Self-Adaptive Differential Evolution Algorithm Unfold Neutron Spectra Obtained from Water-Pumping-Injection Multi-layered Concentric Sphere Neutron Spectrometer

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abstract

To unfold neutron spectra obtained from the Water-Pumping-Injection Multi-layered Concentric Sphere Neutron Spectrometer (WMNS), in this paper, a Self-Adaptive Differential Evolution Neutron Spectrum Unfolding Algorithm (SDENUA) was established. Specifically, the high-quality individuals and failure individuals were introduced in the mutation operation, and the crossover probability and scaling factor were self-adaptively controlled. Furthermore, the maximum fitness of the optimal solution was limited to \(10^6\) to avoid invalid calculation. The readings of the WMNS under 4 different neutron spectra in the IAEA 403 report, including (1) a spectrum of Cf-252 and (2) its spectrum after moderation, (3) a spectrum for BNCT, and (4) a spectrum from a reactor, were obtained by numerical simulation and examined the SDENUA. Results indicate that the solutions of WMNS are not inferior to the MAXED method and GRAVEL method in UMG3.1, and the quality of solutions has increased -2.51\%–30.30\% with an average of 13.06\%. This study further shows that SDENUA does not require complex parameter tuning and without providing a priori default spectrum.

keywords: Water-Pumping-Injection multi-layered spectrometer, Neutron spectrum unfolding, Differential evolution algorithm, Self-Adaptive control

1 Introduction

Since Bonner Sphere Spectrometer (BSS) was the first introduced in 1960 [1], due to its advantages in isotropic response and wide energy range covering, which have been widely used in neutron spectrometry measurements, such as isotopic neutron source filed [2], BNCT [3], and radiation protection near reactors [4]. The Water-Pumping-Injection Multi-layered Concentric Sphere Neutron Spectrometer (WMNS) uses water as moderator [5-7], and the principle of neutron spectrometry measurement is similar to that of BSS. The structure of the WMNS is shown in Figure 1. When

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detecting, an easy-to-replace $^3$He proportional counter was placed in the center, and the water was filled into the gaps between the stainless steel shells to moderate the incident neutrons. Each gap has two states of being filled with water and empty, and 5 gaps have up to 32 combinations of state. In other words, WMNS has 32 measurement combinations to choose from to collect neutron counts. The switching between measurement combinations were realized buy pumping and injecting water with the external Water-Pumping-Injection system [8]. There was also a 1cm lead between the stainless steel shell, which aims to provide expansion for high-energy neutron measurement.

![Figure 1](image)

**Figure 1** Schematic diagram of WMNS structure, the background is the photo of WMNS

The readings of the $^3$He proportional counter are the nuclear reaction event counts of (n, p) under different measurement combinations, which are also called measured neutron counts. The measured counts and response function of the WMNS would be the inputs of neutron unfolding algorithm to unfold neutron spectrometry. The neutron unfolding process could be presented in a discrete form as [9]

$$C_j + \varepsilon_j = \sum_{i=1}^{n} R_{ij} \varphi_i \quad j = 1, 2, 3, \ldots, m \quad (1)$$

Where $C_j$ is the measured neutron count reading from the jth measurement combination, and $\varepsilon_j$ is the reading error of the jth measurement combination, and $R_{ij}$ is the response of jth measurement
combination to the neutron of ith energy group, and $\varphi_i$ is the neutron fluence of ith energy group. Normally, the number of measurement combinations is far smaller than the number of energy groups (in this work, $m=18$, $n=36$).

At present, there are a variety of methods that can be used to unfold neutron spectrum, such as the maximum entropy method [10] and iterative method [11] used in UMG3.1, and the solutions of them were compared with present work. Shahabinejad, H. et al. [12] used a two-step Genetic Algorithm (GA), and then, a Particle Swarm Optimization Algorithm (PSOA) [13] was used with a better solution. Hoang, Sy. Minh. Tuan et al. [14] applied a different two-step GA, the first step in applying in the region from 20 to 35 MeV, whereas the second step covered the whole energy range. Chang, K et al. [6] established a back-propagation artificial neural network neutron spectrum unfolding coed, and its ability was verified by Monte Carlo experiments under 32 neutron spectra. However, the methods in UMG3.1 depended on priori default spectrum, and the parameters tuning in GA and PSOA framework were complicated, and the training of neural networks was also a time-consuming and complex task.

