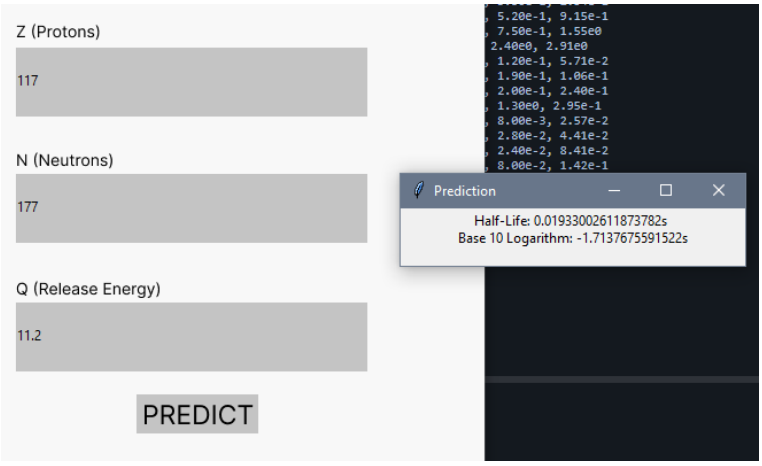
When I inputted everything correctly, it gave me the following output:




```
label = Label(self, text = f"Half-Life: {float(answer)}s \nBase 10 Logarithm: {float(np.log10(answer))}s")
label.pack()
```

This looked ugly so I casted them as floats and added “s” on the end to signify seconds:

This was the output:



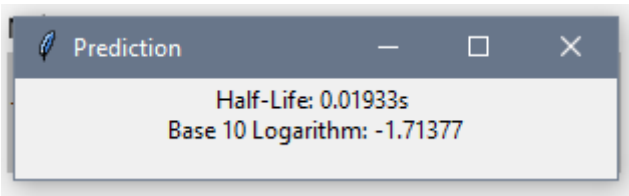
[Evidence for Test v]

I realised that taking the exponent of the half-life and re-logging it will introduce more inaccuracies in my output so I decided to amend this by printing the base 10 log as it was given:

```
loghalflife = ff.feedforward (data)
#halflife = np.float_power (10, loghalflife)

answindow (window, loghalflife)
```

I then changed the output text to the following and rounded to 5 decimal places to make it look better:

```
label = Label(self, text =
    f"Half-Life: {round(float(np.float_power(10, answer)), 5)}s \nBase 10 Logarithm: {round(float(answer), 5)}")
label.pack()
```



The UI was able to output a predicted half-life successfully. The prediction is based on my neural network which was trained via backpropagation to find the base-10 logarithm of alpha-decay half-lives of multiple radioactive isotopes. By saving the states of the weights and biases, I was able to save the state of my trained network and therefore feedforward new input values for new predictions.

This demonstrated that my UI was functional and I was now ready to evaluate the success of my project. Before this, however, I asked my stakeholders for feedback in regards to the GUI.

User Feedback and Updates

I sent my GUI to the stakeholder, along with asking for ratings out of 5 and comments for the following criteria:

- Simplicity: 5/5
    - The GUI is simple and easy to use, it is clear what is wanted from the user and where it is to be entered, and the lack of too many options and boxes make it easy to use
- Understandability: 5/5
    - The software is intuitive to use as the labels for each of the text boxes and the button are very clear in what they are prompting you to do. The prompts for incorrect data are also clear in what they want the user to do as well.
- Design: 4/5
    - The design is clean and simple although could have looked very slightly more polished.
- Other Comments?
    - None, see above.

