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A comparison of back propagation and Generalized Regression Neural Networks performance in neutron spectrometry

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ABSTRACT

The process of unfolding the neutron energy spectrum has been subject of research for many years. Monte Carlo, iterative methods, the bayesian theory, the principle of maximum entropy are some of the methods used. The drawbacks associated with traditional unfolding procedures have motivated the research of complementary approaches. Back Propagation Neural Networks (BPNN), have been applied with success in neutron spectrometry and dosimetry domains, however, the structure and learning parameters are factors that highly impact in the networks performance. In ANN domain, Generalized Regression Neural Network (GRNN) is one of the simplest neural networks in term of network architecture and learning algorithm. The learning is instantaneous, requiring no time for training. Opposite to BPNN, a GRNN would be formed instantly with just a 1-pass training on the development data. In the network development phase, the only hurdle is to optimize the hyper-parameter, which is known as sigma, governing the smoothness of the network. The aim of this work was to compare the performance of BPNN and GRNN in the solution of the neutron spectrometry problem. From results obtained it can be observed that despite the very similar results, GRNN performs better than BPNN.

1. Introduction

Neutron spectrometry is not a trivial problem. The derivation of the spectral information is hard because the unknown is not given directly as result of measurements. The derivation of the spectral information is an ill-posed problem (Vega-Carrillo et al., 2005), it is derived through the discrete version of the Fredholm integral-differential equation of first type (Thomas, 2004). The system of equations that derives the spectral information have no explicit solution, and may have no unique solution. Normally, researchers solve a discrete version of this equation, which gives an ill-conditioned system of equations (Thomas and Alevra, 2002).

Since 60's years, the Bonner Sphere Spectrometer (BSS) has been the most widely used method for radiological protection purposes (Bonner, 1961). The isotropy of the response, the wide energy range (from thermal to GeV neutrons) and the easy operation make these systems still applicable (Thomas and Alevra, 2002). BSS consists of a thermal neutron detector located at the center of several high density polyethylene spheres of different diameters (Alevra et al., 1992). By measuring the count rate of each

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sphere individually, an unfolding process can, in principle, provide some information about the energy distribution of the incident neutrons (Matzke and Weise, 1985a).

However, the most delicate part of neutron spectrometry based on BSS is the unfolding process (Matzke, 2003). The unfolding spectrum of the measured neutrons consist on establishing the rate of energy distribution of fluency, known as response matrix, and the group of measures carried out (Lferde et al., 2004). Because the number of unknowns overcome the number of equations, this ill-conditioned system has an infinite number of solutions (Vega-Carrilo et al., 2006). The process of selecting a meaningful solution for the problem is part of the unfolding process.

To solve the system of equations for BSS unfolding, several approaches have been used: iterative procedures (Miller, 1993; Hertel et al., 2002), Monte Carlo methods (Matzke and Weise, 1985b; Sanna and O'brien, 1971), regularization and maximum entropy methods (Goldagen et al., 2002). However, the drawbacks associated with these traditional unfolding procedures have motivated the research of complementary approaches. Novel methods based on Artificial Intelligence (AI) have been suggested (Kardan, et al., 2003; Braga and Dias, 2002; Freeman et al., 1999; Vega-Carrillo et al., 2005; Vega-Carrilo, et al., 2006; Vega-Carrillo et al., 2007, 2009a, 2009b, 2009a, 2009b, 2010).

In neutron spectrometry, the theory of Artificial Neural Networks (ANN) has offered a promising alternative to the classic calculations over traditional methods (Vega-Carrillo et al., 2005', 2007, 2009a, 2009b, 2009a, 2009b, 2010; Vega-Carrilo et al., 2006). Neural networks are large structured systems of equations (Galushkin, 2007; Arbib, 2003; Mehrotra et al., 1997; Graupe, 2007; Dreyfus, 2005; Fausett, 1993). These systems have many degrees of freedom and are able to adapt to the task they are supposed to do (Gupta et al., 2003). Generally, there are two very different types of neural networks: Back-Propagation Neuronal Networks (BPNN) and Probabilistic neural networks (PNN) (Huang, 1999; Mao et al., 2000; Chtioui et al., 1997).