In this paper, we focus on the need for unfolding neutron spectrum obtained from WMNS. The Self-Adaptive Differential Evolution Neutron Spectrum Unfolding Algorithm (SDENUA) was proposed, which included the mutation containing individual information and parameters self-adaptive control technique. The maximum fitness of the final optimal solution was limited to $10^6$ to automatically restart the SDENUA for controlling the quality of solution and saving calculation time, and Gaussian smoothing was used to further improve the quality of the solution. The 1) spectrum of Cf-252 and 2) its spectrum after being moderated and 3) a spectrum using for BNCT and 4) a spectrum from a reactor in the IAEA 403 report [15] were unfolded as reference spectra to verify the ability of the SDENUA. The solutions of SDENUA were compared with the MAXED and GRAVEL in UMG3.1. The response matrix of WMNS is shown in Figure 2. In this work, 18 measurement combinations were selected and 36 energy groups were divided logarithmically at equal intervals in the range of $10^{-9}$~20MeV.
2 Material and methods

2.1 Self-adaptive Differential Evolution Algorithm

To begin with, we will provide a brief background on the Differential Evolution Algorithm, which was introduced by Storn, R. and Price in 1996 [16], because of the simple framework and powerful global search capabilities, it has captured wide attention and application. The iterative loop of the algorithm includes evolutionary operations, such as initialization, mutation, crossover, and selection. For neutron unfolding, the population in the algorithm was composed of several individuals. The individual corresponds to the neutron spectrum composed of several genes. The positions of the genes corresponded to the positions of the energy group, and the values of the genes were the neutron fluence, which was the variables of the unfolding problem to solve. SDENUA will be introduced as following in detail.

Initialization was achieved by randomly selecting from the neutron fluence estimation interval [17], Scale of the population was 10 times the number of the energy groups [18], that was, PopSize=10*36 in this work.

The mutation operation was executed as

$$v_{i,g} = k_{i,g} + F_i \cdot (x_{best,g}^{PopSize} - k_{i,g}) + F_i \cdot (x_{r,g} - x_{f,g}) \quad (2)$$
where \( \mathbf{v}_{i,g} \) is the \( i \)th temporary individual in \( g \)th generation, \( \mathbf{k}_{i,g} \) is the \( i \)th target individual in \( g \)th generation, \( \mathbf{x}_{\text{best},g}^{\text{PopSize}} \) is the high-quality individual. \( \mathbf{x}_{r,g} \) is randomly selected form \( \mathbf{P} \), and \( \mathbf{x}_{f,g} \) is the failure individual randomly selected form \( (\mathbf{P}_f \cup \mathbf{P}) \). \( F_i \) is the scaling factor.

Before the mutation operation, the individuals in the current population \( \mathbf{P} \) would be sorted in descending order based on the fitness, and high-quality individuals would be randomly selected from the top \( 100 \times B \% \) individuals after the sorting, and \( B \) was a uniform random number on the interval \([0.05, 0.60]\). A set \( \mathbf{P}_f \) was created with the scale of \( L \), which for saving candidate individuals with lower fitness (failure individual) in select operation. When the \( \mathbf{P}_f \) was full, the failure individuals in the \( \mathbf{P}_f \) were updated following the "first in, first out" rule.

Each scaling factor was independently generated according to a normal distribution, that was, \( F_i \sim N(u_F, 0.1) \), and \( u_F \) updated [19] at the end of each generation as

\[
u_F = (1 - c) \cdot u_F + c \cdot \frac{\sum F^2}{\sum F} \quad (3)
\]

where \( F \in S_F \), the set \( S_F \) was used to save \( F_i \) when the fitness of the target individual higher than candidate individual in the select operation, and provided prior historical information for \( u_F \) updating. \( S_F \) would be blanked at the beginning of each iteration. \( c \) is a uniform random number on the interval \([0.05, 0.20]\), and \( u_F = 0.5 \) at the initialization.

