THE UNFOLDING EFFECTS OF TRANSFER FUNCTIONS AND PROCESSING OF THE PULSE HEIGHT DISTRIBUTIONS

by

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This paper deals with the improvements of the linear artificial neural network unfolding approach aimed at accurately determining the incident neutron spectrum. The effects of the transfer functions and pre-processing of the simulated pulse height distributions from liquid scintillation detectors on the artificial neural networks performance have been studied. A better energy resolution and higher reliability of the linear artificial neural network technique have been achieved after implementation of the results of this study. The optimized structure of the network was used to unfold both monoenergetic and continuous neutron energy spectra, such as the spectra of ^{252}Cf and ^{241}Am–Be sources, traditionally used in the nuclear safeguards experiments. We have demonstrated that the artificial neural network energy resolution of 0.1 MeV is comparable with the one obtained by the reference maximum likelihood expectation-maximization method which was implemented by using the one step late algorithm. Although the maximum likelihood algorithm provides the unfolded results of higher accuracy, especially for continuous neutron sources, the artificial neural network approach with the improved performances is more suitable for fast and robust determination of the neutron spectra with sufficient accuracy.

Key words: unfolding, neutron spectra, pulse height distribution, MCNP-PoliMi numerical code, linear ANN, maximum likelihood method

INTRODUCTION

Accurate detection and characterization of nuclear materials are of an urgent need in the area of nuclear non-proliferation and homeland security [1]. Special nuclear materials, as well as several radionuclides, many of which are in regular use in industry, medicine or energy production need to be monitored to avoid risks. Neutron measurements are widely used for nuclear safeguards applications since they do not experience the problem of self-shielding that -rays exhibit in larger samples. A way of detecting neutrons from samples is by using organic scintillation detector because of its good capability to discriminate neutrons against -rays by means of pulse shape. One possible way of a neutron source identification is based on an optimized fast pulse-shape discrimination algorithm in a mixed radiation field [2] or numerical techniques which do not relay on the unfolding technique [3]. Another possibility of detecting and identifying nuclear materials in non-proliferation and homeland security applications is based on the determination of the energy spectrum of the neutron source [4]. Neutron spectrometry by unfolding the light pulse amplitude spectra is appropriate in the field measurements for safeguards purposes. The neutron spectrum is a unique characteristic of each neutron source and therefore it is of high priority for accurate neutron source identification.

Organic scintillators (liquid and plastic) are used in many nuclear applications, including identification and characterization of nuclear materials [5]. Detection of neutrons in such detector is based on multiple scatterings on hydrogen and/or carbon, as the main constituents of the scintillator material. The neutron deposits a portion of its initial energy in the scattering collisions and the energy deposited is converted to scintillation light, which is collected by the photomultiplier tube (PMT) and converted to a measured pulse. Pulse-height distributions (PHD) from the detector based on proton recoil are used to unfold neutron energy spectra.

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Overview of the traditional unfolding techniques (based on least-squares, iterative, and Monte Carlo methods) is given in [6, 7], while the alternative unfolding technique based on neural networks is described in [8-10] and the references therein. One of objects of our investigation was to achieve a better energy resolution and higher reliability of the linear artificial neural network (ANN) technique, since very small deviations from the target values can cause uncertainties of the unfolded results. The improvement of the energy resolution of the linear ANN leads to better performances of the neutron unfolding technique. This paper also deals with comparative analysis of the modified ANN technique with the reference method based on the maximum likelihood expectation-maximization (MLEM) method with one step late (OSL) algorithm, having excellent unfolding performances [11-13].

MONTE CARLO SIMULATION OF THE DETECTOR RESPONSE MATRIX

The response matrix of the detector should be available for the unfolding procedures. The detector response matrix is determined by calculating the pulse height spectra of incoming neutron with various energies. Calculation of such response matrices and their use in unfolding an unknown neutron spectrum has been investigated to a large extent in the past (see [14] and the references therein). The response matrix has been simulated with high-fidelity and accuracy by using the MCNP-PoliMi numerical code based on the Monte Carlo method [15]. This code provides a very accurate simulation of each neutron interaction in a scintillator material. We used a postprocessing Matlab code for the analysis of the interactions occurring in the scintillator material. The measured pulse-height distributions from neutron sources traditionally used in nuclear safeguards experiments were compared to distributions simulated with the MCNP-PoliMi code and very good agreement was achieved [16].