BPNN have been the most popular networks used in neutron spectrometry (Braga and Dias, 2002; Kardan et al., 2003; Sara et al., 2006; Vega-Carrilo et al., 2006; Vega-Carrillo et al., 2010, 2009a, 2009b, 2009a, 2009b, 2007', 2005). BPNN use equations that are connected using weighted factors. The selection of this factors make these neural networks so powerful. However, BPNN uses methods that are not based on statistical methods and take long time, many iterations and feedbacks until it gradually approaches the underlying function (Chtioui et al., 1997). The learning of BPNN can be described as trial and error. This is no longer the case of the PNN. The experience is learned not by trial but by experience others made for the neural network (Zhao et al., 2002).

PNN use a statistical approach in their prediction algorithm (Zhao et al., 2002; Mao et al., 2000) (Huang, 1999). The bases for the statistical approach are given in the Bayes strategy for pattern classification (Specht et al., 1991; Specht and Donald, 1992; Specht et al., 1994; Specht and Donald, 1990', 1988). These strategies can be applied to problems containing any number of categories as in the case of the neutron spectrometry problem. To be able to use the Bayes strategy is necessary to estimate the probability density function accurately. The only available information to estimate the density functions are the training samples.

Opposite to BPNN, PNN use statistical methods to select the equations within the structure and do not weight these functions differently. The Bayes strategy for pattern classification, in which PNN is based, extracts characteristics from the training samples to unfold the knowledge about the underlying function.

The aim of this work, was to compare the performance of BPNN and PNN architectures aiming to solve the neutron spectrometry problem. Results obtained shows that the two architectures solve the neutron spectrometry problem well, with high performance and generalization capabilities, however, Generalized Regression Neural Network (GRNN) outperform BPNN, mainly because GRNN does not produce negative values and oscillations around the target value.

2. Materials and methods

An ANN is a network of simple processing nodes, which is roughly modeled on the human brain (Cheng et al., 1994; Haykin, 2004). ANN consists of a number of nodes, each of this nodes can be thought of as neuron representation (Arbib, 2003; Hornik, 1989). Typically, the network is arranged such that one layer is the input layer, which receives inputs that are yet to be classified (Fausett, 1993). These inputs activate some of the neurons in the input layer, then, those neurons pass signals to the connected neurons, afterwards, the process is repeated in the next layer . In this way, a complex pattern of activations is arranged throughout the network, with final result being that some neurons in the final output layer activate (Dreyfus, 2005).

The connection between neurons are weighted, and by modifying these weights, the neural network can be arranged to perform extremely complex classification tasks such as handwriting analysis (Rehman, 2014), face recognition (Graupe, 2013) or to solve the neutron spectrometry problem.

2.1. Back-propagation neural networks

BPNN consist of neurons organized in one input layer, one output layer and several hidden layer of neurons (Apolloni et al., 2009). Neurons perform some kind of calculation. They use inputs to compute an output that represent the system (Mehrotra et al., 1997). The outputs are then passed to a connecting neuron (Galushkin, 2007). A line indicates to which neuron the output is connected. These lines carry synaptic weights.

Fig. 1 shows the structure of a BPNN. The input vector consists of variables that are used to predict the desired output (that solves the problem being analyzed). The inputs could be for example, the rates count measured with the BSS and the outputs could be the unfolded neutron spectrum.

As can be observed from Fig. 1, the information is given on to the next neuron. Each neuron receives signals coming from n neurons of the m_{j-1} layer, where m_j is the current layer. Each signal is weighted as it is given from the input layer to the first hidden layer. As the new signals reaches a connecting neuron in the hidden layer, all the signals are received by the neuron and are summed up. This process can be seen as a multiplication vector of the weights vector w and the signal vector $y_{previous}$ of the previous layer. In the hidden layer new signals are computed and given on to the next hidden layer. This process continues until the output layer is reached (Fig. 2).

