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ABSTRACT

Free unfolding in neutron spectroscopy means reconstructing energy spectra from experimental data without a priori assumptions regarding their shape. Due to the ill- conditioned nature of the problem, this cannot be done analytically. Neural networks (NN) are here applied to this task and synthetic data is used for training and testing. Results showed very consistent performance especially in the region of low and medium counts, where they fall near the Poisson statistical boundary. Comparison with other unfolding methods validated these results. Application time on the order of ms makes NN suitable for real-time analysis. This approach can be applied to any instrument of which the response function is known.

1. INTRODUCTION

Detectors such as neutron spectrometers generally do not directly measure neutron spectra. The experimental data usually comes folded with the response function (**R**) of the instrument. The energy spectra can be estimated from the experimental data through a backward process called unfolding. An analytic inversion of the response function is rarely possible since the problem is typically ill-conditioned and the experimental data is affected by statistical errors. The finite resolution of the instrument poses additional challenges in the unfolding process as two or more neutron spectra can become degenerate, i.e. indistinguishable once folded with R. Techniques for data unfolding are divided into two main groups. The first one does not rely on any assumption concerning the shape of the energy spectra and is known as free unfolding. The second is referred to as assisted unfolding and is based on a theoretical model or a parametric representation of the solution. While assisted unfolding is generally more accurate for typical cases and well-understood physical models, free unfolding is of interest to spot unforeseen features not yet included in the model. This paper describes a technique for free unfolding of data using artificial Neural Networks (NN) with the aim of providing accurate and real-time performance within the limitations posed by statistics and numerical degeneracy of **R**. The method is here applied to nuclear fusion neutron spectrometers for ITER-relevant conditions, with particular focus to the NE213 liquid scintillator. Assisted unfolding for neutron spectrometers can also be performed with NN with similar characteristics [1].

2. GENERATION OF SYNTHETIC DATA

A set of synthetic random energy spectra has been generated to train the method and evaluate the free unfolding performance. The synthetic data covers the spectra space with a random number (n) of random Gaussians. Each Gaussian features three degrees of freedom, namely amplitude (A), mean (μ) and full width half maximum (FWHM), each varying uniformly in given intervals. These are between 0 and 100% (A), 12 and 17MeV (μ) and 240 to 1880keV (FWHM). The ranges have been chosen to test cases of deuterium-tritium neutron emission for ITER-relevant conditions. Each synthetic experimental data (m) is generated by folding the corresponding energy spectrum (y) with the response function and by normalizing the output to a given number of counts (N). The

application of Poisson statistics on the data bins completes the process and transforms m into a discrete vector of Poisson-perturbed data (m_0), in analogy with the experimental conditions. Log(N) is sampled evenly between 10^4 and 10^8 events. The random Gaussian approximation has been adopted due to memory requirements and training time. Besides, the expansion of neutron energy spectra in a random series of random Gaussians is an experimentally plausible and meaningful approximation in this energy range.

3. NEURAL NETWORK FRAMEWORK

Neural Networks (NN) have been adopted as a free unfolding method due to their speed and robustness as well as their capability of generalization [2]. The architecture chosen for the task is feed-forward with tan-sigmoidal hidden neurons and linear outputs [3]. The network is trained with m0 as input and y as output. The training algorithm used is a regularized version of the Levenberg-Marquardt (LM) method [4], using a Bayesian approach to determine the best coefficients at each epoch [5]. Unfortunately, a large amount of computer memory and processor power is required by this method and a number of techniques have been adopted to comply with the available hardware. The very detailed response function adopted for NE213 has been uniformly rebinned on the data side by a factor three. This reduced the computational load by the same amount without any apparent loss in unfolding performance. The energy side has been reduced as well so that only the interval between approximately 10 and 19 MeV is chosen. The result is then interpolated through 60 cubic splines on a uniform grid yielding interpolation errors around 0.3±0.5% (root-mean-square). This is a small drawback for a more than a factor four reduction in the number of output nodes. The resulting network features 212 inputs and 60 outputs. Finally, six NN have been trained on different ranges of counts rather than on a single one spanning over the entire region. This is found to improve NN generalization and regularization. The network architecture has been limited to a single hidden layer of 16 tan-sigmoidal neurons. The training of each network took about 15-20 hours on a 2.4GHz quad-processor workstation. After this, the application time is in the range of microseconds.