In the response matrix, each row corresponds to a given neutron energy and each column corresponds to a given pulse height. The detector response, the count rates, and the neutron spectrum, are related through the Fredholm integral equation of the first kind. The continuous equation can be reduced to the following discrete form

$$N_j \quad r_{ij}\phi_i \qquad (1)$$

where N_j is the count rate recorded in the j^{th} channel of the pulse height distribution, Φ_i – the incident neutron fluence in the i^{th} energy group, and r_{ij} – the corresponding element of the response matrix. The response matrix of the detector (5 cm 5 cm cylindrical NE-213 scintillator) was calculated by the MCNP-PoliMi numerical code in the energy range between 0 and 15 MeV. The detector response matrix is related to 150 neutron energy groups of 0.1 MeV width and 256 channels for distributions of pulse amplitude for each energy bin. Only one part of the detector response matrix for neutrons in the energy range between 4 MeV and 5 MeV with step of 0.1 MeV is given in fig. 1.

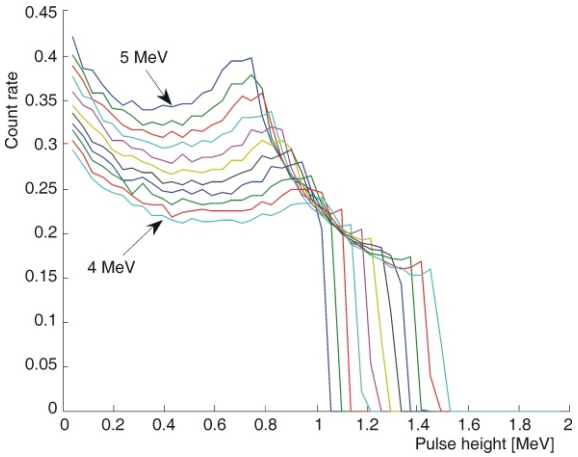

Figure 1. The detector response matrix for neutrons with energies between 4 MeV and 5 MeV with step of 0.1 MeV

CHARACTERISTICS OF THE MLEM AND LINEAR ANN UNFOLDING METHODS

The linear ANN unfolding with improvement of the energy resolution

The results presented in paper [8] have shown that the linear ANN technique can be successfully used for the unfolding of pulse height distributions obtained by the MCNP-PoliMi calculations, or measured by liquid scintillation detectors. The neural network constructed with a transfer function *f*, performs a mapping of the detector data, *y*, to the neutron energy spectrum, *x*, *i. e.*, $x = f(y)$ [17]. One feature of this approach is that continuous spectra can be expressed as a linear superposition of known monoenergetic spectra by using a linear transfer function. The linear network was trained with a large number of light pulse distributions (recorded in 256 channels) for a number of different neutron energies up to 15 MeV (150 energy groups with 0.1 MeV width).

In the previous work [8] it was demonstrated that the best results in the identification of unknown neutron spectra had been achieved with the linear network with the width of energy group of 0.6 MeV, which represented a tradeoff between energy resolution and accuracy of the unfolding procedure. However, we noticed that there were deviations between target and calculated values in the training process that caused some uncertainties in the unfolded monoenergetic and continuous spectra. In this paper we have shown that taking into ac-

count new pre-processing of the input data, *i. e.* derivation of the pulse height spectra with amplification (which was left out in the previous work), the unfolded results can be obtained with both good properties, *i. e.* reduced energy resolution of 0.1 MeV and good agreement with the reference spectral data.

The linear neural network was constructed for unfolding of neutron energy spectra with 150 output neurons for 150 energy groups of 0.1 MeV width. O_j, the output of the j^{th} output neuron is given as

$$O_j \quad f(b_j \quad \sum_i w_{ij} \; x_i) \qquad (2)$$

where f is the linear transfer function of the neurons, $w_{i,j}$ – the weight connecting the i^{th} input neuron to j^{th} output neuron, b_j – a bias, and x_i – the input of the i^{th} neuron in input layer.

We have studied the effect of the transfer function on the linear ANN performance with "purelin", "satlin" and "satlins" transfer functions shown in fig. 2. The unfolded neutron peak with energy of 5 MeV obtained after training process with the transfer functions mentioned before and with bias and no bias is presented in fig. 3. It is obvious that satlin transfer function contributes to the best performances of the ANN approach in the case of one monoenergetic neutron peak. However, in the case of neutron spectra with a few neutron peaks of equal probability at energies of 4, 8, and 12 MeV (shown in fig. 4.), the third peak at energy of 12 MeV disappeared by using satlin transfer functions. All three peaks have been detected by using "purelin" and "satlins" transfer function (deviations between "purelin" and "satlins" unfolding results are negligible). Intensities of the peaks obtained by 'purelin' transfer function are equal up to about 11 MeV but at 12 MeV intensity of the peak is smaller from the target value of 1 for about 30%.