The previous process in the neural network is repeated. The values of the signals along with weights will be different but the process itself will continue similarly. The signals are weighted and then summed up, they cause a reaction of the neuron and the reaction, which is the new signal, will be given on to the next neuron.

The last step is to give the signal to the output layer. The output layer can consist of one or more neurons. More neurons mean that the plane of the neural network has multiple outputs. In the output neuron a calculation is necessary to yield a value that is not normalized in order to have a physical meaning.

One characteristic of BPNN is that they are very flexible. They can be used to solve different problems. Another advantage is that the process is highly parallel, however, BPNN have some

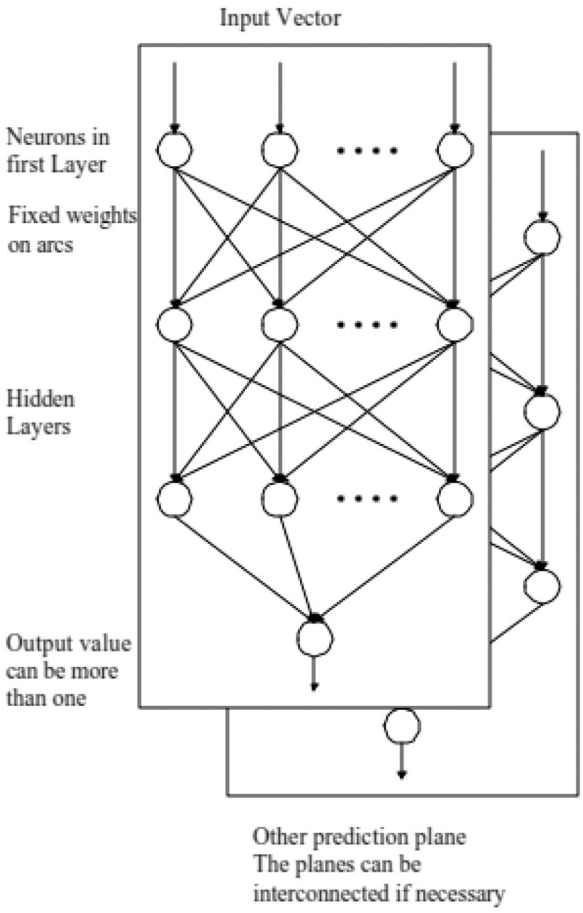

Fig. 1. BPNN architecture.

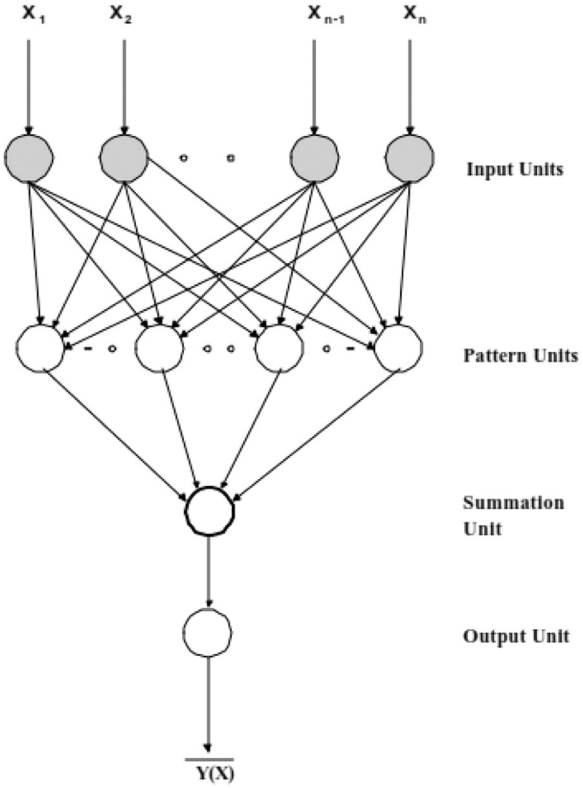

Fig. 2. GRNN architecture.

