Fusion Neutron **Acti**vation Spectra **U**nfolding by **N**eural **N**etworks (FACTIUNN)

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Abstract

A neural network approach to neutron spectrum unfolding was attempted and explained in this thesis. The optimal hyperparemters for such a neural network were found in a grid search.

A value of 5.0178 was obtained when evaluating the mean of the mean-squared deviation of the best-performing neural network's predictions from the true neutron flux in log space(mean MSE in log space). This is too high for practical fusion neutron unfolding, and is a significant improvement from the unfolding results obtained from GRAVEL, where the mean MSE in log space was 10.188 when given only a naive prior (flat *a priori* spectrum). When the neural network's output was used as the *a priori* for GRAVEL instead, it only led to an insignificant improvement in mean MSE down to 9.8994.

Attempts to generalize the knowledge learnt across different type of spectra proved to be a failure, as the neural networks trained on fission data gave nonsensical predictions when faced with reaction rates associated with fusion neutrons, with the best neural network among all giving a mean MSE of 16.768.

The generally poor performance of the neural network is attributed to the small amount of data available. Some improvements upon this experiment are proposed, but their effectiveness will be limited if the fusion neutron spectra size remains small.

Keywords: activation, neutronics, fusion

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1 Introduction

In a fusion reactor, the neutron fluence can go up to as high as $1.7 \times 10^{21} cm^{-2}$[18]. This leads to an unprecedented need of shielding against neutrons of up to 14.1 MeV or higher energies.

Neutrons are notoriously difficult to shield against due to their uncharged nature, and therefore low propensity to interact with matter[21]. To develop effective shielding for various components of the reactor from these high energy neutrons, the energy spectrum of the neutrons created inside the nuclear reactor has to be well understood [8].

It is also important to understand the neutron spectrum inside the reactor in order to develop Tritium breeding modules; a Tritium Breeding Ratio TBR>1 is essential for making fusion a sustainable source of clean energy [20]. Last but not least, the power output of future fusion power plants can only be quantified when the neutron spectrum is characterised [47]. Accurate measurement of the neutron spectrum is required to properly model the energy distribution of neutrons to be used in neutron transport simulations for the above purposes.

All of the above activities relies on having accurate knowledge of the neutron spectrum. Therefore neutron spectroscopy is a key focus in the diagnostic systems in all fusion reactors.

Incidentally, for the same reason that they are difficult to shield against, neutron energy is also difficult to measure. Neutrons, especially high energy neutrons such as the 14.1 MeV neutrons created in fusion reactors, do not easily deposit their full energy into a sufficiently small detection volume to allow direct measurement[21]. Various neutron detectors have been developed to deal with this problem;however, most of them cannot stand this high neutron fluence at the first wall of fusion reactors without additional shielding that changes the flux profile [41]. The extreme temperature and magnetic fields inside the nuclear fusion reactor compound the difficulty of employing other means of neutron measurement as most electronics will not be able to function in such environments effectively. [30]

This is where the technique of activation foil unfolding stands out: By analyzing the level of activations in various elements induced by neutrons, relying on the variation of reaction cross-sections across different elements and energies, one can infer the neutron spectra that was previously present at the first wall.

This is a very robust method as it does not require any active components, thus can be employed for very high neutron fluxes [10], as the total number of neutron activation reactions can be controlled by changing the volume of the activation foils used [12] according to the anticipated neutron fluence in the next irradiation period, so not to paralyze the γ radiation detector. It is also insensitive to γ rays, thus removing most of the challenges facing mixed-field spectrometry. [5]

The disadvantage of this method is that it has to be time-integrated over the whole irradiation period, thus no information about the temporal variation in the neutron spectrum can be extracted from its measurements.

Another disadvantage of using neutron activation as the means of measuring the neutron spectrum in a fusion reactor is that it is an indirect method of measurement, requiring the measured reaction rates to be 'unfolded' back into reaction rates. This is a 'mathematically incorrectly posed ' problem[22], as will be further explained in the next section (2.3), requiring an initial guess spectrum to be provided before the unfolding procedure can take place. This is because the number of reaction channels recorded (usually denoted as M) is fewer than the number of neutron groups (usually denoted as N) whose neutron flux we would like to know, i.e. M<N, thus this problem is underdetermined (the number of constraints is fewer than the number of variables). The *a priori* has to be used to introduce extra information into the problem. However, if this *a priori* spectrum deviates too much from the actual spectrum, then the result of the unfolding will be inaccurate.

To address this problem, an investigation into using neural networks to unfold fusion neutron spectra is presented in this thesis. Neural networks excels in incorporating previous spectra as *a priori* information, without requiring users to explicitly input an *a priori*. Two approaches are proposed. The first one is to use neural networks directly as an unfolding tool; and the second one is to use them as an *a priori* generator, which is then fed into an existing unfolding computer code, from which a solution neutrons spectrum is unfolded out of.

2 Theory

When a nuclide is placed in the activation module at the irradiation position inside a nuclear fusion reactor (or any other neutron sources), it is activated via one or more nuclear reactions with the incoming neutrons. The probability of interacting with the incoming neutron via reaction j is proportional to the microscopic cross-section $\sigma_j(E)$, where E is the neutron's energy, and reaction j is a neutron-induced reaction, i.e. (n,*any*) reaction.

By measuring the activity of reaction j's daughter nuclide in the activation foil (which has a known amount of the initial nuclide) after irradiation, and multiplying it by a correction factor of

$$\frac{1}{1 - exp(\lambda_j T)} \tag{1}$$

the reaction rate Z_{0j} can be obtained. This correction factor accounts for the decay of the daughter nuclide of reaction j which has a half-life of λ_j, over the period T which is the duration between irradiation and measurement. A more complicated correction factor is required if the irradiation period is comparable to the half-life λ_j, or if the population of the parent nuclides for reaction j changes over the course of the irradiation period. This can be done using FISPACT-II, detailed in [38].

The total reaction rate of the j^{th} reaction can then be expressed as a Fredholm integral as follows:

$$Z_{0j} = \int_0^\infty R_j(E)\phi_0(E)dE \tag{2}$$

where the reaction rate Z_{0j} has the unit of s^{-1}, ϕ_0 is the neutron flux (unit: $cm^{-2}s^{-1}eV^{-1}$), which is a function of energy E. The unfolding process aims to find a solution spectrum ϕ which approximates the actual spectrum ϕ_0 as closely as possible.

As for R in the equation above, (which has dimension of area)

$$R_j(E) = \sigma_j(E)\frac{N_A}{A}F_j\rho V \tag{3}$$

assuming that there is no self-shielding/down-scattering inside the foil. N_A is the Advogadro's constant (unit: mol^{-1}), A is the molar mass of the parent nuclide for reaction j (unit: g mol^{-1}), F_j is reaction j's parent isotope's mass fraction in the foil's constituent material (unit: dimensionless), ρ is the density of the alloy (unit: g $barn^{-1}$ cm^{-1}), V is the volume of the foil (unit: cm^3) Note that $\sigma(E)$ (unit: $barn$)is the only energy dependent component in R.

The neutron spectrum can be discretised into N energy bins:

$$Z_{0j} = \sum_{i=1}^{N} R_{ji}\phi_{0i} \tag{4}$$

where ϕ_{0i} is the scalar flux integrated over the energy bin's range

$$\phi_{0i} = \int_{E_{i-1}}^{E_i} \phi_0 d(E) \tag{5}$$

, thus having a unit of $cm^{-2}s^{-1}$.

By assuming that the scalar flux distribution inside each energy bin is relatively flat, equation 4 calculates Z_{0j} by replacing $(R_j(E), E_{i-1} \leq E \leq E_i)$ with

$$R_{ji} = R_j(E_{i-1}) \tag{6}$$

Let there be M neutron-induced reactions whose reaction rate was measured,

$$\begin{aligned} \forall j \in &\{1, ..., M\}, \\ \exists Z_{0j} \in &\mathbb{R}_{\geq 0} \end{aligned} \tag{7}$$

Collecting all reaction rates into a vector $\boldsymbol{Z_0}$ of M-dimensions, one can express eq. 4 as a matrix multiplication equation:

$$\boldsymbol{Z_0} = \underline{\underline{\mathbf{R}}}\boldsymbol{\phi_0} \tag{8}$$

where $\underline{\underline{\mathbf{R}}}$ is a $M \times N$ matrix, termed the *response matrix.* $\boldsymbol{\phi_0}$ is an N-dimensional vector containing the neutron flux in the each of the N bins. The subscripts 0's denote that they are the measured/known quantity, as opposed to the conjectured solutions which will appear later in this text.

For nuclear fusion applications, the number of possible reaction investigated M is very limited [24], as the parent nuclide of each of these reactions must exist in solids which:

- can be manufactured into specified shape and thickness, with well-measured number density and impurity contents,
- are safe to be handled,
- has a threshold energy in the region of interest (in the MeV range),
- has well-characterised cross-section values in nuclear data libraries (see [11])
- has stable parent isotope and daughter isotopes of medium length half-lives such that it can be activated and measured.

in practice, very few types of metals/alloys can be used in these systems. For the ACT project in JET in particular, in recent experiments, only 7 types of foil materials and 11 reactions were examined. [38]

Meanwhile, the number of bins, N, can be arbitrarily high. For some investigations, such as the one in [36] it goes up to 709 bins. This makes the unfolding problem a strongly underdetermined one.

In the mathematical sense of the problem, an inverse does not exist. This is because, theoretically, multiple neutron spectra, say $\boldsymbol{\phi_0}$, $\boldsymbol{\phi_1}$ and $\boldsymbol{\phi_2}$, can give the same set of reaction rates $\boldsymbol{Z_0}$, so there is no correct, unique choice of mapping of $\boldsymbol{Z_0}$ back to $\boldsymbol{\phi_0}$, $\boldsymbol{\phi_1}$ and $\boldsymbol{\phi_2}$.

Such an inverse problem is termed 'mathematically incorrectly posed'. [22]

2.1 General unfolding methods

The most straight-forward way of getting back a solution ϕ is by using the Moore-Penrose inverse matrix. This matrix inversion operation generalizes the usual matrix inversion operation for square matrices, where the $M \times N$ response matrix $\underline{\underline{\mathbf{R}}}$ in equation 8 is inverted into an $N \times M$ matrix $\underline{\underline{\mathbf{R}}}^{\mathbf{-1}}$, so that ϕ can be obtained by $\boldsymbol{\phi} = \underline{\underline{\mathbf{R}}}^{\mathbf{-1}}\boldsymbol{Z_0}$. However, this method is the equivalent of rotating a 2-D photo of a 3-D object from a horizontal position to an upright/tilted position: the solution is still "trapped" in a flat, M-dimensional manifold within the N-dimensional solution space.

Therefore to start the unfolding process, extra information has to be given to the program. This is termed the *a priori* spectrum.

The most general unfolding program can, ideally, find a solution $\boldsymbol{Z}$, $\underline{\underline{\mathbf{R}}}$ and $\boldsymbol{\phi}$ [27], such that their overall deviation from the measured reaction rates ($\boldsymbol{Z_0}$), expected response matrix ($\underline{\underline{\mathbf{R_0}}}$), and the initial guessed neutron spectrum ($\boldsymbol{\phi_0}$), is minimised. The deviation of the solution reaction rates from the measured reaction rate is calculated from its covariance matrix $\underline{\underline{\mathbf{S_Z}}}$, as the $(\chi^2)_Z = Z^T \underline{\underline{\mathbf{S_Z}}}^{-1} Z$. Equivalently the deviation of $\boldsymbol{\phi}$ from $\boldsymbol{\phi_0}$ and $\underline{\underline{\mathbf{R}}}$ from $\underline{\underline{\mathbf{R_0}}}$ can be calculated from their respective covariance matrix..

2.2 Current practice

In practice, there is always uncertainty associated with the cross-section values provided by the nuclear data libraries [28]. This is known as the "ambiguity" of the response matrix. To reduce the complexity of the problem, however, the ambiguity in the response matrix is nearly always ignored, by assuming that the response matrix $\underline{\underline{\mathbf{R_0}}}$ is accurately and precisely defined, fixing the response matrix during the solution search. This reduces the number of dimensions in the solution search by $M \times N$, massively reducing the computational complexity. It also assumes that the covariance matrix of the reaction rates is diagonal, i.e. there are no covariance across different reaction rates.

Some programs, such as GRAVEL[26] and SAND-II[29], simply start their iterative solution search from this *a priori* spectrum, with the aim of minimising the χ^2 (which measures the deviation of $\boldsymbol{Z}$ from $\boldsymbol{Z_0}$); while others, such as MAXED [40] add the deviation of the solution spectrum from the *a priori* spectrum ($\boldsymbol{\phi}$ from $\boldsymbol{\phi_0}$) on top of the deviation of the solution reaction rates from the measured reaction rates ($\boldsymbol{Z}$ from $\boldsymbol{Z_0}$) when evaluating the χ^2.

Current fusion neutron measurements rely on MCNP simulations heavily to supplement their unfolding procedure. They use MCNP model of the reactor to calculate a neutron spectrum, which is used as the *a priori* [25] [23]; and the response matrix is usually obtained in the same way as well [12].

2.3 Neural Networks

Neural networks, on the other hand, learn the relationship between reaction rates and the original neutron spectrum. Ideally, it will make use of information in previous neutron spectra, effectively bypassing the problem of underdetermination.

A typical neural network learns the relationship between the inputs (the two nodes in the leftmost layer in Figure 1) and outputs (the node in the rightmost layer in Figure 1) of a function via training, thus becoming an approximator for that function.

2.3.1 Forward Propagation

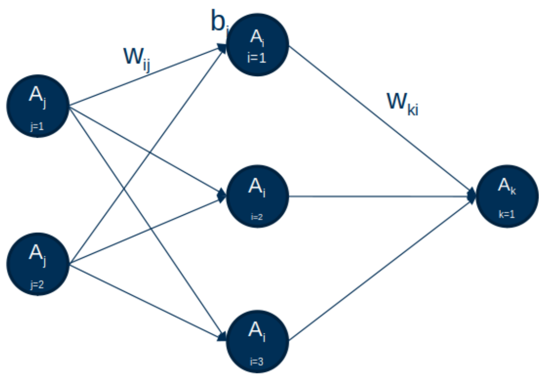


Figure 1: Illustration of the topology of a typical neural network

The inputs to the neural network are known as "features" and the outputs are known as the "labels".

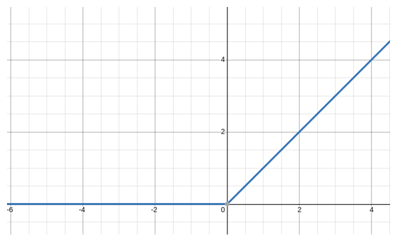


Figure 2: A ReLU function (a rectifying function)
Abscissa=function's input; ordinate=function's output.

In the context of neutron spectrum unfolding using neural networks, there are M features (reaction rates Z_j for $1 \leq j \leq M$) and N labels (neutron flux in each bin ϕ_j for $1 \leq j \leq N$).

The "activation" A_i of the i^{th} node refers to the value that it takes. w_{ij} denotes the "weight" of each connection from the j^{th} node to the i^{th}.

When the activations in the input layer (A_j) are known, the activation in the next layer (in this case, the first hidden layer) is calculated as follows:

$$A_i = \sigma_i \left(\sum_j (w_{ij} A_j) + b_i \right) \tag{9}$$

b_i denotes a "bias" value which will be added onto the sums in front of each node before it is parsed through the activation function σ_i. The activation function is usually denoted as σ_i, i.e. it is possible to use different activation functions for different nodes i; however, the common practice is to use the same type of activation function across the whole layer, or even across all nodes and all layers of the neural network. The typical function chosen is the ReLU function (Figure 2), i.e. for all layers, and for all values of i, as it is one of the simplest non-linear function whose gradient can be computed quickly.

$$\sigma_i(x) = ReLU(x) = \frac{|x| + x}{2} \tag{10}$$

Equation 9 is applied recursively to calculate the activations in the immediate next layer. For example, to calculate the activations in the second layer (i.e. the output layer) in Figure 1 simply by swapping the indices in for the indices of the next layer: $i \mapsto h$, $j \mapsto i$. This process is known as forward propagation.

2.3.2 Backpropagation

The weights w and biases b are known as the parameters of the neural network. This is in contrast with the term "hyperparameters", which are the numbers that describe the topology of the neural network, i.e. the number of layers, number of nodes in each layer, learning rate (see section 2.3.4 below), etc. During the training phase of the neural network, these parameters are adjusted so that the neural network's predicted output values align with the true output values more closely. This deviation of the predicted label from the true label is termed the "loss value", and can be calculated in a variety of manner (see Section 11 for the loss value metrics considered in this investigation). For the moment let's assume it is calculated as the mean-squared value, i.e. same as the χ^2 value familiar to physicists.

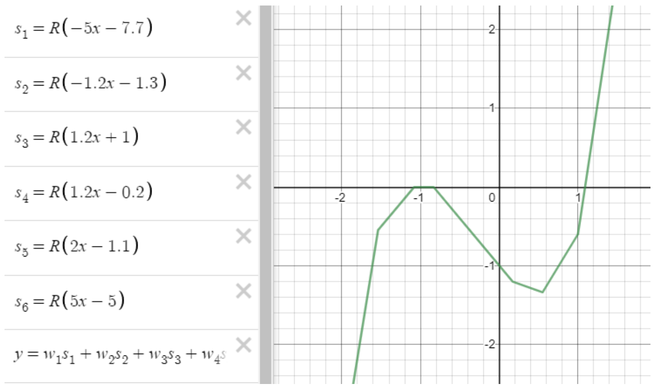
The process of adjusting parameters to reduce the loss value is known as backpropagation, as the 'desired' change to each weight and bias (calculated from the gradient of the loss value with respect to w or b, i.e. $\frac{\partial(loss)}{\partial w}$ or $\frac{\partial(loss)}{\partial b}$) is obtained by tracing the change in the output layer back to the weight and biases of each layer.

For the neural network to converge on a stable set of parameters (i.e. a minimum value of the loss value in the parameter space), features are usually normalized before they are given to the neural network. This reduces the difference in variance across each feature, allowing the neural network to take a more direct path when gradient-descending to the set of parameters that achieves minimum loss value, instead of an oscillatory approach to the minimum loss value[33], thus reducing the number of steps required to train the neural network.

2.3.3 Universal approximation theorem

Before diving into the details of neural network training, it is beneficial to see how a neural network can approximate any function.

The key to its ability to approximate functions lies in the non-linear activation function.



$s_1 = R(-5x - 7.7)$

$s_2 = R(-1.2x - 1.3)$

$s_3 = R(1.2x + 1)$

$s_4 = R(1.2x - 0.2)$

$s_5 = R(2x - 1.1)$

$s_6 = R(5x - 5)$

$y = w_1 s_1 + w_2 s_2 + w_3 s_3 + w_4 s$

Figure 3: A cubic function approximated by a neural network

This neural network has 1 hidden layer containing 6 neurons. Here, R is the alias for the ReLU function (see Figure 2), abscissa is the input layer neuron's activation value (feature); and the ordinate is the output layer neuron's activation value (label), obtained by summing over the product of the activation of the i^{th} neuron (aliased as s_i) with the weight of its connection to the final layer (aliased as w_i). The weights and bias to the first layer are already defined on-screen inside the brackets of the first six lines; while the weights and bias to the second layer (output layer) are defined off-screen.

Figure 3 is a crude representation of how a 1-hidden-layer neural network can approximate a cubic function. A single hidden layer neural network with one scalar input and one scalar output can approximate any non-linear functions, provided that there are enough neurons in the hidden layer.

The weights w_i scales each ReLU function; whereas the bias to the first layer (defined as the second term inside each of the bracket in the first six lines) changes the horizontal offset of each ReLU function. The bias to the second layer controls the vertical offset of the whole function. Summing them up leads to the output in Figure 3.

Even with only six hidden neurons (only 19 parameters: 6 weights and 6 biases for connecting the input layer to the 1^{st} hidden layer; 6 more weights and 1 bias for connecting the hidden layer to the output layer), it is able to reasonably approximate a cubic function within the visualized range of the domain. It is apparent that the accuracy of this approximation to the cubic function can be improved by increasing the number of neurons available in the neural network, provided that there are enough training data to cover the domain densely.

A function with vectorial inputs is then capable of

Armed with this intuition, the notion of a neural network being able to approximate any function becomes conceivable, even if the function has vectorial inputs and outputs.

2.3.4 Training the neural network

Before adjusting the parameters, a fraction of the data is drawn out and reserved for testing. The remaining is used as the training dataset. These "training" and "testing" data are chosen in such a way that they cover the same range of domain and co-domain in the feature- and label-space respectively.

The parameters are adjusted in iteratively to minimise the loss value. Each step requires a calculation of the gradient value over the entire dataset, known as an "epoch", obtained by calculating the average $\frac{\partial(loss)}{\partial w}$ or $\frac{\partial(loss)}{\partial b}$ over the entire training dataset. The parameter are adjusted according to an algorithm known as the "optimizer"; this algorithm may require some more hyperparameters, such as the "momentum", "acceleration" term to be defined. When further training no longer improves the loss value over the training set (i.e. the "training loss"), training can be stopped, and the parameters are then fixed at their final values. The size of each step is calculated as (learning rate)×(gradient of the loss value in parameter space)

The performance of the neural network is then evaluated over the testing set to obtain an average loss value, known as the "testing loss". If the testing loss is much higher than the training loss, it signifies that the neural network was "overfitting", i.e. it reached a minimum training loss by "memorizing" the relationship between training features and training labels, and is unable to generalize these relationships to the testing set. This may suggest that the neural network is too complex, i.e. has too many nodes or neurons.

Apart from reducing the complexity of the model, various techniques exist to reduces overfitting, including weight-regularisation and dropout [2]. Weight regularisation ensures that the numerical values of weights w remains small; while dropout effectively removes a specified fraction of the connections at each layer. However, these techniques are not applied.

But one of the most powerful and widely applied method of reducing overfitting is by measuring the validation loss. A small subset of the training data is reserved and not used for backpropagation during the training, but its loss value (known as the "validation loss") is calculated at each epoch also. This amounts to calculating the loss value of the neural network's prediction on a set of data that it has never seen before as well. When the validation error stops decreasing, then one can be sure that the neural network has stopped identifying general patterns which applies across both the validation set and the training set, and begin memorisation. The training can be stopped at this point.

This method is called "Early Stopping"; it catches the neural network before it begins overfitting aggressively.

2.3.5 Applying neural network to the unfolding problem

To apply neural networks as unfolding tools, we will want neutron spectra as the output and reaction rates as the input, i.e. M features (reaction rates Z_j for $1 \leq j \leq M$) and N labels (neutron flux in each bin ϕ_j for $1 \leq j \leq N$).

By using a neural network to do the unfolding, we are assuming that the inverse equation (below) exists,

$$\boldsymbol{Z} = \underline{\underline{\mathbf{R}}}^{-1}\boldsymbol{\phi} \tag{11}$$

i.e. all reaction rates can be unfolding back to one and only one unique solution spectrum. Ideally, the set of all possible solution for the neutron spectrum $\boldsymbol{\phi}$ can be expressed as a linear sum of M or fewer basis vectors due to the constraints of various physical processes. The role of the neural network is to identify these M- bases vectors and relate them to the M reaction rates.

Several metrics were considered for the neural networks. Since the neural networks' goal is to predict a set of labels (solution spectrum) ϕ_{pred} that is identical to the true spectrum ϕ_0 when given the set of features Z_0 corresponding to the set of labels ϕ_0, the loss function must have a minimum at $\phi_{pred} = \phi 0$.

This loss value is also expected to scale its penalisation according to the true flux ϕ_0. Large deviation when ϕ_0 is large should be penalized by the same amount as with small deviations when ϕ_0 is small. For example, over-predicting the to flux at the 14.1 MeV peak by, say, 10%, in a DD-operation, should be given the same penalty as over-predicting the 14.1 MeV peak flux in a DT-operation by 10%, despite the fact that $\phi_0(E = 14.1 MeV)$ is much smaller for the same TOKAMAK in a DD campaign than in a DT campaign.

Several of such functions come to mind; they include:

- cross entropy, $H(\phi_{pred}, \phi_0) = \sum_i^N \Bigg(\phi_{pred}(E_i)(ln(\phi_{pred}(E_i)) - ln(\phi_0(E_i)))\Bigg)$ (See [43])
- Average distance in L^P log-space $= \Bigg(\sum_i^N (log(\phi_{pred}) - log(\phi_0))^p\Bigg)^{\frac{1}{p}}$ which is a generalisation of mean squared error and mean absolute error.
- mean fractional deviation, $MFD(\phi_{pred}, \phi_0) = \sum_i^N \left|\frac{\phi_{pred}(E_i) - \phi_0(E_i)}{\phi_0(E_i)}\right|$
- mean pairwise squared error:
  $MPSE(\boldsymbol{\phi_{pred}}, \boldsymbol{\phi_0}) = \frac{1}{L}\sum_k^L \sum_i^N \sum_q^N \Bigg((\phi_{pred,k}(E_i)) - \phi_{pred,k}(E_q) - (\phi_{0,k}(E_i)) - \phi_{0,k}(E_q)\Bigg)$

In the end, only the following function was chosen as they were the default functions available from TensorFlow; using these functions minimises the room for human error and development time.

Let there be L features-labels pairs in the dataset. The loss function is defined as:

- mean squared error:

$$MSE(\boldsymbol{\phi_{pred}}, \boldsymbol{\phi_0}) = \frac{1}{L}\sum_k^L \sum_i^N \Bigg(log_{10}\big(\phi_{pred,k}(E_i)\big) - log_{10}\big(\phi_{0,k}(E_i)\big)\Bigg) \tag{12}$$

The neural networks in this investigation differ from the typical neural network, in that the latter has fewer labels than features output ($N \leq M$); and that, since the features are related to the labels via a physical process, the inverse function for turning labels back into features exist (equation 8), and is assumed to be deterministic.

This allows for additional information to be supplied to the neural network during the training stage:

- mean squared error including folded reaction rates:

$$MSE_{\text{including\_folded\_reaction\_rates}} = MSE(\boldsymbol{\phi'_{pred}}, \boldsymbol{\phi'_0}) \tag{13}$$

Where $\boldsymbol{\phi'}$ is the $\boldsymbol{\phi}$ and $\boldsymbol{Z}$ vector concatenated together,

$$\boldsymbol{\phi'} = [\phi_1, ..., \phi_N, Z_1, ..., Z_M] \tag{14}$$

and Z is, in turn, obtained by equation 8:

$$\boldsymbol{Z_{pred}} = \underline{\underline{\mathbf{R}}}\boldsymbol{\phi_{pred}} \tag{15}$$

$$\boldsymbol{Z_0} = \underline{\underline{\mathbf{R}}}\boldsymbol{\phi_0} \tag{16}$$

This is analogous to the technique of regularisation[13] in normal unfolding procedures, where both deviation from the *a priori* spectrum and the reaction rates are calculated and used as the χ^2 value. In this case, the regularisation constant (weight of the neutron flux's deviation relative to the reaction rates' deviation) is simply chosen as 1.

These two metrics will give loss value = 0 when ϕ_{pred} and ϕ_0 matches perfectly; but the neural network will be penalized by an additional amount if it makes a mistakes in the spectrum that leads to a greater deviation of the Z_{pred} from the Z_0 (which is a mistake that other linear/non-linear least-square minimisation unfolding codes such as MAXED and GRAVEL will not make). This is done in the hopes of providing the neural network some information about the physics of the activaiton foil system, thus improving its accuracy.

3 Literature review

There are no previous attempts of unfolding fusion neutron spectra using neural networks.

Some work has been carried out in the field of neutron spectrum unfolding using neural networks, none of which pertains specifically to neutron spectra of fusion neutrons. Only one of them is directly related to the method of activation foil neutron spectrum unfolding [19], which has a more pathological response matrix than the other two methods typically discussed in unfolding (Bonner Spheres and liquid scintillators). The condition number of the response matrix (i.e. the ratio of the maximum to minimum singular value[31]) is likely worse due to the similarities between reaction cross-sections as dictated by nuclear physics; unlike in the other two detectors, where the response matrix is almost guaranteed to be lower-triangular matrix, where the response of each Bonner sphere/ scintillation pulse height is guaranteed to be linearly independent with respect to each other, so that the condition number is to be small, i.e. they are less ill-conditioned than the problem of activation foil neutron spectrum unfolding. Therefore unfolding these two types of spectra are not as difficult as unfolding neutron spectra from activation foil.