Evaluation

Success Criteria

Essential Success Criteria

Criterion	Criterion Met?	Justification of Previous Column	Plans for Future Development
Predictions of the neural network must have better accuracy than the statistical model	Yes - Fully	Evidenced by my network giving a lower standard deviation than the statistical model on 3 separate occasions with random test sets (pg. 42)	There are no plans to update the neural network or how it functions in future development
The network is able to account for updates to the database of isotopes	Yes – Fully	The databasing aspect is completely modular, and none of it is hard-coded, meaning that it is able to account for any additions or removals from the database (pg. 19)	There are no plans to update how the database is managed in future development
User is able to easily navigate the GUI	Yes – Fully	Evidenced by my stakeholder feedback (pg. 47)	Update the GUI based on future developments to allow the GUI to be usable with new features

Desirable Success Criteria

Criterion	Criterion Met?	Justification of Previous Column	Plans for Future Development
User is able to retrain the network on their own with their own specified number of epochs	Partially	The user is able to retrain the network, but only by going into the back-end files and modifying them. If they do not understand the code, this feature will not be available to them.	Add a screen/section in the GUI which allows the user to easily be able to do this.
It is easy for the user to make any adjustments to the network's shape and size	Partially	It is possible, but not easy. The user will have to go into the network files and modify them there.	Add a screen/section in the GUI which allows the user to easily be able to do this.
User is easily able to update the database	No	The user can update the database, but only by going into the back-end files. They also do not know the format of the database, making it even more difficult for them to do so.	Add a screen/section in the GUI which allows the user to easily be able to do this.

Post-Development Testing

Back-End

Test	Success Criteria	Met?	Evidence	Explanation
Accuracy of NN	Better than statistical model consistently	Yes	Page 42	This demonstrates that my NN is a more accurate tool for determining half-lives than existing statistical models

Front-End

Test	Success Criteria	Met?	Evidence	Explanation
Incorrect User Input (Robustness)	Able to catch incorrect input and prompt the user for correct input	Yes	Page 39	This demonstrates that my NN is a more accurate tool for determining half-lives than existing statistical models

Limitations

One of the main limiting features of my program is that it does not let the user interact with the network in any way shape or form. They are unable to modify or train it easily, as there is no option in the interface that allows them to do this. This is something I hope to amend in future development by adding menus and sections in the GUI that allow the user to interact with these things.

One of the limitations of my project as a whole is to do with the problem itself, as I chose a project which focused solely on alpha decay. This limits the capabilities of the program as it can only be used by a very specific group of people who only need to focus on one type of decay. In future, I hope to be able to develop a program which will predict the half-life for any conceivable isotope with any decay mode, with it also telling the user what type of decay it will undergo. For the current project, however, focusing on alpha decay was sufficient in terms of computational complexity, and I believe my solution is effective.

Evaluation Summary

Overall, I believe that my solution was a success as it reached all the essential success criteria, as well as satisfying the stakeholder requirements. I am very happy with the development and the performance of the neural network and the fact that my solution performs better than existing models is also very reassuring to me. Despite this, there are still ways in which my project can be improved, however, I believe that my solution is more than sufficient for the problem specified.

A video of the working code can be found here: https://youtu.be/lB3MoOg_INM
The full code is also available on GitHub with the following link: https://github.com/MAmJ4/CS-Project

Final Code

Back-End

data.py

```
import csv as csv
import numpy as np

import sys
import os
data_dir = os.path.abspath(os.path.join("..","Network and Data"))
sys.path.insert(1, data_dir) # add this path to system path

class Data ():

        def __init__ (self):
                self.data = []
                with open("Database.csv") as database:
                        csvreader = csv.reader (database)
                        for row in csvreader:

        self.data.append([row[0],int(row[1]),int(row[2]),int(row[3]),
                                        float(row[4]),float(row[5]),float(row[6])])

                # Format: Element, Z, N, A, Q, T12, ELDM
                for isotope in self.data:

                        Zdist = min([abs(isotope[1]-2), abs(isotope[1]-8),
                                abs(isotope[1]-20), abs(isotope[1]-28),
                                abs(isotope[1]-50), abs(isotope[1]-82),
                                abs(isotope[1]-126)])
                        isotope.insert (2, Zdist)

                        Ndist = min([abs(isotope[3]-2), abs(isotope[3]-8),
                                abs(isotope[3]-20), abs(isotope[3]-28),
                                abs(isotope[3]-50), abs(isotope[3]-82),
                                abs(isotope[3]-84), abs(isotope[3]-126)])
                        isotope.insert (4, Ndist)

                # Format: Element, Z, ZDist, N, NDist, A, Q, T12, ELDM


        def getZ (self):
                Z = []
                for x in self.data:
                        Z.append(x[1])
                return Z

        def getZDist (self):
                ZDist = []
                for x in self.data:
                        ZDist.append(x[2])
                return ZDist

        def getN (self):
                N = []
                for x in self.data:
                        N.append (x[3])
                return N

        def getNDist (self):
                NDist = []
                for x in self.data:
                        NDist.append(x[4])
                return NDist
```

```
        def getA (self):
                A = []
                for x in self.data:
                        A.append (x[5])
                return A

        def getQ (self):
                Q = []
                for x in self.data:
                        Q.append (x[6])
                return Q

        def getHL (self):
                HL = []
                for x in self.data:
                        HL.append (x[7])
                return HL

        def getModel (self):
                Model = []
                for x in self.data:
                        Model.append (x[8])
                return Model

        def getIsotope (self):
                Isotope = []
                for x in self.data:
                        Isotope.append ([x[1], x[3], x[5], x[6], x[2], x[4]])
                return Isotope
```