drawbacks (Ortiz-Rodriguez et al., 2006; Martinez-Blanco et al., 2006). The structural and learning parameters of the network are often determined using the trial an error technique. This produce networks with poor performance and low generalization capabilities affecting the application of the trained networks in real applications. The training stage can be time consuming in order to gradually approach good values of the weights. The size of the training data has to be very large, thus, often it is almost impossible to provide enough training samples as in the case of the neutron spectrometry problem. Another drawback is that adding new information requires retraining the network and this is computationally expensive for BPNN but not for PNN (Chtioui et al., 1997). PNN have the big advantage that the prediction algorithm works with only few training samples (Specht et al., 1991). Other big advantage is that they are very flexible and new information can be added immediately with almost no retraining.

The learning of BPNN can be described as trial and error. A GRNN has certain differences compared to an BPNN approach (Specht and Donald, 1992). The experience is learned not by trial, is learned by experience others made for the neural network. The biggest advantage is the fact that the probabilistic approach works with one-step-only learning.

2.2. Generalized Regression Neural Networks

GRNN belong to PNN classification. These neural networks use a statistical approach in their prediction algorithm (Specht and Donald, 1990, 1988, 1992). The bases for the statistical approach are given in the Bayes strategy for pattern classification. These strategies can be applied to problems containing any number of categories as in the case of the neutron spectrometry problem. In order to use the Bayes strategy, it is necessary to accurately estimate the probability density function (PDF) (Specht and Donald, 1992). The only available information to estimate the PDF are the training samples. The structure of the calculations for the probabilistic density function has striking similarities to BPNN.

The general structure of GRNN (Zhao et al., 2002) consists of; one input layer and two hidden layers. The first hidden layer contains the pattern units. Each pattern unit represents information on one string sample. Each pattern unit calculates the probability on how well the input vector fits into the pattern unit. In the second hidden layer there is only one summation unit. Here it is decided upon the individual results of each pattern unit in which pattern the input vector finally belongs. The output unit performs again a calculation to give the output which is physically meaningful.

A further difference that exists between BPNN and GRNN is the difference in the process inside the neurons (Zhao et al., 2002; Specht et al., 1991; Specht and Donald, 1988). A GRNN use functions that are based on knowledge resulting from the Bayes strategy for pattern classification. The strength of a probabilistic neural network relay in the function that is used inside the neuron.

In this work, a comparison of the performance obtained in the solution of the neutron spectrometry problem using two different neural network architectures, BPNN and GRNN, is presented. Both, BPNN and GRNN, were trained and tested using the same information: two hundred and fifty-one neutron spectra, extracted from IAEA's compilation. 80% of the whole data set was randomly selected as a training set, the remaining 20% was used as a testing set. 50 neutron spectra were used as testing data set.

The architectural and learning parameters of the PBNN were optimized using a statistical methodology known as Robust Design of Artificial Neural Networks Methodology (RDANNM) (Ortiz-Rodriguez et al., s.f.). In GRNN the only parameter determined was the spread constant value, known as sigma. Customized scientific

computational tools were used for the training, testing, analysis and storing of the information generated in the whole process. From results obtained it can be observed that despite two networks architectures shown very similar performance and generalization capabilities, GRNN perform better than BPNN in the solution of the neutron spectrometry problem. BPNN produce negative values and high oscillations around the target values, which makes this type of network not useful in the solution of the problem mentioned.

3. Results

By using the RDANNM, 50 different network architectures were trained in an average of 150 min, before the selection of the near optimum architecture. By testing different network architectures according RDANNM, each network was trained in 50E3 epochs and 180 s average, stopping the training when the network reached the established mean square error (mse) equal to 1E-4, value used to measure the network performance. After selecting the near optimum architectural and learning parameters of the BPNN, the network was trained and tested using the following values: one hidden layer with 10 neurons, a *trainscg* training algorithm and a learning rate and momentum equal to 0.1 and 0.01 respectively, a detail description is presented in Table 1.

Opposite to BPNN, the spread constant (sigma) was the only value determined in GRNN. Using the same training and testing data sets used for BPNN, 2000 neural networks were trained in an average of 154 s, in order to determine the spread constant equal to 0.2711. Each GRNN was trained in 0.058 s average in only one-step-only learning.