Bonner spheres and liquid scintillator neutron measurement and unfolding cannot be employed to measure the neutron spectra in nuclear fusion reactors, despite its common application in medical physics and fission reactors. This is because very high neutron and γ fluences are present in the former environments, compared to fluences typically present in the latter environments. Due to their low radiation tolerances relative to the method of activation foil, these two method cannot be employed to measure the neutron spectra at the first wall.

However, this does not mean the work of neural network unfolding of neutron spectra from Bonner Spheres measurements [35] [34] [15] [9] and liquid scintillator measurements [17] are not useful for fusion neutron spectrum unfolding. They provide reference points for neural network topologies which are generally useful in neutron spectrum unfolding (Table 1).

They also offer some insight as to how to overcome data the challenge of data scarcity. Namely, with Radial Basis Function Neural Networks (RBFNN) and General Regression Networks (GRNN)[45], which are subsets of Probabilistic Neural Networks (PNN). They are more intricately designed than the typical Feedforward Neural Network (FNN), which is the type of neural network that has been discussed in this thesis so far. But neutron spectrum unfolding with RBFNN[6][52] and GRNN[51][14][52] are more complicated than unfolding with feedforward neural networks, so in this thesis only FNN will be investigated in details; further investigation into using RBFNN and GRNN may follow from this thesis, in an attempt to improve fusion neutron spectrum unfolding performance.

In addition to having a more underdetermined matrix than all of the cases displayed in Table 1 (number of input nodes = 11; number of output nodes = 175), the problem of unfolding fusion neutron spectra comes with the lack of data: There are very few existing nuclear fusion facilities in the world, many of which do not have a first-wall similar to JET, ITER or DEMO, where tritium is expected to be bred, and neutron spectra measurement is paramount. Since the first wall condition will affect the plasma

Source	topology of NN	comment
[35]	7:10:75	optimum: momentum =0.1, learning rate= 0.1, activation function = trainscg
[34]	7:14:31	optimum: learning rate= 0.1, optimal momentum = 0.1, activation function = trainscg (same author as [35])
[15]	6:10:16:6	Fully determined system
[17]	1 input layer : 2 hidden layer : 1 output layer	Fully determined system
[7]	50:50:1	over-determined (for fluence estimation)
[9]	10: 50: 52	used for unfolding monoenergetic and continuous spectra

Table 1: The topology of all of the feedforward neural networks used for neutron spectrum unfolding found in the literature.

physics and the neutron scattering greatly, very few existing fusion neutron spectra are useful for training the neural network. They mainly consist of measurements from JET and modelling results from ITER. (This will be discussed further in Section 5.)

Some of these authors[52] have also attempted to unfold neutron spectra via other artificial intelligence methods, such as Genetic Algorithm (GA). There is some interest on this topic[46][32], but recent work here in CCFE has shown that GA is unpromising for unfolding fusion neutron spectra [53]. For completeness, other AI methods that were considered for neutron spectrum unfolding includes Particle Swamp [42] and Artificial Bee Colony [44]. None of these methods will be considered in detail as it is beyond the scope of this thesis.

4 Proof of concept on simulated spectra

To demonstrate that the neural network can unfold neutron spectra at all, simple synthetic neutron spectra were created and folded through a response function, and neural networks were used to unfold them. These synthetic neutron spectra are simple in the sense that there are no physical processes modelled/considered while creating them, thus cannot be used to represent real-world data.

4.1 Fully determined case

A square response matrix consisting of 5×5 randomly picked numbers (uniformly distributed across $1 \leq R_{ji} \leq 50$) was generated.

A set of 100 spectra, each containing 5 randomly picked numbers (uniformly distributed across the range $1 \leq \phi_i \leq 15$) were also generated. They are regarded as the "true" neutron flux distributions. The "true" reaction rates corresponding to each spectrum was obtained by folding it through the response matrix according to equation 8. These form the features and labels respectively.

A single neural network with 0-hidden layer was able to predict the remaining labels (i.e. labels in the testing set) from the features perfectly after 10000 epochs of training over half the dataset (i.e. the training set consist of the first 50 features-labels pair). Note that at this stage, the neural network has not logarithmised the features' or the labels' numerical values in its pre-processing step, i.e. its loss function calculates the deviation in linear-space instead of log-space in equation 12, and regressing on the original value of the features, instead of log(features). This was done since the features are uniformly distributed within the same magnitude, so feature normalisation is not needed.

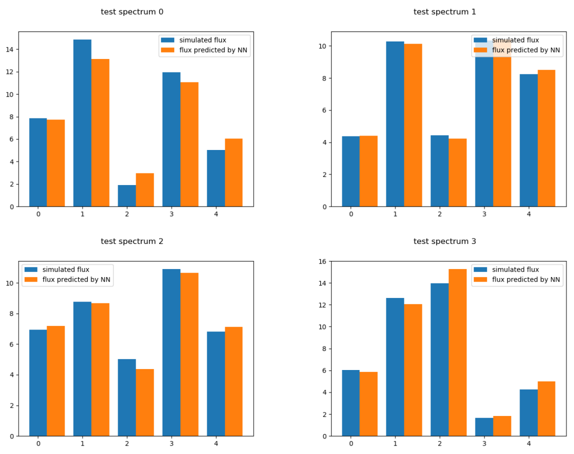


Figure 4: The spectra predicted by a 2-hidden-layers neural network (with 16 nodes per layer) on a fully determined system.
Abscissa: neutron bin number; ordinate: neutron flux (arb. units)
The loss function used is as defined in equation 12.

The perfect replication of the results is an expected and trivial result, as a 0-hidden-layer neural network is merely a matrix multiplication equation. Further examination of the weights (by enabling eager_execution_mode in TensorFlow before re-training the neural network) shows that the weights connecting the input to the output layer form a matrix that is identical to the transpose of the inverse matrix $\underline{\underline{\mathbf{R}}}^{-1}$ up to 3 significant figure. The difference after the 3rd (or more) significant figure were attributed to rounding errors, and the fact that the learning rate (i.e. Adam Optimizer's default learning rate of 0.001) was too big for the neural network to settle into the minimum in the parameter space properly.

The practise of logarithmising the numerical values of features and labels in the pre-processing step was then introduced and tested on this dataset.

Since logarithms destroy the linearity of this problem, two hidden layers were added to account for the increased complexity of the problem. (Preliminary experimentation showed that adding only one hidden layer is insufficient, as the loss value does not go down as far as with the two hidden layer neural network.)

The neural network was still able to reproduce the original spectra with a somewhat satisfactory level of accuracy after training for 10000 epoch at a learning rate=0.001 over the 50 training data. The training was done using the Adam algorithm, which is the default tensoflow algorithm. Figure 4 contains 4 example plots from the testing set, as predicted by the neural network.

As expected, larger deviations were observed when the absolute value of ϕ_{0i} is high, as the loss value contribution from each $\phi_{pred\,i}$ is proportional to $\frac{log_{10}(\phi_{0i})}{log_{10}(\phi_{pred\,i})}$

4.2 Underdetermined case

To demonstrate that the neural network is capable of performing the unfolding procedure in an underdetermined condition, 2100 spectra were made from 7 fusion neutron spectra, and then used to train and test the neural network. The 7 spectra used are listed in Table 2.

The data were rebinned into a modified Vitamin-J group structure, where the last 4 (highest energy) bins are discarded to avoid the need of extrapolating some of the spectra beyond their recorded energy ranges.

Each neutron spectrum was parametrised as a sum of 3-7 normal and log-normal distributions(see Figure 5a). The full table of the parameters used to parametrise the

Code	reactor
JAEA-FNS	JAEA Fusion Neutron Source D-T
Frascati-NG	ENEA Frascati Neutron Generator D-T
ITER-DD	Magnetic confinement fusion, ITER D-D
ITER-DT	Magnetic confinement fusion, ITER D-T
DEMO-HCPB-FW	DEMO fusion concept He-cooled pebble bed, first wall
JET-FW	Joint European Torus, first wall vacuum vessel
NIF-ignition	Inertial confinement fusion, NIF ignited

Table 2: The neutron spectra used as the starting point for creating more simulated fusion neutron spectra, obtained from [49]

spectra is listed in Table 5. The parametrisation was carried out using a parameterised code currently under development at CCFE.

Each simulated new spectrum is created using the following procedure: using the parametrised representation of one of the above spectra, 40% of these distributions in the parametrised representation were randomly selected to have their amplitudes of scaled up/down by a random factor(picked from a lognormal distribution with $\mu = 0, \sigma = 1$), leaving the remaining 60% of them un-perturbed.

This process was repeated 300 times for each spectrum in Table 2, giving the 2100 spectra in Figure 5b.

The purpose of this parametrisation is such that an underlying pattern can be introduced into the spectrum, which the neural networks are expected to identify on its own during the training stage.

Two neural networks were created. An arbitrarily chosen network topology of 11:128:256:175 was used. 80% of the data were randomly selected to become the training set; while the remaining becomes the testing set. The training set is further subdivided such that 20% of it is used as the validation set (i.e. 16% of the original features-labels pair becomes the validation set). The technique of Early Stopping was applied so that if the neural network shows no improvement in validation loss in 1000 epochs, the training will be stopped and the parameters (weight and biases of every layer) will be restored to the values achieved in that epoch which has the minimum validation loss. The maximum number of epoch allowed for the training was set to 10000; however both neural networks finished training (i.e. reached a minimum validation value with no further improvement for 1000 epoch) before reaching the 10000 epochs mark.

The first neural network uses mean-squared-error as the metric for calculating loss value (equation 12); while the second uses mean-squared-error-including-folded-reaction-rates (equation 13).

Interestingly, the latter achieved a slightly lower loss value instead of the former, and finishes training earlier than the former, despite having its loss function sum over a longer vector and therefor more terms to sum over more terms to obtain the loss value. The details are shown in Table 3.

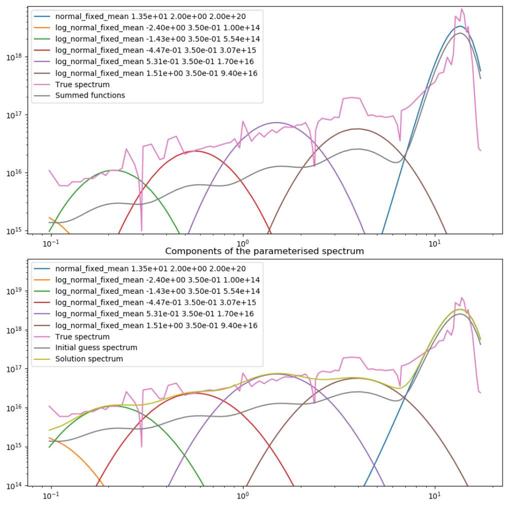
The last row in Table 3 is defined as

$$\text{std-dev-log(C/E)} = \sum_{j}^{M} ln\left(\frac{Z_{pred\,j}}{Z_{0j}}\right) \tag{17}$$

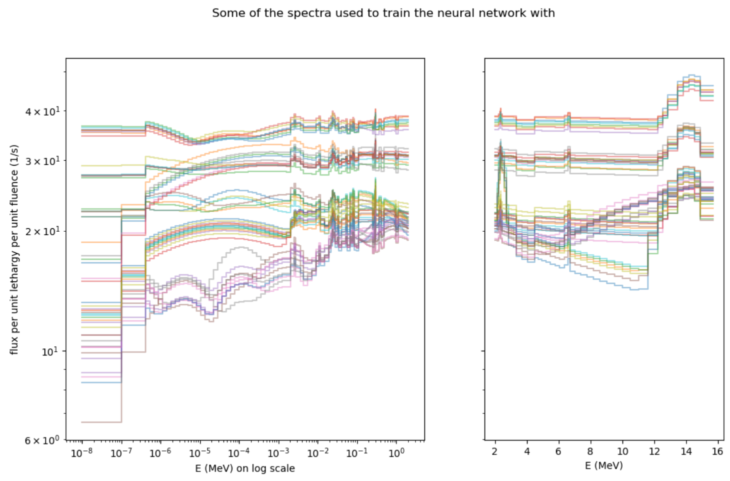
This quantity measures the sum of squares of deviation of reaction rates in log space, where Z_{pred} is obtained via equation 15.

An example of the second neural network's prediction is shown in Figure 6.

The low training loss/MAE/MSE show that the neural networks were able to learn the relationship between the features (reaction rates) and labels (neutron spectra), and then replicate the underlying pattern in the label; while the test loss/MAE/MSE were



(a) An example of parametrisation performed on the NIF spectra. These flux values are the total flux inside each energy bin, *not* divided by the lethargy span of each bin, so they are higher/lower in wider/narrower energy bins. The top plot is the initial guess parametrisation, the bottom plot is the final parametrised spectrum.

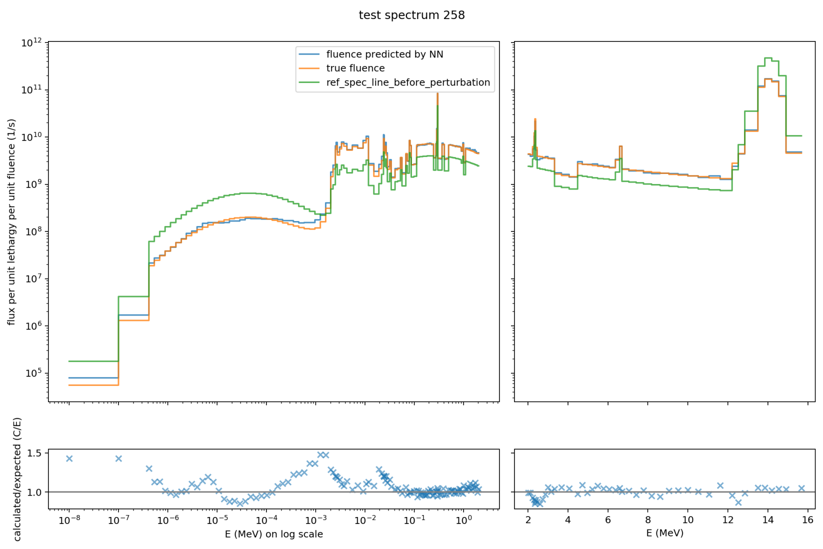


(b) 300 perturbed spectra were generated for each of the 7 original fusion spectra are plotted here, in flux per unit lethargy.

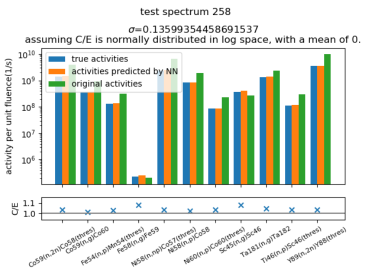
Figure 5: Data augmentation performed to create simulated spectra.

loss value	defined in eq. 12	defined in eq. 13
number of epochs of training required before a minimum val. loss is reached	6607	5078
training loss	0.29554	0.27586
training MAE	0.38083	0.37598
training MSE†	0.29554	0.29201
validation loss	0.34390	0.30682
validation MAE	0.37107	0.36681
validation MSE†	0.34390	0.32596
testing loss	0.45329	0.37592
testing MAE	0.41419	0.40527
testing MSE†	0.45329	0.39924
standard deviation of log of $\frac{Z_{pred}}{Z_0}$ ††	0.34263	0.14875

Table 3: Performance of the two neural networks trained on simulated (171 groups) data
† MAE = mean-absolute-error; MSE = mean squared error. Since MSE is identifically defined as in eq.12, the * loss value in column 2 is equivalent to * MSE.
†† standard deviation of log of $\frac{Z_{pred}}{Z_0}$ (shortened to std-dev-log(C/E) below) is defined with equation 17



(a) The predicted label (neutron flux as unfolded by the neural network) compared with the original flux. Note that the colour scheme is reversed, i.e. the blue bars denote the reaction rates predicted by the neural network instead of the true reaction rates, vice versa.



(b) The reaction rates (features) obtained using equation 15. The neural network was given the true reaction rates, and asked to predict the corresponding fluence (Figure 6a).

Figure 6: An example of the neutron spectrum (a perturbed JET first wall spectrum) as unfolded by the neural network.

only slightly higher than the training loss/MAE/MSE (i.e. it is within a factor of 2 of the latter), suggesting that the neural networks has learnt to do so without loss of generality.

5 Neural networks trained on real spectra

From the result of the previous section, we can expect the neural network to be able to identify the relationship between reaction rates and neutron spectra, while replicating the underlying pattern in the real neutron spectra, when sufficient data is given.

A set of 212 neutron spectra were acquired from the IAEA+UKAEA compendium[37]. 137 of them were identified as fission neutron spectra and 19 of them were identified as fusion neutron spectra. These spectra are listed in the appendices L.

They were rebinned into the Vitamin-J group structure using FISPACT-II[1]. The Vitamin-J group structure was chosen as it is well known and widely used in neutron spectrum unfolding [39] [50] [16]. Using the 11 reactions that are measured by the ACT project [38], the corresponding reaction rates for each spectrum was obtained by folding it through the response matrix (plotted in Figure 7). The method of obtaining the response matrix is explained in Figure 7:

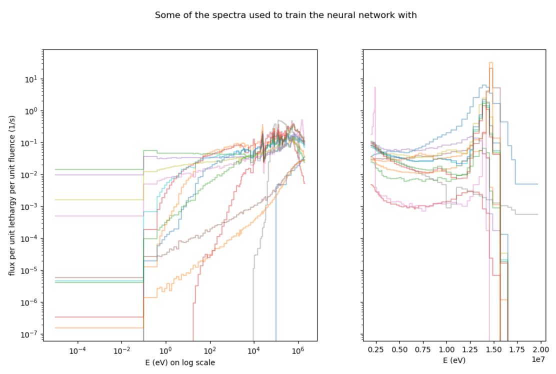


Figure 8: All fusion spectra used, obtained from [37]

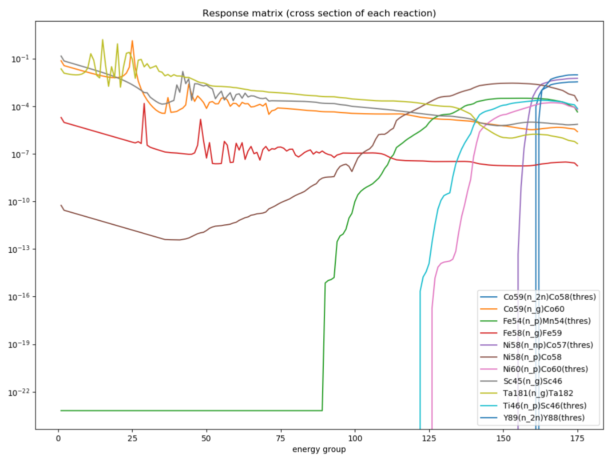


Figure 7: Microscopic cross-section of each reaction
These values are obtained from TENDL15 via FISPACT-II [1] at the left edge of each bin in the Vitamin-J group structure.

By assuming that the flux per unit lethargy inside each bin are relatively flat (energy independent), the reaction rates contributed by the neutron flux in each bin is then proportional to the product of neutron flux with the microscopic. Symbolically,

$$Z_j \propto \sum_i \sigma_{ji}\phi_i \tag{18}$$

Akin to the equation 4. Therefore these microscopic cross-section values were used in place of the response function for each of the reaction, assuming the constant of proportionality in equation 18 is unity.

5.1 Hyperparameter Optimisation

Since the of each neural network varies according to the hyperparameters used and the data that it is trained on, when investigating the real fusion spectra in section 5, multiple neural networks were generated, each with different hyperparameters, to investigate the combination of optimal hyperparameters which may be applied onto this problem.

The following hyperparameters/variables were considered:

- activation function used
- strategies applied to prevent overfitting

    - weight regularisation
    - dropout
- number of layers
- number of nodes in each layer
- number of epochs trained
- optimizer algorithm, which has the following parameters:
    - momentum term (if applicable)
    - acceleration term (if applicable)
    - epsilon (denominator offset parameter) (if applicable)
    - learning rate
- Normalisation techniques applied:
    - logarithmize the numerical values of features
- metric used to evaluate the loss value (See Section 11)
- Training set/testing set

It is nearly impossible to optimize all 14 parameters listed above simultaneously in a grid search as it will be very computationally intensive and laborious. Therefore the following choices were made for each of the hyperparameters to reduce the number of hyperparameters combinations in the grid search:

hyperparameter	choice
activation function	ReLU[3] for nodes in all layers, as it is the most widely used activation fucntion in machine learning and simplest function.
overfitting prevention strategies	Early Stopping (stopping the training when the validation loss does not see improvement in 1000 epochs); while the complexity of the model is restricted by limiting the number of layers to 5 or fewer, so neither dropout or weight regularisation will be applied.
number of epochs trained	10000 (subject to change by TensorFlow's EarlyStopping callback)
number of hidden layers	ranges from 0-5, as this includes all the configurations stated in Table 1.
number of nodes in each layer	with refernce to Table 1, the first hidden layer starts with 32 nodes, and logarithmically increases to the last hidden layer, which has 256 nodes. Therefore the six resulting neural network topologies are 11:175, 11:32:175, 11:32:256:175, 11:32:90:256:175, 11:32:64:128:256:175, 11:32:53:90:152:256:175.
Optimizer algorithm	using the Adam optimizer[4] with its default parameters (except for the learning rate, which is specified below), as it is a widely used algorithm in various machine learning projects.
learning rate	ranges from 10^{-2} to 10^{-2}, logarithmically spaced, 6 steps per decade.
metric used to calculate loss value	ranges from equation 12 to 13
training set	Either fusion spectra or fission spectra is used; if fusion spectra is used, then only 80% (15 spectra) are used as the training set (drawn at random), the remaining 20%(4) are reserved for testing.
testing set	fusion spectra
validation set	20% of the testing set, drawn at random

Table 4: Hyperparameters chosen for building neural networks for investigations

For each combination of variable hyperparameters in Table 4 (highlighted with bold typeface), a neural network is created; all other hyperparameters are fixed according to the rows in Table 4 with plain font.

5.2 Results of predicting using the real spectra

The resulting neural networks were sorted into two groups according to the training set (into "trained on fission" and "trained on fusion"), then each of these groups was sorted into 4 smaller groups according to the loss value used during training.

For each group of the data, the resulting loss value, MAE(mean-absolute-error), and MSE(mean-squared-error), evaluated over the training set, validation set, and testing set, as well as the std-dev-log(C/E) over the testing set, were all plotted as heatmaps (see Figure 9 for example). The main focus of this section is to find the neural networks that give the minimum test loss, as they indicate that these neural networks are able to perform well on data that it has never seen before.

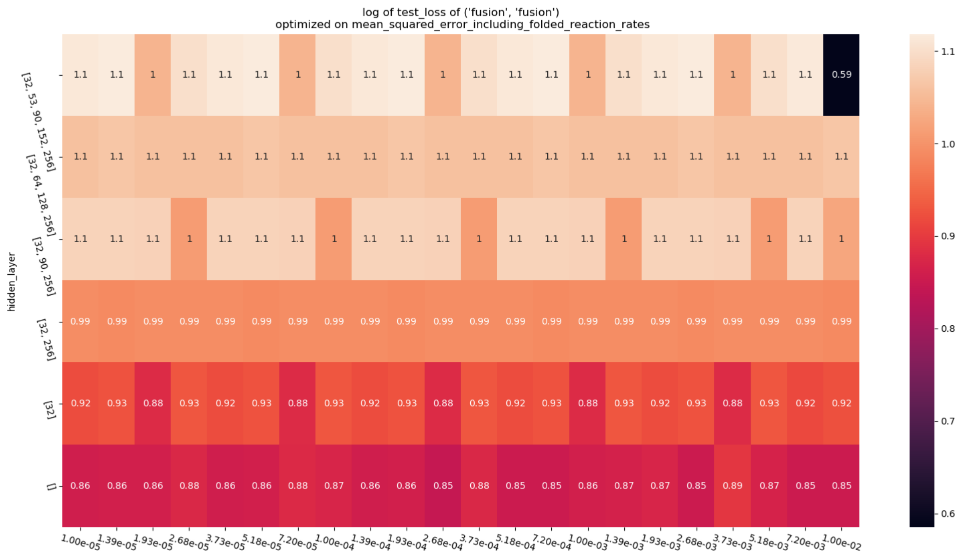


Figure 9: Heatmap visualizing the loss values of the neural networks' prediction on the test dataset.

Each square represents a neural network with a particular set of hyperparameters, i.e. learning rate and number of layers. The learning rate increases logarithmically across the x-axis; while the number of layers increases linearly across the y-axis. The number of nodes per layer is increased logarithmically from 32 to 256 (if the number of hidden layers ≥ 2). Neural networks which perform better have lower loss values, and are represented with darker colours.

General effects of the learning rate and the number of layers were identified in this manner. For all of the dataset and loss function used concerned, a general trend of increasing testing loss was identified as the number of layers increases; while the learning rate has no significant effect on it (except for causing a periodic oscillation in the testing loss as the learning rate increases logarithmically, which was dismissed as an artefact of the Optimizer algorithm Adam).

However, a closer examination of the performance of these few-layer neural networks reveals that their performances are mediocre.

For example, below are some of the predicitons made by these few-layer neural networks.

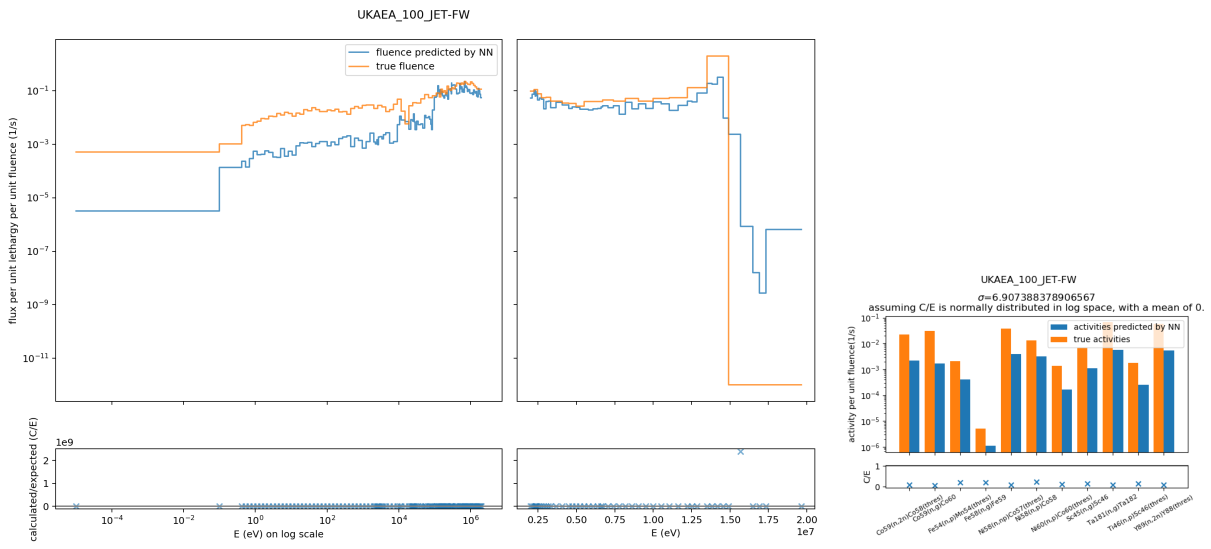


Figure 10: A typical 0-hidden-layer neural network prediction of JET's first wall spectra when trained on fusion spectra (learning rate=0.01)

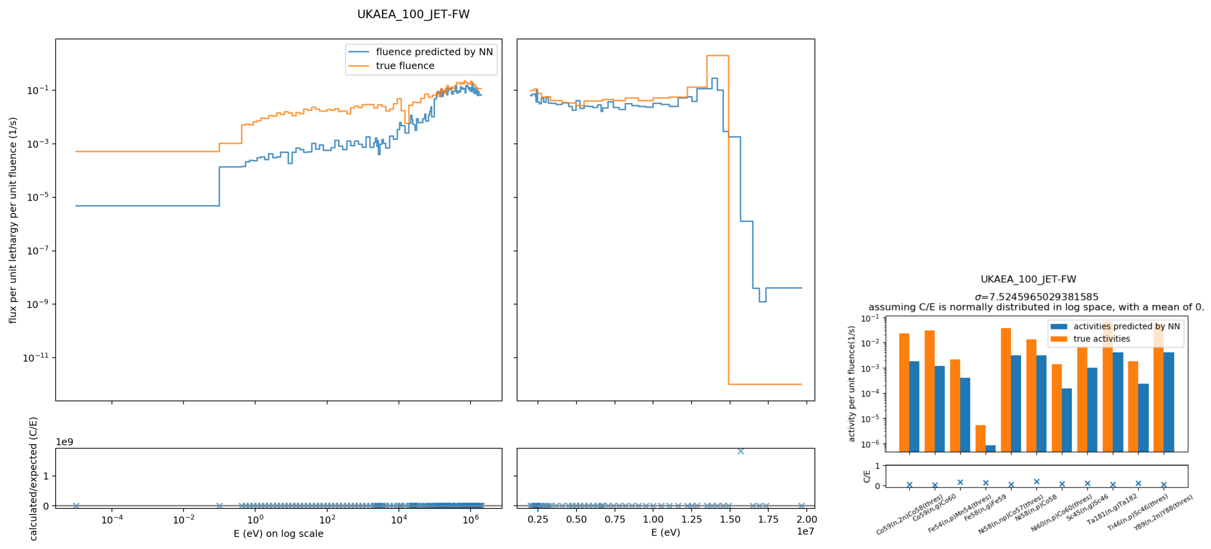


Figure 11: A typical 1-hidden-layer neural network's prediction of JET's first wall spectra when trained on fusion spectra(learning rate=0.01)

They are unable to replicate the 14.1 MeV peak at the correct width, and occasionally massively underestimate the high energy tail.

