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A Case Study on Deep Learning applied to Capture Cross Section Data Analysis

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Abstract. A good data analysis of neutron cross section measurements is necessary for generating high quality and reliable nuclear databases. Artificial intelligence techniques, and in particular deep learning, have proven to be very useful for pattern recognition and data analysis, and thus may be used in the field of experimental nuclear physics. In this publication, we train a neural network in order to improve the capture-to-background ratio of neutron capture data of measurements performed in the time-of-flight facility n_TOF at CERN with the so-called Total Absorption Calorimeter. The evaluation of this deep learning-based method on accurate Monte Carlo simulated measurements with ^{197}Au and ^{239}Pu samples suggests that the capture-to-background ratio can be increased 5 times above the standard method.

1 Introduction

The reliability and quality of the nuclear databases [1–4] is supported on the good practices when analyzing the data from the experiments, which allow these libraries to be used on numerous nuclear applications. One of the most critical aspect of the analysis of a neutron capture cross section measurement is the signal-to-background ratio. This can define, up to great extent, the quality of the final result. During the analysis, different methods can be applied depending on the used experimental setup in order to improve this signal-to-background ratio.

For the particular case of the time-of-flight facility n_TOF at CERN [5], several capture measurements have been performed with the Total Absorption Calorimeter (TAC) [6], an array detector of 40 BaF_2 crystals. This high segmentation of the detector has been used to discriminate capture events from background events (including fission events) based on the different emitted gamma multiplicities followed by a nuclear reaction.

As this problem can be approach as a classification problem between capture and background, it could be a possible application of one of the multiple artificial intelligence and machine learning algorithms, which have been proved to yield good results in related tasks [7]. In addition, the presence of machine learning techniques in the nuclear physics literature [8–11] is continuously growing.

In this context, we propose a deep learning based method trained to discriminate capture from background events, tested on two simulated capture measurements using the geometry and features of the TAC detector at n_TOF with ^{197}Au and ^{239}Pu samples, respectively. Results indicate that the deep learning method may be useful to boost the traditional method used in these type of data analysis and thus obtain a higher signal-to-background ratio. The article is structured as follows. In section 2 the details of the experimental setup chosen to be modeled is described, as well as the procedure to generate a valid dataset to train and test a DL-based model. In section 3, the results of the proposed method are shown and compared with the standard method. Finally, the conclusions are stated in section 4.

2 Capture experiments and signal-to-background ratio

Given the importance of a good signal-to-background ratio in any measurement, and in particular for capture measurements, it is essential to have a good method that allow us to increase this ratio when the original data has an important background contribution. This is typically the scenario of some challenging capture measurements, e.g. the ^{239}Pu measurement, where the fission competes with the neutron capture reactions.

This problem have been usually addressed by means of the different multiplicity in the gamma cascades between capture and other nuclear reactions or background sources. Rejecting those events with specific detected crystal multiplicity and total deposited energy has been the traditional method to obtain a higher signal-to-background ratio in capture measurements. For the particular case of the n_TOF facility at CERN, this method has been applied to the data measured with the Total Absorption Calorimeter (TAC).

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2.1 The Total Absorption Calorimeter at n_TOF

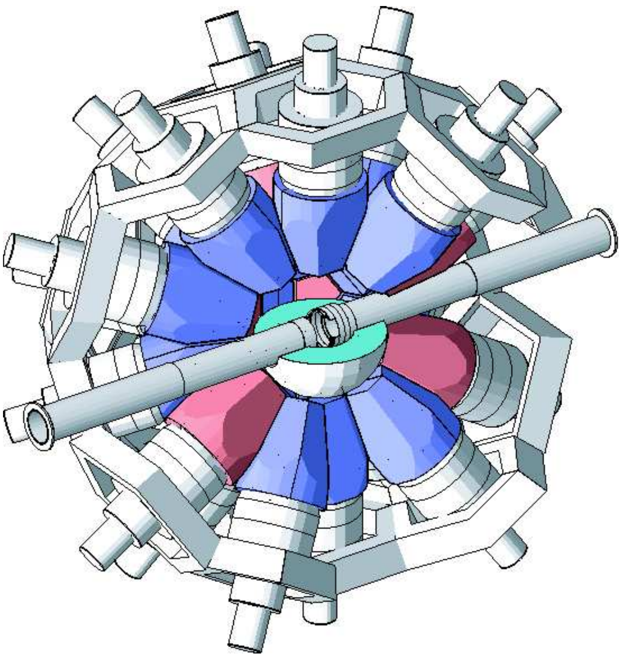

Figure 1. Half-opened 3D model of the TAC detector used at n_TOF for capture measurements.