network.py

```
import numpy as np
import matplotlib.pyplot as plt
import data
from data import Data
import joblib

# miscellaneous functions
sigmoid = lambda x : 1.0/(1.0+np.exp(-x))
sigmoid_prime = lambda z : sigmoid(z)*(1-sigmoid(z))

# database
d = Data()

# network class
class Network ():

        def __init__ (self, structure, learningrate = 0.01):
                d = Data ()
                self.size = len(structure) # set size equal to number of layers
                self.structure = structure # set structure (n of neurons) to match
input

                self.weights = [] # declare weight array
                self.biases = [] # declare bias array
                for x in range (0, (self.size - 1)):
                        # initialise weights and biases with random values
                        self.weights.append(np.asarray(np.random.uniform(-1,1,
                                (structure[x+1],structure[x]))))
                        self.biases.append(np.asarray(np.random.uniform(-1,1,
                                (structure[x+1],1))))

                self.preactive = []

                self.activations = [] # declare activations
                for x in range (0, self.size):
                        # initialise activations with zeros
                        self.activations.append(np.zeros((structure[x],1)))
```

```
        self.learningrate = learningrate

    def feedforward (self, data):

        # min-max normalise all values
        Z = (data[0]-min(d.getZ()))/(max(d.getZ())-min(d.getZ()))
        N = (data[1]-min(d.getN()))/(max(d.getN())-min(d.getN()))
        A = (data[2]-min(d.getA()))/(max(d.getA())-min(d.getA()))
        Q = (data[3]-min(d.getQ()))/(max(d.getQ())-min(d.getQ()))
        Zd = (data[4]-min(d.getZDist()))/(max(d.getZDist())-min(d.getZDist()))
        Nd = (data[5]-min(d.getNDist()))/(max(d.getNDist())-min(d.getNDist()))

        # use normalised inputs as initial activations
        self.activations [0] = np.array([[Z], [N], [A], [Q], [Zd], [Nd]])

        # iterate through hidden layers using weights and biases (except for
        # last)
        for x in range (0, self.size - 1):
                a = self.activations [x]
                mult = np.array([np.matmul(self.weights[x], a)])
                mult = np.reshape(mult, (self.structure[x+1],1))
                presig = mult + self.biases [x]
                self.preactive.append(presig)
                self.activations [x+1] = sigmoid(mult + self.biases[x])

        #manually apply last layer weights and biases to avoid sigmoid

        af = np.array([])
        mult = np.array([np.matmul(self.weights[self.size - 2],
                self.activations [self.size - 2])])
        mult = np.reshape (mult, (self.structure[self.size - 1],1))
        af = mult + self.biases[self.size - 2]

        self.activations[-1] = [af] # was self.activations.append([af])
        self.preactive.append ([af])

        return af

    def backpropagation (self, activation, target):

        deltaBiases = [] # define arrays for change in biases
        deltaWeights = [] # define arrays for change in weights

        learningrate = self.learningrate

        # error in last layer
        error_l = activation - target # getting error
        error_l = np.reshape (error_l, (self.structure[-1], 1))
        # reshaping error to be array
        deltaBiases.insert (0, error_l) # error = delta biases
        deltaWeights.insert (0,
                np.matmul(error_l, self.activations[self.size-2].transpose()))
                # weight delta is error propagated backwards

        for x in range (0, self.size - 2):
                # propagate error backwards
                prop = np.matmul (self.weights[-(x+1)].transpose(), error_l)

                # hadamard product with preactivations
                error_l = np.multiply (prop,
                        sigmoid_prime (self.preactive[-(x+3)]))

                # reshape because numpy is peculiar
                error_l = np.reshape (error_l, (self.structure[-(x+2)] , 1))
                # error = delta bias so add to start
                deltaBiases.insert (0, error_l)
```

```
                        # add delta weights
                        deltaWeights.insert (0, np.matmul(error_l,
                                self.activations[((self.size-3)-x)].transpose()))


                for x in range (0,self.size-1):
                        # adjust each weight by delta weight
                        self.weights [x] = self.weights [x] -
                                (learningrate * deltaWeights[x])

                        # adjust each bias by delta bias
                        self.biases[x] = self.biases [x] -
                                (learningrate * deltaBiases[x])

        def train (self, dataset, targets, epochs):
                for x in range (epochs): # for the specified amount of epochs
                        #print (f"Epoch {x+1}")
                        # for each value in the dataset
                        for y in range (0, len(dataset)):
                                # feed it forward:
                                activation = self.feedforward (dataset[y])
                                # backpropagate against the target:
                                self.backpropagation (activation, targets[y])

        def evaluate (self, dataset, targets):
                predictions = [] # define array for predictions
                errors = [] # define array for errors
                for isotope in dataset:
                        prediction = self.feedforward (isotope)
                        # add predictions to array of predictions:
                        predictions.append(prediction)

                for x in range (len(predictions)):
                        error = predictions[x] - targets[x] # calculate errors
                        errors.append (error**2) # append error^2 to array

                # sigma = (1/n)*(sum of (errors)^2)^(1/2)
                stddev =  (np.sum(errors)**(1/2)) / len(dataset)
                return float(stddev)

        def save (self):
                joblib.dump(self.weights, "weights")
                joblib.dump(self.biases, "biases")
```