This is likely due to the small dataset of fusion data available. This explanation is supported by the small number of epochs required for training to finish: most of the neural networks finished training in fewer than 50 epochs, i.e. showed no further improvement in the validation loss in the next 1000 epoch after that. This is unusually early stopping of compared to the number of epochs the neural network required to be trained in Section 4.2.

However, one particular extremum showed up on some of the graphs. This is the neural network with the hyperparameters of (learning rate=0.01, topology=11:32:53:90:152:256:175, loss function used = mean-squared-error-including-folded-reaction-rates, eq. 13), a particularly loss value is obtained. This neural network is found to be as the neural network with the lowest testing loss and testing MSE. (test loss = 5.0309, test MSE = 5.0178)

This neural network was able to reproduce the same results even when its initial weights and biases were initialized using a different TensorFlow seed. Therefore its low

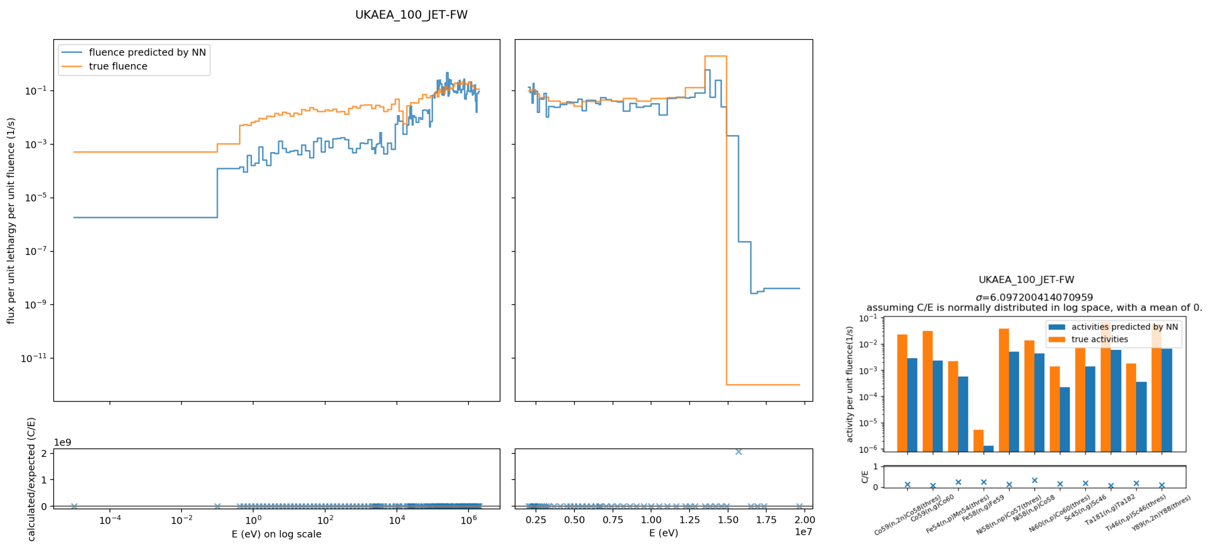


Figure 12: A typical 2-hidden-layer neural network prediction of JET's first wall spectra when trained on fusion spectra (learning rate=0.01)

test loss and test MSE were not coincidental, resulting from a numerical instability. It was thought that the neural network was able to generalize from such small dataset, so its predicted spectra were looked into in closer detail.

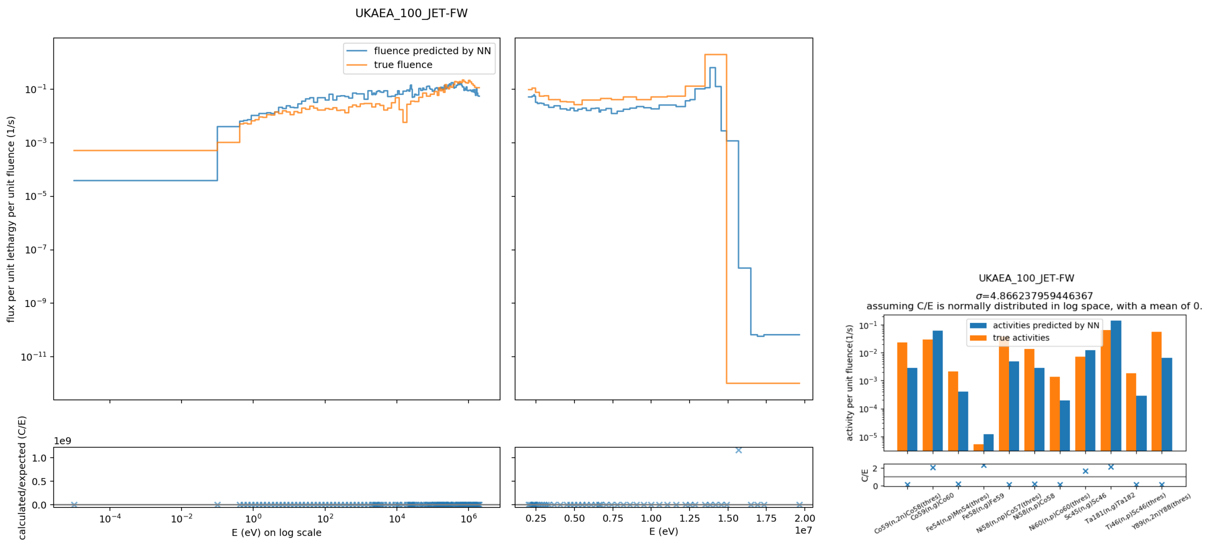


Figure 13: JET first wall spectrum as predicted by the optimally performing NN among all NN trained on fusion data.

But in the end, it was concluded that this 5-hidden-layer neural network likely only achieves the above-average performance serendipitously by re-tracing the same average spectrum. This conclusion is supported by it replicating a very similar spectrum when it attempts to deduce the spectra corresponding to the other two test data.

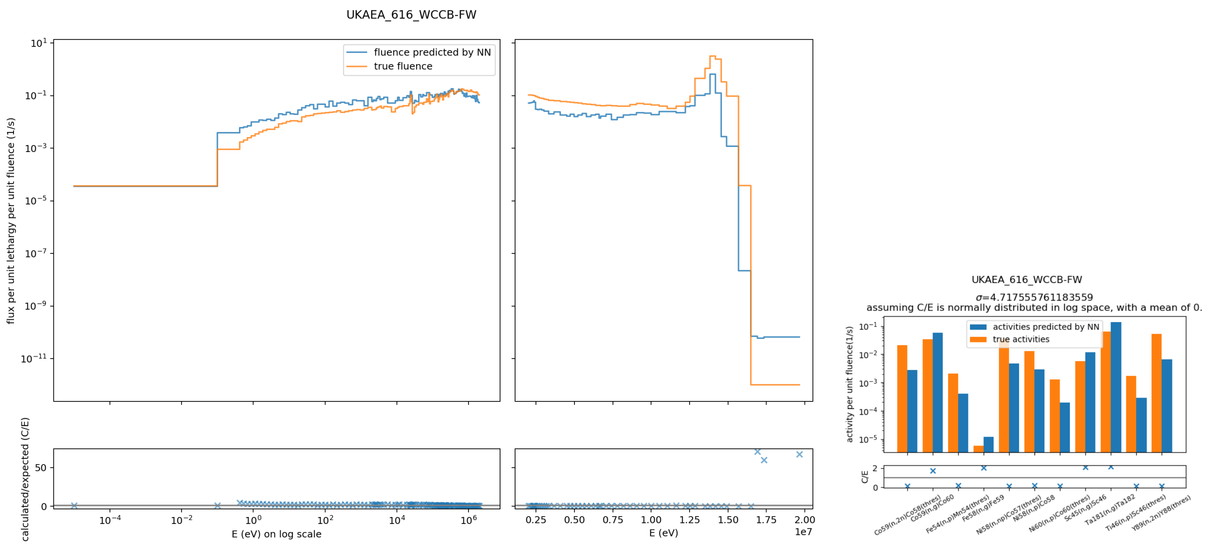


Figure 14: Water-cooled ceramic breeder blanket TOKAMAK's first wall spectrum as predicted by the optimally performing NN among all NN trained on fusion data.

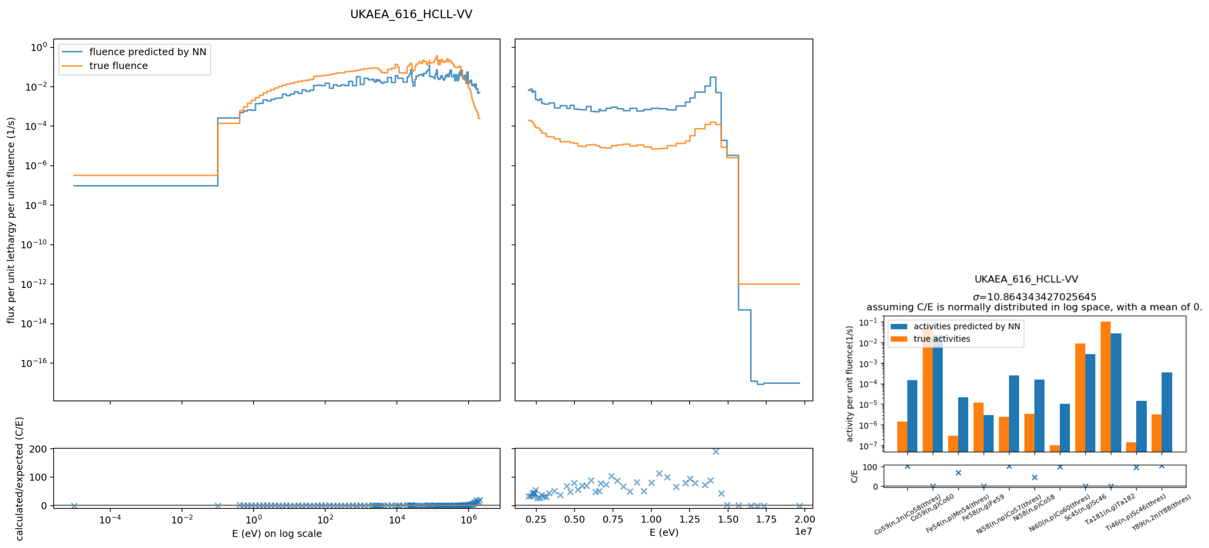


Figure 15: Helium-cooled LiPb TOKAMAK's spectrum at the vacuum vessel, as predicted by the optimally performing NN among all NN trained on fusion data.

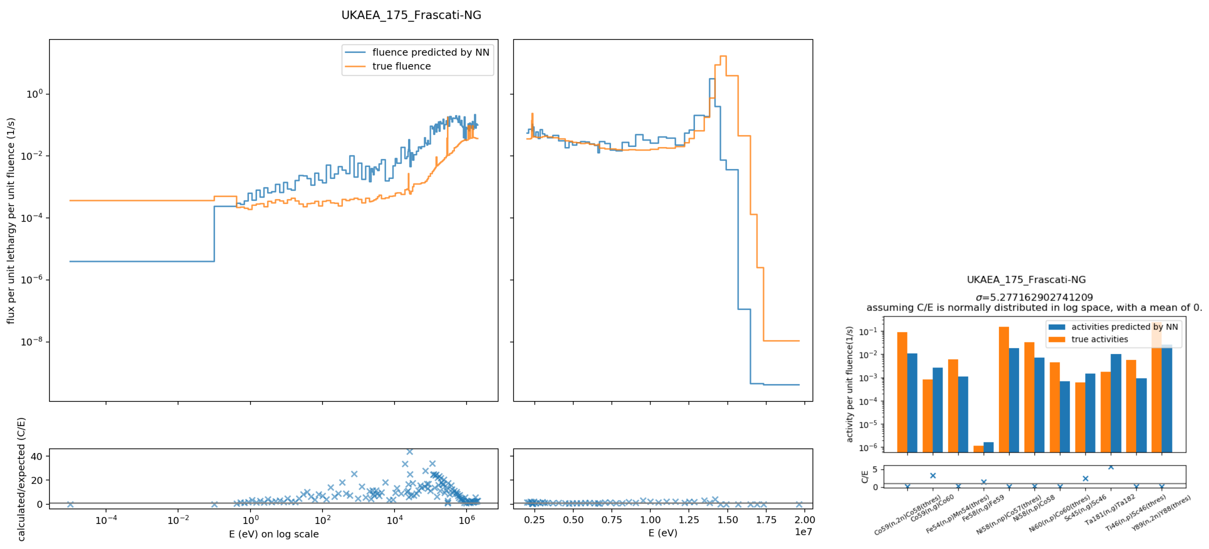


Figure 16: Frascati neutron generator spectrum, as predicted by the optimally performing NN among all NN trained on fusion data.

5.3 Benchmarking against existing codes

5.3.1 As an unfolding tool

The method of unfolding using neural networks has the inherent advantage of not having to provide an *a priori* spectrum; if sufficient training data (with the correct group structure, and with corresponding reaction rates) has been given to it, a neural network is, theoretically, capable of unfolding any set of new reaction rates into a neutron spectrum.

Therefore to fairly compare a neural network against the usual unfolding codes, no meaningful information should be given to the unfolding code in the form of an *a priori* spectrum. Therefore a naive prior of a flat neutron spectrum (i.e. flux in each bin is simply proportional to the "size" (lethargy span) of each bin) will be given to the unfolding code before comparing their performance against the neural network unfolded neutron spectra. The unfolding codes chosen are GRAVEL and MAXED, as they are the two commonly used neutron unfolding code [38] [12]; and a python implementation of them is currently under development in CCFE.

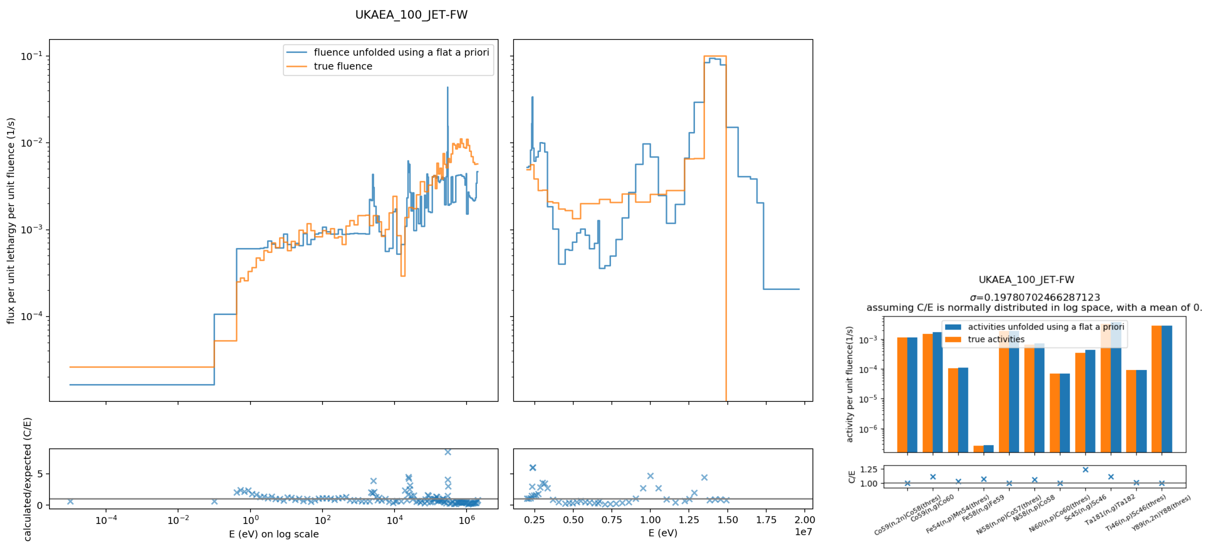


Figure 18: JET first wall spectrum as unfolded by GRAVEL upon using a flat neutron spectrum as the *a priori*

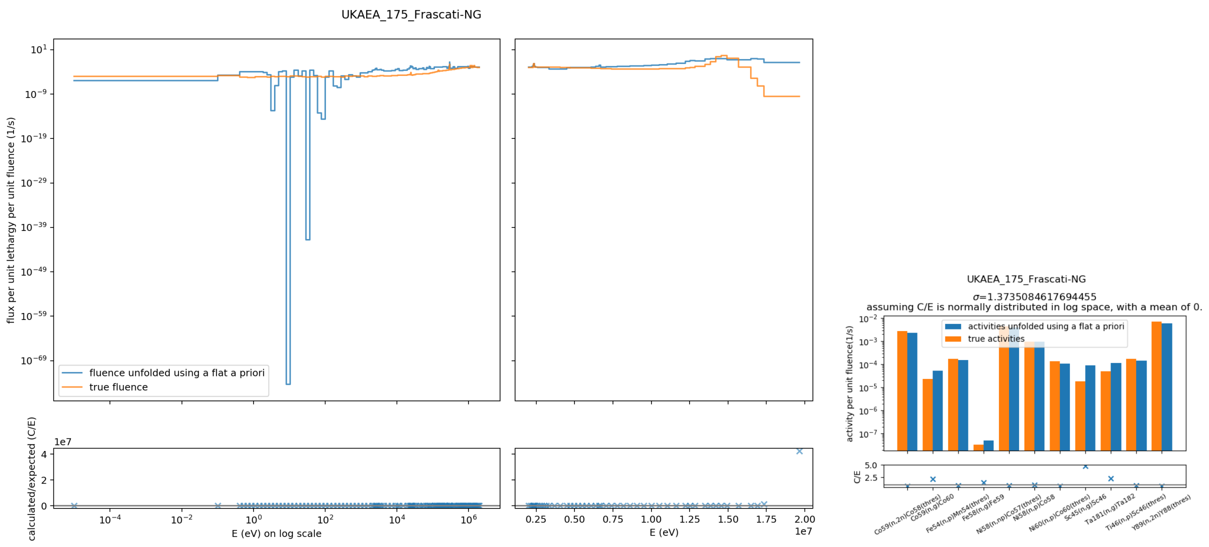


Figure 17: JET first wall spectrum as unfolded by MAXED upon using a flat neutron spectrum as the *a priori*

While MAXED performed very poorly (Figure 17) when given a flat *a priori* (giving a mean MSE value of 53.442406, as defined in equation 12), GRAVEL was able to unfold a neutron spectrum from the flat *a priori*, though with an underestimated low energy region and overestimated high energy range neutrons. A mean MSE value (as defined in equation12) of 10.188233 was obtained when comparing the unfolded spectra against the 4 true spectra in the testing set.

While the best performing neural network (Figure 13) gives a slightly better result, both Figure 13 and Figure 18 are far from being applicable to real neutron spectrum unfolding, where the unfolding accuracy is much higher (currently the unfolded spectrum gives a total flux that differs from measured total flux by $\pm 7\%$[12]). This low accuracy of the solution spectrum is likely due to the small training set of the neural network. This small sample size means that it cannot densely cover the entire domain (feature space) and co-domain (label space) of the fusion neutron spectrum unfolding problem. For the same reason, the neural network's prediction cannot be relied upon for unfolding spectra in new/unknown types of fusion reactor designs, as it has not been shown to extrapolate

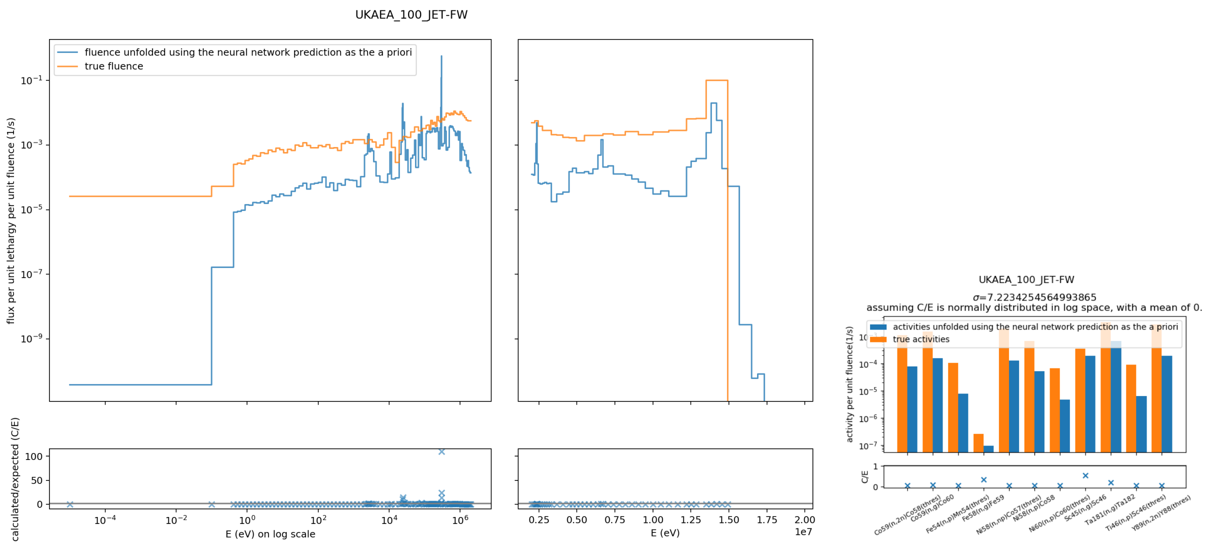


Figure 19: JET first wall spectrum as unfolded by GRAVEL upon using the optimal NN's output as the *a priori* spectrum.

its predictions with satisfactory performance beyond the very short list of fusion spectra in Appendices L.

5.3.2 As an a priori generator

When unfolding, an *a priori* spectrum with a reasonably close match to the original spectrum is required as the starting point for an iterative solution search. Given that the neural network did not yield satisfactory unfolding result in the last section, an attempt of using the neural network's output as an *a prior* was made, with the hopes that the neural network's output will be close enough to the true spectrum such that, with further adjustment by the unfolding code such as GRAVEL and MAXED, a reasonable solution spectrum can be reached.

The motivation of using a neural network's output as the *a priori* is that one can save hours of MCNP calculation in order to obtain the response matrix and *a priori* spectrum.

However, this proves to be rather unpromising as well. Even when with best neural network's predictions (Figure 13, 16, 15, 14), GRAVEL unfolded results that are as poor as when a flat *a priori* was used. A mean MSE value of 9.8994 was achieved.

And MAXED produced results that are also as meaningless as Figure 17, as the log of the flux in some bins tends to negative infinity.

5.4 An attempt at using fission data to predict fusion data

While fusion spectra are scarce, there is an abundant database of fission neutron spectra. Therefore, it would be ideal if neural networks trained on fission spectra can use it to explain fusion spectra, as we will not run into the issue of not having enough data.

Therefore, the results of the second group of neural networks (trained on fission spectra, tested on fusion spectra) were examined. If there is indeed a transferable underlying structure that is common to both fission and fusion spectra, e.g. the Maxwellian distribution at thermal energy, then it should be able to identify them, and piece together semblances of fusion spectra, resulting in a low test loss.

But even the best one among all of these neural networks performed very poorly. It uses an MSE loss value equation 12 giving a testing loss of 16.768. Closer examination of its prediction shows that its predictions are nonsensical.

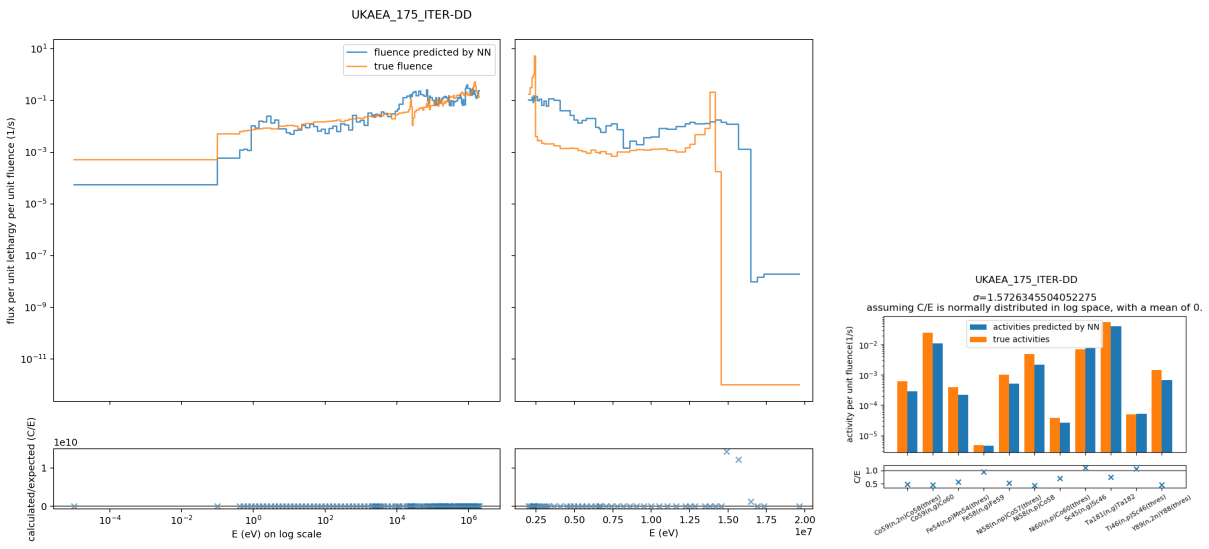


Figure 20: (calculated) ITER spectrum as predicted by the optimal NN among all NN trained on fission spectra

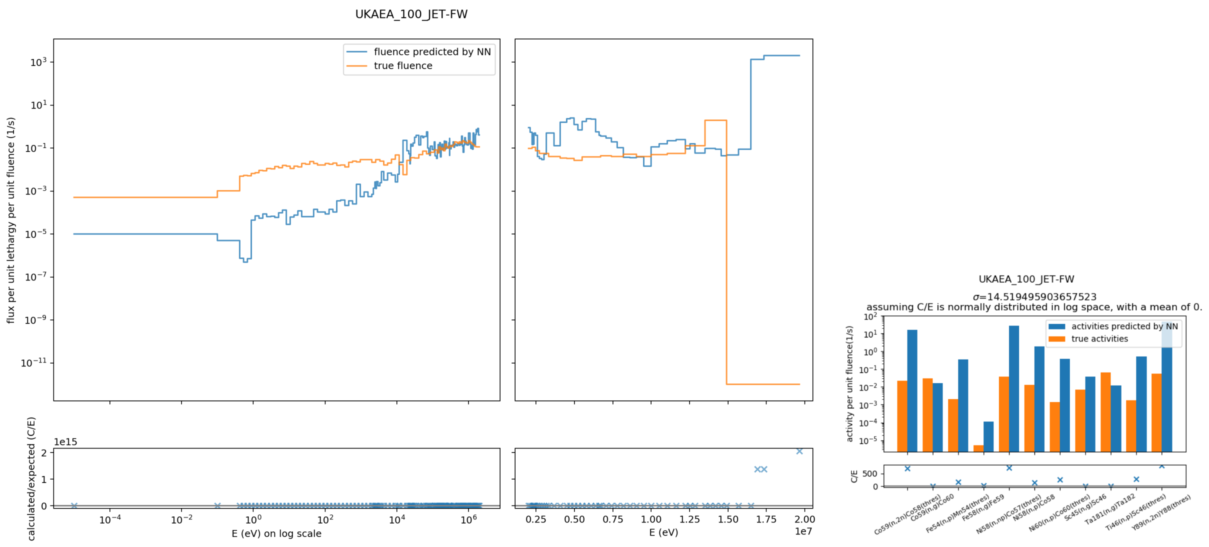


Figure 21: JET first wall spectrum as predicted by the optimal NN among all NN trained on fission spectra

(For the record, this neural network (which performed the best out of all neural networks trained on fission spectra) has very similar hyperparameters as the optimally performing neural network identified in the previous section 5.3.1, differing only in the loss function used. (learning rate = 0.01, topology = 11:32:53:90:152:256:175, loss function used = MSE (eq.12)).)