The temporary individual generated by the mutation operation would be sent to the crossover operation, and then crossover with the target individual as

\[
u'_{i,g} = \begin{cases} v'_{i,g}, & r' \leq CR_j \\ k'_{i,g}, & \text{otherwise} \end{cases} \quad (4)
\]

where \( u'_{i,g} \) is the \( j \)th gene of the \( i \)th candidate individual, \( v'_{i,g} \) is the \( j \)th gene of \( \mathbf{v}_{i,g} \), \( k'_{i,g} \) is the \( j \)th gene of \( \mathbf{k}_{i,g} \), and \( r' \) is a uniform random number on the interval \([0, 1]\).

In the crossover operation, the genes of the temporary individual and the target individual were extracted in an orderly manner according to the crossover probability, and a candidate individual was
generated to transmit the influence of the mutation operation.

Each $CR_i$ was generated as Eq. (5) and updated as Eq. (6)

$$CR_i = \begin{cases} CR_i \sim N(\mu_{CR}, 0.1), & \text{otherwise} \\ CR_i = 0.5, & CR_i < 0.5 \\ CR_i = 0.95, & CR_i > 0.95 \end{cases} \quad (5)$$

$$u_{CR} = (1-c) \cdot u_{CR} + c \cdot S_{CR}^{\text{mean}} \quad (6)$$

where $S_{CR}^{\text{mean}}$ is the average of all elements in the set $S_{CR}$, each $CR_i$ would be sent into the set $S_{CR}$, when the fitness of the target individual higher than candidate individual in the select operation. $S_{CR}$ would be blanked at the beginning of each iteration. $c$ is a uniform random number on the interval $[0.05, 0.20]$, and $u_F=0.5$ at the initialization. To ensure that the genes both of the temporary individual and the target individual could be passed partly on to the candidate individuals, $CR_i$ was truncated to $[0.5, 0.95]$. The selection operation decided to refuse or to allow the candidate individual to enter the population as Eq. (7). This is a mechanism with pros and cons. On the positive side, candidate individual which fail to evolve will be denied entry into the population in time to avoid the reduction of the quality of the population. On the negative side, the algorithm has no predictability and tolerance in the optimization process, and only accepts candidate individuals that have a positive effect on the current population. Therefore, even a potential candidate individual would be immediately affected because of the low fitness value.

$$k_{i+1,g} = \begin{cases} u_{i,g}, & f(u_{i,g}) > f(k_{i,g}) \\ k_{i,g}, & \text{otherwise} \end{cases} \quad (7)$$

Where $f$ is the fitness function as Eq. (8) [14]. The solution was closer to the reference spectrum, and the fitness was higher.

$$f = \left[ \sum_{j=1}^{m} \frac{(C_{j}^{\text{mean}} - C_{j}^{\text{cal}})^2}{(C_{j}^{\text{mean}})^2} \right]^{-1} \quad (8)$$

where $C_{j}^{\text{mean}} = \sum_{i}^{n} R_{ijk}^{\text{ref}}$ is the measured neutron count of jth measurement combination, and due to the limitation of the experimental conditions, we used the counts after convolution of the reference
spectrum and the response matrix to simulate the measured neutron counts obtained by the experimental measurement. $\phi_{i}^{ref}$ is the neutron fluence of the $i$th energy group of the reference spectrum. $C_{j}^{cal} = \sum_{i}^{n} R_{j}^{i} \phi_{i}^{cal}$ is the calculated neutron counts of $j$th measurement combination, $\phi_{i}^{cal}$ is the neutron fluence of $i$th energy group of calculated neutron energy spectrum (solution). In summary, $C_{meas}^{meas} = \left[ C_{1}^{meas} \cdots C_{j}^{meas} \cdots C_{n}^{meas} \right]^{T}$ and $R = \{ [R_{11} \cdots]; \cdots [R_{ij} \cdots]; \cdots [R_{mn}] \}$ were the input of the SDENUA, and $\Phi^{cal} = \left[ \phi_{1}^{cal} \cdots \phi_{i}^{cal} \cdots \phi_{n}^{cal} \right]^{T}$ was the output. The flow of SDENUA is shown in Figure 3.