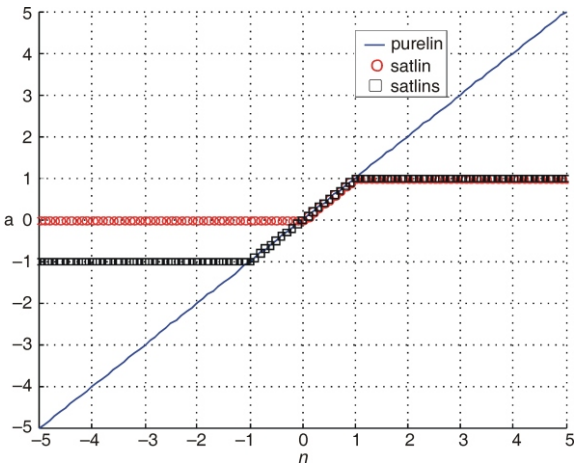

Figure 2. Transfer functions ("purelin", "satlin" and "satlins")

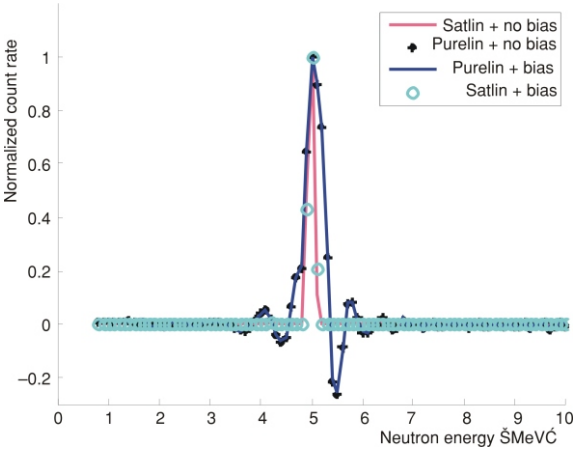

Figure 3. Neutron peak at 5 MeV obtained by the linear ANN with various transfer functions

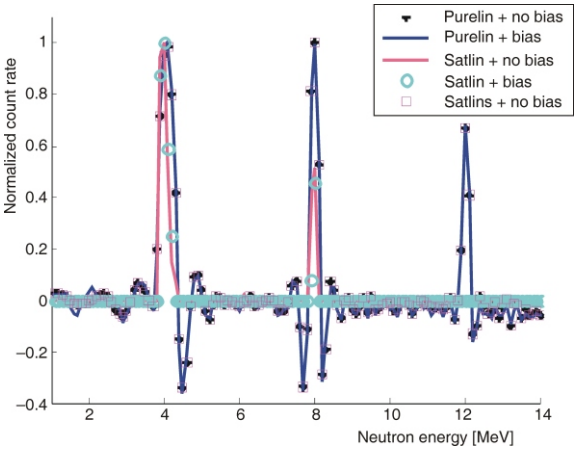

Figure 4. Three neutron peaks of equal probabilities obtained by the linear ANN with various transfer functions

It was demonstrated in ref. [9] that differentiation of neutron response functions led to a highly peaked function so that the unfolding problem became approximately linearly separable problem. In this paper the effect of the way of pre-processing of the input data on the ANN unfolding results has been investigated with pulse

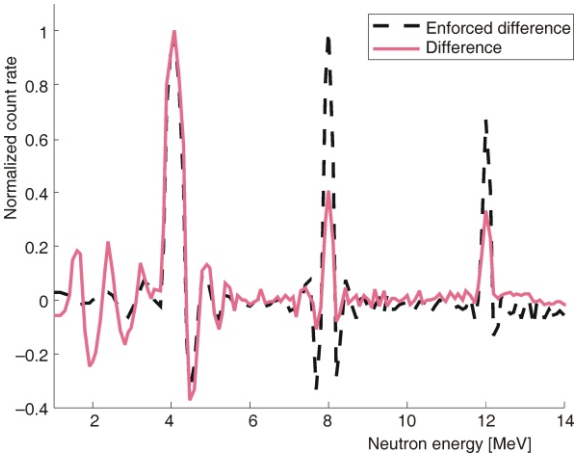

Figure 5. Three neutron peaks of equal probabilities obtained by pre-processing the training data in two ways

height distribution for neutron spectra with three peaks. Figure 5 shows the unfolded results obtained after applying the simple derivation of the pulse height spectra and amplification of the input data derivations, *i. e.,* after making larger the first difference between neighbouring pulse height channels. It is obvious from fig. 5 that the latter method of pre-processing of the input data contributes to the improvement of the linear ANN performances taking into account less oscillations and more accurate intensities of the peaks.