This suggests that the inverse function required to unfold fission-induced reaction rates in the activation foils is a different inverse function than the inverse function required to unfold the fusion-induced reaction rates in the activation foils.

6 Potential Future improvements

The technique of neural network classification is best applied when the dataset is large, which is not the case with fusion neutron spectra.

To improve upon the results observed in this thesis, a larger dataset, consisting the neutron spectra for magnetic confinement fusion with various plasma and first wall conditions, and potentially of other inertial confinement fusion, should be attained. These data may be obtained by numerical simulations with MCNP, or actual measurements of neutron spectra at various TOKAMAK's and various other fusion facilities; but one has to recognize that neural networks trained on a set of data can only make predictions that are as reliable as its training data. In other words, if the training data consists of numerical simulations made from MCNP modelling which may be inaccurate, the neural networks will also make inaccurate predictions.

Other possible directions of investigation are listed below:

- Repeat this experiment using RBFNN or GRNN, as explained in section 3, which are known to perform better under low sample number conditions. However, it is doubtful as to whether these neural networks will be able to generalize their predictions to new types of fusion reactors.
- Transfer learning[48]: train the neural network with fission data, fix the weights and biases in the half of the neural network, and then train the weights and biases in the remaining half of the neural network using fusion data. This makes use of much large, similar, dataset of fission spectra, to complete half of the training process, reducing the amount of information required to train the neural network.
- The method of RDANNM proposed in [34] uses Orthogonal Arrays instead of grid searching the entire hyperparameter space, as well as fractional factorial instead of full factorial combinations when performing the optimisation. This can reduce the amount of time required for the experimentation; or extend the range of hyperparameter space searched in the same amount of time. This may reveal a combination of hyperparameters that leads to a better neural network design for fusion neutron spectrum unfolding than the existing optimal design found in this thesis.
- Since the best hyperparameter occured at the extrema of the search ranges (at the maximum number of layers and minimum learning rate), it is possible that a better set of hyperparameter lies outside of this search range. As [35] has shown the optimal learning rate may be 0.1, which is beyond the searched range in the current investigation. Therefore another possible way of improving the unfolding accuracy of the neural networks is via expanding the search range.

Lastly, as uncertainty of the neutron spectra needs to be known for the application of fusion neutron measurements, once an optimally performing neural network has been identified, a global sensitivity analysis can be performed on the neural network using a Monte Carlo approach: by repeatedly adding in noise δZ_j into the reaction rates Z_j and allowing the neural network to carry out its prediction (forward propagation), the Monte Carlo program will be used to infer the resulting changes $\delta\phi_i$ associated with the neural network's predictions (ϕ_i), thus propagating uncertainty in the measurements of reaction rates σZ to uncertainties in the spectrumσ_ϕ. An unfolding code suite is already under development in CCFE to allow this to be done systematically.

7 Conclusion

A neural network unfolding approach to neutron spectrum unfolding was examined.

A prototype neural network unfolding code was made for a simulated 5 reaction channels$\times$5 energy bins, fully determined system with synthetic data; and then again with an 11 reaction channels $\times$ 171 energy bins, underdetermined system with synthetic data, as proofs of concept. They behaved as expected, unfolding the simulated spectra from the reaction rates without being given the response matrix explicitly.

Then, 19 fusion neutron spectra were acquired. They were rebinned into the Vitamin-J group structure and folded through the response matrix to obtain the corresponding reaction rates.

To find the best hyperparameters for unfolding these neutron spectra, a grid search for the optimal hyperparameters for the neural network was performed over 4 dimensions (training set used, learning rate, number of layers, and loss function used). Some of the neural networks with the best test losses were examined in detail.

Two loss functions were examined: one is a simple MSE in log space (eq. 12), one is a modified MSE in log space, which takes into account the physics of the unfolding process as well (eq. 13); while the number of hidden layers used in the neural networks examined ranges from 0-5. The learning rate for the Optimizer Adam used ranges from 0.01 to 10^{-9}.

Among all neural networks trained on fusion data, the optimal one achieved the best mean MSE value of 5.0178. It has a topology of 11:32:53:90:152:256:175. However, it is thought that the neural network is being overtrained, as it was a very complex model with lots of parameters, but very few data points; and training finished in very few epochs as well, leading to the speculation that it was only "memorizing" the average fusion neutron spectra. Therefore this model requires much more scrutinous examination and validation before it can be deployed for predicting neutron spectra of novel fusion reactor designs.

Also, it does not significantly improve the unfolding accuracy compared to traditional neutron spectrum unfolding codes when they are given naive priors. The fusion neutron spectra unfolded from by GRAVEL, when flat *a priori*'s were given, unfolds to give a mean MSE value of 10.188 over the same dataset.

When outputs from the optimal neural network (with the topology of 11:32:53:90:152:256:175) were used as the *a priori* for GRAVEL instead, an average RMS value of 9.8994 was obtained. This is an insignificant improvement, and shows that the optimal neural network's predictions do not make good *a priori*'s for unfolding.

When fission spectra are used as the training data for the neural networks instead, then the performance of them greatly reduces. In this case, the optimal neural network gives a very poor result of mean MSE = 16.768, and the spectra that it predicts were nonsensical. This shows that neural networks trained to unfold fission spectra cannot be used to unfold fusion spectra directly without at least some attempts of retraining.

In conclusion neutron spectrum unfolding with feedforward neural network is not a suitable technique for unfolding neutron spectra given the small number of fusion neutron spectra available, as it is a technique designed for big data. Techniques such as RBFNN, GRNN and Transfer Learning can be applied to minimise the impact of the insufficiency of data, while RDANNM may offer a faster approach to searching through a wider range of hyperparameters for the best hyperparameter. However, the validity of these techniques requires further examination beyond the scope of this thesis.

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Appendices

A Neural network building functions tailored for the purpose of neutron spectrum unfolding

The following contains the class in which the neural network is built.