![Flowchart of SDENUA](image)

**Figure 3** The flow of SDENUA

### 2.2 Termination criterion

The termination criterion of the iteration loop has an important impact on the quality of the solution and the effective running time. In the current literature [9, 12] on the neutron spectrum unfolding algorithms based on the fitness function, the authors empirically defined a maximum number of
iterations. To improve the probability of convergence and obtain high-quality solutions, a larger estimate of the maximum number was usually made. However, an overestimation would increase too much invalid calculation time, and an underestimation would cause to output the optimal solution before converging.

For describing, Spectrum quality factor (QS) [9] was used to evaluate the quality of the solution as

$$QS = 100 \cdot \sqrt{\frac{\sum_{i=1}^{n} (\varphi_{i}^{ref} - \varphi_{i}^{cal})^2}{\sum_{i=1}^{n} (\varphi_{i}^{ref})^2}}$$

where $\varphi_{i}^{ref}$ and $\varphi_{i}^{cal}$ are the same as Eq. (8). A perfect solution gives QS=0.

In the process of neutron spectrum unfolding, it was expected that the quality of the optimal solution would improve with iteration and roughly conform to the monotonic non-increasing trend. However, we discovered that the quality (QS) of the optimal solution fluctuated with iteration greatly, and the QS of the final optimal solution was almost not the lowest value. But, the fitness of the optimal solution of each generation continues to increase and finally converged. A quintessential relationship between QS and fitness is shown in Figure 4. The increase in the fitness of the optimal solution may (high probability) reduce the quality of the optimal solution, and in that case, the invalid calculation was production. After a large number of experiments, the fitness of the optimal solution was limited to $10^6$ as the iteration termination criterion in this work, which helped to save the running time and increase the quality of the final optimal solution.

![Figure 4](image_url)  
**Figure 4**  A quintessential relationship between QS and fitness
The final optimal solution was based on the average over 20 independent runs, and then Gaussian smoothing adopted to overcome the oscillations [12,13,20] in the neutron spectrum unfolding problem.

3 Results and discussion

As shown in Figure 5, the termination generations distribute in a large range when the fitness of the optimal solution reaches $10^6$. Although it seems that "For BNCT" and "Reactor" concentrate around 500 generations, however, it’s not shown that the 500 is the reasonable estimate of the maximum number of iterations, because as shown in Figure 4, the quality of the optimal solution around the 500th generation changes drastically. Therefore, limiting the fitness of the optimal solution as the iteration termination criterion is more conducive to controlling the quality of the output solution and saving running time.

![Figure 5](image-url)  
**Figure 5**  The termination generation of the final optimal solution of 20 runs

To take into account both the dependence of the methods on the priori default spectrum in UMG 3.1 and the performance of SDENUA, all the full-spectra fluence of the priori default spectra were set to the median of the corresponding reference spectra, that were, $\phi_i^{\text{priori}} = \text{Median}(\phi_i^{\text{ref}})$, and Chi-squares were set to $10^{-5}$ in UMG 3.1. Figure 5 shows the unfolding results of the four spectra in the IAEA 403 report.
Figure 6  The neutron spectra unfolding results, where a) is the spectrum of the isotope source of Cf-252, and b) is the spectrum of Cf-252 source after moderated, and c) is the spectrum used for BNCT, and d) is the spectrum of a certain reactor from Germany, and the results of the SDENUA have 95% confidence error bars (the red dots).