Table 1 shows the obtained values after training the two networks architectures being compared in this work. As can be seen, when the trial-and-error technique is used it is very difficult to determine if the performance of the network is good or bad, mainly because is not used a scientific and systematic methodology for determining the near optimum learning and architectural values as when RDANNM is used.

Table 1
Comparison between BPNN and GRNN values in neutron spectrometry.

Network parameters	BPNN [trial and error]	BPNN [RDANNM]	GRNN
Networks tested before training	Undetermined	50 in 150 min	2000 in 154 s
Hidden layers	Undetermined	1	Fixed architecture
Neurons in hidden layer	Undetermined	10	According input
Training algorithm	Undetermined	Trainscg	Statistical methods
Learning rate	Undetermined	0.1	–
Momentum	Undetermined	0.01	–
Spread constant	–	–	0.2711
Performance [mse]	Undetermined	2.12E-4	2.48E-4
Training time [s]	Several hours	170.40	0.058
Epochs	Often millions	50E3	1
Best Chi-square test BPNN		2.3525	0.049
Statistical margin 34.7			
Best Correlation test BPNN		0.9928	0.99571
Statistical margin 1			
Worst Chi-square test BPNN		0.44704	0.3223
Worst Correlation test BPNN		0.2926	0.46023

As is shown in Table 1, after training both network architectures, BPNN optimized using RDANNM and GRNN, the performance measured by mse reached by the two networks is very similar between both strategies. In BPNN networks, the mse is a value optimized by the network designer using RDANNM, in a GRNN network the value is automatically obtained by the network based on the training information. Said differences, demonstrates the powerful of RDANNM in the optimization of the near optimum values of BPNN architectures.

Fig. 3 shows that at testing stage, the chi-square and correlation tests are very close in both, BPNN and GRNN network architectures. The same 50 neutron spectra were used for testing the two networks. At testing stage, only the count rates were fed to the trained networks. The output produced by the networks was compared with the expected neutron spectrum taken from IAEA's compilation by means of chi-square and correlation tests. In the trained networks, two spectra are above the statistical margin of the chi-square test. In correlation tests, both BPNN and GRNN obtained 0.2926 and 0.46023 respectively. This shows the high performance of the networks.

As can be seen from Fig. 3, the 50 chi-square and correlation tests of trained networks are very similar. In both cases the average value is around 0 and 0.8 respectively, which is near of the optimum values equal to 0 and 1. This demonstrate the high performance of BPNN and GRNN, generalization capabilities, and demonstrates the effectiveness of the RDANNM in the design of near optimum architectures of BPNN.

As before mentioned, 50 neutron spectra were randomly selected at testing stage. The same training and testing data sets were used to train and to test the performance and generalization capabilities of the networks. The best and the worst cases for both, BPNN and GRNN, are showed in Figs. 4–7. Figs. 4 and 5 show the best cases observed at testing stage for BPNN and GRNN respectively. From these figures it can be observed that the chi-square test for both, BPNN and GRNN, are 2.3525 and 0.0490 respectively, the correlations for BPNN and GRNN are 0.9928 and 0.99571 respectively, which means that the compared neutron spectra are very similar.

As can be appreciated in Figs. 4–7, despite the good results obtained with BPNN, one drawback is that the calculated neutron spectra produce negative values, said values have no meaning in real problems. These negative values are eliminated from the output produced by the network, however, when the BPNN is applied in real workplaces, Due the training received, the network tends to produce negative values and oscillations around the target value. GRNN networks do not produce these negative values and oscillations, therefore the performance is better than BPNN in the solution of the neutron spectrometry problem.

Figs. 6 and 7 show the worst case observed at testing stage for BPNN and GRNN networks respectively. As can be seen from these figures both, BPNN and GRNN, selected the same neutron spectra as the worst. This could be because the 50 energy bins that the neural networks calculate, 49 values are very similar and only one value is far from the expected target value, this causes that the chi-square and correlation tests produce low values. From Figs. 6 and 7 can be observed that in the GRNN architecture the output is closer than the target values of the neutron spectra when compared with BPNN. This shows that in the worst case, GRNN outperformance BPNN.