The Total Absorption Calorimeter (TAC) is a 4π array of 40 BaF_2 crystals with high efficiency, located in the 185m flight path of the neutron time-of-flight facility n_TOF at CERN. The modeled geometry can be seen in Figure 1. The TAC has been used on many neutron cross-section capture measurements for applications like nuclear technology and stellar nucleosynthesis. Thanks to its features, the TAC allows to discriminate events based on the total deposited energy and the crystal multiplicity, thus increasing the signal-to-background ratio of the acquired data.

An example of the effect of applying these restrictions can be seen in Figure 2, which shows the deposited energy spectrum from a ^{197}Au (n,γ) measurement with the TAC. As it can be seen, rejecting events with crystal multiplicity m_{cr} = 1 or higher produces a significant noise reduction at lower energies. However, due to the limited efficiency and other physical effects, we also lose some capture events by making this event selection, so a balance has to be found. For the case of the ^{197}Au capture measurement, the optimal event conditions are $m_{cr} > 2$ and $2.5 < E_{sum} < 7$ MeV.

From the point of view of machine learning, this specific task would be equivalent to a binary classification problem between capture and non-capture. This lead us to the possibility of using one of these algorithms to help improving the performance of this event selection for the TAC.

2.2 Building and training a Neural Network for classification

Depending on the application and nature of the problem to solve, different machine learning classifiers can be used,

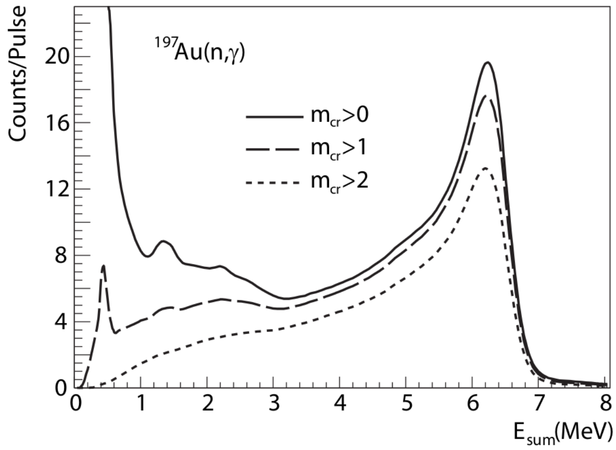

Figure 2. Deposited energy spectrum for a ^{197}Au neutron capture measurement with the TAC, applying different cuts in the crystal multiplicity of the events.

such as clustering algorithms (kNN, kmeans), support-vector machines (SVM) or deep neural networks. The latter, also known as Deep Learning (DL), has become very popular in the last years thanks to the development of computer processing power and their many capabilities, e.g. pattern recognition, and applications of multiple nature. In addition, neural networks are the best option when the data has high dimensionality and the size of the dataset is relatively big. These are typically the characteristics found in the data recorded with the TAC detector in a capture experiment.

In order to use a neural network for our classification problem, we generated a labeled dataset using Monte Carlo simulations based on the n_TOF flight path properties and the TAC geometry. An incident neutron energy range of 10^{-2} to 10^5 eV has been used in the simulation, as well as the real dimensions and canning type of the samples measured at n_TOF. Each sample of the generated dataset is composed of 40 values corresponding to the energy deposited in each of the BaF_2 crystals.

For the architecture of the neural network, the best configuration found is a model with 5 dense –or Fully Connected– layers with a decreasing number of neurons from 200 to 1, with a Batch Normalization [12] layer and Leaky ReLu [13] activation between two consecutive dense layers (see Figure 3). Finally, a sigmoid activation is applied to the output in order to obtain a value between zero and one.