4. ANALYSIS AND RESULTS

To quantify the unfolding performance two metrics have been introduced. These are here referred to as Q and M and describe errors on the energy and data side respectively, as in Eq. (1). The Q-metric consists of the sum of the absolute errors between each unfolded (y_{NN}) and correct (y) energy spectrum, normalized in percent to the area of the latter. Q should be as low as possible for best unfolding performance. The second Metric (M) is a measure of the statistical plausibility of the unfolded spectrum. It measures the root-mean-square error ratio between the folded NN solution ($m_{NN} = \underline{\mathbf{R}} \cdot y_{NN}$) and the unperturbed data. This is then compared with the one due to the Poisson perturbation. When M is near 1, the solution folds back very close to the unperturbed data, with errors that are comparable to the Poisson statistics. In this case, the solution should be considered statistically plausible, regardless of what lies on the energy side. Cases when M^{a}1 and Q>>1 are

examples of numerical degeneracy, where two significantly different energy spectra do not produce any statistically significant difference on the data side and thus cannot be resolved. Conversely, when Q is low and M is considerably smaller than unity the errors on the data side are smaller than the Poisson statistics. This is an indication that additional constraints (e.g. assumptions on the shape of the solution) have been adopted. Similar considerations can be drawn from metrics based on Bayesian analysis of m_{NN} [6].

$$Q = \frac{\sum \left| y^i_{NN} - y^i_{NN} \right|}{\sum y^i} \cdot 100 \qquad M = \frac{\sqrt{\langle (m_{NN} - m)^2 \rangle}}{\sqrt{\langle (m_0 - m)^2 \rangle}} \tag{1}$$

Figure 1a provides Q and M metrics for NE213 free unfolding with NN. The mean and standard deviation of Q are plotted in the top and middle panels respectively, while the mean M value is reported at the bottom. The curves are derived through combined use of all the networks trained for different levels of statistics and the merging points manifest as small discontinuities in the slopes. This plot describes the average results obtained for any shape of random spectra (dots) and a particular case of Gaussian 20keV DT bulk plasma neutron emission [7] (crosses). The latter is of particular interest to ITER fusion plasmas. Figure 1b illustrates the same information for another type of fusion neutron spectrometer called Magnetic Proton Recoil upgrade (MPRu) [8]. The ranges have been adjusted for the increased performance per count of this instrument and its response function (roughly a factor 100).

5. DISCUSSION

The results obtained in Figure 1 highlight the main features of NN free unfolding. The first aspect concerns the capability of generalization, with implications onto the reliability of the results. The small difference in Q value between the dotted and crossed curves proves that NN performs on a simple Gaussian case as well as on spectra of more general shape. This is true for NE213 but also for other spectrometers, e.g. MPRu. The high degree of consistency comes thanks to the Bayesian regularization of the training algorithm and the type of training used. As expected, the standard deviation is smaller in the 20 keV trace since only one shape is considered. The behavior in the M metrics shows another characteristic of NN, with M very close to unity until 10^6 (NE213) and 10^4 (MPRu) counts. This implies that the NN results are here in fact statistically plausible and in line with the Poisson errors introduced in the data. Significant deviations from M = 1 take place on the right side of the plots. In these conditions the reduction of the statistical error $<(m_0 - m)^2>$ is faster than the reduction of the NN error on the data side $<(m_{NN} - m)^2>$, causing M to rise. This effect has been observed for all networks studied and indicates that the network is no longer making optimal use of the statistical information in the data. One possible way to optimize the results at higher statistics is the introduction of the Cash statistic (C-Stat) [6] of the folded solution in the NN performance function. Another one is to post-process the solution using a variational principle aimed at minimizing the C-Stat of mNN. The latter technique has been tested more in detail. Although

this has been proved to enhance results in cases of assisted unfolding at high counts, it did not provide any significant improvement for free unfolding due to the large number of variables, i.e. the energy bins.