4. Discussion

Statistical methods tend to emphasis on the structure of the data. For neural network methods the structure of the data is secondary. Therefore, the amount of data needed for statistical

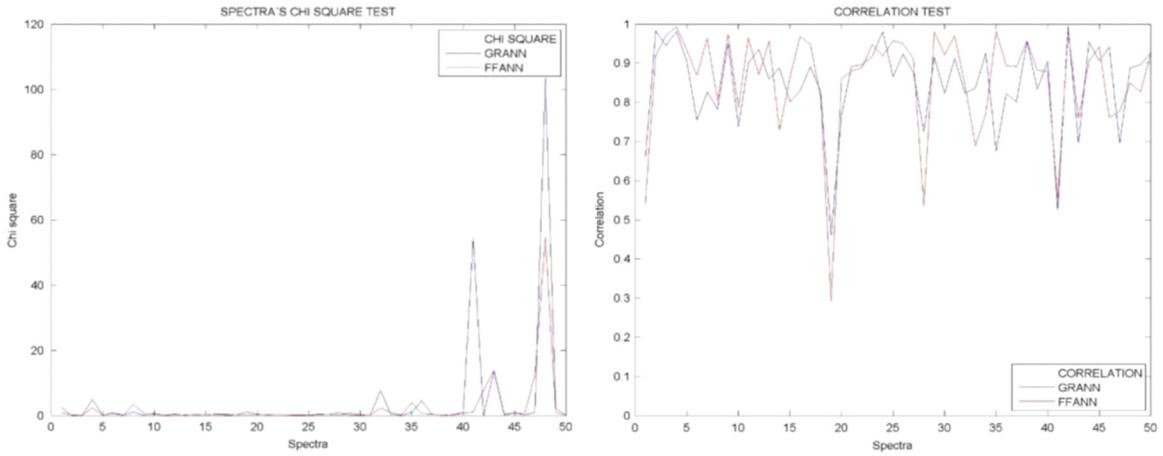

Fig. 3. Chi-square and correlation tests comparison for BPNN and GRNN.

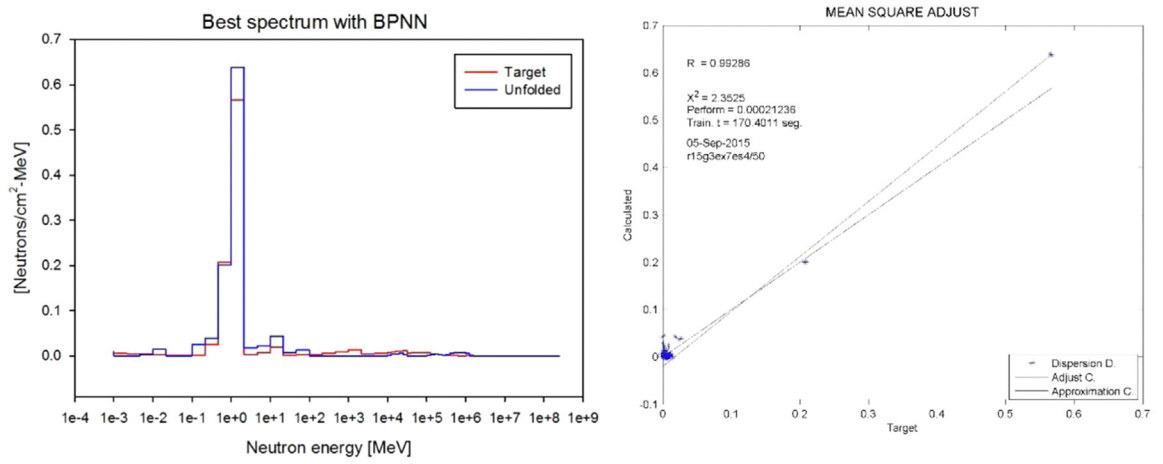

Fig. 4. Best chi-square and correlation tests obtained with BPNN.

