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The criteria for selecting a method for unfolding neutron spectra based on the information entropy theory

Qingjun Zhu [a,b,*], Fengquan Song [b], Jie Ren [c], Xueyong Chen [d], Bin Zhou [e]

[a] Engineering Physics Research Center, National University of Defense Technology, Changsha 410073, China
[b] University of Science and Technology of China, Hefei, Anhui 230027, China
[c] China Institute of Atomic Energy, Beijing 102413, China
[d] Radiation Environmental Protection Consultation Center of JiangSu Province, NanJing, JiangSu 210000, China
[e] Institute of High Energy Physics, Chinese Academy of Sciences, Beijing 100049, China

HIGHLIGHTS

- Two neutron spectra unfolding methods, ANN and MEM, were compared.
- The spectrum's entropy offers useful information for selecting unfolding methods.
- For the spectrum with low entropy, the ANN was generally better than MEM.
- The spectrum's entropy was predicted based on the Bonner spheres' counts.

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ABSTRACT

To further expand the application of an artificial neural network in the field of neutron spectrometry, the criteria for choosing between an artificial neural network and the maximum entropy method for the purpose of unfolding neutron spectra was presented. The counts of the Bonner spheres for IAEA neutron spectra were used as a database, and the artificial neural network and the maximum entropy method were used to unfold neutron spectra; the mean squares of the spectra were defined as the differences between the desired and unfolded spectra. After the information entropy of each spectrum was calculated using information entropy theory, the relationship between the mean squares of the spectra and the information entropy was acquired. Useful information from the information entropy guided the selection of unfolding methods. Due to the importance of the information entropy, the method for predicting the information entropy using the Bonner spheres' counts was established. The criteria based on the information entropy theory can be used to choose between the artificial neural network and the maximum entropy method unfolding methods. The application of an artificial neural network to unfold neutron spectra was expanded.

1. Introduction

Neutron spectra provide critical information for shielding designs (Huang et al., 2003, 2001), radiation dose monitors (Sarkar, 2010) and more (Chen and Wu, 2000; Liu et al., 2007; Zhang et al., 2006). The Bonner sphere spectrometer has been widely used to measure the neutron spectra in the field of radiation protection (A.V. Alevra et al., 1992; McDonald et al., 2002; Wiegel et al., 2009; Wiegel and Alevra, 2002); it is a set of n different diameter moderating spheres with a thermal neutron detector located in their centers that is used to measure the neutron spectrum through the solution of equation system shown in Eq. (1).

$$B_i = \sum_{j=1}^{m} R_i(E_j)\Phi(E_j) \tag{1}$$

where B_i is the count rate of the ith Bonner sphere, $R_i(E_j)$ is the response of ith Bonner sphere to the jth energy bin, $\Phi(E_j)$ is the fluence in the jth energy bin, m is the number of energy bins, n is the number of Bonner sphere, Because $m > n$, the equation system is ill-conditioned and the spectrum must be obtained using an unfolding method.

Many unfolding methods have been developed including the maximum entropy method (MEM) (M. Reginatto and Goldhagen,

* Corresponding author. University of Science and Technology of China, Hefei, Anhui 230027, China. Tel.: +86 551 5595293.
E-mail addresses: qjzhu@mail.ustc.edu.cn, qingjunzhu@yahoo.com (Q. Zhu).

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1998; Reginatto et al., 2002), the artificial neural network (Braga and Dias, 2002; Vega-Carrillo et al., 2007, 2006a, 2006b, 2010) and so on (Matzke, 2003; Reginatto, 2010). The MEM is an unfolding method to maximize entropy I of Eq. (2) under the restrictions given by Eqs. (3) and (4).

$$I = -\sum_{j=1}^{m}\left(\Phi(E_j)\ln\left(\frac{\Phi(E_j)}{\Phi^{\mathrm{DEF}}(E_j)}\right)+\Phi^{\mathrm{DEF}}(E_j)+\Phi(E_j)\right) \tag{2}$$

$$B_i + e_i = \sum_{j=1}^{m} R_i(E_j)\Phi(E_j) \tag{3}$$

$$\sum_{i=1}^{n}\frac{e_i^2}{\sigma_i^2} = n \tag{4}$$

where B_i is the counts of the ith Bonner sphere, $\Phi(E_j)$is the fluence in jth energy bin of the solution spectrum, $\Phi^{\mathrm{DEF}}(E_j)$is the fluence in jth energy bin of the guess spectrum, e_i is the difference between the predicted value and B_i, $R_i(E_j)$ is the response of ith Bonner sphere to the jth energy bin, σ_i is the standard deviation of the ith Bonner counts, n is the number of the Bonner spheres. The method of Lagrange multipliers was applied to solve this constrained optimization problem (M. Reginatto and Goldhagen, 1998; Reginatto et al., 2002). The MEM is a popular unfolding method, however, there is an unavoidable weakness in the MEM. In the MEM unfolding application, the accuracy of the solution spectrum $\Phi(E_j)$ strongly depends on the guess spectrum $\Phi^{\mathrm{DEF}}(E_j)$(Vega Carrillo and de la Torre, 2002).