Figure 2 reports on the comparison between NN and another free unfolding method, i.e. MAXED, [9] in the region between 10^4 and 10^7 counts. Tests performed with different target χ^2 yielded different results. In the particular case of the 20keV shape, results have shown that target $\chi^2 < 1$ would enhance the low-counts region with drawbacks in the high-counts side. Higher values tend to achieve the opposite result [10]. This result is not necessarily true for any spectral shape, so the comparison has been performed using target $\chi^2 = 1$, which is the statistically most probable value. MAXED has been used with a flat starting guess. From the plot it can be seen that there is a significant advantage for NN at any counts both in consistency and in Q value. This is about a value 5-30 Q reduction for the general case and up to 20 for the Gaussian shape. The curves, however, suggest that the edge off NN becomes smaller at higher statistics, which is in agreement with what was discussed above for the M values in this region. The performance advantage of NN can be explained by the network being trained on an ensemble of data rather than on single events, such as MAXED. This permits a more effective filtering of statistical oscillations for NN through the Bayesian regularization. At higher counts random fluctuations become less important and the gap narrows. In the limit of infinite counts MAXED is bound to become more accurate than NN without post-processing, due to its iterative nature on the χ^2 of the solution. From a computational time point of view, MAXED took from between 2-3 to 30-40 minutes per spectrum, depending on the particular shape and counts. By comparison, NN performed unfolding of the 80000 events test set in a fraction of a second, suggesting mean time per sample is in the order of few ms. This is several orders of magnitude faster and suitable for real-time analysis.

CONCLUSION

Results presented in this paper have shown that NN can efficiently and consistently perform free unfolding of spectroscopic data. This method can be applied to any instrument of which the response function is known, with all the features discussed in section 5. The use of a Bayesian-regularized LM method allowed for efficient training and produced networks that can cope even with large random fluctuations in the data. This aspect was refined further by joint application of several networks trained on different levels of statistics. The combined use of the Q and M metrics has allowed for analyzing the statistical plausibility of the NN results within the statistical boundaries set by N. The fact that M was very close to unity until 10^6 (NE213) and 10^4 (MPRu) counts is an indication that the network has made efficient use of the information available, producing results that lie near the statistical boundary. Comparison with MAXED confirmed this, showing a significant Q performance lead for NN in this region. The increase in M values for higher statistics suggests that the NN response is no longer optimal and could be enhanced. Post-processing based on C-Stat minimization, however, did not show substantial improvement for this case. Computational speed

proved to be another advantage of NN with respect to other methods such as MAXED, as the mean time per sample is in the range of microseconds. This makes NN a valid candidate for real-time free unfolding of experimental data of virtually any kind.