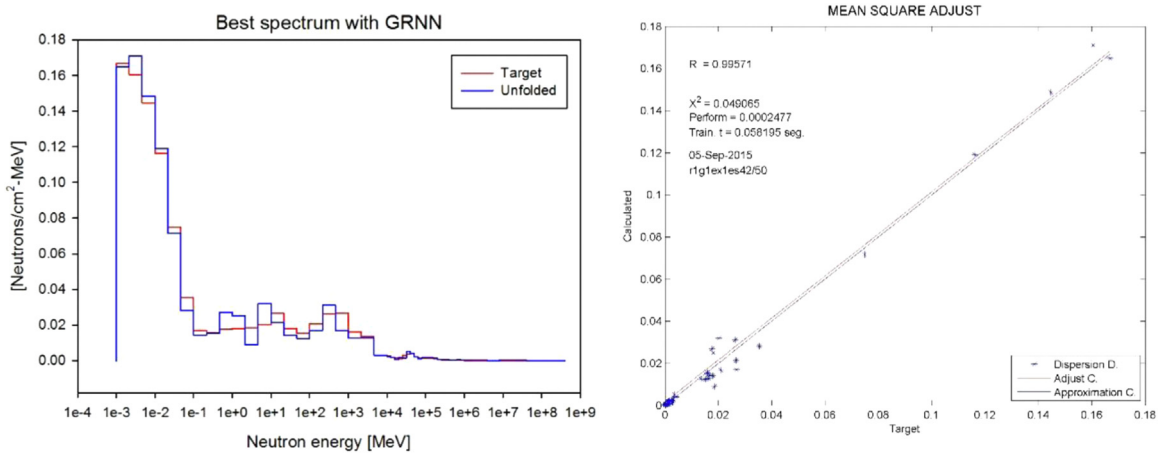

Fig. 5. Best chi-square and correlation tests obtained with GRNN.

methods is a smaller than the amount of data needed for ANN approaches.

Most methods are asymptotically good, nevertheless most of them have severe drawbacks as well. BPNN need a large number of training samples and the weights refinement is time consuming. Adding of new information requires retraining and this is computationally expensive for BPNN but not for PNN. PNN have the big advantage that the prediction algorithm works with only a few training samples. Other advantage is that they are very flexible and new information can be added immediately with almost no retraining.

PNN use a statistical approach in their prediction algorithm. The bases for the statistical approach are given in the Bayes strategy for pattern classification. These strategies can be applied to problems containing any number of categories as in the case of the neutron spectrometry problem. To be able to use the Bayes strategy it is necessary to estimate the probability density function accurately. The only available information to estimate the density

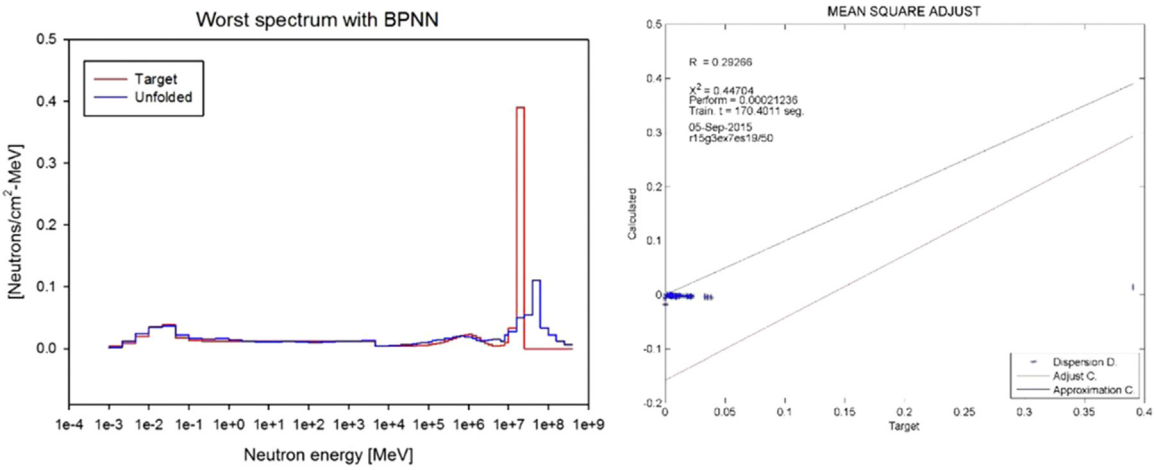

Fig. 6. Worst chi-square and correlation tests obtained with BPNN.