An artificial neural network (ANN) has been used to unfold neutron spectra using prior knowledge and without the guess spectrum $\Phi^{\mathrm{DEF}}(E_j)$. Some unfolding codes has been developed based on the ANN techniques, and the application results showed that these ANN unfolding codes had high performance and generalization capability (Martinez-Blanco et al., 2009; Rosario et al., 2008). These ANN unfolding codes were also compared with the classical iterative unfolding method (Guimaraes et al., 2012; Ortiz-Rodriguez et al., 2013). In order to improve the accuracy and robustness of ANN unfolding model, the methodology for optimizing the design of ANN model was also researched (Manuel et al., 2008; Ortiz-Rodriguez et al., 2006). These ANN unfolding models were off-line trained, so the unfolded spectra can be output directly from ANN model without the iterative procedure. The application results of previous researches showed that the ANN was a promising unfolding method.

Each method has both weaknesses and strong points; however, it remains unclear which method achieves better unfolding results. Therefore aim of this work was to develop an ANN model to unfold the neutron spectra and to compare with the unfolding results obtaining with the MEM; based on these results, the selection criteria for choosing between the ANN and MEM unfolding methods were proposed.

2. Materials and methods

2.1. Data collection and the unfolding model building

251 neutron spectra and the corresponding responses of Bonner spheres were collected from an IAEA report (IAEA, 2001), to broaden the diversity of the neutron spectra, we imported 5 1/E-shaped spectra, 5 Mx spectra and 5 quasi mono-energetic spectra into the database; as a result, the total number of spectra in the database was increased to 266. The neutron spectra ranged from thermal energies to 630 MeV in 60 energy bins, the neutron with the energy over 25.1 MeV(the 53 th energy bin) was defined as the high energy neutron, there are 68 spectra with the high energy neutrons in the total 266 spectra. The conventional Bonner spheres spectrometer (CBSS) was not suitable to measure these 68 high energy spectra, so the extended range Bonner spheres spectrometer (ERBSS) was needed (Esposito et al., 2010; Goldhagen et al., 2002; Wiegel et al., 2009). In order to have a comprehensive comparison of ANN and MEM, the ANN and MEM unfolding methods were compared based on the two kinds of the Bonner spheres spectrometer, CBSS and ERBSS. According to the previous research (Zhu et al., 2012), the CBSS which was composed of the 11 conventional Bonner spheres, these 11 Bonner spheres consists of He3 proportional counter and polyethylene spheres with diameters,0, 2.5, 3.5, 4, 4.5, 5, 6, 8, 9.5, 12 and 18 inches. The building of the ERBSS was based on the CBSS. According to the suggestions of building the ERBSS (Vylet, 2002), the Bonner spheres with the diameter over 18 inches were not used, so the 18 inches Bonner spheres in the CBSS was excluded, then 2 special Bonner spheres in the IAEA report, 12inch + Pb, 15ich + Pb were added into the rest 10 Bonner spheres of the CBSS to build the ERBSS, so the number of the Bonner spheres in the ERBSS was 12.

For comparing the unfolding methods based on the ERBSS, the total 266 spectra which composed by 60 energy bins were used as the spectra database. In order to build ANN unfolding model, the 266 spectra were randomly divided into a training set (226, 85%) and a testing set (40, 15%). Using the counts from the 12 Bonner spheres as the input data and the values of the 60 energy bins as the desired data, a feed-forward neural network 12-45-60 was selected after several trials. The transfer functions 'logsig', 'purelin' were chosen. The initial weights and thresholds of the network were optimized using the genetic algorithm. The K-fold cross-validation methods ($K = 10$) were used to avoid overtraining. When the number of epochs reaches 1000 or the *MSE*s of the cross-validation set began to increase after 6 iterations, the training was stopped. To avoid spectra with negative values, the value of the energy bin was set to 0 if the output from the ANN model was lower than 0. After the training process, the weights and thresholds were saved. The counts of the 12 Bonner spheres from the testing set were then input into the ANN model, and the outputs of the ANN model were the predicted neutron spectra. Then the MEM was used to unfold these 266 spectra. The maximization of I of Eq. (2) with constraints given by Eqs. (3) and (4) is equivalent to maximization of a potential function $Z(\lambda_k)$(Reginatto et al., 2002)

$$Z = -\sum\Phi^{\mathrm{DEF}}(E_j)\exp\Big\{-\sum\lambda_k R_{ij}\Big\} - \Big(n\sum(\lambda_k\sigma_i)^2\Big)^{0.5} - \sum C_i\lambda_k \tag{5}$$

since λ_i is the solution for Maximum of $Z(\lambda_k)$, the solution spectrum $\Phi(E_j)$ can be obtained by

$$\Phi(E_j) = \Phi^{\mathrm{DEF}}(E_j)\exp\Big(-\sum\lambda_i R_i(E_j)\Big) \tag{6}$$

According to the suggestions (M. Reginatto and Goldhagen, 1998), the simulated annealing algorithm was used to maximize the potential function $Z(\lambda_k)$. The maximum number of iterations was 1×10^6, and the annealing factor was 0.01, the default spectrum $\Phi^{\mathrm{DEF}}(E_j)$ was set as a uniform distribution in the 60 energy bin, the standard deviation σ_i were set to 1×10^{-3}.

For comparing the unfolding methods based on the CBSS, due to the 68 high energy spectra were excluded from the 266 spectra, and the rest 198 spectra without the high energy neutron. Of these 198 spectra, all the values of the energy bin which over 53rd energy bin were the 0, so it can be regarded that these 198 spectra were