Both UMG 3.1 and SDENUA, the error between the calculated neutron counts and the measured neutron counts were limited artificially to a small range. As shown in Figure 6(a) and Figure 6(b), in the energy range where the fluence of the reference spectra approaches 0, the fluence of the calculated spectra have no space to decrease due to the non-negative value of neutron fluence. As mentioned above, to ensure a small error between measured counts and calculated counts, the algorithm can only make the fluence of the calculated spectrum close to 0 in these energy ranges, prompting both SDENUA and UMG 3.1 to give better results. As shown in Figure 5, however, when the fitness of the final optimal solution reaches $10^6$, the corresponding termination generation has a large span distribution between 500 and 2000 in the case of the unfolding of Cf-252, which means that this energy ranges with 0 fluence increase the search cost of SDENUA. On the contrary, for Figure 6(c) and Figure 6(d), even the same counting errors were given, the final optimal solution fluctuates in a relatively
large range around the true value, which obstructed the agreement between the final optimal solution and the reference spectrum. However, the fitness of the final optimal solution was accelerated to reach $10^6$, as shown in Figure 5.

The optimal solution of SDENUA smoothed by the Gaussian method, which artificially increases the error of the energy groups at "sharp peak", so, as shown in Figure 6, the optimal solutions of SDENUA were underestimated at the peak position. However, early-stage experimental studies have examined that the positive effect of Gaussian smoothing was much greater than the increased error, and the final solution was acceptable. For the average results over 20 independent runs, only short error bars can be seen obviously in Figure 6(c), indicating that SDENUA has good robustness.

![Figure 7 The QS of the solutions](image)

The estimation of a superior priori default spectrum depends on the user's understanding of neutron field. When measuring activities in an unknown neutron field, a superior priori default spectrum was given, even for an experienced user, it is challenging. Therefore, the prior default spectra set in this article were quite different from the reference spectrum, so, the output results were not profoundly optimal. As shown in Figure 7, For the neutron energy spectrum of Cf-252, the QS given by SDENUA and UMG 3.1 were equivalent, but the results of the rest of the neutron energy spectra were significantly better than UMG 3.1.
As shown in Figure 8, when the calculated solution (spectrum) were folded back to neutron count, the errors of UMG 3.1 were almost within ±2%. We limited the fitness of the solution in SDENUA, as known from the fitness function as Figure (5), the errors between the measured counts and calculated counts would be limited too. Consequently, the errors of SDENUA were bigger than UMG 3.1. However, in the neutron unfolding problem, we usually pay more attention to obtaining a suitable spectrum instead of a smaller counting error [12]. Combining Figure 6 and Figure 7, we hold the view that the counting errors given by SDENUA are acceptable.

4 Conclusion

Finally, conclusions and further work are summarized. The Self-Adaptive Differential Evolution Neutron Spectrum Unfolding Algorithm has achieved promising results for the Water-Pumping-Injection Multi-layered Concentric Sphere Neutron Spectrometer. In the mutation operation, the information of both high-quality individuals and failure individuals was used to improve the guidance of the evolution direction of the population, so that the fitness of the final optimal solution can quickly reach the $10^6$, which improves the quality of the solution and shortens the running time. Historical experience information was adopted to perform the Self-adaptive control of scaling factor and
crossover probability. The constructed self-adaptive difference algorithm was used to unfold (1) spectrum of Cf-252 and (2) its spectrum after being moderated, and (3) a spectrum using for BNCT and (4) a spectrum from a reactor in the IAEA 403 report, which obtained from Water-Pumping-Injection Multi-layered Concentric Sphere Neutron Spectrometer by the numerical simulation experiment. The unfolding results demonstrate that in the absence of a priori default spectrum, the quality of the calculated spectra of the SDENUA for Water-Pumping-Injection Multi-layered Concentric Sphere Neutron Spectrometer is better than the MAXED method and the GRAVEL method in UMG 3.1, and the quality increased -2.51%~30.30% with an average of 13.06%.

5 Further work

In further work, we will study how to reduce the error caused by smoothing, and the influence of different measurement combinations on the neutron spectrum unfolding.

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