After implementation the results of the study mentioned above, we have constructed the optimized network with a better energy resolution of 0.1 MeV, which is comparable to the energy resolution obtained by using the MLEM method, explained below. Optimization of the network for unfolding both monoenergetic and continuos spectra was performed by using "purelin" transfer function and enlarging first differences of the input pulse height distributions.

Unfolding by the MLEM method with OSL algorithm

Maximum likelihood method is a popular statistical method used to make inferences about parameters of the underlying probability distribution of a given data set. The method increases the likelihood that the neutron spectrum estimate will generate the measured data until an absolute maximum during each iteration. Neutron spectrum is constrained to remain positive in each iteration. The MLEM [11] algorithm takes into account the Poisson nature of the noise in the amplitude distribution data. This features of MLEM algorithm lead to the neutron spectra that are not noise. However, neutron spectrum reconstruction is slow, especially when accurate response matrices are used.

A possible way to model the Poisson nature of the measurements is to treat the data as stochastic variables and not as exact measures. This is the usual case in unfolding for a Poisson distribution, without making any *a priori* assumptions about neutron spectrum distribution. The log likelihood function is

$$\ln P_r \quad \sum_{i\ 1}^{I} \left(\sum_{j\ 1}^{J} r_{ij} x_j \right) \quad y_i \ln \sum_{j\ 1}^{J} r_{ij} x_j \quad \ln(y_i !) \quad (3)$$

where y_i are binned count rates, x_j – the incident neutron fluence in the i^{th} energy group, and r_{ij} – the corresponding element of the response matrix. The MLEM is used to find non-negative values of each x_j.

The MLEM has a drawback that it generates noisy neutron energy spectra when the iterations proceed. This sort of over-fitting can be avoided if the iterations are stopped before the convergence. This approach suffers from a noise-bias trade-off. If the convergence is reached, the solution is too noisy. On the other hand, if a small number of iterations are used, the solution is less noisy, but the quantitative level of solution values are biased towards the initial solution.

The solution is required not to fit with the data as well as possible, but also be consistent with additional criteria in order to make an ill-posed reconstruction problem to a well-posed one. The objective function to be maximized is not the likelihood (eq. 3) but a posteriori probability density function (PDF).

The prior is described by the Gibbs distribution $P(x) \quad \exp[\ \beta U(x)]$ [12], the penalty term, where β is a scalar weighting parameter, and $U(x)$ – the energy function.

One of the Bayesian formulations, OSL algorithm, uses a current estimate $x^{(k)}$ when calculating the value of the derivative of the energy function U [13]. The OSL update can be solved as

$$x_k^{k\ 1} \quad \frac{x_j^k}{\sum_{i\ 1}^{I} r_{ij} \quad \beta \dfrac{\partial U(x,j)}{\partial x_j}} \sum_{i\ 1}^{I} r_{ij} \frac{y_i}{\sum_{l\ 1}^{J} r_{il} x_l^k}, \qquad j \quad 1,\ldots, J \quad (4)$$

where $U(x, j)$ is energy function chosen as

$$U(x,j) \quad \sum_{b\ N_j} w_{jb} v(x_j \quad x_b) \quad (5)$$

where w_{jb} is the weight of energy bin b in the neighbourhood of energy bin j and parameter β expresses the confidence of the prior. The Gibbs distribution and energy are mathematical constructs and they are not related to real physical quantities. In our investigations we used a well-known choice of quadratic prior $v(r) = r^2$. The regularization parameter β controls the degree to which the models of the prior are accentuated, and keeps constant during the iterations. An appropriate value for parameter β should be empirically selected. For $\beta = 0$, the OSL is reduced to the usual MLEM algorithm.

