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A neutron spectrum unfolding code based on generalized regression artificial neural networks

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HIGHLIGHTS

- Main drawback of neutron spectrometry with BPNN is network topology optimization.
- Compared to BPNN, it's usually much faster to train a (GRNN).
- GRNN are often more accurate than BPNN in the prediction. These characteristics make GRNNs to be of great interest.
- This computational code, automates the pre-processing, training and testing stages.

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ABSTRACT

The most delicate part of neutron spectrometry, is the unfolding process. The derivation of the spectral information is not simple because the unknown is not given directly as a result of the measurements. Novel methods based on Artificial Neural Networks have been widely investigated. In prior works, back propagation neural networks (BPNN) have been used to solve the neutron spectrometry problem, however, some drawbacks still exist using this kind of neural nets, i.e. the optimum selection of the network topology and the long training time. Compared to BPNN, it's usually much faster to train a generalized regression neural network (GRNN). That's mainly because spread constant is the only parameter used in GRNN. Another feature is that the network will converge to a global minimum, provided that the optimal values of spread has been determined and that the dataset adequately represents the problem space. In addition, GRNN are often more accurate than BPNN in the prediction. These characteristics make GRNNs to be of great interest in the neutron spectrometry domain. This work presents a computational tool based on GRNN capable to solve the neutron spectrometry problem. This

Abbreviations: BPNN, back propagation neural networks; GRNN, generalized regression neural network; BSS, Bonner Spheres System; ANN, Artificial neural networks; PNN, Probabilistic neural networks; RBF, Radial Basis Function; IAEA, International Atomic Energy Agency; MSE, mean square error

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computational code, automates the pre-processing, training and testing stages using a k-fold cross validation of 3 folds, the statistical analysis and the post-processing of the information, using 7 Bonner spheres rate counts as only entrance data. The code was designed for a Bonner Spheres System based on a ^{6}LiI(Eu) neutron detector and a response matrix expressed in 60 energy bins taken from an International Atomic Energy Agency compilation.

1. Introduction

Spectrometry and dosimetry of neutron radiation is one of the most complicated tasks in radiation protection (Kardan et al., 2004a, 2004b). The monitoring of radiation exposure of neutron fields is mainly done with passive detection systems, among those systems, track detectors, film dosimeters i.e. albedo dosimeters are the most common type detector (Fehrenbancher et al., 1999). These detector use foil filters to detetect said neutron fields, nevertheless, these dosimetric systems have a response that strongly depends upon neutron energy.

A special type of neutron dosimeters, commonly known as Bonner Spheres System (BSS), is also utilized as multi-element system where each element has a particular response to neutrons (Bonner, 1961; Alevra et al., 1992; Awschalom and Sanna, 1985). Usually these dosimeters have better detection efficiency in a wide energy range, allowing a better dose assessment (Fehrenbancher et al., 1999). The detection is achieved using the integral counts obtained by the active detector, said counts are weighted by factors that belong to each element (Alberts et al., 1997), The integral counts can also be used to unfold the neutron spectrum that is multiplied by neutron fluence-to-dose conversion coefficients. With the neutron spectrum information, different dose quantities can be estimated i.e. Hp(10), H*(10) (International Commission on Radiation Units and Measurements, 2001).

Nevertheless, BSS have some drawbacks, the weight computation is a time consuming procedure, low resolution spectrum and the necessity of an unfolding procedure. The BSS response matrix, the count rates and the neutron spectrum are related through the discrete version of the Fredholm integro-differential equation, which is an ill-conditioned system with an infinite number of solutions. (Vega-Carrillo et al., 2002).