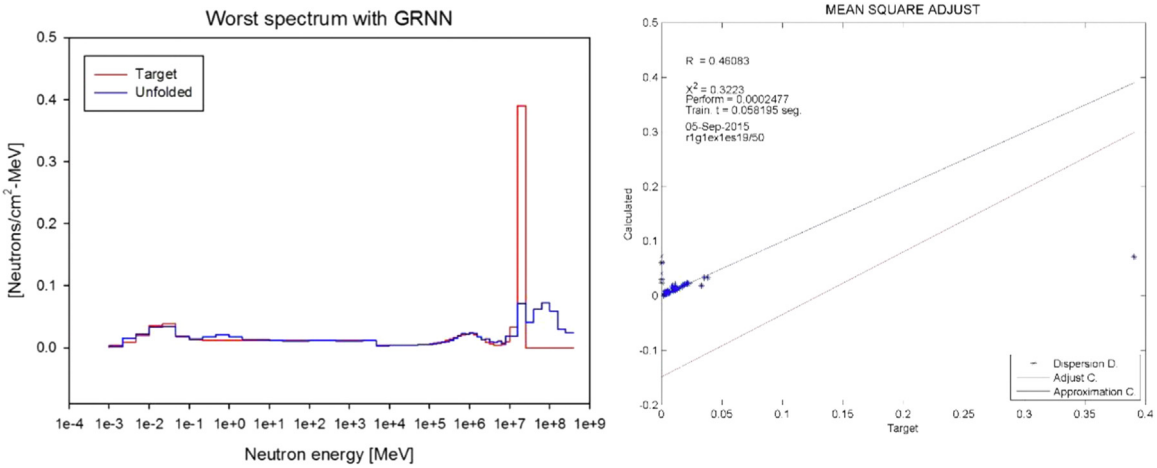

Fig. 7. Worst chi-square and correlation tests obtained with GRNN.

functions are the training samples.

The structure of the calculations for the PDF has striking similarities to a back-propagation feed-forward neural network. PNN are frequently used to classify patterns based on learning from examples. PNN algorithm uses the Bayes strategy for pattern classification. Different rules determine patterns statistics from the training samples. BPNN uses methods that are not based on statistical methods and need a long time to compute and many iterations and feedbacks until it gradually approaches the underlying function. It would be desirable to approach the parameters in one-step-only approach. The Bayes strategy for pattern classification extracts characteristics from the training samples to come to knowledge about underlying function.

5. Conclusions

In this work, two different Artificial Neural Networks architectures, BPNN and GRRN, were trained and tested using the same information. The performance of the networks was compared. From results obtained it can be observed that GRNN perform better than BPNN in the solution of the neutron spectrometry problem.

Different approaches exist to model a system with the data available. Each one of them has its very own qualities and therefore advantages. GRNN falls into the category of PNN. This neural network like other PNNs needs only a fraction of the training samples as a BPNN would need. The data available from measurements of an operating system is generally never enough for a BPNN. Therefore, the use of GRNN is especially advantageous due to its ability to converge to the underlying function of the data with only few training samples available. The additional knowledge needed to fitting in a satisfying way is relatively small and can be done without additional input by the user.

PNN have a very simple structure, therefore very stable procedures. PNN perform very well for even only a few available training samples, nevertheless the quality increases as the number of training samples increases. This makes GRNN a useful tool to perform predictions and comparisons of system performance in practice. GRNN is a promising technological tool that can be applied to solve with high efficiency problems related with neutron spectrometry.

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