neuralnetworklibrary.py

```
import glob
import sys
import os
# Import commonly used numerical processing and plotting functions
import pandas as pd
import matplotlib as mpl
mpl.use("agg") #for using this script on the cumulus server of ukaea
from matplotlib import pyplot as plt
import numpy as np
from numpy import e
from numpy.fft import fft, ifft
import tensorflow as tf
from tensorflow import keras
from tensorflow.keras import layers, activations
import time
from shutil import get_terminal_size
import fcntl

def read_NN_weights(session_name):
    '''returns the weights and biases read from a h5 file'''
    import h5py
    path_to_file = ".checkpoints/" + session_name.split("/")[-1] + ".h5"
    weights, biases = {}, {}
    keys = []
    with h5py.File(path_to_file, 'r') as f:  # open file
        f.visit(keys.append)  # append all keys to list by visiting each
        for k in keys:
            if ':' in k:  # Filter out all keys that is
                # Get the layer number
                name_splitted = f[k].name.split("/")
                layer = name_splitted[1]

                layer_num = "".join(d for d in layer if d.isdigit())
                if layer_num == "": layer_num = "1"  # if there is no digit in
                                                        the layer name: it must'
                                                        ve been layer 1.

                # Decide whether it's bias or weight according to the last
                                                        element in the
                                                        name_splitted list
                if "kernel" in name_splitted[-1]:
                    weights["layer_" + layer_num] = f[k].value
                elif "bias" in name_splitted[-1]:
                    biases["layer_" + layer_num] = f[k].value
    return weights, biases

def _find_matching_braces(list_of_lines):
    '''given a collection of text lines stored as a list, find out the indices
                                      of the lines where matching braces
                                      occurs'''
    # copying the design pattern of finding matching paranthesis.
    brace_stack = []  # stack
    d = {}
    # d stores the opening and closing braces' line numbers
    for l_num, line in enumerate(list_of_lines):
        if "{" in line: brace_stack.append(l_num)
        if "}" in line:
            try:
                d[brace_stack.pop()] = l_num
            except IndexError:
                print("More } than {")
    if len(brace_stack) != 0: print("More { than }")
    return d

def convert_str_value(string):
    if ("[" in string) and ("]" in string):  # filter out the list
        splitted_list = string.strip("[]").split(",")
        # filter out the empty list case:
        if len(splitted_list) == 1:
            if splitted_list[0] == "":
                # return an empty list [] instead of a [None]
                return []
        return_list = [convert_str_value(elem.strip()) for elem in
                       splitted_list]  # recursively call itself on the
                                                   elements of the
                                                   list
        return return_list
    if string.startswith('"') and string.endswith('"'):  # filter out the
                                      strings
        assert string.count('"') == 2, "too many quotation marks!"
        return string[1:-1]
    if string.startswith("'") and string.endswith("'"):  # filter out the
                                      strings
        assert string.count("'") == 2, "too many quotation marks!"
        return string[1:-1]
    if "False" in string: return False  # filter out the booleans and None's
    if "True" in string: return True
    if "None" in string: return None
    if ("." in string) or ("e-0" in string):  # filter out the floats
        try:
            return float(string)
        except ValueError:  # filter out the function objects
            if ("<" in string) and (">" in string) and ("object" in string):
                raise ValueError("Cannot input a method object as a string; but
                                                can try using string e.
                                               g. 'AdaGrad'")
    return int(string)  # only integers should be left

def cut_file_in_halves(filename):
    '''
    return two lists, one containing the first dictionary;
    the other contains all other files.
    '''
    with open(filename, "r") as f:
        data = f.readlines()
    braces = _find_matching_braces(data)
    try:
        first_pair = next(iter(braces.items()))
    except StopIteration:
        sys.exit("No more dictionaries in file")
    first_dict = []
    for line in data[first_pair[0]:first_pair[1] + 1]:
        if ":" in line:
            line = line.strip().strip("{}").strip()
            if line[-1] == ",": line = line[:-1]  # remove the rightmost comma
            first_dict.append(line)
    rest_of_the_lines = data[first_pair[1] + 1:]
    return first_dict, rest_of_the_lines

def convert_lines_to_dict(lines):
    dictionary_to_be_returned = {}
    for line in lines:
        # split the "sentence" down the middle at the ':'
        key, value = [arg.strip() for arg in line.split(":")]
        # must ensure that none of these are empty
        assert not len(key) == 0, "Must have a key before the :"
        assert not len(value) == 0, "Must have a value after the :"
        dictionary_to_be_returned[key] = convert_str_value(value)
    return dictionary_to_be_returned

def overwrite_file_by_removing_first_dict(filename, lines):
    # fcntl.flock(filename, fcntl.LOCK_EX | fcntl.LOCK_NB)
    with open(filename, "w") as f:
        for line in lines:
            f.write(line)
    # fcntl.flock(filename, fcntl.LOCK_UN)

def fold_and_append(response_matrix, label, log_label):
    if log_label: #exponentiate, multiply, and then take log again:
        label_in_linear = tf.math.pow(e,label)
        pred_feature_in_linear = tf.matmul(label_in_linear, response_matrix.T.
                                 astype("float32"))
        pred_feature = tf.math.log(pred_feature_in_linear)
    elif not log_label:
        pred_feature = tf.tensordot(response_matrix, label)
    return tf.concat([label, pred_feature], axis=1)

def convert_str_to_loss_func(string, response_matrix, log_label):
    include_folding_string = "_including_folded_reaction_rates"
    if string.endswith(include_folding_string):
        loss_func = convert_str_to_loss_func( string.replace(
                                              include_folding_string,""),
                                              response_matrix, log_label=
                                              log_label) #use to get one of
                                              the following
        return lambda lab, pred : loss_func( fold_and_append(response_matrix,
                                              lab, log_label=log_label),
                                              fold_and_append(response_matrix,
                                              pred, log_label=log_label)) #
                                              return a wrapped function
        #This assumes that each element of the folded reaction rate has the
```

```
                                                       same weight in terms of
                                                       deviation from the label.
    elif string=="mean_squared_error":
        return tf.compat.v1.losses.mean_squared_error
    elif string=="mean_pairwise_squared_error":
        return tf.compat.v1.losses.mean_pairwise_squared_error
    elif string=="cosine_distance":
        return lambda lab,pred : tf.losses.cosine_distance(lab,pred,axis=0)
    else:
        return string


class NeuralNetwork():
    #This class contains all the read- and write information required to pre-
                                                   process and post-process inputs to
                                                   the neural network.
    #It allows for all types of input imaginable, except for the
    def __init__(self):
        # List of parameters for pre- and post-processing
        self.data_preparation_options = {
                "log_feature"    : True,
                "log_label"      : True,
                "lower_limit"    : 1E-12, # any flux value below lower_limt will
                                                              be clipped to
                                                             lower_limt
                "label_already_in_PUL" : False, #labels needs to be converted
                #from total flux per bin to average flux per unit lethargy (PUL
                                                             ) across the bin before
                                                             training/handled by the
                                                             NN.
                #total flux needs to be divided by the difference in lethargy
                                                             of the upper and lower
                                                             limit to be converted
                                                             into flux PUL.
                "ft_label"       : False, # Do not apply fourier transform
                                                             before processing the
                                                             data by default.
                # apply log on both sides (the RR and the flux) before
                                                             processing the data, by
                                                             default
        }

        # options of how to rearrange the data before reading it in.
        self.data_reordering_options = {
                "shuffle_seed"       : 0,
                "startoff"           : None,
                "cutoff"             : None, #number of data lines to accept
                                                             from the next file.
                "train_split"        : 0.8,
                "validation_split"   : 0.2,
        }

        # metadata recording the training time. These will be auto-generated as
                                                        the NeuralNetwork training
                                                       begins.
        self.timing = {
                "start_time_raw"     : time.time(), #give in unix time
                "start_time"         : time.strftime("%I:%M%p %d-%m-%Y").lower()
                                                             ,
                "run_time_seconds"   : 0.0,
        }

        start_time_global = self.timing["start_time_raw"]

        # hyperparameter describing the architecture of the NN
        self.hyperparameter = {
            "tf_seed"        : 0,
            "act_func"       : [],
            "hidden_layer"   : [],
            "learning_rate"  : 0.001,
            "loss_func"      :
                             "mean_pairwise_squared_error",
                             # "cosine_distance", # chi^2 calculated as
                                                                       normalized
                                                                       unit sum of
                                                                       squared
                                                                       values #this
                                                                        one is
                                                                       weird and I
                                                                       can never
                                                                       get it to
                                                                       work.
                             # "mean_squared_error", #chi^2 calculated as mean
                                                                       of squares
                                                                       of deviation
                                                                        from true
                                                                       labels.
            "metrics"        : ['mean_absolute_error', 'mean_squared_error'], #
                                                        "precision_at_thresholds"
                                                        only works with boolean,
                                                        therefore is not used.
            "num_epochs"     : 10000,
        }
        self.hyperparameter["optimizer"] = tf.keras.optimizers.Adam(self.
                                              hyperparameter["learning_rate"])

        #loss values to be filled in later
        self.losses = {
        }
        # for key in self.hyperparameter['metrics']:
        #     self.losses.update({key: 0})

        self.session_name = ""

        self.callbacks_applied = ["PrintEpochInfo"]#, "TensorBoard"]

        # list the parameters to be saved
        self.settable_property_list = list(self.__dict__.keys())

        ################################################### Everything above
                                              may be tweaked manually before
                                              starting building and training;
        ################################################### Everything below
                                              will be automatically generated
                                              and shared across the class.

        # class instances of callbacks; used for monitoring training in real
                                              time/reviewing it afterwards..
        class _PrintEpochInfo(keras.callbacks.Callback):  # inherits from keras
                                              .callbacks.Callback,
        # which is a dummy class specifically designed for creating objects
                                                         that goes into callbacks
                                                        argument in tf.model.fit();
        # This is a local class that will not need to be reused outside of
                                                        the function.
        start_time_global = self.timing["start_time_raw"]#grab the global
                                                        start time from the timing
                                                        dictionary above.
        def on_epoch_end(self, epoch, logs):  # redefine the function so
                                                        that it prints only a dot,
                                                        regardless of verbosity
                                                        level.
            # ignore the logs (which logs the mae and mse)
            terminal_width = get_terminal_size().columns

            output_string = "{:>7} epochs finished;"\
                        "loss-value (mse) = {:0.9f};"\
            "validation loss-value (mse) = {:0.9f};"\
            "program has ran for = {:04.2f} s".format(
                    epoch + 1, logs["loss"], logs["val_loss"], time.time()
                                                                      -
                                                                      start_time_global
                                                                      )
            prompt_wider = "please make the terminal wider!"
            if terminal_width>=len(output_string):
                print( output_string ,end="\r", flush=True)  # make sure
                                                                the screen is wide
                                                                enough to print all
                                                                of this in a single
                                                                line; otherwise it
                                                                will overflow into
                                                                the next line then
                                                                the "\r" and flush
                                                                operation will not
                                                                extend back onto the
                                                                 first line, and the
                                                                 flush behaviour won
                                                                't occur.
            elif len(prompt_wider)<=terminal_width<len(output_string):
                print( prompt_wider, end="\r", flush=True)
            else:
                pass #don't print anything.


    if not os.path.exists(".checkpoints/tb_logs/"): os.makedirs(".
                                                     checkpoints/tb_logs/")
    self.callback_objects_available = {
        "PrintEpochInfo" : _PrintEpochInfo(), #just to print the epoch info
                                                         to screen.
        "TensorBoard" : tf.keras.callbacks.TensorBoard(log_dir=".
                                                        checkpoints/tb_logs/
                                                        latest_run", histogram_freq=
                                                        1), #overwrites the
                                                        previously saved TensorBoard
                                                         file.
        "EarlyStopping" : tf.keras.callbacks.EarlyStopping(patience=1000,
                                                        restore_best_weights=True),
        "ProgbarLogger" : tf.keras.callbacks.ProgbarLogger(),
        "ReduceLROnPlateau": tf.keras.callbacks.ReduceLROnPlateau(),
    }
```

```
        self.keep_showing_figure = True #this has to be kept in order to make
                                              things simple and modular.

        self.folder = "test"

        #recording the model itself
        self.model = None

        # A list of variables used for sharing numerical data/object across
                                              methods.
        self.data_input = {
            # This dictionary only stores the corresponding data,
            # all of which are stored in the format of DataFrame
            "feature_before_preprocessing" : None,
            "train_feature" : None,
            "test_feature"  : None,

            "label_before_preprocessing"   : None,
            "train_label"   : None,
            "test_label"    : None,

            "true_spec" : None, # in usual operation, post-processing "
                                                  test_label" will give "
                                                  true_spec";
                                # i.e. the testing split of the trimmed "
                                                                      label_before_prep
                                                                      " is
                                                                      identical
                                                                       to
                                                                      true_spec
                                                                      .
            "ref_spec"  : None, # a THIRD line to be plotted on the graph. This
                                                   is only utilized when
                                                  predicting the demo data.
            "ref_info"  : None, # dataframe from which the title text is loaded
                                                  .

            "group_structure" : None,
            "response_matrix" : None,
        }

        self.evaluation_output = {
            # this is a hybrid dictionary that stores data in various formats (
                                                  numpy.array, pandas.
                                                  DataFrame, list).
            "hist_df" : None,
            "predicted_labels_array_before_post_processing": None, # Holds the
                                                  prediction values (from file
                                                   or from test set)
            "predicted_labels_array_after_post_processing" : None,
            "error" : [],  # list of elementwise error
        }

    def interactive_neural_network_maker(self):
        key_input_prompt = "input the any key or attribute whose value that you
                                              'd like to change, or input 'c'
                                              to exit:"
        for d in self.settable_property_list:
            print("{0} :".format(d))
            print(getattr(self,d), "\n")
        while True:
            key_input = input(key_input_prompt)
            if key_input=="c":
                break
            for d in self.settable_property_list:
                val_input_prompt = "input the value for {0} as you would in
                                                python script ('quotes'
                                                around str, [brac]
                                                around lists, etc.):".
                                                format(d)
                if type(getattr(self,d))==dict:
                    keys = getattr(self,d).keys()
                    for k in keys:
                        if key_input.strip()==k:
                            val_input = convert_str_value(input(
                                                            val_input_prompt
                                                            ))
                            dict_copy = getattr(self,d)
                            dict_copy[k]=val_input
                            setattr(self,d,dict_copy)
                            print(d, "now takes the value of ", dict_copy)
                elif key_input.strip()==d:
                    val_input = convert_str_value(input(val_input_prompt))
                    setattr(self,d,val_input)
                    print(d, "now takes the value of ", val_input)

    def try_to_update_attribute(self, test_k, value):
        if hasattr(self, test_k):
            setattr(self, test_k, value)
            return
        else:
            dictionaries = [ i for i in dir(self) if type( getattr(self,i) )==
                                                    dict] #get the list of
                                                    attributes which are
                                                    dictianaries.
            for dic_name in dictionaries:
                if test_k in getattr(self,dic_name).keys(): # if the input key
                                                        is found in the
                                                        dictionary.
                    dic_copy = getattr(self, dic_name) #get a copy of the
                                                        dictionary
                    dic_copy[test_k] = value # change the corresponding value
                    setattr(self, dic_name, dic_copy)
                    return # only stop retun the method if we stop the case.
            raise KeyError("no attribute or key named", test_k)

    def load_data(self, csv_file, data_input_key):
        '''
        Retrieve data from .csv in the same directory without normalziation;
        Usual use case is
        nn.load_data("reaction_rate.csv","feature_before_preprocessing")
        nn.load_data("flux.csv", "labels_before_preprocessing")
        '''
        df = pd.read_csv(csv_file, delimiter=",", header=None, comment="#")

        # Error-checking:
        # Ensure that the data obtained are of the correct size before saving
                                            it as a class attribute.
        if "label" in data_input_key:
```

```
        opposite_key = data_input_key.replace("label", "feature")
    elif "feature" in data_input_key:
        opposite_key = data_input_key.replace("feature", "label")
    elif data_input_key=="ref_spec":
        opposite_key = "feature_before_preprocessing"
    elif data_input_key=="true_spec":
        opposite_key = "test_label"
    elif data_input_key=="group_structure":
        pass #ignore this case
    elif data_input_key=="response_matrix":
        df = pd.read_csv(csv_file, header=None, index_col=0) #redo the read
                                        , including the indices name
                                         for each row.
    elif data_input_key=="ref_info":
        df = pd.read_csv(csv_file, header="infer") #redo the read,
                                        including the column headers
        opposite_key="label_before_preprocessing"
    else:
        raise KeyError( "data_input_key='{0}' not found".format(
                                        data_input_key) )

    #by asserting that the opposite entry is of the same shape if it has
                                    been loaded:
    if data_input_key=="group_structure": #specific treatment for loading
                                    group_structure.
        num_boundaries = len(df.values.flatten())
        assert num_boundaries == max( np.shape(df) ), "The .csv where the
                                        group_structure is stored"\
            "must contain only a single line of data, stored vertically or
                                            horizontally"

        if type(self.data_input["label_before_preprocessing"])!=type(None):
            label_num_col = len(self.data_input["label_before_preprocessing
                                            "].columns)
        elif type(self.data_input["train_label"])!=type(None):
            label_num_col = len(self.data_input["train_label"].columns)
        try:
            assert num_boundaries== ( label_num_col+1 ), "there must be N+1
                                            "\
                "group boundaries value provided for N flux values provided
                                                ; "\
                "But at the moment the group_structure has length = {1} "\
                "which doesn't match the second dimension of train_label's
                                                boundary "\
                "{0}".format( num_boundaries , np.shape(self.data_input["
                                                train_label"]) )
                #Check that the shape of group_structure corresponds with
                                                the labels.
        except UnboundLocalError as E:
            if "label_num_col" in str(E):
                pass # this means the group structure was loaded before "
                                                train_label" or "
                                                label_before_preprocessing
                                                "
    elif data_input_key =="response_matrix":
        index_len, columns_len = df.shape
        if type(self.data_input["label_before_preprocessing"])!=type(None):
            label_col_len = len(self.data_input["label_before_preprocessing
                                            "].columns)
            assert label_col_len==columns_len, "number of columns in the
```

```
                                                              response matrix({1})
                                                              must equal to the number
                                                               of neutron groups({0})"
                                                              .format(label_col_len,
                                                              columns_len)
            if type(self.data_input["feature_before_preprocessing"])!=type(None
                                                          ):
                feature_col_len = len(self.data_input["
                                                              feature_before_preprocessing
                                                              "].columns)
                assert feature_col_len==index_len, "number of activites in
                                                              features({0}) must equal
                                                               to the number of rows
                                                              in the response matrix({
                                                              1}).".format(
                                                              feature_col_len,
                                                              index_len)
        elif type(self.data_input[opposite_key]) != type(None):
            assert len(self.data_input[opposite_key].index) == len(df.index
            ),  "The entries in {0} must have one-to-one correspondance" \
                "with the entries in {1}. But they have shape {2} and {3}" \
                "respectively".format(data_input_key, opposite_key, np.shape(df
                                                              ),
                np.shape(self.data_input[opposite_key]))
        assert not (df.isnull().values.any()), "NaN value(s) found inside
                                                       dataframe!"

        #saving the dataframe as an attribute to be used across the class.
        self.data_input.update({data_input_key:df})

    def _preprocess_numerical_values(self, df_or_array, datatype):
        assert (datatype=="feature") or (datatype=="label"), "The datatype must
                                                        be specified either as 'label'
                                                       or 'feature'."
        if datatype=="feature":
            if self.data_preparation_options["log_feature"]:
                df_or_array = np.log(df_or_array)
                df_or_array = np.clip(df_or_array, np.log( self.
                                                              data_preparation_options
                                                              ["lower_limit"] ), None)
                                                               #
        if datatype=="label":
            if not self.data_preparation_options["label_already_in_PUL"]:
                df_or_array = self._convert_to_PUL(df_or_array)
            if self.data_preparation_options["log_label"]:
                df_or_array = np.log(df_or_array)
                df_or_array = np.clip(df_or_array,np.log( self.
                                                              data_preparation_options
                                                              ["lower_limit"] ), None)
                                                                #clip all values to
                                                              above zero to prevent -
                                                              inf's when taking log.
            if self.data_preparation_options["ft_label"]:
                df_or_array = fft(df_or_array)
        return df_or_array

    def trim_data(self): # self.data_reordering_options["cutoff"]
        '''
        Cut out unused data from self.data_input["feature"] and self.data_input
                                                        ["label"]
        using self.data_reordering_options["cutoff"]
        '''
        cutoff_point = self.data_reordering_options["cutoff"] #copying the
                                                 global cutoff variable to a
                                                 shorter expression.
        startoff_point = self.data_reordering_options["startoff"]
        if (cutoff_point==None) and (startoff_point==None): print("trim_data
                                                 called but data is not trimmed
                                                 since startoff and cutoff=None")
        self.data_input["feature_before_preprocessing"] = self.data_input["
                                                 feature_before_preprocessing"][
                                                 startoff_point:cutoff_point]
        self.data_input["label_before_preprocessing"] = self.data_input["
                                                 label_before_preprocessing"][
                                                 startoff_point:cutoff_point]
        if type(self.data_input["ref_spec"])!=type(None): #if ref_spec is not
                                                 empty:
            self.data_input["ref_spec"] = self.data_input["ref_spec"][
                                                     startoff_point:cutoff_point]
        if type(self.data_input["ref_info"])!=type(None):
            self.data_input["ref_info"] = self.data_input["ref_info"][
                                                     startoff_point:cutoff_point]

    def shuffle(self): # self.data_reordering_options["shuffle_seed"]
        '''
        shuffle the *_before_preprocessing DataFrames in self.data_input to a
                                                 random but reproducible order
        using self.data_reordering_options["shuffle_seed"]
        '''
        assert len(self.data_input["feature_before_preprocessing"])==len(
            self.data_input["label_before_preprocessing"]), "features and
                                                     labelsmust have 1-to-1
                                                     correspondance."
        indices = np.arange(len(self.data_input["feature_before_preprocessing"]
                                                 ))
        if self.data_reordering_options["shuffle_seed"] != None:
            np.random.seed(self.data_reordering_options["shuffle_seed"])
            np.random.shuffle(indices)  # operate in-place
        else:
            print("shuffle is called but data is not shuffled since
                                                     shuffle_seed=None")
        self.data_input["feature_before_preprocessing"]= self.data_input["
                                                 feature_before_preprocessing"].
                                                 loc[indices]
        self.data_input["label_before_preprocessing"]  = self.data_input["
                                                 label_before_preprocessing"].loc
                                                 [indices]
        if type(self.data_input["ref_spec"]) != type(None):
            self.data_input["ref_spec"] = self.data_input["ref_spec"].loc[
                                                     indices]
        if type(self.data_input["ref_info"]) != type(None):
            self.data_input["ref_info"] = self.data_input["ref_info"].loc[
                                                     indices]

    def split_into_sets(self): # self.data_reordering_options["train_split"]
        '''
        populate train_* and test_*
        by splitting *_before_preprocessing in two parts
        according to the fraction determined by self.data_reordering_options["
                                                 train_split"]
        '''
        print("populating sets from *_before_preprocessing...")
        sample_size = len(self.data_input["feature_before_preprocessing"].index
                                              )
        # Use the first part as training data, the second part as
        num_train = round(self.data_reordering_options["train_split"] *
                                              sample_size)

        self.data_input["train_feature"] = self.data_input["
                                              feature_before_preprocessing"].
                                              iloc[:num_train]
        self.data_input["test_feature"] = self.data_input["
                                              feature_before_preprocessing"].
                                              iloc[num_train:]

        self.data_input["train_label"] = self.data_input["
                                              label_before_preprocessing"].
                                              iloc[:num_train]
        self.data_input["test_label"] = self.data_input["
                                              label_before_preprocessing"].
                                              iloc[num_train:]
        if type(self.data_input["ref_spec"])!=type(None):
            self.data_input["ref_spec"] = self.data_input["ref_spec"][num_train
                                                  :]
        if type(self.data_input["ref_info"])!=type(None):
            self.data_input["ref_info"] = self.data_input["ref_info"][num_train
                                                  :]

    def preprocess_input(self): # self.data_preparation_options
        '''
        Transform the numerical values inside the dataframe (in self.data_input
                                              ) (reversibly)
        using the options listed in self.data_preparation_options
        '''
        #pick out ONLY the test_* and train_* labels and features; leaving the
                                              *_before_preprocessing alone.
        df_list = [ df_key for df_key in self.data_input.keys() if ("_feature"
                                              in df_key) or ("_label" in
                                              df_key) ]
        for k,v in self.data_input.items():
            if type(v) != type(None): # filter out all empty cases
                if "feature" in k:
                    v = self._preprocess_numerical_values( v , "feature")
                if "label" in k:
                    v = self._preprocess_numerical_values( v , "label")
                self.data_input.update({k:v})

    def _print_module_name(self): # dependent on whether build_model is called
                                          with print_pretty_logo=True or False
                                          .

        print("'|.   '|'                                  '||  ")
        print(" |'|   |    ....  ... ...  ... ..   ....    ||  ")
        print(" | '|. |  .|...||  ||  ||   ||' '' '' .||   ||  ")
        print(" |   |||  ||       ||  ||   ||     .|' ||   ||  ")
        print(".|.   '|    '|...'  '|..'|. .||.    '|..'|' .||. ")
        print("                                                ")
        print("                                                ")
        print("'|.   '|'           .                               '||      ")
        print(" |'|   |    ....  .||.  ... ... ...   ...   ... ..   ||  ..  ")
        print(" | '|. |  .|...||  ||    ||  ||  |  .|  '|.  ||' ''  || .'   ")
        print(" |   |||  ||       ||     ||| |||   ||   ||  ||      ||'|.   ")
        print(".|.   '|   '|...'  '|.'    |   |     '|..|' .||.    .||. ||. ")

    def build_model(self, print_pretty_logo=True): # self.hyperparameter
        '''
        using arguments saved in self.hyperparameter
        (which includes tf_seed,hidden_layer,act_func,learning_rate,
                                               loss_func,metrics)
        a model is generated.
        '''
        tf.random.set_random_seed(self.hyperparameter["tf_seed"])

        # act_func should be a list
        act_func_iter = iter(
            [activations.linear, ] + self.hyperparameter["act_func"])  # ensure
                                                that the first layer is a
                                               purelin activation

        def get_next_activation_function():  # create a short method to iterate
                                              through activation functions
            try:
                act = next(act_func_iter)
            except StopIteration:
                act = activations.relu  # if user hasn't given enough
                                                   activation functions,
                                                   pad the rest using relu.
            return act

        neural_network_structure = []
        for n in self.hyperparameter["hidden_layer"]:
            if type(n) == int: # if it is an integer, interpret it as "numebr
                                               of nodes to insert into the
                                               next layer",
                neural_network_structure.append(layers.Dense(n, activation=
                                                   get_next_activation_function
                                                   ())) # and match it to
                                                   the next activation
                                                   function on the list.
            elif type(n) == float:
                assert 0 < n < 1, "a float value is interpreted as a drop out
                                                   rate, thus must be a
                                                   fraction between 0 and 1
                                                   ."
                neural_network_structure.append(layers.Dropout(n))

        # The zeroth and last layer have linear activation functions
        # and shape corresponding to the input and output respectively.
        neural_network_structure.append(layers.Dense(len(self.data_input["
                                               train_label"].columns),
                                               activation=activations.linear))
        # first_layer_size = first integer value, otherwise if there are no
                                               hidden layers, then it equals
                                               the number of labels
        first_layer_size = len(self.data_input["train_label"].columns)
        for n in self.hyperparameter["hidden_layer"]:
            if type(n) == int:
                first_layer_size = n
                break
        # forcefully overwrite the first layer to have a purelin activation
                                               function,
        # and make sure the zeroth layer understands the input shape to be of
                                                  shape=self.num_feature
        neural_network_structure[0] = layers.Dense(first_layer_size,
                                                  input_shape=[len(self.data_input
                                                  ["train_feature"].columns)],
                                                        activation=activations.



        #getting the loss function:
        loss_func = convert_str_to_loss_func(self.hyperparameter["loss_func"],
                                                  self.data_input["response_matrix
                                                  "], self.
                                                  data_preparation_options["
                                                  log_label"])

        model = keras.Sequential(neural_network_structure)
        model.compile(
            # loss="mean_squared_error",
            # loss="logcosh",
            loss=loss_func,
            # Mean squred error is the most sensible and widely chosen option
                                                       among all loss functions in
                                                       this case,
            # where where we're preforming a regression with no other boundary
                                                       condition (e.g. area under
                                                       graph =1) applied.
            # But perhaps later we may wish to define some functions to
                                                       penalize for discontinuity
                                                       between bins,
            # e.g.
            # def loss(x): return abs(np.diff(x)))
            optimizer=self.hyperparameter["optimizer"],  # use the RMS
                                                       propagation algorithm listed
                                                        above
            metrics=self.hyperparameter["metrics"] #******Look at changing the
                                                       loss function and metrics!!!
            # save these parameters into the history object such that the
                                                       accuracy of the NN to the
                                                       validation set can be
                                                       tracked.
        )
        if print_pretty_logo:
            self._print_module_name()
        # save these parameters as the class attributes
        self.optimizer = model.optimizer  # save the optimizer
        self.model = model

    def _print_params_as_dictionary(self): # dependent on whether train_model
                                                  is called with
                                                  print_dict_before_training=True or
                                                  False.
        '''print all non-numerical parameters and hyperparameters to stdout'''
        dictionary_of_params = {}
        for k in self.settable_property_list:
            dictionary_of_params[k] = getattr(self, k)
        for k, v in dictionary_of_params.items():
            print(k, ":", v, "\n")

    def train_model(self, print_dict_before_training = True, verbose=0): # "
```

```
                                                     num_epochs", "validation_split",
                                                     callbacks_applied
    '''
    self.data_reordering_options["validation_split"]
    self.hyperparameter["num_epochs"]
    self.callbacks_applied, which contains the keys
        PrintEpochInfo
        TensorBoard
        EarlyStopping
        ProgbarLogger
        ReduceLROnPlateau
    usually only the first two are used.
    '''
    if print_dict_before_training:
        self._print_params_as_dictionary()

    print("using {0} training samples, which consist of a validation split
                                                         = {1}, begin training for #
                                                         epochs = {2}...".format(
        len(self.data_input["train_feature"].index), self.
                                                             data_reordering_options["
                                                             validation_split"], self.
                                                             hyperparameter["num_epochs"]
                                                             ) )

    history = self.model.fit(

        self.data_input["train_feature"],
        self.data_input["train_label"]  ,

        epochs = self.hyperparameter["num_epochs"],
        validation_split = self.data_reordering_options["validation_split"]
                                                             ,
        verbose = verbose,
        callbacks = [ self.callback_objects_available[k] for k in self.
                                                             callbacks_applied ],

    )
    print("\ntraining complete!\n")  # skip a line to avoid overwriting the
                                                          previous lines.

    hist_df = pd.DataFrame(history.history)
    epoch_of_interest = -1
    if 'EarlyStopping' in self.callbacks_applied:
        epoch_of_interest = hist_df["val_loss"].idxmin()
        self.hyperparameter["num_epochs"] = epoch_of_interest
    self.losses.update(dict(hist_df.iloc[epoch_of_interest]))

    hist_df['epoch'] = history.epoch # a column handle for plotting
    print(hist_df.tail())
    self.evaluation_output["hist_df"] = hist_df
    self.timing["run_time_seconds"] = time.time() - self.timing["
                                                         start_time_raw"]

def auto_generate_session_name(self): # add stuff in front of self.
                                                     session_name
    all_non_dropout_layers = [l for l in self.hyperparameter["hidden_layer"
                                                         ] if type(l) == int]

    num_layer_str = str(len(all_non_dropout_layers)) + "_layer" #
```

```
                                                characterise the session by the
                                                number of layers used.

    datetime_str = time.strftime("%m%d_%H%M") + "_" # add the date and time
                                                 to prevent name conflict

    #Sort these into folders according to their loss values.
    '''
    loss_value = list(self.evaluation_output["hist_df"]["val_loss"])[-1] #
                                                get the validation loss from the
                                                 hist_df, which is guaranteed to
                                                 have been generated and
                                                recorded at the training stage.
    if self.losses["loss"]!=0: #if the test loss has been recorded:
        loss_value = self.losses["loss"]
    '''
    self._evaluate_against_test_set() #force _evaluate_against_test_set to
                                                be run so that the self.losses['
                                                test_loss'] takes a non-zero (
                                                meaningful) value.
    rounddown_loss_magnitude = np.floor(np.log10(self.losses['test_loss']))
                                                .astype(int) #sort the .png's
                                                into folders according to their
                                                numbers.
    dir_str = "lossabove1e"+ str(rounddown_loss_magnitude) + "/"
    if not os.path.exists(dir_str): os.makedirs(dir_str)

    # sort by 1. loss value, 2. time,     3.hyperparameter,    4. custome
                                                name
    session_name = dir_str + datetime_str + num_layer_str + self.
                                                session_name

    self.session_name = session_name
    print("this session's details are saved in", session_name)

def save_params_as_dictionary(self): #Overwrite old *_params.txt dictionary
                                             if present
    '''save all non-numerical parameters and hyperparameter into a .txt
                                                file.'''
    original_params_txt = self.session_name.split("layer")[-1]+"_params.txt
                                                " #always save at the CURRENT
                                                working directory; by ignoring
                                                all that *layer etc. stuff
                                                generated.
    f = open(original_params_txt, "w")
    f.write("{\n")
    def _write_datum(datum):
        if type(datum)==str:
            f.write("'")
            f.write(datum)
            f.write("'")
        else:
            f.write(str(datum))
    for k_1 in self.settable_property_list:
        entry = getattr(self, k_1)
        if type(entry)==dict:
            for k_2 in entry:
                f.write(k_2)
                f.write(" : ")
                _write_datum(entry[k_2])
                f.write("  ,\n")
        else:
            f.write(k_1)
            f.write(" : ")
            _write_datum(entry)
            f.write("  ,\n")
    f.write("}")
    f.close()

def save_NN_weights(self):
    if not os.path.exists(".checkpoints/"): os.makedirs(".checkpoints/")  #
                                                    make sure .checkpoint/ exist
    self.model.save_weights(".checkpoints/" + self.session_name.split("/")[
                                                   -1] + ".h5")  # save the NN in
                                                   the .checkpoints directory,
                                                   ignoring the lines before it.

def plot_history(self, show_plot_instead_of_saving = False):  # self.
                                              session_name+"_loss_value.png" will
                                              become the name of the saved plot
    num_metrics = len(self.hyperparameter["metrics"])+1 # loss + metrics =
                                                   total number of metrics that
                                                   will get outputted
    df = self.evaluation_output["hist_df"]  #get the hist_df in form of a
                                                   shorter variable name.
    columns = df.columns[:-1] #ignoring the last column, which is the epoch
                                                    number.
    optimal_epoch = self.hyperparameter["num_epochs"]

    fig, axes = plt.subplots(num_metrics, 1, sharex=True)  # Vertically
                                                   stack the graphs
    if num_metrics==1:
        axes = [axes,] #wrap the single element into a list so that it can
                                                       also be iterated through as
                                                       well.

    axes[0].set_title("Performance of the neural network wrt. training
                                                   progress")
    for i in range(num_metrics):
        train = columns[i]
        valid = columns[num_metrics+i]
        axes[i].set_ylabel( " ".join(columns[i].replace("squared","sq.").
                                                       replace("absolute","abs.").
                                                       replace("error","err.").
                                                       split("_")) ) #replace the _
                                                        with space. and abbreviate.
        axes[i].semilogy(df["epoch"], df[ train ], label="train. error" )
        axes[i].semilogy(df["epoch"], df[ valid ], label="val. error")
        axes[i].legend()
        y_scatt = (df[train][optimal_epoch], df[valid][optimal_epoch])
        axes[i].scatter( np.ones(2)*optimal_epoch, y_scatt, color="r",
                                                       marker="x")
    axes[-1].set_xlabel("# epochs")

    if show_plot_instead_of_saving:
        plt.show()
    else:
        plt.savefig(self.session_name + "_error_variation.png")
    plt.clf()
    plt.close()
```

```
def _evaluate_against_test_set(self):
    # Print loss values when evaluated against test set
    losses_output = self.model.evaluate(self.data_input["test_feature"],
                                        self.data_input["test_label"]) #
                                        use tf.model.evalulate to get
                                        the loss values of the
                                        predictions.
    if type(losses_output) == list:
        for i in range(len(losses_output)):
            key = list(self.losses.keys())[i]
            self.losses.update({"test_"+key: losses_output[i]})
    else:
        self.losses.update({"test_loss": losses_output})
    self.save_params_as_dictionary() #overwrite existing dictionary with a
                                        very
    print("The loss values and other metrics when evaluated against the
                                        test set are obtained as {0}".
                                        format(self.losses) )
    # find the element-wise error
    self.evaluation_output["predicted_labels_array_before_post_processing"]
                                         = self.model.predict(self.
                                        data_input["test_feature"]) #use
                                         tf.model.predict to get the
                                        actual prediction themselves.
    self._postprocess_output() # popularte using the program self.
                                        postprocess_numerical...
    self.evaluation_output["error"] = self.evaluation_output["
                                        predicted_labels_array_before_post_proces
                                        "].flatten() - self.data_input["
                                        test_label"].values.flatten()
    #   use the difference between prediction and true values BEFORE
                                        postprocessing as the deviation/
                                        error list.
    #= self.evaluation_output["predicted_labels_array_after_post_processing
                                        "].flatten() - self.data_input["
                                        true_spec"].values.flatten()
    #   instead of using the difference of their respective values AFTER
                                        postprocessing.

# compute how far off each label is, element-wise
def plot_test_results_histogram(self, show_plot_instead_of_saving=False):
    prepend_in_bracket = ""
    if self.data_preparation_options["log_label"]:
        prepend_in_bracket += "log of "
    if self.data_preparation_options["ft_label"]:
        prepend_in_bracket += "fourier coefficients of "
    if len(self.evaluation_output["error"]) == 0:
        self._evaluate_against_test_set()#ensure that the error list isn't
                                                empty before continuing with
                                                 the rest of the current
                                                method"
    plt.hist(self.evaluation_output["error"], bins=25)
    plt.suptitle("Prediction error on each element of the label, (i.e. " +
                                        prepend_in_bracket + "flux PUL"+
                                         ")")
    plt.title("loss function(prediction, test_label)={0}".format(self.
                                        losses["test_loss"]))
    plt.xlabel("Error")
    plt.ylabel("Count")
```

```
        if show_plot_instead_of_saving:
            plt.show()
        else:
            plt.savefig(self.session_name + "_error_distribution.png")
        plt.clf()
        plt.close()

    def _postprocess_numerical_values(self, df_or_array, datatype): #datatype
                                          states whether it's 'label' or '
                                          feature' that's being processed.
        assert (datatype=="feature") or (datatype=="label"), "The datatype must
                                               be specified either as 'label'
                                              or 'feature'."
        if datatype=="feature":
            if self.data_preparation_options["log_feature"]:
                df_or_array = e**df_or_array
        if datatype=="label":
            if self.data_preparation_options["ft_label"]:
                df_or_array = ifft(df_or_array)
            if self.data_preparation_options["log_label"]:
                df_or_array = e**df_or_array
            if not self.data_preparation_options["label_already_in_PUL"]:
                gs = self.data_input["group_structure"].values.flatten()#
                                                      shorten the group
                                                      structure list into 'gs'
                lethargy_span = np.diff(np.log(gs))                    #
                                                      calculate the lethargy
                                                      span of each bin
                df_or_array = df_or_array*lethargy_span                #
                                                      multiply the label (
                                                      representing flux PUL)
                                                      by lethargy span to get
                                                      total flux instead.
        return df_or_array

    def _postprocess_output(self):
        self.evaluation_output["predicted_labels_array_after_post_processing"]
                                              = self.
                                              _postprocess_numerical_values(
                                              self.evaluation_output["
                                              predicted_labels_array_before_post_proces
                                              "], "label")
        self.data_input["true_spec"] = self._postprocess_numerical_values(self.
                                              data_input["test_label"], "label
                                              ") #un-log and un-fourier
                                              transform the data to get it
                                              back into the correct form.

    def _convert_to_PUL(self, flux):
        gs = self.data_input["group_structure"].values.flatten() #shorten the
                                              variable name into 'gs'
        lethargy_span = np.diff(np.log(gs)) #calculate the lethargy span of
                                              each bin
        flux = flux/lethargy_span
        return flux

    def _split_line_at_threshold(self, flux, upper_or_lower = "lower",
                                          threshold = 2):
        '''
        covnert flux to flux PUL,
        and chop it, leaving only the half that's above/below the threshold
                                                  energy value.
        '''
        gs = self.data_input["group_structure"].values.flatten()
        # flux = self._convert_to_PUL(flux) #the flux has already been
                                                  converted to PUL when inputting
                                                  it.
        thres_ind = abs(gs - threshold).argmin() #find the index of the closest
                                                  to the threshold
        if upper_or_lower =="lower":
            gs_cut = gs[:thres_ind+1]
            flux_cut = np.hstack([flux[0], flux[:thres_ind]])
        elif upper_or_lower=="upper":
            gs_cut = gs[thres_ind:]
            flux_cut = np.hstack([flux[thres_ind], flux[thres_ind:]])
        return gs_cut, flux_cut

    def _side_by_side_plot(self, press, ind, true_line, predicted_line ,
                                                ref_spec_line=None, ref_info_line=
                                                None):
        '''
        make two plots,
            ax1 compares total flux in each bin according to bin number, by
                                                  plotting predicted flux and
                                                  true_flux side-by-side
            ax2 plots the flux in each bin.
        '''
        fig, (ax1, ax2) = plt.subplots(1, 2, sharey=True)
        # label the axes.
        ax1.set_xlabel("bin number"); ax1.set_ylabel("flux per unit lethargy
                                                  per unit fluence (1/s)")
        ax2.set_xlabel("energy (MeV)")#; ax2.set_ylabel("flux (per unit
                                                  lethargy)")
        # make the plot on the right a log-log plot,
        # ax1.set_yscale("log")
        ax2.set_yscale("log"); ax2.set_xscale("log")

        #add titles
        ax1.set_title("smooth plot of spectrum for comparison purpose."); ax2.
                                                  set_title("log-log plot of
                                                  spectrum")
        plt.suptitle("test spectrum " + str(ind))
        if type(ref_info_line)!=type(None):
            plt.suptitle(ref_info_line["title"]) #overwrite the suptitle
        # link up to the press() function (defined locally within the scope of
                                                  self.compare_individual_spectra
                                                  ())
        fig.canvas.mpl_connect('key_press_event', press)
        #actual plotting
        ax2.step(*self._split_line_at_threshold(true_line, "upper", threshold=0
                                                  ), label="true fluence", alpha=0
                                                  .8)
        ax2.step(*self._split_line_at_threshold(predicted_line, "upper",
                                                  threshold=0), label="fluence
                                                  predicted by NN", alpha=0.8)
        ax1.semilogy(true_line, label="true fluence", alpha=0.8)
        ax1.semilogy(predicted_line, label="fluence predicted by NN", alpha=0.8
                                                  )
        #plotting the original spectrum if it exist.
        if type(ref_spec_line)!=type(None):
```

```
        ax2.step(*self._split_line_at_threshold(ref_spec_line), label="
                                                original flux before
                                                perturbation", alpha=0.8)
        ax1.semilogy(ref_spec_line, label="original flux before
                                                perturbation", alpha=0.8)
    #apply legends
    ax1.legend()
    ax2.legend()
    #maximize window
    mng = plt.get_current_fig_manager()
    if hasattr(mng, 'frame'):  # works with ubuntu
        mng.frame.Maximize(True)  # try to maximize the window
    else:
        try:
            mng.window.showMaximized()
            # mng.resize(*mng.window.maxsize())
        except:
            pass  # ignore this if python cannot maximize window; it has to
                                                     be maximized manually.
    plt.show()
    plt.clf(); plt.close() #show an then close.

def _C_E_plot(self, press, ind, true_line, predicted_line, ref_spec_line=
                                          None, ref_info_line=None, threshold=
                                          2):
    '''
    Plot the original spectrum and the NN's prediction on the same graph,
                                              and show the C/E value of each
                                              point below it.
    '''
    # naming axes according to the scale at x and y axes.
    fig, ([log_data, lin_data],
          [log_ce,     lin_ce]) = plt.subplots( 2, 2, sharex='col', sharey=
                                                  'row',
                                                  figsize=(12, 8),
                                                  gridspec_kw={   '
                                                                  '
    plt.suptitle("test spectrum " + str(ind))
    if type(ref_info_line)!=type(None):
        plt.suptitle(ref_info_line["title"])
    log_data.set_xscale("log")
    lin_data.set_xscale("linear")
    log_data.set_yscale("log")
    log_data.set_ylabel("flux per unit lethargy per unit fluence (1/s)")
    log_ce.set_ylabel("calculated/expected (C/E)")
    unit="eV"
    if threshold<100: unit="MeV"
    log_ce.set_xlabel("E ({0}) on log scale".format(unit) )
    lin_ce.set_xlabel("E ({0})".format(unit) )
    log_ce.axhline(1,color="gray")
    lin_ce.axhline(1,color="gray")

    def plot_data(flux, label):
        log_data.step(*self._split_line_at_threshold(flux, "lower",
                                                threshold), label=label,
                                                alpha=0.8)
        lin_data.step(*self._split_line_at_threshold(flux, "upper",
                                                threshold), label=label,
                                                alpha=0.8)

    def plot_ce(ce):
        log_ce.scatter(*self._split_line_at_threshold(ce, "lower",
                                                threshold), marker="x",
                                                alpha=0.6) #fmt="C0x"
        lin_ce.scatter(*self._split_line_at_threshold(ce, "upper",
                                                threshold), marker="x",
                                                alpha=0.6) #fmt="C0x"

    plot_data(predicted_line, label="fluence predicted by NN")
    plot_data(true_line, label="true fluence")
    if type(ref_spec_line)!=type(None):
        plot_data(ref_spec_line, label="ref_spec_line_before_perturbation")
                                                      #overwrite the suptitle
    plot_ce(predicted_line/true_line)

    # add legend to the graph
    log_data.legend()
    fig.tight_layout(rect=[0, 0, 1, 0.95]) # top right hand corner of 'rect
                                           '
    # has the coordinate (1,0.95) to prevent the suptitle clipping into the
                                                graph
    plt.savefig(self.session_name + "_test_" + str(ind).zfill(3) + "
                                              _fluence.png", dpi=180)
    plt.clf()
    plt.close()

def _reaction_rate_compare(self, press, ind, true_line, predicted_line ,
                                          ref_spec_line=None, ref_info_line=
                                          None, save_or_not=True):
    if type(ref_spec_line)!=type(None):
        ref_spec_line = np.array(ref_spec_line)

    response_matrix = np.array(self.data_input["response_matrix"])
```

```
assert np.ndim(response_matrix)==2, "Please load the response matrix
                                        before doing self.
                                        _reaction_rate_compare()!"
true_activities = response_matrix.dot(true_line)
predicted_activities = response_matrix.dot(predicted_line)
num_activites = np.arange( len(response_matrix) )

dist_in_log_space = np.log(predicted_activities/true_activities)
mu = 0
sigma = sum(np.sqrt( (dist_in_log_space-mu)**2 /len(dist_in_log_space)
                                        ))
# chi2_dof = sum( (dist_in_log_space-0)**2 )/len(dist_in_log_space)
# chi2txt = r"total $\frac{\chi^2}{DoF}$="+ str(chi2_dof) +"\n"+"
                                        assuming C/E is lognormally
                                        distributed around 1."
if save_or_not:
    fig, (bar, ce) = plt.subplots(2,1, sharex=True,
                    gridspec_kw={'height_ratios': [6, 1]})

    reaction_names = [ i.replace("_",",") for i in self.data_input["
                                            response_matrix"].index ]

    ce.set_xticks(num_activites)
    ce.set_xticklabels(reaction_names, rotation=30, fontdict={"fontsize
                                            ":8})

    num_bars = 2
    if type(ref_spec_line)!=type(None):
        ref_activites = response_matrix.dot(ref_spec_line)
        num_bars = 3
    width = 0.8/num_bars

    bar.set_ylabel("activity per unit fluence(1/s)")
    bar.bar(num_activites + width , predicted_activities, label="
                                            activities predicted by NN",
                                             width=-width, align="edge")
    bar.bar(num_activites, true_activities, label="true activities",
                                            width=-width, align="edge")
    if type(ref_spec_line)!=type(None):
        bar.bar(num_activites + 2*width, ref_activites, label= "
                                                original activities",
                                                width=-width, align="
                                                edge")
    bar.legend()
    bar.set_yscale("log")

    ce.axhline(1,color="gray")
    ce.scatter(num_activites, predicted_activities/true_activities,
                                            marker="x")
    ce.set_ylabel("C/E")

    sigmatxt = r"$\sigma$="+ str(sigma) +"\n"+"assuming C/E is normally
                                             distributed in log space,
                                            with a mean of 0."
    bar.set_title(sigmatxt)

    plt.suptitle( "test spectrum " + str(ind) )
    if type(ref_info_line)!=type(None):
        plt.suptitle(ref_info_line["title"]) #overwrite the suptitle
```

```
            # fig.text( 0.5, 0.0 , chi2txt, va="bottom", ha="center")
            # link up to the press() function (defined locally within the scope
                                                       of self.
                                                      compare_individual_spectra()
                                                      )
            fig.tight_layout(rect=[0, 0.03, 1, 0.95])
            plt.savefig(self.session_name + "_test_" + str(ind).zfill(3) + "
                                                      _activities.png", dpi=100)
            plt.clf()
            plt.close()
        return sigma

    def _renormalize_prediction(self, fluxPUL):
        if self.hyperparameter["loss_func"]=="mean_pairwise_squared_error":
            n = np.ndim(fluxPUL)
            fluxPUL = ((fluxPUL).T/np.sum(fluxPUL, axis=n-1)).T
        return fluxPUL

    def compare_individual_spectra(self, using_simple_data=False, threshold = 2
                                              , save_C_E_plots = True,
                                              save_reaction_rate_comparisons=True,
                                               silent_mode=False):
        def press(event): #for stopping the plot comparison program when the
                                                    key 'q' is pressed
            if event.key == 'q':
                self.keep_showing_figure = not self.keep_showing_figure
                print("Pressed 'q' to toggle self.keep_showing_figure to {0}".
                                                              format(self.
                                                              keep_showing_figure))

        does_ref_spec_exist = not (type(self.data_input["ref_spec"]) == type(
                                                    None))

        # Need to compare the self.data_input["true_spec"] against the
                                                    evaluation_output["
                                                    predicted_labels_array_after_post_process
                                                    "].
        # Therefore the next part gets the evaluation_output["
                                                    predicted_labels_array_after_post_process
                                                    "]
        if type(self.evaluation_output["
                                                    predicted_labels_array_after_post_process
                                                    "])==type(None): #in case the
                                                    _evaluate_against_test_set hasn'
                                                    t been ran
            #(such that _postprocess_output hasn't been called to populate
                                                      evaluation_output properly)
            print("postprocessing test_label and predicted_labels to get
                                                      true_spec and predicted
                                                      spectrum respectively.")
            self._evaluate_against_test_set()

        #shorten the names
        true_spec = self.data_input["true_spec"].values
        predicted_labels = self.evaluation_output["
                                                    predicted_labels_array_after_post_process
                                                    "]
        if does_ref_spec_exist:
            ref_spec = self.data_input["ref_spec"].values
        ref_info = self.data_input["ref_info"]
```

```
does_ref_info_exist = not type(ref_info)==type(None)

#covnert to PUL if not already in PUL.
if (not using_simple_data) and (not self.data_preparation_options["
                                    label_already_in_PUL"]):
    predicted_labels = self._renormalize_prediction(self.
                                        _convert_to_PUL(
                                        predicted_labels))
    true_spec = self._renormalize_prediction(self._convert_to_PUL(
                                        true_spec))#The true
                                        spectrum is left in the raw,
                                         non-PUL state until now.
    if does_ref_spec_exist:
        ref_spec = self._renormalize_prediction(self._convert_to_PUL(
                                            ref_spec))
sigma_list = []
for ind in range(len(predicted_labels)):
    if using_simple_data:
        fig, ax1 = plt.subplots()
        ax1.bar(np.arange(5), true_spec[ind], label="true fluence",
                                            width=0.4)
        ax1.bar(np.arange(5) + .4, predicted_labels[ind], label="
                                            fluence predicted by NN"
                                            , width=0.4)
        ax1.legend()
        plt.suptitle("test spectrum " + str(ind))
        fig.canvas.mpl_connect('key_press_event', press)
        # link up to the press() function (defined locally within the
                                            scope of self.
                                            compare_individual_spectra
                                            ())
        plt.show()
        plt.clf(); plt.close()
    else:
        ref_spec_line = None
        if does_ref_spec_exist:
            ref_spec_line = pd.DataFrame(ref_spec).iloc[ind]

        ref_info_line = None
        if does_ref_info_exist:
            ref_info_line = pd.DataFrame(ref_info).iloc[ind]
        if not silent_mode:
            self._side_by_side_plot(press, ind, true_spec[ind],
                                                predicted_labels[ind
                                                ], ref_spec_line=
                                                ref_spec_line,
                                                ref_info_line=
                                                ref_info_line)
        if save_C_E_plots:
            self._C_E_plot(press, ind, true_spec[ind], predicted_labels
                                                [ind], ref_spec_line
                                                =ref_spec_line,
                                                ref_info_line=
                                                ref_info_line,
                                                threshold=threshold)
        sigma = self._reaction_rate_compare(press, ind, true_spec[ind],
                                             predicted_labels[ind],
                                            ref_spec_line=
                                            ref_spec_line,
                                            ref_info_line=
                                                          ref_info_line,
                                                          save_or_not =
                                                          save_reaction_rate_comparisons
                                                          )
                #will not save if save_reaction_rate_comparisons is False; in
                                                          which case it will
                                                          simply return the sigma
                                                          to be appended to the
                                                          sigma_list below:
                sigma_list.append(sigma)
            if not self.keep_showing_figure:
                break #condition to stop showing more figures if 'q' is pressed
                                                           (self.
                                                          keep_showing_figure is
                                                          set by the locally
                                                          defined function 'press
                                                          ')
        mean_sigma = np.mean(sigma)
        self.losses.update({'std_of_log_of_C_over_E_reaction_rates':mean_sigma}
                                                    )
        '''
        #THIS IS A BODGE to insert a line into the _params.txt.
        if not save_C_E_plots:
            original_params_txt = self.session_name.split("layer")[-1]+"_params
                                                      .txt"
            with open(original_params_txt,"r") as f:
                lines = f.readlines()
            for i in range(len(lines)):
                if "}" in lines[i]:
                    brace_line_num = i
            with open(original_params_txt,"w") as f:
                [ f.write(l) for l in lines[:brace_line_num] ]
                f.write('std_of_log_of_C_over_E_reaction_rates : '+str(
                                                          mean_sigma)+' ,\n')
                [ f.write(l) for l in lines[brace_line_num:] ]
        '''
        self.save_params_as_dictionary()

    def predict_from_additional_file(self, prediction_file_name):
        raw_unlabelled_features = pd.read_csv(prediction_file_name, header=None
                                                    , comment="#")
        processed_unlabelled_features = self._preprocess_numerical_values(
                                                    raw_unlabelled_features, "
                                                    features")
        prediction_label_array_before_post_processing = self.model.predict(
                                                    processed_unlabelled_features)
        return self._postprocess_numerical_values(
                                                    prediction_label_array_before_post_proces
                                                    , "feature")

    def plot_training_spectra(self,threshold):
        processed_train_label_df = pd.DataFrame(self.data_input["train_label"])
        max_num_plots=None
        if len(processed_train_label_df)>200: max_num_plots=50

        fig, (log_data, lin_data) = plt.subplots( 1, 2, sharey=True,
                                                         figsize=(12, 7),
                                                         gridspec_kw={'width_ratios'
        log_data.set_xscale("log")
        lin_data.set_xscale("linear")
        log_data.set_yscale("log")
        log_data.set_ylabel("flux per unit lethargy per unit fluence (1/s)")
        unit="eV"
        if threshold<100: unit="MeV"
        log_data.set_xlabel("E ({0}) on log scale".format(unit))
        lin_data.set_xlabel("E ({0})".format(unit))

        for flux in processed_train_label_df.iloc[:max_num_plots].iterrows():
            log_data.step(*self._split_line_at_threshold(flux[1], "lower",
                                                       threshold=threshold), alpha=
                                                       0.4)
            lin_data.step(*self._split_line_at_threshold(flux[1], "upper",
                                                       threshold=threshold), alpha=
                                                       0.4)
        plt.suptitle("Some of the spectra used to train the neural network with
                                                      ")
        plot_name = self.session_name+"_training_spectra"
        if hasattr(self, "train_label_file"): plot_name = ".".join(getattr(self
                                                      , "train_label_file").split(".")
                                                      [:-1])
        plt.savefig(plot_name+".png")
```