evaluate.py

```
import numpy as np
from network import Network
import data
from data import Data

d=Data()

def getSets ():
        global stddevModel

        isotopes = d.getIsotope()
        halflives = d.getHL()

        # number of training isotopes = len(dataset) * 0.8 rounded down
        numTrain = len(isotopes)*8//10
        numTest = len(isotopes)-numTrain # number of testing is what remains

        # all the possible indices I can use for isotopes
        totalNums = np.arange(len(isotopes))

        randomNums = np.random.choice (len(isotopes), numTrain, replace = False)
        # replace: whether or not a sample is returned to the sample pool
```

```
        # define testing indices to be whatever is left after getting rid of training
        testingNums = np.delete(totalNums, randomNums)

        trainSet = []
        trainLabels = []

        for x in range (numTrain):
                trainSet.append (isotopes[randomNums[x]])
                trainLabels.append (np.log10(halflives[randomNums[x]]))

        testSet = []
        testLabels = []

        for x in range (numTest):
                testSet.append (isotopes[testingNums[x]])
                testLabels.append (np.log10(halflives[testingNums[x]]))

        model = d.getModel()
        errors = []

        for x in range (numTest):
                actual = np.log10(halflives[testingNums[x]])
                models = np.log10(model[testingNums[x]])
                error = models - actual
                errors.append(error**2)

        stddevModel =  (np.sum(errors)**(1/2)) / (numTest)
        #print (f"Statistical Model Error: {stddevModel}")

        return trainSet, trainLabels, testSet, testLabels, stddevModel

trainSet, trainLabels, testSet, testLabels, stddevModel = getSets ()

net = Network ([6,16,20,20,16,1])

print ("Training...")
net.train(trainSet, trainLabels, epochs = 500) # train network
print ("Training Complete")

print ("Round 1")
stddevNetwork = net.evaluate(testSet, testLabels) # evaluate network on given test set
print (f"Network Deviation: {stddevNetwork}") # print net score
print (f"Stat Model Deviation: {stddevModel}") # print model score

if stddevNetwork < stddevModel: # if net is better than model
        print("Round 2") # round 2
        # fresh sets
        trainSet, trainLabels, testSet, testLabels, stddevModel = getSets ()

        # evaluate using already trained weights and biases
        stddevNetwork = net.evaluate(testSet, testLabels)

        print (f"Network Deviation: {stddevNetwork}") # print net score
        print (f"Stat Model Deviation: {stddevModel}") # print model score

        if stddevNetwork < stddevModel:
                print("Round 3")
                # repeat above
                trainSet, trainLabels, testSet, testLabels, stddevModel = getSets ()

                stddevNetwork = net.evaluate(testSet, testLabels)
                print (f"Network Deviation: {stddevNetwork}")
                print (f"Stat Model Deviation: {stddevModel}")

                if stddevNetwork < stddevModel: # if net IS better than model 3 times
                        print ("Saving")
                        net.save() # save weights and biases
```

```
''' CODE FOR COMPARING ERRORS
errors = []

epochs = 2000

print (f"Error Before Backpropagation: {net.feedforward (isotopes[i]) - np.log10
(d.getHL()[i])}")

for x in range (0, epochs):
        activation = net.feedforward (isotopes[i]) - np.log10 (d.getHL()[i])
        net.backpropagation (activation, np.log10 (d.getHL()[i]))
        error = activation - np.log10 (d.getHL()[i])
        errors.append(float(error))
        if x == (epochs-1):
                print (f"Final Error in BackProp: {error}")
                print (f"Log 10 of Predicted Half Life = {activation}")
                print (f"Log 10 of Actual Half Life = {np.log10 (d.getHL()[i])}")

print (f"Error After Backpropagation: {float(net.feedforward (isotopes[i])) -
float(np.log10 (d.getHL()[i]))}")
'''
```