To unfold the neutron spectrum, several methods have been proposed such as Monte Carlo (Lindemann and Zech, 1995), regularization (Routti and Sandberg, 2001), parameterization, iterative methods (International Commission on Radiation units and Measurements, 2001) and maximum entropy (Reginatto et al., 2002) procedures. Each of them has difficulties that have motivated the development of complementary procedures (Vega-Carrillo et al., 2002; Vega-Carrillo and Iñiguez, 2002; García-Domínguez et al., 1999). Artificial neural networks (ANN) methods have been proposed (Feherembacher et al., 1999), Braga et al. proposed the "Stuttgart Neural Network Simulator", using a Back Propagation Neuronal Network (BPNN) to unfold the neutron spectra, the methodology was tested in twenty-two spectra with a reported error of 0.0014, however the methodology required 3×10^{5} iterations to achieve said performance. (Braga and Dias, 2002; Kardan et al., 2003). Recently, Suman et al. proposed a new approach using the Monte Carlo methodology to unfold the spectra and as a fitness function, then using a genetic algorithm several Monte Carlo solutions were gathered and merged into the final solution to unveil the spectra, a set of 37 spectra were used to test the system, a reported a 2.32×10^{-3} Chi-square was obtained, after up to 1000 generations (Suman et al., 2014). However, the application of ANN to unfold actual neutron spectra still has some problems. Significant work is still to be done in order to assets the feasibility of the ANN for the spectrum unfolding problem (Braga and Dias, 2002).

ANN are a large structured system of equations (Haykin, 1999). These systems have many degrees of freedom and are able to adapt to the task they are supposed to do (Galushkin, 2007; Apolloni et al., 2009). Generally, the most common type of ANN, falls into two different types: Back Propagation Neuronal Networks (Graupe, 2007; Mohan et al., 1997; Jain et al., 1996) and probabilistic neural networks (PNN) (Chtioui et al., 1997; Huang and Zhao, 2005; Mao et al., 2000; Huang, 1999). BPNN use equations that are connected using the weight factors (Arbib, 2003; Hammer and Vilmann, 2003). The selection of the weighting factors makes these neural networks so powerful. On the other hand, PNN uses a statistical approach to select the equations within the structure and do not weight these functions (Mao et al., 2000; Huang, 1999; Specht, 1998).

Previous research of ANN in neutron spectrum unfolding indicate that BPNN perform well (Braga and Diaz, 2002; Kardan et al., 2004a, 2004b; Fehrenbacher et al., 1999; Hernandez-Davila et al., 2005; Vega-Carrillo et al., 2009). However, BPNN have serious drawbacks in neutron spectrometry; the proper determination of the network architecture, the long training periods, another drawback is the lack of available neutron spectra data to train and test the networks, said BPNN networks usually require huge data to train (Ortiz-Rodríguez et al., 2013). Even that Generalized Regression Neural Network (GRNN) and BPNN are complementary versions of the same ANN architecture, GRNN is usually much faster to train (Chtioui et al., 1997; Mao et al., 2000).

The GRNN may converge even with a fraction of the training samples as a BPNN typically needs (Mao et al., 2000) (Huang, 1999; Specht, 1998). Therefore, the use of a GRNN is especially advantageous due to the ability to converge with only few training samples available. The additional knowledge needed to get the fit in a satisfying way is relatively small and can be done without additional input by the user. GRNN only require the spread constant parameter, opposite to BPNN in which, before the training stage, it is necessary to determine many learning and architectural parameters of the network (Ortiz-Rodríguez et al., 2013).

A GRNN is a feed forward neural network based on non-linear regression theory consisting of four layers: the input layer, the pattern layer, the summation layer and the output layer. Said GRNN function as an approximation for complex tasks such as system modeling and prediction. The neurons in the first three layers are fully connected, each output neuron of said layer is connected only to some processing units in the summation layer, a schematic ot a GRNN is shown in Fig. 1.

As can be seen from Fig. 1, the first layer is the input layer and is fully connected to the pattern layer. The second layer is the pattern layer and has one neuron for each input pattern. The neuron stores the values of the predictor variables along with the target value.