B Neural network abstractions and controller

The following contains the higher level abstractions, as well as functions which walks the user through the process of creating a neural network interactively.

neuralnetworktrainer.py

```
from neuralnetworklibrary import *
from matplotlib import pyplot as plt
#This files contains the toolsets for doing the following three things:
#1. To demonstrate that neural network works when using_simple_data
#   (i.e. using the 5 reaction_rates obtained by folding the 5 randomly
                                      generated flux values through a 5x5 non-
                                      singular matrix, therefore giving a
                                      fully determined problem.)
#2. To demonstrate the neural network works when trying to unfold the simulated
                                       data.
#3. To investigate what hyperparameters is required if we were to invert the
                                      real data.
'''
#######Higher level automations############
This program offers two warpper method, which does all of the above methods all
                                       at once:
run_real_spectra / run_demo
'''
class NeuralNetworkHandler(NeuralNetwork):
    def __init__(self):
        super().__init__()
        self.using_simple_data=False # assume, by default, that we're not
                                       reading the simple, 5x5 case
                                       data.
        self.reactor_prefix=""
        self.activation_system=""

    def read_demo_data(self, using_simple_data=False):
        self.using_simple_data = using_simple_data
        if self.using_simple_data:
            print("using simple, 5x5, non-singular (fully determined) data ..."
                                         )
            self.reactor_prefix="simple_"
            self.activation_system=""
            self.data_preparation_options["label_already_in_PUL"] = True
        else:
            self.reactor_prefix="GS_eq_1_JAEA_FNS_"
            self.activation_system="ACT_"
        feature_file= self.reactor_prefix + self.activation_system + "RR.csv"
        label_file  = self.reactor_prefix + "spectra.csv"
        ref_spec_file=self.reactor_prefix + "reference_spectra.csv"
        response_matrix_file=self.reactor_prefix+self.activation_system+"
                                       Response_Matrix.csv"
        gs_file = "demo_gs.csv"
        self.load_data(feature_file, "feature_before_preprocessing")
        self.load_data(label_file,   "label_before_preprocessing")
        if not self.using_simple_data:
            self.load_data(ref_spec_file, "ref_spec")
            self.load_data(gs_file, "group_structure")
            self.load_data(response_matrix_file,"response_matrix")

    # higher level methods: methods that uses other lower level methods; read
                                     these for a summary of the program
    def cast_and_preprocess_data(self):
        '''
        Condense the whole data preparation stage into a single, more compact
                                       method.
        First trim the data (according to the self.data_re_ordering_options)
        '''
        # read the raw data
        if type(self.data_input["train_feature"])==type(None): #only do the
                                       splitting and shuffling if the
                                       train/test sets haven't been
                                       populated yet.
            self.trim_data()  # trim the data
            self.shuffle()  # shuffle the DataFrames
            self.split_into_sets()  # split the DataFrames into training sets
                                         and testing sets.
        self.preprocess_input()  # Take log and fourier analyse

    def build_and_train_model(self, quietly=False):
        self.build_model(print_pretty_logo = not quietly)
        self.train_model(print_dict_before_training = not quietly)

    def plot_performance(self, show_plot_instead_of_saving=False):
        self.plot_history(show_plot_instead_of_saving=
                                       show_plot_instead_of_saving)
        self.plot_test_results_histogram(show_plot_instead_of_saving=
                                       show_plot_instead_of_saving)
```

```
def show_results_of_training(self): #without saving
    # plot and save its performance
    self.plot_performance(show_plot_instead_of_saving = True)
    #Examine the weight matrix (as compared to the weights matrix)
    self.compare_individual_spectra(using_simple_data=self.
                                      using_simple_data,
                                      save_C_E_plots= False)

def compare_with_known_inverse(self, response_matrix_file_name="
                                  demogenerator/simple_response_matrix
                                  .csv"):
    '''
    Compare the  weights obtained for the linear regresser
    against the inverse of the non-singular matrix for the simplecase.
    '''
    assert self.using_simple_data, "This method is only used for the 5x5
                                      fully-determined case!"
    weights, biases = read_NN_weights(self.session_name)
    response_matrix = np.matrix(pd.read_csv(response_matrix_file_name,
                                      header=None))
    # Compare the analytically obtained inverse with the weights matrix
    import seaborn as sns
    sns.heatmap(response_matrix.I.T, annot=True)
    plt.savefig("true_inverse.png")

    plt.cla(); plt.clf(); plt.close() #clear everything

    sns.heatmap(weights["layer_1"], annot=True)
    plt.savefig("NN_weights_emulating_inverse_matrix.png")
    print("See the newly saved *.png ('true_inverse' and '
                                      NN_weights_emulating_inverse_matrix
                                      ') to compare how well the NN
                                      emulated the weights matrix of
                                      the 1st layer")
    print("Additionally, the biases in the 1st layer are \n", biases["
                                      layer_1"])
    return response_matrix, weights["layer_1"], biases["layer_1"]

def save_metrics_and_compare_reproducibly(self, threshold, save_plots=True,
                                   silent_mode=False):
    self.auto_generate_session_name()
    self.save_NN_weights()
    self.save_params_as_dictionary()
    self.plot_performance()
    if self.using_simple_data:
        #Examine the weight matrix (as compared to the response matrix's
                                          inverse)
        self.compare_with_known_inverse()
        self.compare_individual_spectra(using_simple_data=True)
    else:
        # opening up each predicted spectrum and plotting it side-by-side
                                          with the true spectrum and
                                          original spectrum
        self.compare_individual_spectra(threshold=threshold, save_C_E_plots
                                          =save_plots,
                                          save_reaction_rate_comparisons
                                          =save_plots, silent_mode=
                                          silent_mode)
def run_demo(self, using_simple_data=False):
    self.using_simple_data = using_simple_data
    self.read_demo_data()
    self.cast_and_preprocess_data()
    self.build_and_train_model()
    self.save_metrics_and_compare_reproducibly(threshold=2)

def run_real_spectra(self, save_plots=True, silent_mode=False):
    #self.condense_into_one_csv(directory)
    self.cast_and_preprocess_data()
    self.build_and_train_model()
    self.save_metrics_and_compare_reproducibly(threshold=2E6, save_plots=
                                               save_plots, silent_mode =
                                               silent_mode)

##Tutorials for new users

def program_structure(self):
    print("# To run a process successfully, the following methods have to
                                               be run:")
    print("# 0. Setting hyperparameters")
    print("interactive_neural_network_maker #alternatively, these can be
                                               changed manually by using
                                               setattr().")
    print("# 1. load and pre-processing")
    print("load_data('feature_before_preprocessing','
                                               label_before_preprocessing','
                                               group_structure')")
    print("# or in case of using demo data:")
    print("read_demo_data")
    print("trim_data (optional)")
    print("shuffle (optional)")
    print("split_into_sets (can skip if data is directly loaded into '
                                               train_*' and 'test_*' instead of
                                                splitting from '*
                                               _before_preprocessing' in the
                                               load_data() step)")
    print("preprocess_input")
    print("    # All of section 1 above, except load_data, is summarized by
                                                the method of
                                               cast_and_preprocess_data.")
    print("# 2. build and train model")
    print("build_model")
    print("train_model")
    print("    # These are summarized by build_and_train_model in
                                               NeuralNetworkHandler")
    print("# 3. for saving data (optional)")
    print("auto_generate_session_name")
    print("save_params_as_dictionary")
    print("save_NN_weights")
    print("# 4. for plotting (optional)")
    print("plot_history")
    print("plot_test_results_histogram")
    print("compare_individual_spectra")
    print("    # 3 and 4 are summarized by show_results_of_training and
                                               save_metrics_and_compare_reproducibly
                                                in NeuralNetworkHandler")
    print("")
    print("######### Alternatively section 1-4 above can be replaced by the
                                                single method")
    print("run_demo # for running the demonstrative data")
    print("# or in case of running a real data:")
    print("run_real_spectra")

def input_instructions(self):
    print("The data are inputted in the form of csv's,")
    print("each row representing one spectrum or its reaction rate.")
    print("The file containing the spectra should be loaded as the
                                               feature_file;")
    print("while the file containing the corresponding reaction rates
                                               should be loaded as the
                                               label_file.")
    print("A single line csv (horizontal or vertical) containing all the
                                               boundaries of the bins should be
                                                loaded as the gs_file")

def tutorial_demo(self):
    # print("This interactive tutorial is designed to be used in an
                                               interactive python environment (
                                               e.g. ipython).")
    print("This method walks the user through the process of creating a
                                               neural network, and then trains
                                               and runs this neural network on
                                               the demo data.")
    print("\n")
    print("The following is a list of options and hyperparameters to be
                                               inputted into the neural network
                                               .")
    self.interactive_neural_network_maker()
    print("Please state whether you would like to use the 5x5 fully-
                                               determined case, or the
                                               simulated 11x171 response matrix
                                                case.")
    while True:
        using_simple_data_y_n = input("type 'y' for fully-determined case,
                                                'n' for 11x171")
        if using_simple_data_y_n=="y":
            using_simple_data=True
            break
        elif using_simple_data_y_n=="n":
            using_simple_data=False
            break
    print("running the demo...")
    self.run_demo(using_simple_data=using_simple_data)

def interactive_menu(self):
    '''start here'''
    print("0. program_structure")
    print("1. input_instructions")
    print("2. tutorial_demo")
    print("3. interactive_neural_network_maker (to set the options and
                                               hyperparameters for this neural
                                               network)")
    while True:
        x = input("choose a number from the menu above:")
        if x in [str(i) for i in range(4)]:
            break
        print("input not accepted.")
    print("
                                               -----------------------------------------
```

```
                                                        ")
        if x=="0":
            self.program_structure()
        elif x=="1":
            self.input_instructions()
        elif x=="2":
            self.tutorial_demo()
        elif x=="3":
            self.interactive_neural_network_maker()

def continuous_neural_network_runner(filename, demo=False, using_simple_data=
                                        False):
    import shutil as shu
    print("_"*shu.get_terminal_size().columns) # print a separation line
                                            between each run.
    first_dict_lines, rest_of_the_lines = cut_file_in_halves(filename)
    dictionary_read = convert_lines_to_dict(first_dict_lines)
    #instantiate a NeuralNetworkHandler()
    nn = NeuralNetworkHandler()
    for k, v in dictionary_read.items():
        print(k, ":", v)
        if k.endswith("_file"):
            assert k[:-5] in nn.data_input.keys(), "File type not found"
            setattr(nn, k, v)
            nn.settable_property_list.append(k)
            nn.load_data(v, k[:-5])
        else:
            nn.try_to_update_attribute(k,v)
    #overwrite only if the attributes are set without raising any errors.
    overwrite_file_by_removing_first_dict(filename, rest_of_the_lines)
    if demo:
        nn.run_demo(using_simple_data=using_simple_data)
    else:
        nn.run_real_spectra(save_plots=False, silent_mode=True)

if __name__=="__main__":
    if len(sys.argv)==1:
        while True:
            continuous_neural_network_runner("real_hyperparameter_tweaking.txt"
                                                        , demo=False)
        while False:
            continuous_neural_network_runner("pre-presentation-demos.txt", demo
                                                        =True)
    elif len(sys.argv)>1:
        try:
            int(sys.argv[1])
            while True:
                continuous_neural_network_runner("job_number_"+sys.argv[1]+".
                                                txt", demo=False)
        except ValueError:
            filename = "real_hyperparameter_tweaking.txt"
            if sys.argv[1]=="debug":
                first_dict_lines, rest_of_the_lines = cut_file_in_halves(
                                                filename)
                dictionary_read = convert_lines_to_dict(first_dict_lines)
                nn = NeuralNetworkHandler()
                for k,v in dictionary_read.items():
                    print(k,":",v)
                    if k.endswith("_file"):
                        assert k[:-5] in nn.data_input.keys(), "File type not
```

```
                                                                    found"
                        setattr(nn, k, v)
                        nn.settable_property_list.append(k)
                        nn.load_data(v, k[:-5])
                    else:
                        nn.try_to_update_attribute(k,v)
                overwrite_file_by_removing_first_dict(filename,
                                                      rest_of_the_lines)
                nn.run_real_spectra(save_plots=True, silent_mode=False)
                nn.plot_training_spectra(threshold=2e6)
```

C Code for benchmarking

This code uses 'unfoldingsuite', which contains implementations of MAXED and GRAVEL in python, developed locally at CCFE, to unfold spectra from various a priori. Their performance can then be used as benchmarks for the neural network unfolding results to be compared against.

comparison_with_existing.py

```
import numpy as np
import pandas as pd
import shutil
from unfoldingsuite.datahandler import UnfoldingDataHandler_2
from unfoldingsuite.nonlinearleastsquare_2 import SAND_II_2, GRAVEL_2
from unfoldingsuite.maximumentropy_2 import MAXED_2
from unfoldingsuite.parameterised_2 import Parameterised_2
'''
from unfoldingsuite.tools.unfolding_data_handler import UnfoldingDataHandler
from unfoldingsuite.nonlinearleastsquares.sand2 import SAND_II
from unfoldingsuite.nonlinearleastsquares.gravel import GRAVEL
from unfoldingsuite.maximumentropy.maxed import MAXED
'''
def conver_to_PUL(vector, group_structure):
    assert len(group_structure)-1==len(vector), "must have N+1 boundaries for
                                                vector length N={0}, but instead {1}
                                                 boundary values are found".format(
                                                len(vector), len(group_structure))
    leth_span= np.diff(np.log(group_structure))
    return vector/leth_span

DATASET="fusion_test"
A_PRIORI_IS_FLAT=True
# true_spec_list = pd.read_csv("../real_"+DATASET+"_normed.csv",header=None)
reaction_rates_list = pd.read_csv("../real_"+DATASET+"_normed_ACT.csv",header=
                                        None)
response_matrix = pd.read_csv("../response_matrix_ACT_175_gs.csv", header=None,
                                        index_col=[0])
group_structure = pd.read_csv("../175_gs.csv",header=None).values.flatten()

maxed_solution=[]
gravel_solution=[]

for i in range(len(reaction_rates_list.index)):
    rr_line = reaction_rates_list.iloc[i]
    unfolder = UnfoldingDataHandler_2()
    unfolder.set_vector('reaction_rates', list(rr_line) )
    unfolder.set_vector_uncertainty('reaction_rates', np.full( len(rr_line),0.
                                                05 ).tolist() )
    unfolder.set_matrix('response_matrix', response_matrix.values)
    # unfolder.load_vector('a_priori')
    if A_PRIORI_IS_FLAT:
        unfolder.set_vector('a_priori', np.ones( np.shape(unfolder.get_matrix('
                                                        response_matrix'))[1] ).tolist()
                                                         )# set flux PUL a priori to be
                                                        a flat spectrum, dimension =
                                                        number of energy bins.
    else:
        unprocessed_a_priori = pd.read_csv("real_"+DATASET+"_a_priori.csv",
                                                        header=None).values[i]# find the
                                                         i-th line of the a priori in
                                                        the a priori file.
        a_priori = conver_to_PUL(unprocessed_a_priori, group_structure)
        unfolder.set_vector('a_priori',a_priori.tolist())
    gravel=GRAVEL_2(verbosity=0)
    gravel.set_all_parameters(unfolder)
    try:
        gravel.run('n_trials', [10000]) #run until we reach num_trials = 1000
    except:
        break
    gravel_solution.append(gravel.get_vector('solution'))
    print("finished line", i)

    maxed=MAXED_2()
    maxed.set_all_parameters(unfolder)
    maxed.run('basin_hopper',[]) #emtpy list to denote use all default
                                                    parameters of the basin hopper
                                                    algorithm.
    maxed_solution.append(maxed.get_vector('solution'))
if A_PRIORI_IS_FLAT:
    np.savetxt("real_"+DATASET+"_gravel_"+"flat"+"_a_priori_solution.csv",
                                                    gravel_solution, delimiter=",")
    np.savetxt("real_"+DATASET+ "_maxed_"+"flat"+"_a_priori_solution.csv",
                                                    maxed_solution, delimiter=",")
else:
    np.savetxt("real_"+DATASET+"_gravel_"+ "nn" +"_a_priori_solution.csv",
                                                    gravel_solution, delimiter=",")
    np.savetxt("real_"+DATASET+ "_maxed_"+ "nn" +"_a_priori_solution.csv",
                                                    maxed_solution, delimiter=",")

ref_info_file = "real_"+DATASET+"_normed_ref_info.csv"
shutil.copyfile("../"+ref_info_file, ref_info_file)
```

D Fully determined simulation data generation

Creates a 5 energy-bins fluence vector, which is then folded through a 5 × 5 response matrix; both of which are randomly generated. Each element both were picked from a uniform random distribution larger than 1. The upper bound of the elements in the vector were chosen as 15 and the upper bound of the elements in the response matrix were chosen to be 50.

simple_non_singular_case.py

```
from unfoldingsuite.nonlinearleastsquares.gravel import GRAVEL
import numpy as np

SIZE = 5                            # Shape of square response matrix =(SIZE x
                                        SIZE)
```

```
RESPONSE_RANGE = (1.0, 50.0)       # Range response matrix values can take
FLUX_RANGE = (1.0, 15.0)           # Range flux values can take
NUMBER_OF_SPECTRA = 100    # For training the neural network

# Generate a random response matrix, checking that it is full rank.

response = np.matrix([np.zeros(5) for row in range(SIZE)])

np.random.seed(0)#Make sure we get the same response matrix every time.

while np.isinf(np.linalg.cond(response)):#Make sure that the response matrix is
                                                  not singular.
    for row in range(SIZE):
        for col in range(SIZE):
            response[row, col] = RESPONSE_RANGE[0] + (np.random.rand() * (
                                                  RESPONSE_RANGE[1] -
                                                  RESPONSE_RANGE[0]))

# Generate random spectra, and fold into reaction rates

def generate_N_spectra_and_reaction_rates(N):
    spectra, reaction_rates = [], []
    for spectra_index in range(N):
        spectrum = np.matrix([np.zeros(1) for row in range(SIZE)])
        for row in range(SIZE):
            spectrum[row] = FLUX_RANGE[0] + (np.random.rand() * (FLUX_RANGE[1]
                                                  - FLUX_RANGE[0]))
        spectra.append(spectrum)
        reaction_rates.append(response * spectrum)
    print(np.shape(spectra))
    return np.reshape(spectra,[-1,SIZE]), np.reshape(reaction_rates,[-1,SIZE])

# Print out random spectra, their response functions and check that the inverse
                                                  can be found

print("R=",response)
if __name__=="__main__":
    np.savetxt("for_test_spectra.csv",response, delimiter=",")  #Saving this
                                                  response matrix just for reference
                                                  purpose.
    spectra, reaction_rates = generate_N_spectra_and_reaction_rates(
                                                  NUMBER_OF_SPECTRA)

    np.savetxt("../simple_spectra.csv",spectra, delimiter=",") #Features
    np.savetxt("../simple_RR.csv",reaction_rates, delimiter=",") #Labels
```

E Underdetermined simulation data generation

For each of the 14 FISPACT reference spectra, each is parametrised into a list of peaks. The height of these peaks were then perturbed to form a ‘new’ spectrum. This ‘new’ spectrum is then folded through a corresponding response matrix.