Front-End

gui.py

```
from pathlib import Path
designPath = Path ("GUI Images/")
import predictor as ff
from tkinter import *
import numpy as np

class errorWindow(Toplevel):

    def __init__(self, master = None, message = "Error"):

        super().__init__(master = master)
        self.title("Error")
        self.geometry("300x50")
        label = Label(self, text = message)
        label.pack()

class ansWindow (Toplevel):

    def __init__ (self, master = None, answer = "Error"):
        super().__init__(master = master)
        self.title("Prediction")
        self.geometry("300x50")
        label = Label(self, text =
            f"Half-Life: {round(float(np.float_power(10, answer)), 5)}s \n
               Base 10 Logarithm: {round(float(answer), 5)}")
        label.pack()

def btn_clicked():
    data = []

    try:
        Z = int (entry0.get())
    except ValueError:
        # print ("Please enter an integer number of Protons")
        entry0.delete (0,END)
        errorWindow (window, "Please enter an integer number of Protons")
        return

    try:
        N = int (entry1.get())
    except ValueError:
        # print ("Please enter an integer number of Neutrons")
```

```
        entry1.delete(0,END)
        errorWindow (window, "Please enter an integer number of Neutrons")
        return

    try:
        Q = float (entry2.get())
    except ValueError:
        # print ("Please enter a number for Energy Release")
        entry2.delete(0,END)
        errorWindow (window, "Please enter a number for Energy Release")
        return

    A = Z+N
    Zdist = min ([abs(Z-2), abs(Z-8), abs(Z-20), abs(Z-28),
        abs(Z-50), abs(Z-82), abs(Z-126)])
    Ndist = min ([abs(N-2), abs(N-8), abs(N-20), abs(N-28),
        abs(N-50), abs(N-82), abs(N-84), abs(N-126)])
    data.append(Z)
    data.append(N)
    data.append(A)
    data.append(Q)
    data.append(Zdist)
    data.append(Ndist)

    loghalflife = ff.feedforward (data)
    # halflife = np.float_power (10, loghalflife)

    ansWindow (window, loghalflife)

window = Tk()
window.title("α-Predictor")
window.geometry("502x526")
window.configure(bg = "#ffffff")
canvas = Canvas(
    window,
    bg = "#ffffff",
    height = 526,
    width = 502,
    bd = 0,
    highlightthickness = 0,
    relief = "ridge")
canvas.place(x = 0, y = 0)

background_img = PhotoImage(file = designPath / "background.png")
background = canvas.create_image(
    251.0, 268.0,
    image=background_img)

entry0_img = PhotoImage(file = designPath / "img_textBox0.png")
entry0_bg = canvas.create_image(
    247.0, 153.5,
    image = entry0_img)

entry0 = Entry(
    bd = 0,
    bg = "#c4c4c4",
    highlightthickness = 0)

entry0.place(
    x = 94, y = 124,
    width = 306,
    height = 57)

entry1_img = PhotoImage(file = designPath / "img_textBox1.png")
entry1_bg = canvas.create_image(
    247.0, 263.5,
    image = entry1_img)
```

```
entry1 = Entry(
    bd = 0,
    bg = "#c4c4c4",
    highlightthickness = 0)

entry1.place(
    x = 94, y = 234,
    width = 306,
    height = 57)

entry2_img = PhotoImage(file = designPath / "img_textBox2.png")
entry2_bg = canvas.create_image(
    247.0, 375.5,
    image = entry2_img)

entry2 = Entry(
    bd = 0,
    bg = "#c4c4c4",
    highlightthickness = 0)

entry2.place(
    x = 94, y = 346,
    width = 306,
    height = 57)

img0 = PhotoImage(file = designPath / "img0.png")

b0 = Button(
    image = img0,
    borderwidth = 0,
    highlightthickness = 0,
    command = btn_clicked,
    relief = "flat")

b0.place(
    x = 199, y = 426,
    width = 106,
    height = 34)

window.resizable(False, False)
window.mainloop()
```