The function of the pattern layers of the GRNN is a Radial Basis Function (RBF) (Specht, 1998; Specht and Shapiro, 1991), typically a Gaussian kernel function, as can be seen in Fig. 2, the activation of pattern units characterizes the distance of the center of a RBF to produce; localized, bounded, and rapidly symmetric activations, those activations rapidly decrease with the distance from the

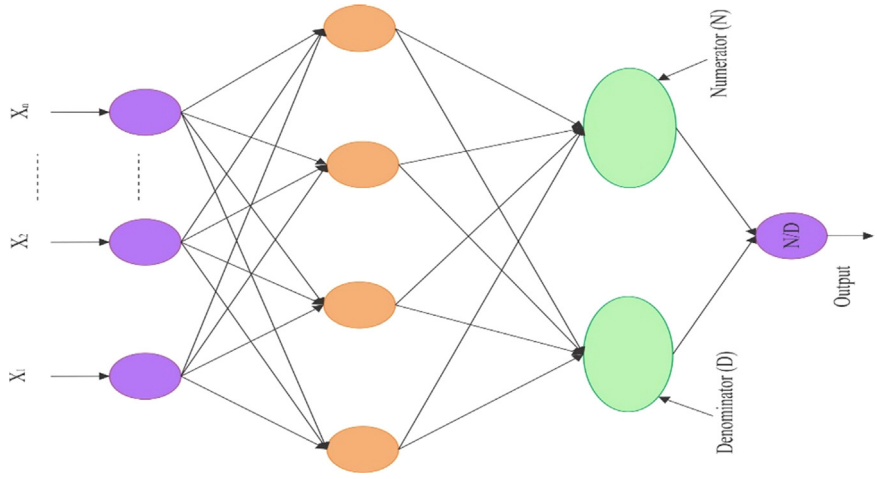

Fig. 1. General structure of GRNN.

function´s center. The RBF is named because the radius distance is the argument to the function, as seen in Fig. 2.

The width of a RBF of the pattern units, also known as the spread constant σ, is an important parameter allowing the user to influence the generalization capabilities of the GRNN. Said spread parameter σ, determines the spread of the function RBF; that is, how quickly the function declines as the distance increased from the point of the Radial Basis Function, therefore, with larger sigma values, distant points have a greater influence. In general, larger values of the spread constant results in a smoother interpolation of the output vectors values among the values corresponding to the centers of RBF of the individual pattern units.

The summation layer has two different types of processing units: the summation units and the single division unit. The number of the summation units is always the same as the number of the GRNN output units. The summation unit adds up the weight values coming from each of the pattern neurons. The division unit only sums the weighted activations of the pattern units without using any activation function.

Another useful characteristic of GRNN, which makes it faster in the training stage, is that there is only the linear output layer beyond the first hidden layer; this guarantees that the network will converge to a global minimum, provided that the optimal value of spread has been determined and that the dataset adequately represents the problem space. In addition, for some specific problems, GRNN may be more accurate than BPNN in the prediction (Ma. del Rosario Martinez-Blanco et al., 2016). These characteristics makes GRNN good candidates in the neutron spectrometry research area. However, since this is an emergent research field, one drawback is the lack of scientific knowledge and technological tools to train ant test GRNN in the neutron spectrometry field.

The aim of this work is to train a GRNN capable to solve with high efficiency the neutron spectrum unfolding problem. To achieve the before mentioned, a neutron spectrum unfolding computational tool based on a GRNN methodology was designed. This computer code was developed under the Matlab programming environment (MATLAB and Statistics Toolbox Release, 2012), automates the stages of: pre-processing the information used to train and test the network, the selection of the spread constant, the training and testing stages of the network, the analysis of the performance of the trained network and the storing of information produced before, during and after training and testing stages for further analysis. The automated algorithm saves a lot of time, and potentially human induced errors.

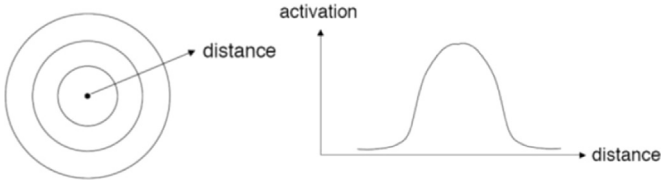

Fig. 2. Radial Basis Function (RBF).

In order to assess the performance of the proposed methodology, a 3k-fold cross validation strategy was used, two thirds of the data were used to train the GRNN, and the rest of the data was used to assess the performance. To determine the optimum spread constant value, around 2000 neural networks were trained in 157 s average. The final GRNN was trained and tested in 0.058 s average using the calculated optimum spread constant by each fold. After training, the performance of the network was analyzed by comparing the output of the trained network with the expected value. In this work, the best and the worst cases are shown by each fold. Results of the trained GRNN for neutron spectrometry shows high efficiency and generalization capability.