spectrumrandomizer.py

```
import numpy as np
import pandas as pd
from matplotlib import pyplot as plt
import warnings
from numpy import sqrt, pi, exp, log
```

```
import copy
import time
start_time = time.time()

def reshape_data_for_smooth_spectrum_plotting(bin_boundaries, bin_heights,
                                              log_scale=False):#For SMOOTH plotting,
                                              for easier visualization in linear scale
                                              , since histogram-like graphs looks ugly
                                               in non-.
    from scipy.stats.mstats import gmean
    '''
    reshape data into a format such that, when plugged into
    plt.plot(x,y), gives a smooth plot.
    The reshape_data_for_histogramic_spectrum_plotting function defined above
                                                  gives very jagged-edges;
    in contrast, this reshape_data_for_smooth_spectrum_plotting function is
                                                  equivalent to applying anti-aliasing
                                                   technique on the spectrum,
    smoothing out the spectrum.
    '''
    assert len(bin_heights)+1==len(bin_boundaries)
    bin_boundaries=np.hstack(np.array(bin_boundaries))
    #If plotting on a linear x-axis scale, the arithmatic mean is used as the
                                                  class mark.
    class_marks=bin_boundaries[:-1]+np.diff(bin_boundaries)/2
    if log_scale:
        #If plotting on a log-x scale, the geometric mean is used to find the
                                                      class mark instead.
        class_marks= gmean([bin_boundaries[:-1], bin_boundaries[1:]])
    return class_marks, bin_heights #return the x, y values requried

def reshape_data_for_histogramic_spectrum_plotting(bin_boundaries, bin_heights)
                                              :
    '''
    reshape data into a format such that, when plugged into
    plt.plot(x,y), gives a histogram-like, square-edges plot.
    i.e. uniform height within each bin.
    '''
    assert len(bin_heights)+1==len(bin_boundaries)# The bin_boundaries variable
                                                   includes both upper and lower
                                                  bounds for each bin
    bin_boundaries,bin_heights=np.array(bin_boundaries),np.array(bin_heights)
    Intercalation = np.repeat(np.arange(len(bin_boundaries)), 2)[:-1] #indices
                                                  to be used in the next line.
    return bin_boundaries[Intercalation[1:]],bin_heights[Intercalation[:-1]] #
                                                  return the x, y values requried

def get_group_structure(reactor):
    '''read a csv of the correct name in the same directory'''
    group_structure_csv_suffix="_Group_Structure.csv"
    return np.genfromtxt(reactor+group_structure_csv_suffix,delimiter=",")

def convert_to_centroid_values(energy_group_structure):
    from scipy.stats.mstats import gmean
    class_marks= gmean([energy_group_structure[:-1], energy_group_structure[1:]
                                                  ])
    return class_marks

def preprocess_df(df, n_sample=1, keep_fixed_fraction=0.6):
    distilled_df = df[["distribution","a_true","b_true","amplitude_true"]] #
```

```
                                                only extract the four values that
                                                matters
    num_func = len(df.index)
    output_df_list = []
    numTrues = int(np.round(keep_fixed_fraction*num_func))
    numFalses= num_func-numTrues
    #Duplicate it up to n_sample of them
    for n in range(n_sample): #The following loop can be sped up by using numpy
                                                 arrays better and perhaps storing
                                                the data as a dataframe instead of a
                                                 list.
        keep_fixed_bool_vector = np.random.choice( [True,]*numTrues + [False,]*
                                                    numFalses , size=num_func,
                                                    replace=False)
        new_df = distilled_df.copy()
        new_df["keep_fixed"] =  pd.Series(keep_fixed_bool_vector, index=new_df.
                                                    index)
        output_df_list.append(new_df)
    return output_df_list #a list of dataframes whose len==n_sample; each has
                                                these columns: "distribution",
                                                a_true","b_true","amplitude_true,"
                                                keep_fixed"

def param_randomizer(df, vary_only_amp = True):
    randomized_df = df.copy()
    for index, line in df.iterrows():
        dist_type = line["distribution"]
        params = np.asarray(line[["a_true","b_true","amplitude_true"]])
        if not line["keep_fixed"]: #must have an added a column with boolean
                                                    values indicating to fix this
                                                    particular function or not.
            #must make sure that amplitude is nonzero, and if dist_type=="
                                                        maxwellian", must be non-
                                                        zero
            if vary_only_amp:
                randomized_df.loc[index, "amplitude_true"] = np.random.
                                                            lognormal() *
                                                            randomized_df.loc[index,
                                                             "amplitude_true"]
            else:
                randomized_df.loc[index] = np.random.multivariate_normal(
                                                            params, get_covar_mat(
                                                            dist_type,params) )
    return randomized_df

def get_covar_mat(dist_type,params):#dist_type is a string
    df_dx_i_list = get_df_dx_i[dist_type](params)
    num_params = len(df_dx_i_list)
    #?unfinished
    return
def spectrum_generator(function_dataframe): #a 2D dataframe input
    function_list = []
    for index, line in function_dataframe.iterrows():
        dist_type = line["distribution"]
        params = line[["a_true","b_true","amplitude_true"]]
        function_list.append( function_pointers[dist_type]( *list(params) ) )
    return lambda x: sum([ f(x) for f in function_list ])

def return_AA1(params):
    return [params[2], params[2], 1]
```

```
def return_A1(params):
    return [params[1], 1]
def return_Watt_params(params):
    a,b,A = params #unpack list
    area = sqrt(pi/2)*A*sqrt(a**3 * b) * exp(a*b/4)
    return [area*(a+6)/(4*a) , area*(b+2)/(2*b), area*1/A]

get_df_dx_i = {
'normal'                 : return_AA1,
'normal_fixed_mean'      : return_AA1,
'log_normal'             : return_AA1,
'log_normal_fixed_mean': return_AA1,
'maxwellian'             : return_A1,
'maxwellian_fixed_mode': return_A1,
'watt_spectrum'          : return_Watt_params,
}

#parameterising functions that return lambda function objects
def normal_dist(*args):
    mu, sigma, amplitude = args[-3:]
    return lambda x: amplitude/sqrt(2*pi* sigma**2) * exp(-(x-mu)**2 / (2*sigma
                                        **2) )
def lognormal_dist(*args):
    mu, sigma, amplitude = args[-3:]
    return lambda x: amplitude/(x*sigma*sqrt(2*pi)) * exp( -(log(x)-mu)**2 /(2*
                                        sigma**2)  )
def maxwellian_dist(*args):
    mode, amplitude = args[-2:]
    a = mode/sqrt(2)
    return lambda x: amplitude*sqrt(2/pi) * (x**2/a) * exp(  -(x**2)/ (2 * (a**
                                        2) ) )
def watt_spec(*args):
    a, b, amplitude = args[-3:]
    return lambda x: amplitude* exp( -x/a ) * np.sinh( sqrt(b * x) )

def save_numpy_array_with_comment_as_csv(fname, comment, array):
    comment = comment.split("\n")
    comment[0] = "#"+comment[0]
    comment[-1]= comment[-1]+"\n"
    comment = "\n#".join(comment)
    array = np.clip(array, 1, None)
    with open(fname,"a") as f:
        f.write(comment)
    with open(fname,"b+a") as f:
        np.savetxt(f,array,delimiter=",")
    return

def get_comment(for_spectra=True):
    if for_spectra:
        comment = ["Each row of this file list ONE spectrum",
        "each column corresponds to the flux value of a specific an energy bin.
                                        ",
        "These will act as the labels with which the neural network will be
                                        trained on /tested on."
        ]
    else: #otherwise this would be used to generate comments for csv files.
        comment = ["Each row of this file list the reaction rates obtained
                                        after folding ONE spectrum",
        "each column corresponds to the activities of a specific energy bin.",
        "This will act as the features with which the neural network will be
```

```
                                                        trained on /tested on."
        ]
    return "\n".join(comment)

function_pointers={  #dictionary that when called with the appropriate string,
                                       acts as an alias to the function
'normal'                :normal_dist,
'normal_fixed_mean'     :normal_dist,
'log_normal'            :lognormal_dist,
'log_normal_fixed_mean':lognormal_dist,
'maxwellian'            :maxwellian_dist,
'maxwellian_fixed_mode':maxwellian_dist,
'watt_spectrum'         :watt_spec,
}

if __name__=="__main__":
    #initialize parameters:
    Reactor_list = ["1_JAEA_FNS","2_Frascati_NG","3_ITER_DD","4_ITER_DT","
                                            5_DEMO_HCPB_FW","6_JET_FW","
                                            7_NIF_Ignition",
    "8_IFMIF_DLi","9_BWR_UO2_15","10_BWR_MOX_15","12_PWR_MOX_15","13_Cf252","
                                            14_Maxwellian"]
    #<edit here>
    seed_val=0
    PLOT=False #Decide whether to show the plots or not
    target_gs = Reactor_list[0]
    save_file_prefixes = "../"+"GS_eq_"+target_gs
    save_file_prefixes +="_reference"
    n_sample = 300 #Choose number of feature:label pairs to be created
    keep_fixed_fraction = 1.0
    #choosing data soruce
    #</edit here>
    for Rxr in Reactor_list:
        method_list=["ACT","TBMD","VERDI"]
        # Rxr = Reactor_list[5]

        np.random.seed(seed_val)
        parameter_csv_suffix="_optimal_parameters.csv"
        df = pd.read_csv(Rxr+parameter_csv_suffix)
        response_matrix_suffix="_Response_Matrix.csv"


        #csv parameter's format is as follows:
        #for the case of normal distributions, a=mu, b=sigma; case of
                                                        maxwellian: b=mode;
        #unused parameters becomes 'nan' or 1

        #The true values to be plugged into various distributions are as
                                                        follows:
        df['a_true'] = df.a_fixed*df.a_corr
        df['b_true'] = df.b_fixed*df.b_corr
        df['amplitude_true'] = df.amplitude_fixed*df.amplitude_corr
        #except with the two cases where amplitudes were scaled logarithmically
                                                         using the correction factor:
        df.loc[df.distribution=="normal",            "amplitude_true"] = df.
                                                        amplitude_fixed * 10**(df.
                                                        amplitude_corr-1)/sqrt(2*pi)
        df.loc[df.distribution=="normal_fixed_mean", "amplitude_true"] = df.
                                                        amplitude_fixed * 10**(df.
                                                        amplitude_corr-1)/sqrt(2*pi)
        df.loc[df.distribution=="log_normal",           "amplitude_true"] = df
                                            .amplitude_fixed * 10**(2*(df.
                                            amplitude_corr-1))
        df.loc[df.distribution=="log_normal_fixed_mean", "amplitude_true"] = df
                                            .amplitude_fixed * 10**(2*(df.
                                            amplitude_corr-1))

        #Obtain the group structure
        gs = get_group_structure(target_gs)#get the flux values corresponding
                                            to the target group structure
        groups_centroids = convert_to_centroid_values(gs)

        #start reading and processing the function parameters
        list_of_df = preprocess_df(df, n_sample=n_sample, keep_fixed_fraction=
                                            keep_fixed_fraction) #
                                            preprocess_df outputs a list of
                                            dataframe with len=n_sample
        randomized_list_of_df = [ param_randomizer(df_i) for df_i in list_of_df
                                             ]
        print("Randomized {0} dataframes of parameters for {1}".format(n_sample
                                            , Rxr))

        target_spectra = [ spectrum_generator(randomized_df)(groups_centroids)
                                            for randomized_df in
                                            randomized_list_of_df ] #
                                            generate the features
        file_structure_comment=get_comment()
        save_numpy_array_with_comment_as_csv(save_file_prefixes+"_spectra.csv",
                                             file_structure_comment,
                                            target_spectra)
        # np.savetxt(save_file_prefixes+"_spectra.csv",target_spectra,delimiter
                                            =",")
        print("Finished generating {0} spectra for {1}, using the group
                                            structure of {2}".format(
                                            n_sample,Rxr,target_gs))

        response_matrix = {} #create dictionary to store the matrices
        method_comment = get_comment()
        for method in method_list:
            response_matrix[method] = np.genfromtxt(target_gs+"_"+method+
                                                response_matrix_suffix,
                                                delimiter=",")
            spectrum_file, reaction_rates_file=[], [] #spectrum file, reaction
                                                rate files
            reaction_rates = [ response_matrix[method].dot(spec) for spec in
                                                target_spectra ] #fold to
                                                get the labels
            save_numpy_array_with_comment_as_csv(save_file_prefixes+"_"+method+
                                                "_RR.csv", method_comment,
                                                reaction_rates)
            print("Folded each sample through the {0} system".format(method))

print("time taken in seconds =",time.time()-start_time)
```

F Training and evaluating neural networks on the underdetermined simulation data

A demonstration of applying neuralnetworktrainer.py on the data generated by spectrum-randomizer.py .

script_for_demo.py

```
#!/home/ocean/anaconda3/bin/python3
from neuralnetworktrainer import *

inc="_including_folded_reaction_rates"
mse = "mean_squared_error"
mpse = "mean_pairwise_squared_error"

modification=[] #create empty list to store dictionaries, each specifying what
                                       modification to make to the default demo
                                        NN.
# modification.append(
#     {"session_name":"test", "loss_func":mse, "callbacks_applied":['
                                       EarlyStopping'], "hidden_layer":[128,
                                       256], "cutoff": 10})
modification.append(
    {"session_name":"_128_256_mse", "loss_func":mse, "callbacks_applied":['
                                           EarlyStopping'], "hidden_layer":[128
                                           , 256], "cutoff": 1800})
modification.append(
    {"session_name":"_256_256_mse", "loss_func":mpse, "callbacks_applied":['
                                           EarlyStopping'], "hidden_layer":[256
                                           , 256], "cutoff": 1800})
modification.append(
    {"session_name":"_128_256_mse_inc", "loss_func":mse+inc, "callbacks_applied
                                           ":['EarlyStopping'], "hidden_layer":
                                           [128, 256], "cutoff": 1800})
modification.append(
    {"session_name":"_256_256_mse_inc", "loss_func":mpse+inc, "
                                           callbacks_applied":['EarlyStopping']
                                           , "hidden_layer":[256, 256], "cutoff
                                           ": 1800})

if __name__=="__main__":
    for mod in modification:
        nn=NeuralNetworkHandler()
        nn.session_name=mod["session_name"]
        nn.hyperparameter["loss_func"]   = mod["loss_func"]
        nn.hyperparameter["hidden_layer"]= mod["hidden_layer"]
        nn.callbacks_applied = mod["callbacks_applied"]
        nn.data_reordering_options["cutoff"] = mod["cutoff"]
        nn.read_demo_data()
        nn.trim_data()
        nn.shuffle()
        nn.split_into_sets()
        nn.preprocess_input()
        nn.build_model()
        nn.train_model()
        nn.auto_generate_session_name()
        nn.save_params_as_dictionary()
        nn.save_NN_weights()
        nn.plot_history()
        nn.plot_test_results_histogram()
        nn.compare_individual_spectra(silent_mode=True)
        # nn.plot_training_spectra(threshold=2)
```

G Selecting from UKAEA and IAEA compendium

Rebinned spectra from the 212 IAEA + UKAEA compendium [37] were sorted into various training and testing sets using the following python program.

getrealdata.py

```
import numpy as np
import pandas as pd
TRAIN_SPLIT = 0.8
SHUFFLE_SEED= 0
'''
# will save one for each of the following
fusion
mcf
fission
commercial_fission
watt
high_energy
activations
every
'''

'''
This file collect all the spectra in generator into a single csv file,
#NORMALIZE THEM,
and then fold them all through the three activation system's response matrices
                                        to get the activation rates.
'''

# Assume all *.txt files in this directory belongs to the spectrum.


def get_ACT_TBMD_VERDI_matrix(absolute_path):
    import os
    matrices = {} #store the three matrices in a dictionary.
    activation_system = ["ACT", "TBMD", "VERDI"]

    for system in activation_system:
        for file in os.listdir(absolute_path):
            if (system in file) and ("response_matrix" in file):
                labelled_matrix = pd.read_csv(absolute_path+file, header=None,
                                                        index_col=0)
                matrices[system] = np.array(labelled_matrix) # add
                                                        reponsematrix to
                                                        dictionary
                # print(system, "has response matrix of shape", matrices[system
                                                        ].shape)
    return matrices #return a dictionary storing the matrices as numpy array in
                                                  the values, corresponding to the
                                                  system name stored in the keys.

def normalize(one_dim_array):
    total = sum(one_dim_array)
    return one_dim_array/total, total

# set(list(spec_index["type"]))
# Want the numbers in PUL, so that the neuralnetworktrainer.run_real will use a
                                        default of label_already_in_PUL=True
# Add the "ref_info" into neuralnetworktrainer.run_real as well.
# # save 1 metadata file + 1 spectra norm.csv file + 3 reaction rates for each
                                       of the following:
'''
{'BT',  # bombardment/Boron target
 'CR',  # cosmic ray
 'HEA', # high energy activation
 'IS',  # instantaneous source (Americium)
 'MA',  # microtron activation
 'PR',  # Pressurized Reactor
 'RFT', # reprocessing fuel technology
 'UKAEA_FIS', # fission
 'UKAEA_FUS', # fusion
 'UKAEA_HEA',
 'UKAEA_IS',
 'UKAEA_PR'}
'''
spec_index = pd.read_csv("real_spectrum_index.txt", sep="\t")
types = spec_index["type"] # shorten the variable name
descriptions = spec_index["description"]

def get_matching_type(*strings):
    matching_loc = ( types=="" ) #get a list of all false
    for pattern in strings:
        if pattern.startswith("*"):
            pattern=pattern[1:]# remove the *
            matching_loc = np.logical_or (matching_loc, types.str.match("UKAEA_
                                                        "+pattern) )
        matching_loc = np.logical_or (matching_loc, types.str.match(pattern) )
                                                    #add these matching patterns
    return matching_loc

def search_in_description(*strings):
    matching_loc = ( descriptions=="" )
    for pattern in strings:
        matching_loc = np.logical_or (matching_loc, descriptions.str.contains(
                                                    pattern) )
    return matching_loc

def get_rebinned_data(file_whole_path, gs):
    E, fluence =np.genfromtxt(file_whole_path).T
    assert all(E==gs[:-1]), "The energy group doesn't match the lower bound of
                                                the reference group!"
    return fluence

def shuffle(truth_value_series): #reproducibly shuffle the dataframe
    #truth_value_series is a pd.Series object with one boolean value
                                                corresponding to each row of the
                                                dataframe, to represent whether or
                                                not it's selected.
    np.random.seed(SHUFFLE_SEED)
    indices = list(truth_value_series[truth_value_series].index) #this extracts
                                                 the rows whose boolean values are "
                                                True".
    np.random.shuffle(indices)
    return indices

if __name__=="__main__":
```

```
spectra_classifications = {
#fusion spectra
"every" : shuffle(search_in_description("")),
"fusion" : shuffle(get_matching_type("*FUS")),  #19 of such spectra
"mcf" : shuffle(search_in_description("-FW", "-VV", "ITER")),   #13 of such
                                               spectra

#fission spectra
"fission" : shuffle(get_matching_type("*FIS", "RFT", "BT", "*PR", "*IS")),
                                               #133 of such spectra
"commercial_fission" : shuffle(get_matching_type("*FIS", "*PR")),   #88 of
                                              such spectra
"watt" : shuffle(get_matching_type("IS", "UKAEA_IS")), #watt spectra
                                              without apparent moderating medium
#   5 of such spectra

#miscellaneous
"high_energy" : shuffle(get_matching_type("*HEA", "CR", "MA")), # spectra
                                              containing a significant amount of
                                              high energy particles
#   56 of such spectra
"activations" : shuffle(get_matching_type("*HEA", "MA", "RFT")), # spectra
                                              of activated materials.
#   82 of such spectra

# assert sum(fusion + fission + high_energy + activations) == len(
                                              spec_index), "Some doesn't belong to
                                               any of the above categories!"
}
#For a few kinds of classifications of interest,
for specific_kind in ("every","fusion", "fission"):
    sample_size = len(spectra_classifications[specific_kind])
    train_rows = round(TRAIN_SPLIT * sample_size)
    spectra_classifications[ specific_kind+"_train"] =
                                                   spectra_classifications[
                                                   specific_kind][:train_rows]
    spectra_classifications[ specific_kind+"_test" ] =
                                                   spectra_classifications[
                                                   specific_kind][train_rows:]

directory = "All_spectra_in_175/data_package_175convert/"

response_matrix = get_ACT_TBMD_VERDI_matrix(directory+ "../../")

gs = np.genfromtxt(directory + "175_gs.csv")
for selection_name, classification in spectra_classifications.items():
    #placeholder for the output dataframe.
    output_fluence = []
    output_rr = dict( [ (system,[]) for system in response_matrix.keys() ]
                                                   )
    normalization_constant_list = [] #placeholder for normalization
                                                   constants to be added to the
                                                   metadata dataframe.

    selected = spec_index.iloc[classification].copy()
    for f in selected["title"]: # read the strings from the title column
        raw_line = get_rebinned_data(directory+f+".txt", gs) #grab the
                                                       original line, and then
                                                       noramlize it.
        norm_line, norm_const = normalize(raw_line)
```

```
            #save the normalized output, normalization constant, and the 3
                                                    respective response rates.
            output_fluence.append( norm_line )
            for system, rr in output_rr.items():
                rr.append( response_matrix[system].dot( norm_line))
            normalization_constant_list.append( norm_const )

        # save the files outputted
        save_name = "real_"+selection_name+"_normed"
        pd.DataFrame(output_fluence).to_csv(save_name+".csv", header=False,
                                                index=False)

        selected["normalization_constant"] = normalization_constant_list
        selected.to_csv(save_name+"_ref_info.csv", header=True, index=False)

        for system, rr in output_rr.items():
            df = pd.DataFrame(rr)
            df.to_csv(save_name+"_"+system+".csv", header=False, index=False)
```

H hyperparameter input controller

Input files for hyperparametertrainer.py using the following code, by iterating through a list of hyperparameters of interest, thus effectively performing a grid search over all hyperparameters.

hyperparameterinput.py

```
import numpy as np
# from matplotlib import pyplot as plt
import pandas as pd
from itertools import product
import hashlib
import sys
import glob
import os
import shutil

def generate(*filename):
    sheet = pd.DataFrame([], columns=["loss_func", "hidden_layer", "
                                          learning_rate", "num_epochs", "files
                                          ", "session_name",
                                    "train_loss","train_mae","train_mse",
                                    "val_loss" , "val_mae" , "val_mse" ,
                                    "test_loss", "test_mae", "test_mse",
                                    "std_CE_rr", "optimal_epoch"])

    #loss functions
    loss_func_list = ["mean_squared_error",
                      # "cosine_distance",
                      "mean_pairwise_squared_error",
                      "mean_squared_error_including_folded_reaction_rates",
                      "
                                                      mean_pairwise_squared_error
                                                      "]

    #hidden layers
    hidden_layer_list=[]
    '''
    #discarded choices of hidden_layers as listed as follows:
```

```
hidden_layer_list.append([])
hidden_layer_list.append([256])
hidden_layer_list.append([128, 256])
hidden_layer_list.append([64, 128, 256])
for n in range(1,6):
    hidden_layer_list.append([256,]*n)
'''
for n in range(6):
    increasing_node_list = np.logspace(5,8, n ,base=2).astype(int)
    hidden_layer_list.append( list(increasing_node_list) )

#learning rate
learning_rate_list = np.logspace( -2,-9, 43)
# learning_rate_list = list(np.logspace(-6, -9, 10))

#training and testing set.
files_list = [  #self verifying
            ("every", "every"),
            ("fusion", "fusion"),
            ("fission", "fission"),
            #cross verifying
            ("fission", "fusion"),
            ("fusion", "fission"),
            #generalization within each category
            ("mcf", "fusion"),
            ("commercial_fission", "fission"),
            #cross verifying
            ("activations", "high_energy"),
            ("high_energy", "activations"),
            #the fission spectra should already contain enough information
                                    to deduce the watt
                                    spectrum
            ("fission","watt"),
            #for fun, see if the fusion spectra contain enough information
                                    to deduce the watt
                                    spectrum
            ("fusion", "watt"),]

p = product(loss_func_list, hidden_layer_list, learning_rate_list,
                                    files_list)
while True:
    try:
        loss_func, hidden_layer, learning_rate, files = next(p)
    except StopIteration:
        break

    #hash out a name:
    line = str(loss_func) + str(hidden_layer) + str(learning_rate) + str(
                                    files)
    name = hashlib.shake_256( line.encode("utf-8") ).hexdigest(6)

    # num_epochs = int( np.clip(10**( round(len(hidden_layer))-1 ) * round(
                                    1/learning_rate), 10, 1E5) ) #
                                    limit the number of epoch to
                                    100000.
    num_epochs = 10000
    #add these data into the end of the spreadsheet
    sheet.loc[ len(sheet.index) ] = [ loss_func, hidden_layer,
                                    learning_rate, num_epochs, files
                                    , name, 0., 0., 0., 0., 0., 0.,
                                                    0., 0., 0., 0., 10000 ] #will
                                                    leave the loss columns empty.

    assert len(set(sheet["session_name"]))==len(sheet.index), "there are
                                                 repetitions of the hashed names; try
                                                  using a longer hexdigest size."
    print("number of rows saved =", len(sheet.index) )
    if len (filename)==0:
        fname = "hyperparameterlist.csv"
    else:
        fname = filename[0]
    sheet.to_csv(fname, index=False)
    print("saved as", fname)

def _write_one_dict_with_EarlyStopping(f, row):
    f.write("\n{\n")
    f.write('response_matrix_file : "response_matrix_ACT_175_gs.csv"' +",\n")
    f.write('group_structure_file : "175_gs.csv"'          + ",\n")
    f.write("loss_func : "+'"'+ str(row["loss_func"])+'"' + ",\n")
    f.write("hidden_layer : " + str(row["hidden_layer"] ) + ",\n")
    f.write("learning_rate : "+ str(row["learning_rate"]) + ",\n")
    f.write("num_epochs : "    + str(row["num_epochs"]    ) + ",\n")
    train, test = [ i.replace("(","").replace(")","").strip("'") for i in row["
                                                 files"].split(", ") ]
    if train==test:
        train=train+"_train"
        test=test+"_test"
    f.write('train_feature_file: "real_'+train+'_normed_ACT.csv"'   +",\n")
    f.write('train_label_file  : "real_'+train+'_normed.csv"'       +",\n")
    f.write('test_feature_file : "real_'+test+'_normed_ACT.csv"'    +",\n")
    f.write('test_label_file   : "real_'+test+'_normed.csv"'        +",\n")
    f.write('ref_info_file     : "real_'+test+'_normed_ref_info.csv"'+",\n")
    f.write('session_name : "'+ str(row["session_name"] )+'"'+ ",\n")
    f.write("callbacks_applied : ['EarlyStopping'] ,") #this callback by
                                                 default restores the best weight.
    f.write("}\n")

def append_dict(*filename):
    if len (filename)==0:
        fname = "hyperparameterlist.csv"
    else:
        fname = filename[0]
    sheet = pd.read_csv(fname, index_col=None)
    with open("real_hyperparameter_tweaking.txt", "a") as f:
        for _, row in sheet.iterrows():
            _write_one_dict_with_EarlyStopping(f,row)

def split_dict(num_jobs, *filename):
    assert num_jobs<=999, "current filename syntax restricts the number of jobs
                                                  to 3 digits"
    if len (filename)==0:
        fname = "hyperparameterlist.csv"
    else:
        fname = filename[0]
    print("reading from {1}, splitting into {0} dictionaries".format(num_jobs,
                                                 fname))
    sheet = pd.read_csv(fname, index_col=None)
    num_rows = len(sheet.index)

    rows_per_file = int(np.ceil(num_rows/num_jobs))
    for n in range(num_jobs):
        with open("job_number_"+str(n).zfill(3)+".txt", "w") as f:
            for _, row in sheet.iloc[ rows_per_file*n : rows_per_file*(n+1) ].
                                                        iterrows():
                _write_one_dict_with_EarlyStopping(f,row)

def search_in_df(*args):
    sheet = pd.read_csv("hyperparameterlist.csv", index_col=None)
    with open("hyperparameterlist.csv") as f:
        lines = f.readlines()[1:] #ignore the header line

    mask = [True,]*len(sheet.index)
    for arg in args:
        new_mask = [ (arg in line) for line in lines ]
        print(sum(new_mask), "matches for ", arg)
        mask = np.logical_and(mask, new_mask)

    if sum(mask)==0:
        print("No matching results!")
        return
    elif sum(mask)>1:
        print("Multiple lines are found to match. the first five are as follows
                                                      :")
    print(sheet[mask].head())
    return

if __name__=="__main__":
    print("This version of hyperparamterinput.py applies EarlyStoppping to
                                                  prevent overfitting.")
    try:
        arg = sys.argv[1]
    except IndexError:
        print("type one of the following words after the program name:")
        print("generate")
        print("write")
        print("split")
        print("search")
        exit()

    if arg=="generate":
        generate(*sys.argv[2:])
    elif arg=="write":
        append_dict(*sys.argv[2:])
    elif arg=="split":
        if len(sys.argv)==2:
            split_dict(132) #by default split into 132 dictionaries
        else:
            split_dict(int(sys.argv[2]), *sys.argv[3:])
    elif arg=="search":
        search_in_df(*sys.argv[2:])
```

This program can be used to split the into multiple jobs, which can then be submitted to a cluster, parallellizing the process and massively reducing the training and evaluation time of the neural networks. This is done by calling the program with `python hyperparameterinput.py split`

I hyperparameter optimisation searching

List the hyperparameter, training- and testing-sets used to evaluate the neural network on, when the hash_name of the neural network is given.