The dataset, generated by Monte Carlo simulation, can be extended as needed. For example, for the study of neutron capture in ^{197}Au, 9.1×10^7 samples were generated for background events, and 3.3×10^7 were generated for capture events. Different trainings were carried out by filtering the original dataset under different conditions in m_{cr} and E_{sum}, with the same model architecture and training parameters. These variations of the original dataset aim to achieve a signal-to-background ratio that favors the classification made by the deep learning model. This combi-

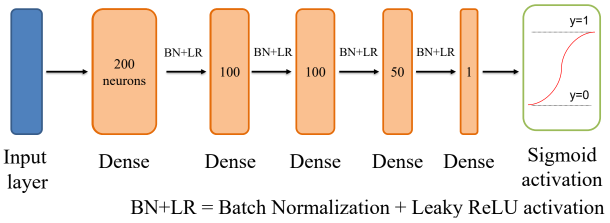

Figure 3. Scheme of the neural network architecture use in this work.

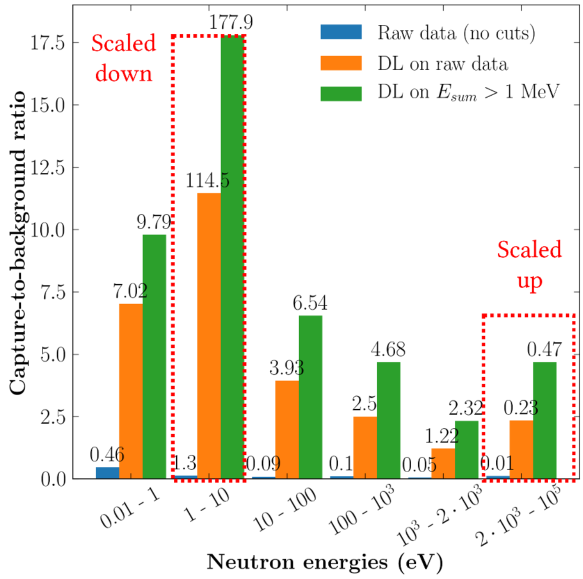

Figure 4. Capture-to-signal ratios for the simulation with ^{197}Au and different neutron energy intervals. Note that the bars in some intervals have been scaled up or down to fit the drawing area. For clearance, the real values are shown above each bar.

nation of cuts in the dataset and subsequent classification with the neural network has been found to be the best strategy to obtain higher signal-to-background ratios.

Each filtered dataset was divided into two separate subsets: one for training and another for testing the performance of the trained model. The neural network was trained with the ADAM optimizer and a binary cross-entropy loss function using the Keras API on Tensorflow. To minimize bias in the trained model due to the imbalance between the two classes in the training dataset, class weights were applied to the loss function for each training sample.

The metric used to evaluate the training and testing of the model was the so-called *balanced accuracy*, as typically defined for binary classification problems. After a few epochs of training, the models converged to balanced accuracies around 70%, with similar values for the tests.

3 Results

The proposed DL-based model has been tested with two Monte Carlo simulated datasets with two different target samples: ^{197}Au and ^{239}Pu.

3.1 Capture classification in a virtual ^{197}Au(n,γ) measurement

Figure 4 shows the capture-to-background ratios for the original dataset as obtained directly from simulations (blue bars) and the ratios for two methods with the deep learning method. Some bars in the figure have been scaled up/down for illustration purposes, but the real values can be seen on top of each bar. For one of the DL-based methods, the original dataset has been modified by only taking events with $E_{sum} > 1$ MeV (green bars). As seen in the figure, using DL trained and tested on the modified dataset increase the capture-to-background ratios in every energy interval. This indicates that using only DL without any prior cut on the dataset is not the best option, at least with a simple model as the one used here.

The best combination of cuts in the dataset and classification with the trained model is shown in Figure 5. Here can be seen that using DL with cuts in the dataset overcome the result of using the standard method, which consists on selecting events with $m_{\mathrm{cr}} > 2$ and $2.5 < E_{\mathrm{sum}} < 7$ MeV.