2. Materials and methods

As previously mentioned, GRNN applied in neutron spectrometry is an emergent research field, in which one drawback is the lack of scientific knowledge and technological tools to train, test and to evaluate the performance of the knowledge acquired by the networks trained. In this work, a GRNN was trained in order to solve the neutron spectrometry problem by using a customized designed tool.

In this work, a neutron spectrum unfolding computer tool based on neural nets technology was designed to train a GRNN capable to solve the neutron spectrum unfolding problem with high performance and generalization capabilities. The code automates the preprocessing, training, testing, validation and post processing stages of the information generated by the GRNN. The code is capable to train, to test and validate GRNN. After training and testing the neural net, the code analyzes, graph and stores the results obtained.

In order to train GRNNs, the code uses 251 neutron spectra extracted by the International Atomic Energy Agency (IAEA) compilation (IEAE, 2001). The IAEA's compendium contains a large collection of detector responses and spectra. The report aims to provide specific technical information that could be used by radiation protection specialists for proper selection of dosimeters

and survey instruments, and for interpretation of data obtained with these detectors.

At this stage of development, the customized technological tool designed to train GRNNs for neutron spectrometry uses 251 neutron spectra and three response matrix from IAEA´s compilation. The designed technological tool automates the following activities:

- Read the neutron spectra data set coming from the IAEA's compendium, which are expressed in 60 energy bins.
- Read a response matrix used to train the neural network.
- Because the neutron spectra coming from IAEA's compendium are expressed in lethargy units, the code converts these spectra in energy units.
- The neutrons expressed in energy units are multiplied by the selected response matrix in order to calculate the count rates.
- To train the GRNN, the code uses the 251 calculated count rates as entrance data and their corresponding neutron spectra expressed in energy units as the output data, Fig. 3 shows an example of neutron spectra.

- A *k-fold* cross validation of 3 folds is used to measure the performance of the methodology, two thirds of the data are used for the train stage, and the remaining is used in the test stage at each fold. Fig. 4 shows an example of the neutron spectra data set used on testing stage, compared with target spectra.
- Using the before calculated information, the following stage was to determine the spread constant value. To calculate this value, the computer tool trains several neural networks varying this value from 0 in increments of 0.01 through 2 and compare the mean square error (mse) which is used to determine the performance of the network. The minimum value obtained is selected as the spread constant value. 2000 GRNN were trained to determine in 157 s average, an optimum value equal to 0.2711 was selected, Fig. 5 shows the optimum spread constant value.

- To assess the performance, in each fold: Using the calculated spread constant value, a final GRNN was trained and tested in 0.058 s average in only one epoch. At testing stage the code compares and analyze the output of the trained neural network with the expected spectrum, showed in Fig. 4. At testing stage 82 neutron spectrum, randomly selected, were used to analyze the performance of the trained network, performing chi square and correlation tests. In this work, the best and the worst cases are shown from Figs. 6 through 9.

At testing stage, the 82 counts rates randomly selected in the preprocessing stage, are used to test the performance and generalization capabilities of the trained network, no target output is proportionated to the network. The designed code analyzes and compare the output of the network with the neutron spectrum expected as is shown in figures 6–9.

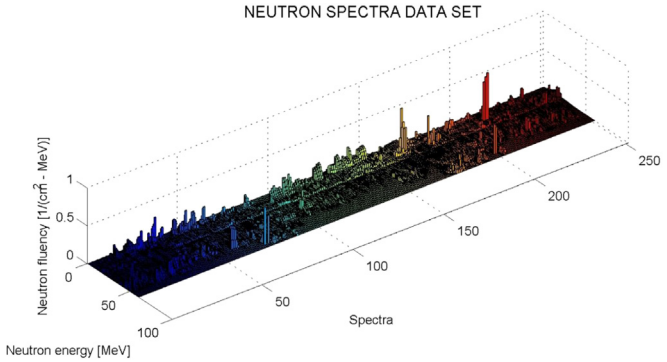

Fig. 3. Neutron spectra data set, expressed in energy units, used to train the GRNN.