THE RESULTS OF UNFOLDING BY THE OSL AND LINEAR ANN

Monoenergetic neutron sources

The responses of the OSL and ANN to the input data are shown in fig. 6. We investigated three neutron peaks of equal probability with energies of 4 MeV, 8 MeV, and 12 MeV. It can be seen that the MLEM method with OSL exactly predicts energy of sharply unfolded neutron peaks with energy resolution of 0.1 MeV, but the intensities of the peaks are not equal. The peak at 4 MeV is correctly estimated, but the peak at 8 MeV is about 80% of the reference peak by its intensity, and the intensity of the peak at 12 MeV is 85% of the reference peak intensity. It can be noticed that the peaks obtained by the OSL are slightly narrower compared to the ones obtained by the linear ANN.

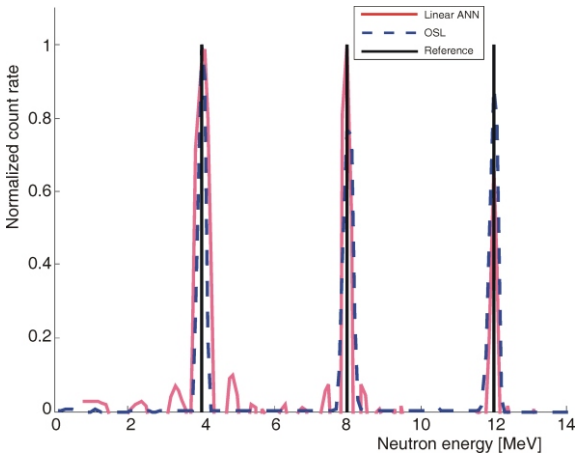

Figure 6. The unfolded spectra from the simulated data with three neutron peaks

The linear ANN method identifies the peaks with energies of 4 MeV, 8 MeV, and 12 MeV with the energy resolution comparable with the energy resolution obtained by the maximum likelihood method. It is obvious that the energies of the neutron peaks have been correctly identified, however, their intensities deviate somewhat from the target values, but still less compared to the peak intensities obtained by the MLEM method with OSL algorithm. Maximum deviation of about 25% was detected for the third peak at 12 MeV, while the intensities of the first two peaks achieved the target values. On the other hand, the linear ANN results show more oscillations than the MLEM unfolded results. It can be expected that application of an appropriate smoothing procedure can reduce the ANN oscillations.

It can be noticed that both unfolding approaches correctly identify energies of neutron peaks, while their intensities deviate somewhat from the reference data.

Continuos neutron sources

The MLEM method and linear ANN have been also applied to continuous spectra, such as the spectra of the ^{252}Cf and ^{241}AmBe neutron sources, traditionally used in the nuclear safeguards experiments. The results of the unfolding of the simulated pulse height distributions from the ^{252}Cf neutron source, obtained by the linear neural network, trained only with the simulated monoenergetic neutron sources, are shown in fig. 7. A fairly good agreement can be seen between ^{252}Cf neutron source spectrum obtained by the linear ANN and the reference spectrum. The results obtained by the reference OSL algorithm are also presented in fig. 7. In can be noticed that the best agreement with the reference data is obtained by the MLEM with OSL method. The ANN approach still provides the unfolded neutron spectra with sufficient accuracy, although the linear ANN unfolded results show larger deviations from the reference spectrum compared to the OSL results.

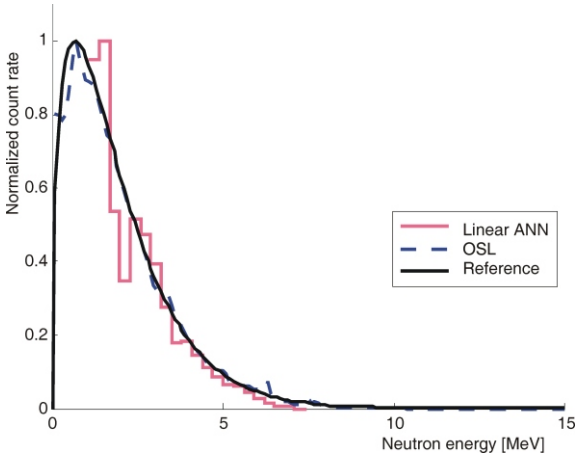

Figure 7. Unfolded spectra of ^{252}Cf source from the simulated data by using the MLEM with OSL and linear ANN compared with the reference data