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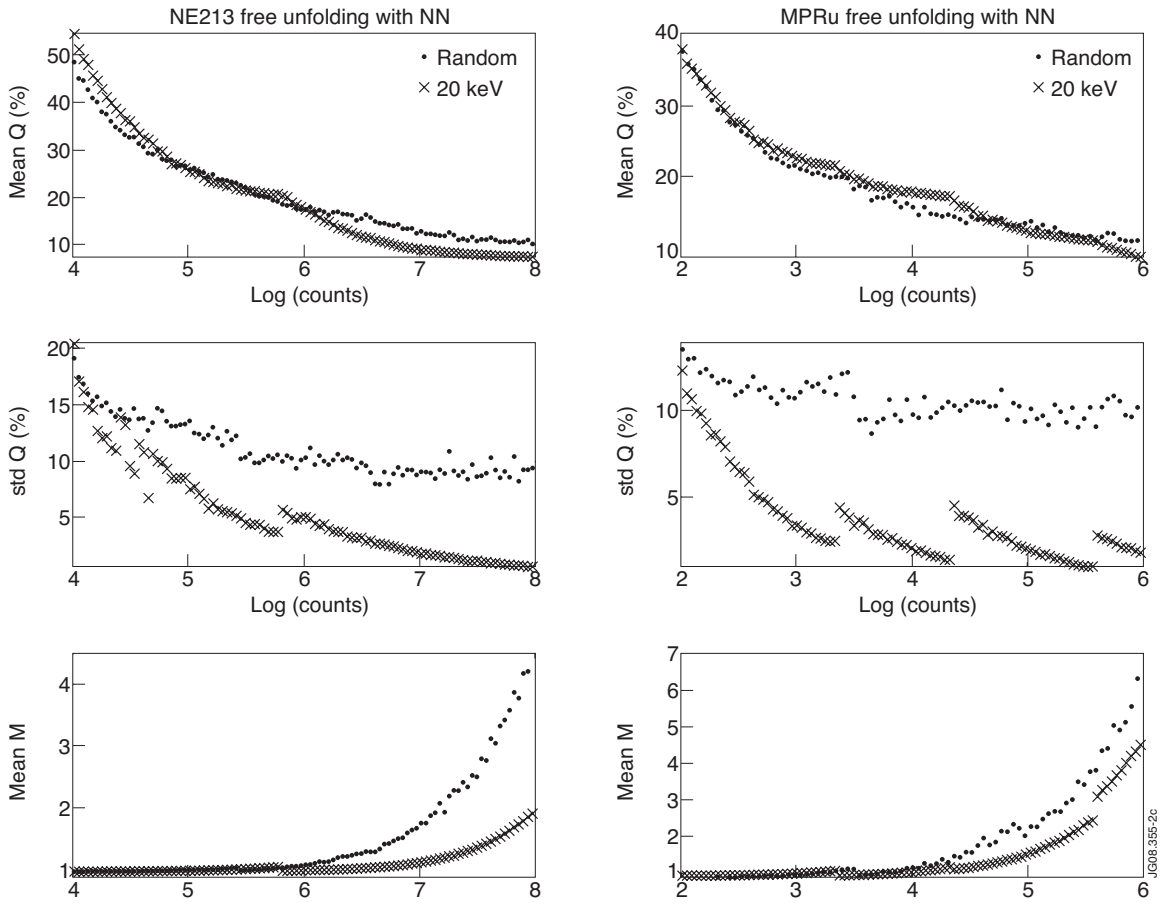

Figure 1: (a) (left). Free unfolding results for NN with NE213 for random spectra (dots) and 20keV DT fusion bulk emission profile (crosses). The first and second panels from top illustrate the average and the standard deviation of Q for each level of counts. The bottom plot reports on the mean M value. Figure 1: (b) (right). Same type of M and Q and M results for NN free unfolding with MPRu.

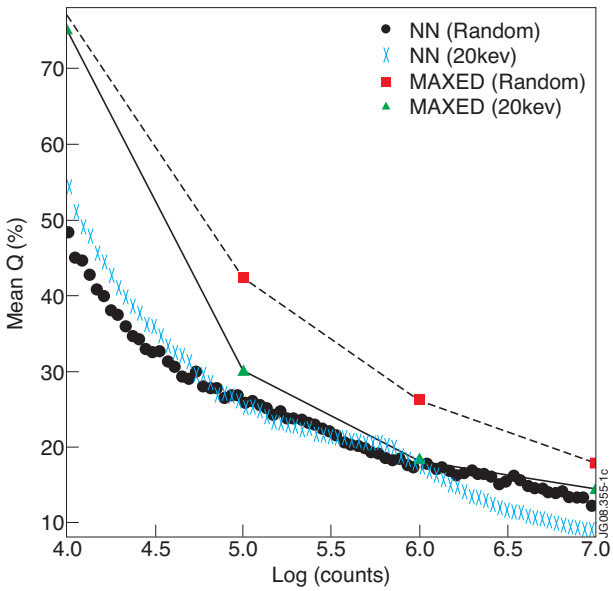

Figure 2. Comparison of NN and MAXED free unfolding performance with NE213 on random shapes and on a fixed 20keV neutron emission profile.