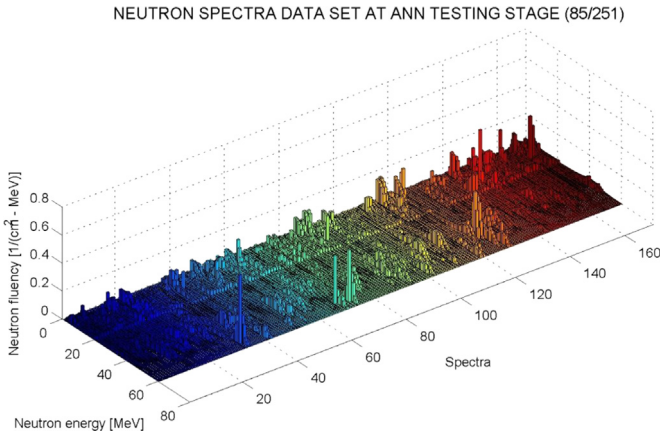

Fig. 4. Neutron spectra data set used on testing stage, compared with target spectra.

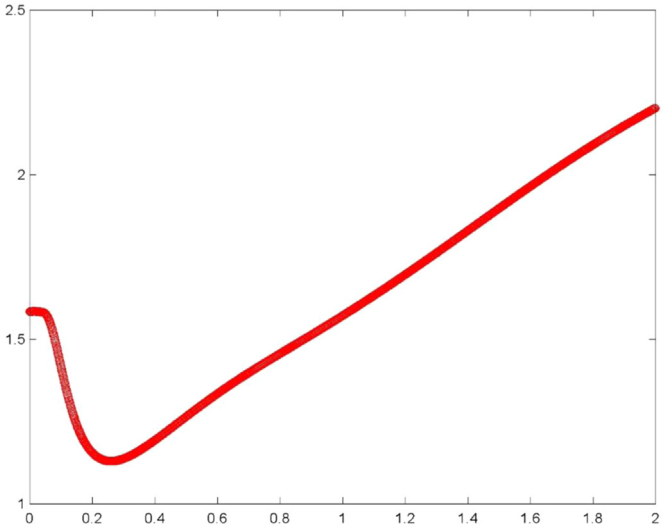

Fig. 5. Optimum spread constant value, sigma, determination.

3. Results

Fig. 6, shows the best spectrum observed at the testing stage in all the folds, compared with the expected output. The values showed in Figures 6 through 9 were calculated and graphed with the customized technological computer code.

As can be seen from Fig. 6, with the proper selection of the spread constant value, the trained GRNN calculated the 60 energy bins values of the spectrum, said values are around the target value (the spectrum from the IAEA's compendium). Opposite to BPNN, non-negative values and oscillations around the target value are generated when GRNN are used.

As can be appreciated in Fig. 6, the performance of the trained network was 2E-4. The chi-square test was 0.33636, near to the optimum value and far from the statistical margin. The correlation test was 0.99856, meaning that the GRNN calculated value and the expected spectra are very similar, therefore, the network performance is high.

Fig. 7 shows the chi-square and the correlation test of the best spectrum at the testing stage. From this figure it can be seen that the predicted and expected values, are very similar, for this experiment, a chi-square of 0.33636 was obtaining in the test stage

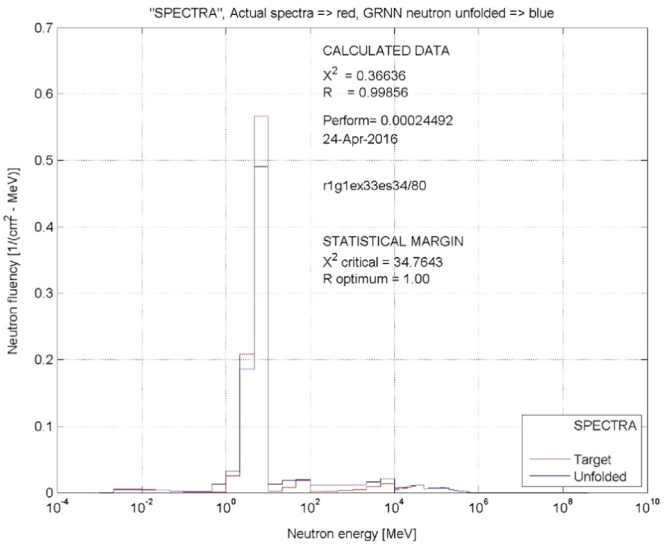

Fig. 6. Best spectrum obtained at the testing stage compared with target spectrum.

with a correlation of 0.99856, the calculated and target spectrum is very similar, the trained GRNN exhibited a high performance and generalization capabilities.