hyperparameteroutput.py

```
import numpy as np
# from matplotlib import pyplot as plt
import pandas as pd
from itertools import product
import sys
import glob
import os
import shutil

def search_in_df(*args):
    verbose=False
    sorting=False
    sheet = pd.read_csv("hyperparameterlist.csv", index_col=None)
    with open("hyperparameterlist.csv") as f:
        lines = f.readlines()[1:] #ignore the header line

    mask = [True,]*len(sheet.index)
    for arg in args:
        if arg=="-v":
            print("Setting verbose to True")
            verbose=True
        elif arg=="-s":
            print("Sorting the outputted dataframe according to the last
                                                    argument provided={}".format
                                                    (args[-1]))
            sorting=True
        else:
            if not sorting:
                new_mask = [ (arg in line) for line in lines ]
                print(sum(new_mask), "matches for ", arg)
                mask = np.logical_and(mask, new_mask)

    if sum(mask)==0:
        print("No matching results!")
        return
    elif sum(mask)>1:
        print("{0} lines are found to match. the first five are as follows:".
                                                format(sum(mask)))
    region_of_interest = sheet[mask]
    if sorting:
        region_of_interest=region_of_interest.sort_values(by=[arg])
    if verbose:
        print(region_of_interest)
        print("with the name(s)")
        print(region_of_interest["session_name"])
    else:
        print(region_of_interest.head())
        print("with the name(s)")
        print(region_of_interest["session_name"].head())
    return

def fill_in_loss_values():
    sheet = pd.read_csv("hyperparameterlist.csv", index_col=None)
    #try to find the hash in the filename
    for ind, row in sheet.iterrows():
        name = row["session_name"]
        matching_txt = glob.glob(name+"_params.txt")
        if len(matching_txt)==0:
            print("Params file for neural network with hash='{0}' is not found/
                                                               not generated yet.".format(
                                                              name), end='\r', flush=True)
            continue
        elif len(matching_txt)>1:
            print("Warning: multiple params*.txt of hash={0} is found!".format(
                                                              name))
            [ print(i) for i in matching_txt]
            print("Using the loss value in the last one.")
        with open(matching_txt[-1]) as f:
            lines = f.readlines()
        def find_in_file(word):
            error_message_line = [line.strip() for line in lines if line.
                                                              startswith("session_name :")
                                                              ]
            loss_lines = [ line.strip() for line in lines if line.startswith(
                                                              word+" :")] #choose the
                                                              matching line
            if len(loss_lines)!=1:
                print("\nNumber of matching lines found ="+str(len(loss_lines))
                                                                  +" !")
                if word=="std_of_log_of_C_over_E_reaction_rates": #only let it
                                                                  slip if it's because the
                                                                   folding process messed
                                                                  up and created a
                                                                  negative value.
                    print("    Ignoring the missing C/E value for line "+
                                                                          error_message_line[0
                                                                          ])
                    print("    continuing 'fill' action")
                    print("    |")
                    print("    |")
                    print("    |")
                    print("    |")
                    print("    |")
                    return
                else:
                    exit()
            loss_value = float(loss_lines[0].split(":")[1].strip().strip(",") )
                                                               #take the part after the
                                                              ':', and remove the '\n' and
                                                               ','
            if not np.isfinite(loss_value):
                print("\n"+error_message_line[0]+"has a non-finite value of {0}
                                                                  ={1}".format(word, str(
                                                                  loss_value)) )
            return loss_value
        #below is an extremely inefficient way of filling in the loss values.
        sheet.at[ind,"train_loss"]=find_in_file("loss")
        sheet.at[ind,"train_mae"]=find_in_file("mean_absolute_error")
        sheet.at[ind,"train_mse"]=find_in_file("mean_squared_error")
        sheet.at[ind,"val_loss"] =find_in_file("val_loss")
        sheet.at[ind,"val_mae"]  =find_in_file("val_mean_absolute_error")
        sheet.at[ind,"val_mse"]  =find_in_file("val_mean_squared_error")
        sheet.at[ind,"test_loss"]=find_in_file("test_loss")
        sheet.at[ind,"test_mae"] =find_in_file("test_mean_absolute_error")
        sheet.at[ind,"test_mse"] =find_in_file("test_mean_squared_error")
        sheet.at[ind,"std_CE_rr"]=find_in_file("
                                               std_of_log_of_C_over_E_reaction_rates
                                               ")
        sheet.at[ind,"num_epochs"]=int(find_in_file("num_epochs"))
    sheet.to_csv("hyperparameterlist.csv", index=False) #overwrite the old file
                                           .

def copy(source_list, dest):
    if len(source_list)!=1:
        assert len(source_list)>0, "no matching files found!"
        print("multiple matching files found, they are listed below. Using the
                                               last one... \n{0}".format("\n".
                                               join(source_list)))
    shutil.copy(source_list[-1], dest)

def rearrange(*cols): #rearrange folder structure according to the column name
    sheet = pd.read_csv("hyperparameterlist.csv", index_col=None)
    for col in cols:
        assert col in sheet.columns, "column {0} not found!".format(col)
    top_level_name = "sort_by_"+"-".join([str(col) for col in cols])

    sets = [list(set(sheet[col])) for col in cols]
    #converting the above sets into folder names
    folder_name = []
    for s in sets:
        new_row = []
        for i in s:
            i=i.replace("'","").strip("[]").strip("()").replace(", ","-")
            if i =="": i="empty"
            new_row.append(i)
        folder_name.append(new_row)
    # folder_name = [ [i.replace("'","").strip("[]").strip("()").replace(",
                                           ","-") for i in s] for s in sets] #
                                           turn each item in the set into a
                                           folder name
    # folder_name = [ [elem for elem in row if elem!="" else "empty"] for row
                                           in folder_name]

    #use for loop and the itertools.product function to create all
                                           subdirectories
    path_name = [ [ top_level_name,],]
    for i in range(len(cols)):
        next_level_names = [ os.path.join(*pair) for pair in product(path_name[
                                               -1],folder_name[i]) ]
        path_name.append(next_level_names)
        for folder in path_name[-1]:
            try:
                os.mkdir(folder)
            except FileExistsError:
                pass

    #select the matching hashed names and pull them into the correct folder
    j = 0
    for matching_criteria in product(*sets):
        mask = [True,]*len(sheet.index)
        for i in range(len(matching_criteria)):
            mask = np.logical_and(mask,sheet[cols[i]]==matching_criteria[i])
        matching_names = sheet[mask]["session_name"]
        folder = path_name[-1][j]
        folder_errorvar = os.path.join(folder,"errorvar")
        folder_deviationdistr = os.path.join(folder,"deviationdistr")
        try:
            os.mkdir(folder)
            os.mkdir(folder_errorvar)
            os.mkdir(folder_deviationdistr)
        except FileExistsError:
            pass
        for name in matching_names:
            matching_txt = glob.glob("*"+name+"_params.txt")
            copy(matching_txt , folder)
            matching_errorvar = glob.glob("lossabove1e*/errorvar/*"+name+"*.png
                                          ")
            copy(matching_errorvar, folder_errorvar)
            matching_deviationdistr = glob.glob("lossabove1e*/deviationdistr/*"
                                          +name+"*.png")
            copy(matching_deviationdistr, folder_deviationdistr)
        j+=1
    # assert j==len(next_level_names), "at this point j should equal to the
                                       number of lowest level files"


if __name__=="__main__":
    try:
        arg = sys.argv[1]
    except IndexError:
        print("type one of the following words after the program name:")
        print("fill")
        print("search")
        print("sort")
        exit()

    if arg=="fill":
        fill_in_loss_values()
    elif arg=="search":
        search_in_df(*sys.argv[2:])
    elif arg=="sort":
        rearrange(*sys.argv[2:])
```

J Loss value visualizer

When given the names of the training- and testing-set, the following code show the loss values (and other metrics) of the neural networks with different hyperparameters achieved on them. This is plotted as a heat map, over the two dimensions of hyperparameters varied, which are ‘number of layers’ (y-axis) and ‘learning rate’ (x-axis) respectively.

hyperparameteroptimizer.py

```
import matplotlib.pyplot as plt
import pandas as pd
import seaborn as sns
import sys
import glob
import os
import numpy as np

def plot3d(*args):
    sheet = pd.read_csv("hyperparameterlist.csv", index_col=None)
    file_list = list(set(sheet["files"]))
    folder_list = [ i.replace("'","").strip("[]").strip("()").replace(", ","-")
                                                for i in file_list ] # get it as
                                               the prettier names.
    matching_file_pairs = []
    for arg in args:
        for i in range(len(folder_list)):
            if folder_list[i].startswith(arg):
                matching_file_pairs.append(file_list[i])
    for train_test in matching_file_pairs:
        raw_data = sheet[sheet["files"]==train_test].drop(columns=["files", "
                                                    num_epochs", "session_name"])
    set_of_loss_func = ['mean_squared_error',
                        'mean_squared_error_including_folded_reaction_rates',
                        'mean_pairwise_squared_error',
                        '
                                                                        mean_pairwise_squared_err
                                                                        ',]
    for loss_func_name in set_of_loss_func:
        print("showing plots of loss_func="+loss_func_name)
        show_each_metric(raw_data[raw_data["loss_func"]==loss_func_name],
                                                    train_test, loss_func_name)

def pivot_and_plot_heatmap(df,metric):
    pivot_table = df.pivot(index="hidden_layer", columns="learning_rate",
                                               values=metric)
    pivot_table.columns=np.array2string(pivot_table.columns, precision=2).strip
                                               ('[]').split() #bodged together in a
                                                hurry.
    pivot_table = pivot_table.reindex([ #reorder the pivot table rows so that
                                               it goes ascending.
    '[32, 53, 90, 152, 256]',
    '[32, 64, 128, 256]',
    '[32, 90, 256]',
    '[32, 256]',
    '[32]',
    '[]'
    ])
    pivot_table = np.log10(pivot_table) #taking log10 to normalize the loss-
                                               values.
    handle= sns.heatmap(pivot_table, annot=True)
    handle.set_xticklabels(handle.get_xticklabels(), rotation=-15)
    handle.set_yticklabels(handle.get_yticklabels(), rotation=-75)
    return handle

def show_each_metric(result_of_training_on_one_loss_func, train_test,
                                         loss_func_name):
    metrics_that_i_care_about = ['val_loss', 'val_mse', 'test_loss', 'test_mse'
                                               , 'std_CE_rr']
    for metric in result_of_training_on_one_loss_func.columns[-10:]:
        if metric in metrics_that_i_care_about:
            pivot_and_plot_heatmap(result_of_training_on_one_loss_func, metric)
            plt.title("log of "+metric+" of "+train_test+"\n optimized on "+
                                                         loss_func_name)
            plt.show()
if __name__=="__main__":
    plot3d(*sys.argv[1:])
```

K Parametrisation of the FISPACT reference spectra

distribution	μ	σ	A	μ_{corr}	σ_{corr}	A_{corr}
log-normal	-1.48e+01	1.20e+00	1.00e+00	1.0	0.6536070787201796	0.6465171468399362
log-normal	-1.17e+01	1.20e+00	5.54e+01	1.0	0.6923014193474084	0.41834840464375106
log-normal	-8.61e+00	1.20e+00	3.07e+03	1.0	0.5802541895436414	0.3391941243798774
log-normal	-5.52e+00	1.20e+00	1.70e+05	1.0	0.769982827091882	0.5451675762326162
log-normal	-2.43e+00	1.20e+00	9.40e+06	1.0	0.6705439760036781	0.6056530392573959
log-normal	6.55e-01	1.20e+00	5.20e+08	1.0	0.6485812808091918	0.6213932412543168
log-normal	3.74e+00	1.20e+00	2.88e+10	1.0	0.33687762989691133	1.754564218248171
log-normal	-1.44e+01	1.50e+00	1.00e+09	1.0	1.1087020488776023	1.2837241483881578
log-normal	-8.60e+00	1.50e+00	3.22e+11	1.0	0.7012835343191862	0.6774642293787084
log-normal	-2.83e+00	1.50e+00	1.04e+14	1.0	0.9732542967472964	1.0011605034609532
log-normal	2.94e+00	1.50e+00	3.33e+16	1.0	0.9872173030484698	0.99379684387792
normal	1.41e+01	4.00e-01	1.00e+19	1.023	1.0500657332932959	1.128662095083972
log-normal	-1.54e+01	1.10e+00	1.00e+03	1.0	1.0295086712444834	1.0871973190897086
log-normal	-1.18e+01	1.10e+00	3.59e+04	1.0	1.0470576309590907	1.1133327728488918
log-normal	-8.26e+00	1.10e+00	1.29e+06	1.0	0.9512570373593815	1.0428424889188541
log-normal	-4.67e+00	1.10e+00	4.64e+07	1.0	1.1561895212201019	1.1532829852822521
log-normal	-1.09e+00	1.10e+00	1.67e+09	1.0	1.0181223850843093	1.018626898626218
normal	1.41e+01	4.00e-01	1.00e+10	1.0	1.32722437503459	1.8671520930196117
normal	2.45e+00	1.00e-01	1.00e+12	1.0	0.8152984470618088	0.5530754449242801
log-normal	-1.26e+01	2.00e+00	1.00e+05	1.0	1.094149298940297	1.17454890924765
log-normal	-7.12e+00	2.00e+00	2.47e+07	1.0	1.7120265659905378	1.12525321665773
log-normal	-1.61e+00	2.00e+00	6.08e+09	1.0	1.2209065015914118	1.5577920026942778
log-normal	3.89e+00	2.00e+00	1.50e+12	1.0	1.0538009149767102	1.5525710802981993
normal	1.41e+01	4.00e-01	1.00e+14	1.0	0.9946385566258605	1.1958058458498946
log-normal	3.00e+00	2.00e+00	1.00e+13	1.0	0.985831182477408	1.191099325784018
log-normal	-3.20e+00	2.00e+00	1.00e+11	1.0	1.0163826189572225	1.037504496747917
normal	1.41e+01	4.00e-01	1.00e+14	1.0	1.132214159680078	1.3221159758391146
log-normal	-5.60e+00	2.30e+00	4.00e+05	1.0	0.912896343655827	0.9707283164160951
log-normal	-4.80e+00	5.00e-01	1.00e+06	1.0	0.9724734344690737	1.3093741751167056
log-normal	3.00e+00	1.80e+00	5.00e+09	1.0	1.1626572027366295	0.8373153796607655
normal	1.41e+01	4.00e-01	1.00e+10	1.0	1.1868044101095476	1.555176012813058
normal	1.35e+01	2.00e+00	2.00e+20	1.0	1.0094598165344801	1.0398929376955228
log-normal	-2.40e+00	3.50e-01	1.00e+14	1.0	0.9999755394847119	1.0437028488962274
log-normal	-1.43e+00	3.50e-01	5.54e+14	1.0	1.0040524756949494	1.2576232255047286
log-normal	-4.47e-01	3.50e-01	3.07e+15	1.0	1.0213050801706227	1.2668031933646988
log-normal	5.31e-01	3.50e-01	1.70e+16	1.0	1.0185780833110203	1.3543132306863206
log-normal	1.51e+00	3.50e-01	9.40e+16	1.0	1.0622261078184665	1.1481233202529897

Table 5: In descending order: each section represents the parameters used to parametrise the spectra of: JAEA-FNS, Frascati-NG, ITER-DD, ITER-DT, DEMO-HCPB-FW, JET-FW, NIF-Ignition. The 2-4th columns indicate the guess value inputted, while the last 3 columns indicate the correction factor multiplied onto them. E.g. $\mu_{final} = \mu * \mu_{corr}$

L neutron spectra extraed from the IAEA + UKAEA compendium

List of all fission data

title	type	Measured/Calculated
PR_PWR_CZECH_6	PR	Czech PWR, circ. pumps, near cold side, p2
PR_BWR_DUNG_1	PR	BWR, Dungeness, boiler cell
RFT_PU_3	RFT	Pu reprocessing plant, fuel pin assembly
RFT_MOX_4	RFT	Fresh MOX, borated water shield
PR_GCR_1	PR	CH1 GC reactor
RFT_PU_2	RFT	Pu reprocessing plant, well shielded
PR_PWR_CZECH_2	PR	Czech PWR, check room, under reactor, p5
PR_BWR_SW_4	PR	BWR (Switzerland), under access
PR_GCR_3	PR	Trawsfynydd GC reactor, position S3
PR_PWR_CZECH_4	PR	Czech PWR, check room, under reactor, p13
PR_BWR_SW_13	PR	PWR (Switzerland), behind generator
UKAEA_029_EBR-2	UKAEA_PR	EBR-2 spectra in 29 energy groups
PR_BWR_SW_8	PR	BWR (Switzerland), near lock, closed
PR_PWR_CZECH_7	PR	Czech PWR, circ. pumps, hot side, p3
PR_BWR_SW_16	PR	PWR (Switzerland), 33 cm behind door
UKAEA_1102_BWR-MOX-Gd-0	UKAEA_PR	BWR-MOX-Gd-0 spectra in 1102 energy groups
UKAEA_100_HFIR-lowres	UKAEA_PR	HFIR-lowres spectra in 100 energy groups
UKAEA_1102_PWR-MOX-15	UKAEA_PR	PWR-MOX-15 spectra in 1102 energy groups
BT_FRM_2	BT	FRM II beam, unfiltered
RFT_PU_1	RFT	Pu reprocessing plant, little shielding, location 1
PR_BWR_SW_14	PR	PWR (Switzerland), at reactor axis
PR_PWR_WOLFCREEK_3	PR	PWR, Wolf Creek, power 50%, 2026 level by valves
RFT_PU_USA_4	RFT	TRU plant, at conduit exit, less shielding
PR_PWR_CZECH_13	PR	Czech PWR, reactor hall, near cap, p10
IS_TRU_6	IS	TRU plant, 25 g AmO2 in container
PR_BWR_SW_2	PR	BWR (Switzerland), at bend of maze
PR_BWR_CAORSO_8	PR	BWR, Caorso, position 4
PR_PWR_WOLFCREEK_1	PR	PWR, Wolf Creek, power 50%, at PH 2047 level
UKAEA_1102_PWR-UO2-Gd-15	UKAEA_PR	PWR-UO2-Gd-15 spectra in 1102 energy groups
PR_BWR_DUNG_3	PR	BWR, Dungeness, on the walkway
PR_BWR_CAORSO_3	PR	BWR, Caorso, position 3
PR_BWR_SW_5	PR	BWR (Switzerland), at stairwell
BT_LVR15_1	BT	LVR-15, epithermal beam
UKAEA_1102_BWR-MOX-Gd-15	UKAEA_PR	BWR-MOX-Gd-15 spectra in 1102 energy groups
PR_PWR_CZECH_10	PR	Czech PWR, reactor hall, at cap, p7
IS_TRU_9	IS	25 Ci Am ceramics, no shield
RFT_WWER_CASK_3	RFT	Transport cask C30/KB54, in corridor at 45 cm
RFT_WWER_CASK_1	RFT	Transport cask C30/KB54, in a hall at 45 cm
PR_GCR_2	PR	CH2 GC reactor
BT_BMRR_1	BT	BMRR spectra, filtered by 34 cm Al/AlF3
UKAEA_172_Phenix	UKAEA_PR	Phenix spectra in 172 energy groups
PR_TRAWS_1	PR	Trawsfynnydd, filter gallery
RFT_TN12_1	RFT	TN-12 fuel container at Valognes
RFT_PU_USA_1	RFT	TRU plant, lightly shielded glovebox 1
RFT_VALDUC_1	RFT	Pu reprocessing at Valduc
RFT_PU_USA_2	RFT	TRU plant, heavily shielded glovebox 1
PR_HINKLEY_2	PR	Hinkley Point, filter gallery
BT_ACCEPI_1	BT	Accelerator based epithermal beam

PR_RINGHALS_3	PR	Ringhals, point P
UKAEA_616_HFR-high	UKAEA_PR	HFR-high spectra in 616 energy groups
PR_BWR_SW_15	PR	PWR (Switzerland), 40 cm behind door
PR_BWR_CAORSO_4	PR	BWR, Caorso, position 4
PR_BWR_SW_6	PR	BWR (Switzerland), 16 m level, near pump
BT_BMRR_1_1	BT	BMRR beam
PR_BWR_SW_10	PR	PWR (Switzerland), in front of containment
PR_BWR_CAORSO_7	PR	BWR, Caorso, position 3
RFT_MOX_2	RFT	MOX transport cask, ver. 03
UKAEA_198_PWR-RPV	UKAEA_PR	PWR-RPV spectra in 198 energy groups
UKAEA_407_Bigten	UKAEA_FIS	Bigten spectra in 407 energy groups
UKAEA_1102_BWR-UO2-Gd-40	UKAEA_PR	BWR-UO2-Gd-40 spectra in 1102 energy groups
BT_BMRR_2	BT	BMRR spectra, filtered by 22 cm 7LiF
UKAEA_1102_PWR-UO2-15	UKAEA_PR	PWR-UO2-15 spectra in 1102 energy groups
BT_BMRR_3	BT	BMRR spectra, filtered by 17 cm D2O
RFT_1393_2	RFT	Transport cask 1393(2)
BT_BNCT_PETTEN_1	BT	BNCT in Petten, HB11 filtered beam
BT_FRM_3	BT	FRM II beam, filtered
UKAEA_1102_BWR-UO2-Gd-15	UKAEA_PR	BWR-UO2-Gd-15 spectra in 1102 energy groups
PR_PWR_GOSGEN_1	PR	PWR, Gosgen, position 1
UKAEA_198_BWR-RPV	UKAEA_PR	BWR-RPV spectra in 198 energy groups
RFT_PU_USA_5	RFT	TRU plant, lightly shielded glovebox 2
PR_RINGHALS_4	PR	Ringhals, point B2
IS_TRU_7	IS	TRU plant, 244Cm in glovebox, no shield
PR_BWR_CAORSO_2	PR	BWR, Caorso, position 2
RFT_PU_USA_3	RFT	TRU plant, at operator desk
UKAEA_1102_PWR-UO2-0	UKAEA_PR	PWR-UO2-0 spectra in 1102 energy groups
PR_RINGHALS_5	PR	Ringhals, point B4
PR_BWR_CAORSO_5	PR	BWR, Caorso, position 1
PR_PWR_WOLFCREEK_2	PR	PWR, Wolf Creek, power 50%, 2 m from PH 2047 level
PR_RINGHALS_1	PR	Ringhals, point D
PR_BWR_CAORSO_6	PR	BWR, Caorso, position 2
PR_BWR_SW_7	PR	BWR (Switzerland), 16 m level, near tap
UKAEA_172_Paluel	UKAEA_PR	Paluel spectra in 172 energy groups
RFT_POLLUX_2	RFT	Pollux container above ground level
PR_BWR_CAORSO_1	PR	BWR, Caorso, position 1
PR_PWR_CP_1	PR	CP reactor, site 5, SPUNIT code
PR_PWR_CZECH_8	PR	Czech PWR, circ. pumps, near door, p4
PR_BWR_SW_9	PR	BWR (Switzerland), near lock, open
RFT_MOX_1	RFT	MOX transport cask, ver. 02
PR_PWR_CP_2	PR	CP reactor, site 6, SPUNIT code
PR_PWR_CZECH_3	PR	Czech PWR, check room, in middle, p12
RFT_WWER_CASK_4	RFT	Transport cask C30/KB54, in corridor at 2 m
PR_PWR_CZECH_11	PR	Czech PWR, reactor hall, at valve, p8
IS_TRU_8	IS	AmBe sources in gloveboxes in line
PR_BWR_SW_11	PR	PWR (Switzerland), 1 m from platform
UKAEA_070_Cf252	UKAEA_IS	Cf252 spectra in 70 energy groups
UKAEA_1102_PWR-MOX-40	UKAEA_PR	PWR-MOX-40 spectra in 1102 energy groups
PR_PWR_CZECH_12	PR	Czech PWR, reactor hall, at generator, p9
UKAEA_1102_PWR-MOX-0	UKAEA_PR	PWR-MOX-0 spectra in 1102 energy groups
PR_HINKLEY_1	PR	Hinkley Point, pile cap
BT_ACC_2	BT	Gantry spectrum
PR_PWR_WOLFCREEK_4	PR	PWR, Wolf Creek, power 100%, at PH 2047 level

PR_PWR_CZECH_9	PR	"Czech PWR, circ. pumps, 4 & 4, p11 "
PR_BWR_SW_3	PR	BWR (Switzerland), at drywell
UKAEA_1102_BWR-UO2-Gd-0	UKAEA_PR	BWR-UO2-Gd-0 spectra in 1102 energy groups
BT_ACC_1	BT	Accelerator based spectrum, 2.5 MeV protons on 7Li
RFT_POLLUX_1	RFT	Pollux container in salt mine
RFT_LK100_1	RFT	LK-100 fuel container at La Hague, position1
UKAEA_616_HFR-low	UKAEA_PR	HFR-low spectra in 616 energy groups
RFT_MOX_5	RFT	Fresh MOX, no shield
RFT_NTL_1	RFT	Transport cask NTL-111, at 115 cm
RFT_HANAU_1	RFT	Fission material deposition, BS measurements
PR_PWR_WOLFCREEK_5	PR	PWR, Wolf Creek, power 100%, 2026 level at loop penetrati
UKAEA_172_Superphenix	UKAEA_PR	Superphenix spectra in 172 energy groups
RFT_WWER_CASK_2	RFT	Transport cask C30/KB54, in a hall at 2 m
RFT_MOX_3	RFT	New MOX at 20 cm, no shield
PR_PWR_CZECH_5	PR	Czech PWR, check room, corridor, p6
PR_PWR_CP_4	PR	CP reactor, site 4, YOGI code
RFT_HANAU_2	RFT	Fission material deposition, LS measurements
UKAEA_1102_PWR-UO2-40	UKAEA_PR	PWR-UO2-40 spectra in 1102 energy groups
PR_GCR_4	PR	Trawsfynydd GC reactor, position S4
UKAEA_1102_PWR-UO2-Gd-40	UKAEA_PR	PWR-UO2-Gd-40 spectra in 1102 energy groups
PR_RINGHALS_2	PR	Ringhals, point E
BT_SPALL_1	BT	Spallation source, 72 MeV protons on W
RFT_LK100_2	RFT	LK-100 fuel container at La Hague, position 2
PR_BWR_SW_12	PR	PWR (Switzerland), 3 m from platform
PR_PWR_GOSGEN_2	PR	PWR, Gosgen, position 2
UKAEA_1102_PWR-UO2-Gd-0	UKAEA_PR	PWR-UO2-Gd-0 spectra in 1102 energy groups
RFT_PU_5	RFT	Pu reprocessing plant, little shielding, location 5
RFT_NTL_2	RFT	Transport cask NTL-111, at 367 cm
RFT_PU_4	RFT	Pu reprocessing plant, little shielding, location 4
PR_PWR_CP_3	PR	CP reactor, site 4, SPUNIT code
PR_PWR_CZECH_1	PR	Czech PWR, circ. pumps, cold side, p1
PR_BWR_DUNG_2	PR	BWR, Dungeness, on the roof
BT_FRM_1	BT	FRM I beam
RFT_1392_1	RFT	Transport cask 1392(1)
UKAEA_1102_BWR-MOX-Gd-40	UKAEA_PR	BWR-MOX-Gd-40 spectra in 1102 energy groups
PR_BWR_SW_1	PR	BWR (Switzerland), at maze entrance

List of all fusion data used as the training set

title	type	description	Measured
UKAEA_616_DEMO-HCPB-VV	UKAEA_FUS	DEMO-HCPB-VV spectra in 616 energy groups	M
UKAEA_150_NIF-ignition	UKAEA_FUS	NIF-ignition spectra in 150 energy groups	M
UKAEA_616_DEMO-HCPB-BP	UKAEA_FUS	DEMO-HCPB-BP spectra in 616 energy groups	M
UKAEA_616_WCLL-VV	UKAEA_FUS	WCLL-VV spectra in 616 energy groups	M
UKAEA_616_HCPB-VV	UKAEA_FUS	HCPB-VV spectra in 616 energy groups	M
UKAEA_616_WCCB-VV	UKAEA_FUS	WCCB-VV spectra in 616 energy groups	M
UKAEA_175_JAEA-FNS	UKAEA_FUS	JAEA-FNS spectra in 175 energy groups	M
UKAEA_175_ITER-DD	UKAEA_FUS	ITER-DD spectra in 175 energy groups	M
UKAEA_161_LMJ-g	UKAEA_FUS	LMJ-g spectra in 161 energy groups	M
UKAEA_175_ITER-DT	UKAEA_FUS	ITER-DT spectra in 175 energy groups	M
UKAEA_616_HCPB-FW	UKAEA_FUS	HCPB-FW spectra in 616 energy groups	M
UKAEA_616_DEMO-HCPB-FW	UKAEA_FUS	DEMO-HCPB-FW spectra in 616 energy groups	M
UKAEA_175_TUD-NG	UKAEA_FUS	TUD-NG spectra in 175 energy groups	M
UKAEA_616_WCLL-FW	UKAEA_FUS	WCLL-FW spectra in 616 energy groups	M

UKAEA_616_HCLL-FW	UKAEA_FUS	HCLL-FW spectra in 616 energy groups	M

List of all fusion data used as the testing set

title	type	description	Measured/Calculated
UKAEA_175_Frascati-NG	UKAEA_FUS	Frascati-NG spectra in 175 energy groups	M
UKAEA_100_JET-FW	UKAEA_FUS	JET-FW spectra in 100 energy groups	M
UKAEA_616_WCCB-FW	UKAEA_FUS	WCCB-FW spectra in 616 energy groups	M
UKAEA_616_HCLL-VV	UKAEA_FUS	HCLL-VV spectra in 616 energy groups	M