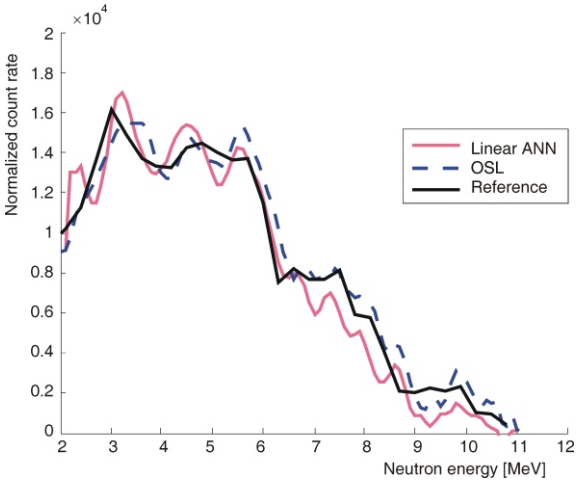

Figure 8. Unfolded spectra of the ^{241}AmBe source from the simulated data by using the MLEM with OSL and linear ANN compared with the reference data

Figure 8 shows the reference spectrum and the unfolded spectrum of the ^{241}AmBe neutron source from the simulated data. Very good agreement between the MLEM with OSL results and the reference spectral data can be noticed, whereas the results obtained by the linear ANN show slightly higher deviations from the reference spectrum.

CONCLUSIONS

This paper deals with the fast and robust unfolding method based on the linear ANN approach with improved characteristics for evaluation of neutron energy spectra obtained by the organic scintillation detector. We have considered the application of linear ANNs in neutron spectrometry with the aim of optimizing a network that could be used for the identification of both monoenergetic and continuous energy

spectra. By using the principle of superposition, continuous spectra can be expressed as linear combinations of monoenergetic spectra so that the unfolding of continuous spectra can be performed using a network that is trained only with monoenergetic spectra.

Implementation of the results regarding the effects of transfer functions as well as pre-processing of the input data has provided construction of the network with the optimized unfolding performances. Thus, the linear ANN with "purelin" transfer function and with amplification of the pulse height derivatives was used to unfold both monoenergetic and continuous neutron spectra.

It was demonstrated that the linear ANN approach can be efficiently used for the unfolding of pulse height distributions obtained by the MCNP-PoliMi simulation of incident neutron interactions with liquid scintillation materials for either monoenergetic or continuous neutron sources. The MLEM method with OSL algorithm has been chosen as a reference unfolding method, because of its excellent unfolding performances. Analysis of the results has shown that the MLEM with OSL method provides the unfolded results with very good energy resolution and with correctly identified neutron energies for monoenergetic neutron peaks as well as for continuos neutron spectra. On the other hand, a drawback of the MLEM method is that neutron spectrum reconstruction is slow since the great number of iterations is required, especially when accurate response matrices are used. The ANN technique with the improved performances is more suitable for fast and robust determination of the neutron spectra with good energy resolution and sufficient accuracy. The modified ANN approach represents a trade-off between accuracy and time consumption in unfolding procedure.

Recently it has been suggested [18] that the analytical method developed supplies a fast and computationally simple method for generating such training sets. It is planned in the next stage of research to compare the results obtained by analytical and numerical training data.

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АНФОЛДИНГ ЕФЕКТИ ПРЕНОСНЕ ФУНКЦИЈЕ И ОБРАДЕ АМПЛИТУДСКЕ РАСПОДЕЛЕ ИМПУЛСА

У овом раду је разматрано побољшање перформанси линеарне неуралне мреже у циљу постизања тачније евалуације упадног неутронског спектра. Испитивани су ефекти преносних функција и обраде симулираних амплитудских расподела импулса из течног сцинтилационог детектора на перформансе конструисане линеарне мреже. Постигнута је боља енергетска резолуција и већа поузданост неуралне мреже после имплементације резултата испитивања. Оптимизована структура мреже је коришћена за анфолдинг моноенергетских и континуалних неутронских енергетских спектара, као што су спектри ^{252}Cf и ^{241}Am–Be извора, који се традиционално користе у експериментима нуклеарне сигурности. У овом раду је показано да је постигнута енергетска резолуција линеарне мреже од 0.1 MeV упоредива са енергетском резолуцијом која је добијена применом референтног анфолдинг метода који је базиран на примени метода максималне веродостојности, а имплементиран користећи ОСЛ алгоритам. Мада метода максималне веродостојности обезбеђује већу тачност резултата анфолдинга са спором реконструкцијом неутронског спектра, посебно у случају континуалних неутронских извора, линеарна неурална мрежа са побољшаним перформансама је погоднија за брзу и робустну евалуацију неутронског спектра са довољном тачношћу.

Кључне речи: анфолдинг, неутронски спектри, амплитудска расподела импулса, MCNP-PoliMi нумерички код, линеарна вештачка неурална мрежа, метода максималне веродостојности