predictor.py

```
import numpy as np
import joblib

import os
import sys

data_dir = os.path.abspath (os.path.join("..","Network and Data"))
# find directory to current file
# go to parent directory ("..")
# from parent, add "Network and Data" to the path
sys.path.insert(1, data_dir) # add this path to system path

from data import Data
d = Data()

sigmoid = lambda x : 1.0/(1.0+np.exp(-x))

weights = joblib.load("weights")
biases = joblib.load ("biases")
activations = []

structure = [6,16,20,20,16,1]
size = len(structure)
for x in range (size):
```

```
    activations.append(np.zeros((structure[x],1)))

def feedforward (data):
    # min-max normalise all values
    Z = (data[0]-min(d.getZ()))/(max(d.getZ())-min(d.getZ()))
    N = (data[1]-min(d.getN()))/(max(d.getN())-min(d.getN()))
    A = (data[2]-min(d.getA()))/(max(d.getA())-min(d.getA()))
    Q = (data[3]-min(d.getQ()))/(max(d.getQ())-min(d.getQ()))
    Zd = (data[4]-min(d.getZDist()))/(max(d.getZDist())-min(d.getZDist()))
    Nd = (data[5]-min(d.getNDist()))/(max(d.getNDist())-min(d.getNDist()))

    activations [0] = np.array([[Z], [N], [A], [Q], [Zd], [Nd]])


    # iterate through hidden layers using weights and biases (except for last)
    for x in range (0, size - 1):
        a = activations [x]
        mult = np.array([np.matmul(weights[x], a)])
        mult = np.reshape(mult, (structure[x+1],1))
        presig = mult + biases [x]
        activations [x+1] = sigmoid(mult + biases[x])

    #manually apply last layer weights and biases to avoid sigmoid
    af = np.array([])
    mult = np.array([np.matmul(weights[size - 2], activations [size - 2])])
    mult = np.reshape (mult, (structure[size - 1],1))
    af = mult + biases[size - 2]
    activations.append ([af])
    return af
```