Fig. 8 shows the worst spectrum observed at the testing stage. From this figure it can be seen that the predicted energy bins spectrum are around of the target value. The chi square and correlation tests, 0.15759 and 1.0072 were obtained respectively.

As can be seen from Figs. 8 and 9, the values for the worst GRNN are less close from expected values, however, even on the worst case the values still predict the expected value in a reasonable way, therefore, demonstrating the power of a GRNN for the solution of the neutron spectrum unfolding problem, using only a limited amount of information extracted from the IAEA's compendium.

Table 1, shows the complete set of values gathered during the cross validation experiment, all the values presented were obtained during the test set, an average correlation of 0.99608 was obtained for the three best GRNN's with an average χ^2 of 0.37382 for said networks. The worst correlation and χ^2 values are also shown, an average correlation of 0.30043 was obtained for the three worst GRNN's, an average χ^2 of 0.97455 was achieved for said networks.

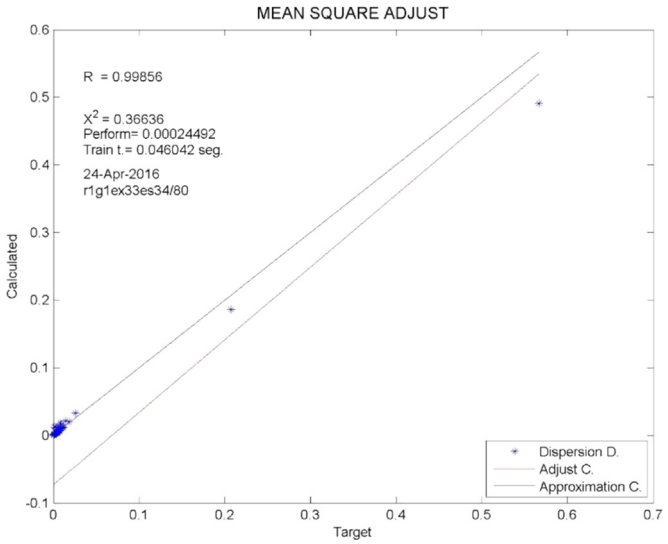

Fig. 7. Best correlation test obtained at the testing stage.

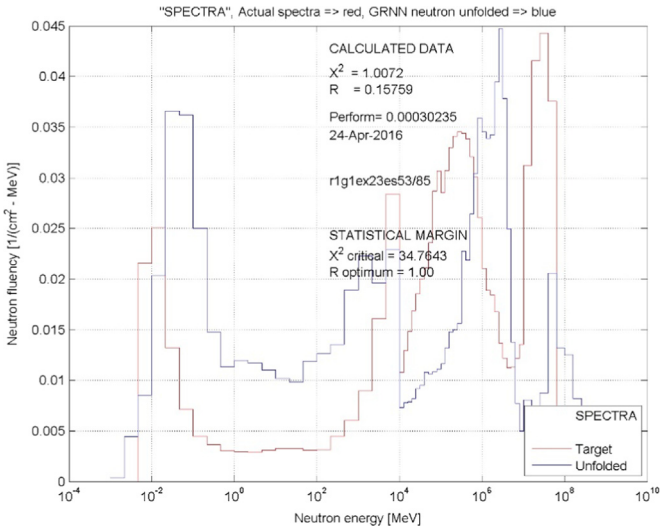

Fig. 8. Worst spectrum obtained at the testing stage compared with target spectrum.