The weaker event restrictions $0.6 < E_{\mathrm{sum}} < 6.75$ and $m_{\mathrm{cr}} > 1$ were found by analyzing the properties of the generated dataset with the goal of fine-tuning the standard cuts. Using DL on these optimized cuts provides similar results in the signal-to-background ratios as using DL on the standard cuts of ^{197}Au. Additionally, as the optimized cuts are less restrictive than the standard ones, the number of true capture events that remain at the end of the classification process is higher. This is preferable, as a higher number of events leads to smaller statistical uncertainties in the subsequent analysis.

The superiority of using DL-based method can also be evaluated qualitatively by the deposited energy spectra shown in Figure 6. In the left panel, the resulting spectrum that would be obtained after applying the standard cuts for the selected events is drawn in black. The red curve represent the ground truth, i.e. the true capture events obtained in the simulation, and the blue one, the rest of gamma contributions detected by the TAC. In the right panel of the same figure, the spectra obtained after applying the DL model is shown. It can be clearly seen that the obtained spectrum is closer to the capture one than in the previous case without DL.

3.2 Capture classification with fission background: the case of ^{239}Pu

For the case of the fissile sample ^{239}Pu, the effect of applying DL with different cuts in the dataset can be observed in Figure 7. Independently of the cuts, using DL improves the total signal-to-background ratio of the data with values around 5 times higher. Even with the more relax constraints in the data, when using DL the capture-to-signal ratio is improved compared with the most restrictive cuts without DL.

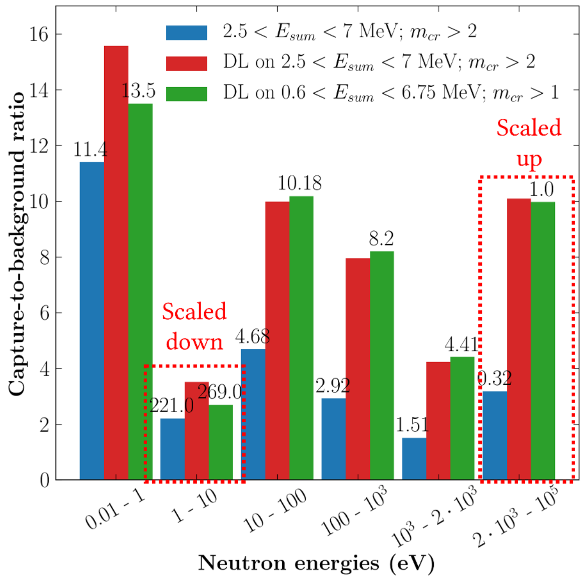

Figure 5. Capture-to-signal ratios for the simulation with ^{197}Au and different neutron energy intervals, comparing the most competitive methods. Note that the bars in some intervals have been scaled up or down to fit the drawing area. For clearance, the real values are shown above each bar.

This improvement can also be seen in the deposited energy spectrum in a more illustrative manner, as shown in Figure 8. Similarly to the gold case, the background reduction in the DL-based method is more effective than the standard method, producing higher quality data for the posterior analysis.

4 Conclusion

Some neutron capture measurements present a challenging data analysis when there are different and important background contributions. Therefore, specific techniques have to be applied during the analysis to improve the quality of the data, e.g. through the capture-to-background ratio. In the particular case of the capture measurements with the Total Absorption Calorimeter in the n_TOF time-of-flight facility at CERN, the standard method consisted in applying specific cuts on the properties of the detected events to reduce the undesired background.

In this article we proposed using a DL-based method that combines the traditional method with a Neural Network classifier for capture events. Using a rather simple neural network architecture to this purpose, we proved that is possible to improve the capture-to-background ratio of a Monte Carlo simulated dataset up to a factor of 3 for the case of a ^{197}Au sample and a factor of 5 for a ^{239}Pu sample.

This intends to prove the validity of using modern machine learning techniques and open the door for its applicability to the field of experimental nuclear data analysis, as it has already been done in many other scientific fields.