Joblib Dumps

Weights

```
8004 95b0 0000 0000 0000 005d 9428 8c13
6a6f 626c 6962 2e6e 756d 7079 5f70 6963
6b6c 6594 8c11 4e75 6d70 7941 7272 6179
5772 6170 7065 7294 9394 2981 947d 9428
8c08 7375 6263 6c61 7373 948c 056e 756d
7079 948c 076e 6461 7272 6179 9493 948c
0573 6861 7065 944b 104b 0686 948c 056f
7264 6572 948c 0143 948c 0564 7479 7065
9468 0768 0e93 948c 0266 3894 8988 8794
5294 284b 038c 013c 944e 4e4e 4aff ffff
ff4a ffff ffff 4b00 7494 628c 0a61 6c6c
6f77 5f6d 6d61 7094 8875 62e3 977a e6ed
86d1 bf37 2713 b885 30d0 bf45 4967 d524
81f2 bf6d d6a1 2b06 70ee 3fa3 d6fb d33f
9cbe 3fd4 362a d7ec 6ef2 bfb6 ee9b 39bc
9bee bf7f 66ac 51c7 9be4 3f88 3632 5faa
d2de bffc 47bb dc0e 44e3 bfb2 1828 5cf2
00dc bf22 b531 4f17 dee5 bf19 fb71 cb14
0cfa 3f48 50d4 1daa 52d2 3f1e 85ba e970
```