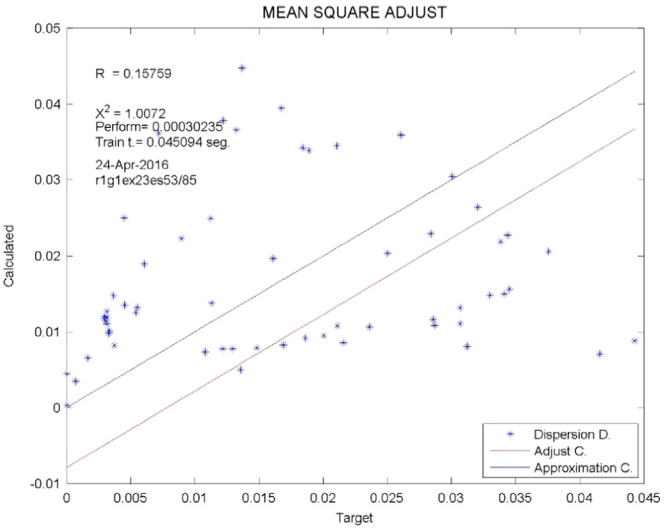

Fig. 9. Worst correlation test obtained at the testing stage.

Table 1
Performance of the methodology using 3 K-fold cross validation.

Fold	Best R	χ^2	Worst R	χ^2
1	0.99158	0.13164	0.28016	1.18
2	0.99811	0.65348	0.15759	1.0072
3	0.99856	0.33636	0.46355	0.73647
Average	0.99608	0.37382	0.30043	0.97455

Values for the best and worst GRNN by each fold are presented.

4. Discussion

ANN technology is widely recognized as a powerful modeling tool. An ANN is a massively parallel distributed processor, that trough a learning process acquires experiential knowledge, making available for use. In general, an ANN is a set of input nodes that links directly to a series of output nodes or indirectly through one or more hidden layers. The use of an ANN requires the training of the network and the testing of the trained network. During the

training, a set of synaptic weights is obtained, where the knowledge is stored.

GRNN is a special case of PNN. Compared with its competitor, i.e. BPNN, GRNN has several advantages: First of all, the structure of a GRNN is relatively simple and static with 2 layers, namely pattern and summation layers. Once the input goes through each unit in the pattern layer, the relationship between the input and the response would be "memorized" and stored in the unit. As a result, the number of units in the pattern layer is equal to the number of observations in the training sample. This type of network, is able to learn from the training data by "1-pass" training, this training represents a fraction of the time it takes to train BPNN. The spread constant value, is the only free parameter in the network. Unlike standard BPNN, GRNN estimation is always able to converge to a global solution and won't be trapped by a local minimum.

The use of GRNN to unfold the neutron spectra from the count rates measured with the BSS is a promising alternative procedure, which has been applied with success in this work. However, one of the main drawbacks was the lack of scientific and technological tools based on this technology. Therefore, a scientific computational tool was designed to train, to test, to analyze and to validate GRNN in this research domain.

5. Conclusions

An ANN simulates a highly interconnected parallel computational structure, with many individual processing elements or neurons. It learns trough an iterative process of adjustments to its synaptic weights and thresholds. A defined set of rules for the solution of a learning problem is the learning algorithm.

GRNN is one of the simplest neural network, in term of network architecture and learning algorithm. The training pattern can be considered as the center of Gaussian function and the target output could be considered as a multiplier of the probability density function. Another advantage is that the learning is instantaneous, which mean require no time for training. In this work, around 2000 neural networks were trained in 154 s average to determine the best performing network. Each network was trained in 0.058 s average.

The purpose of this work was to apply GRNN to predict the neutron spectrum using the count rates data from a BSS. Two hundred and fifty-one different types of neutron spectra, a limited amount of IAEA´s information were used as training dataset. A *k-fold* cross validation of 3 folds was used to measure the performance of the methodology. a customized computer tool was designed in Matlab to train and test a GRNN for the neutron spectrum unfolding, said tool, automates the preprocessing and the post processing information in the training and testing stages.

In the GRNN testing stage 82 spectra were predicted using the trained GRNN at each fold. Comparison with the standard spectra shows that the trained GRNN has high performance and generalization capabilities, indicating that ANN technology could be used as a promising alternative with high accuracy in neutron spectrum unfolding techniques.

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