Acknowledgements

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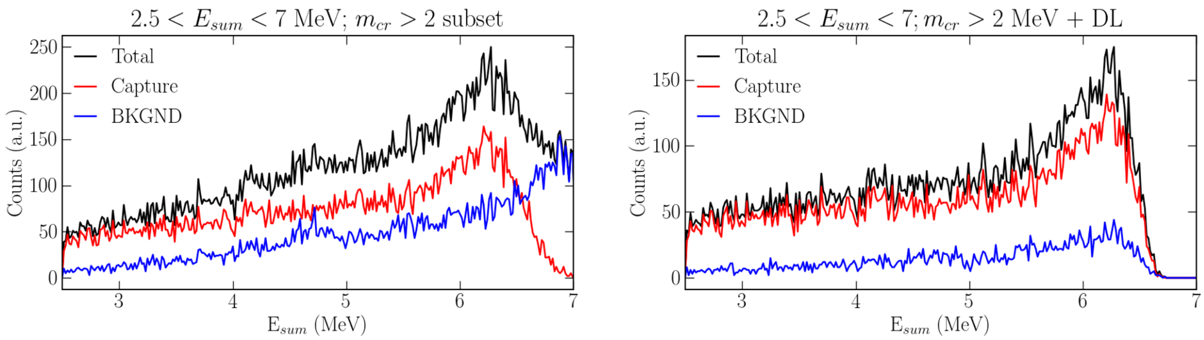

Figure 6. Deposited energy spectra of a simulated ^{197}Au neutron capture experiment with the TAC using standard cuts without DL (left) and with DL (right).

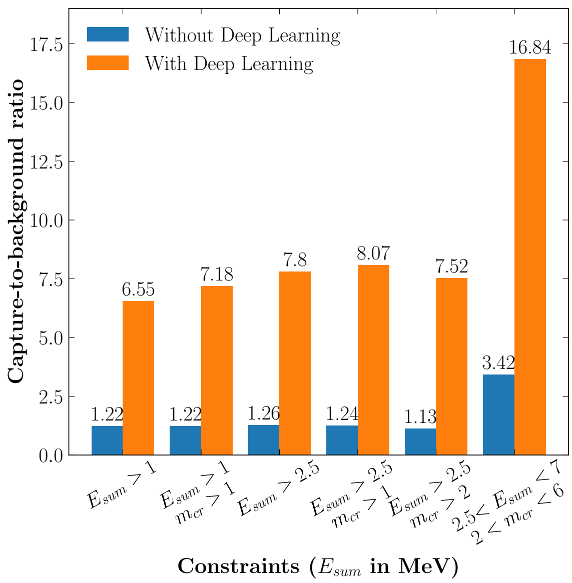

Figure 7. Effect of using DL on the capture-to-signal ratios for the ^{239}Pu sample using different constraints in the dataset.

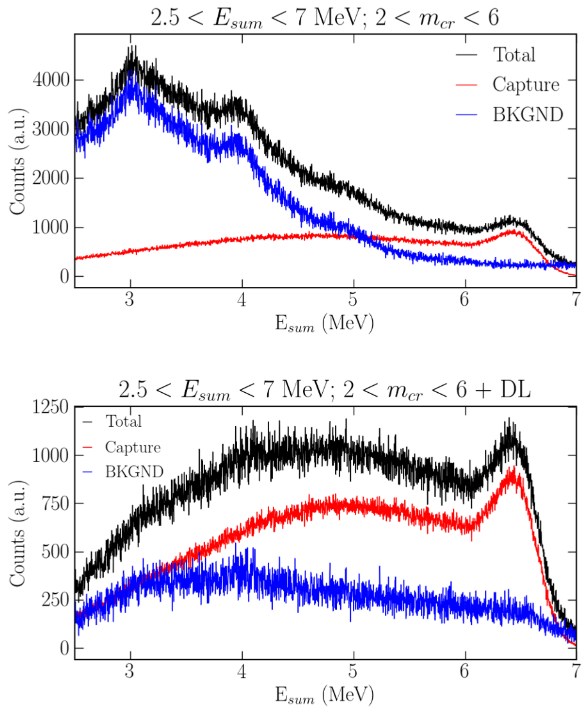

Figure 8. Deposited energy spectra of a simulated ^{239}Pu neutron capture experiment using standard cuts without DL (top) and with DL (bottom).