61e0 3fef d49d 1d6b 1c02 c03a d157 1cfd

02ab bf85 12fc 0288 c2f5 3fe0 ea59 89c5

24f0 bfbe e0b8 f9ee 8bd3 bf04 31b1 4e34

7ae4 bf21 9ed3 884b af01 40e8 8e88 a8bc

bbd1 bf82 952d 0328 01b1 bf14 a58f a1d4

77e7 bf51 eb45 1e49 40e6 bfee 1240 ba24

0ccd 3f94 3e0e 5c94 e4ec 3f58 bbf7 91e8

cfe7 bf56 d680 1ae3 0fd5 3f06 5ac7 aa25

f8e3 3f3b 6204 e25f 27e7 3f9b b270 80a5

95e5 3fd2 155e f9ec b4e5 3f71 7432 fca6

27f4 3fb3 7394 8b05 d3f4 bfa2 648c 1321

83fb bfd0 82d8 6db9 b1fb bfed 8548 5a71

44ec bf01 5842 5aaf ec15 405e 0992 92cd

afe6 bf23 59a9 f42c f2e8 3f7c a584 1321

2dc7 bf03 1642 089b ced5 3f3e 1876 3eb7

10c4 3f04 c485 277b d9fb bf45 eba9 813e

c8c9 3f0c 2b45 16ff efe5 3fba 4f66 724f

55e6 3fb9 9fc2 7611 4de7 3f64 b77d 5b1e

55ca 3fb2 f60f c9aa edde bfa3 aa8b 58d8

56d6 bf35 4d61 61b9 64db bffb 680e f7eb

edfd bf06 2a29 4542 1bc7 bf79 d63e b944

3cf4 bf2e 620c 46bc 1309 402b 3fd5 e2fc

18c8 bfda 1f09 65aa d8f5 bfc2 ad0d f03b

fbe0 bf3c 2e99 54e7 5ed8 bff9 847a 740f

aef0 bf58 db18 1cf2 c4e5 bf30 d4f9 2f1b

70f4 bfae 2540 65ad 0ed8 3f61 f69e 271e

6de9 3feb 98e4 af19 77e9 bfb0 7caf 2582

ccef 3ff7 e371 400d 4a00 c082 5bad 6d11

b0e9 3f7f 13a6 4e7a ade9 bfea ad26 abce

c1e7 bf2e b583 3a6c 01c1 bfbd b974 a80d

7bde 3fdf 014b f517 acfb bf66 c574 2912

bbce bf0c f80e 11a5 14ec bf8c 4f6c 83f7

33f6 bfb4 1a53 1e0a b0c9 bf19 ef04 98cd

8af7 bfbc 8507 a551 c4fc 3f62 0dc2 0797

119f 3fbb b300 fff9 e3f1 bff6 9705 be69

63bf bfe4 0573 16e7 d9e5 3f37 c3c3 e0b5

3de2 bfc3 baa9 e405 710d c0f2 3365 aeaf

7ae4 bf80 3c0c 54f3 61de 3f70 1b19 c726

f7e4 bfa9 131e 2f92 47e7 bf04 5bff 4815

d1e6 bf8b 7c95 935b 8dfc 3fad 576a 19c2

37c9 3faa 2e78 319a 31de 3f95 2100 0000

0000 0000 6803 2981 947d 9428 6806 6809

680a 4b14 4b10 8694 680c 680d 680e 6812

6815 8875 62a9 b721 bf9b b8a9 3fe8 1743

d4b0 2cbc 3f5b fea2 cdc1 81f0 bf77 9141

7d9c dad7 bf03 f2a1 1c13 00e5 3f30 dc36

12ef 29e0 bff9 d522 29b6 d1e0 3f16 861e

5dbc 5aea 3fc6 64ff efb6 87e1 3fea 8941

b1b6 61c5 3faa 8d60 2cd3 6ef2 bf5f 0040

26aa 75ed bf17 1002 ff92 03df 3fe4 cb99

1cc1 d285 3f3f 5fea f0e9 8bdc bfc0 460e

c2f9 afb5 bfa1 3dfe 4c98 51c9 3f4b 6297

8e1f 5ae5 3f2f 5e19 0da5 e0bf bf09 9abb

f400 b9dc 3f33 f531 38ab a2df 3f05 b1e3

739e 1ae0 bf67 6976 9f83 37df 3f84 b9e6

9293 51be bf9c 6417 cf5d af98 3f32 d9bd

d264 dbf1 3f9c ed41 8b8d a2ea 3fdd 3319

3ad9 45f0 bfdb 4b16 5bcd ce74 bf7d 8782

a768 72c5 bf7d 34dd 7fba bde5 3f31 1192

7bf7 aee9 bff5 b90b 3708 c7d4 bfc9 6d0f

684b 53dc bfdb 542b 1511 b3a1 3fb2 4d69

4a66 e2e9 3f19 b3cc a4e5 82e1 3f33 4369

0603 f7c3 3fe8 13f8 eee0 bbee bfd7 5334

8e16 a0d8 bf90 5546 6629 a0ad bfd8 5692

1ab5 cdf0 bf08 b411 828c 22ef bfe4 3f89

ca68 1acd 3f66 ca1e 30ca f7dc 3fe5 e9e6

8295 c7ef bf8b 398d 15d1 09e4 3f0c e6b3

4379 5bde 3f8f 1e43 6c41 88e3 3fa7 7b41

724a 0be9 3f15 22e9 0649 8fd8 bf4c 0943

41f3 c9bb bfbd 2c50 a793 9ea2 3feb 914c

fa66 0bd8 3fbf 7825 ece5 77b9 bfce 6e26

0513 87c7 bfd4 3bfb 0531 d2e8 3fab 93d0

a7d2 d4ea 3f4a d97d ae2e 0eef bfc3 4eee

3169 47e1 3ff7 b4af 90df ccb8 bfaf 9c66

c9a4 07b7 3fcb 4ffe b6b4 83ea 3fe7 7a02

1243 2fd4 3fee 4343 6695 dde3 bfb5 cbee

d521 9bbb bf83 7c01 dd87 41e0 3f13 3230

e6cb bf77 3fba c922 8f99 c1dc 3fc8 b32a

6466 49ea bf40 d4b2 817d e2f3 bf87 bc69

e343 4de7 3f66 5110 326c 7bd8 bf28 0204

419f 9fa6 bf0d 7435 0a1e 4bd6 3f8d 9529

f678 0ea2 bfaf 4f35 e6a2 ad6a bfad 0aa1

9115 cdc3 3f50 66ab fa59 82e9 3fef 57e1

67c2 f6ef bf14 6c3c 5de5 b6e6 3fa2 f099

5fd1 5ce4 bfac 95dd a3a2 f3bb bfcb dbb8

4118 b1f3 3fce eef3 38d3 27e2 3f03 4a63

3a00 81e9 bf86 b1a9 cc53 50fa 3ffa 1574

2a2d 64d2 3fd9 4d62 1503 98b3 3fb1 0d4b

8af3 53e0 3fdb 8942 abf5 3bea 3fe5 09b5

4d61 aee0 bf21 a5d2 1a29 21e4 3f89 23c5

6fe1 a1ee 3f8b 7d6e c317 0cf0 bfe8 6004

097b 15d7 3fb6 8166 ef8b 52e7 3f55 42e0

afc8 8fe5 3f1b 1873 5559 3ac2 bff4 01d9

d605 d8e6 3ff0 4d78 794e bee7 bf8f 8ea8

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Biases


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