

Adaptive Prior Spectrum Estimation Method for Neutron Spectrum Unfolding Based on Pattern Recognition

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Abstract

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Full Text

Preamble

Adaptive Prior Spectrum Estimation Method for Neutron Spectrum Unfolding Based on Pattern Recognition Hong-Fei Xiao¹, Qing-Xian Zhang¹, , Rui Yang², Biao Jiang¹, Zi-Yang Wang¹, Bin Shi³, Jun Chen³, Zhi-Qiang Cheng¹, Jian Zhang¹ *1Applied Nuclear Technology in Geosciences Key Laboratory of Sichuan Province, Chengdu University of Technology, Chengdu 610059,*

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Abstract: Accurate reference spectra are often required as prior information for neutron spectrum unfolding algorithms. However, predicting the prior neutron spectrum in unknown radiation fields remains a significant challenge. To address this, this paper proposes a prior spectrum estimation method based on pattern recognition. Specifically, this method employs iterative spectral dimensionality reduction to achieve feature fuzzification, enabling the automatic extraction and identification of the optimal prior spectrum from a reference database via fuzzy matching and residual analysis. Subsequently, a hybrid PSO-MLEM algorithm is utilized to perform the final high-precision neutron spectrum unfolding. The performance of the proposed methodology was validated using Monte Carlo simulations of a Bonner Sphere Spectrometer (BSS). Additionally, experimental measurements were conducted using a diamond detector system to acquire thermal and epithermal neutron data. Experimental results demonstrate that, compared with the identified reference spectra, the unfolding results for thermal and epithermal neutrons both exhibit a correlation coefficient of 0.999, with Euclidean distances of 0.007 and 0.139, respectively.

Key words: Neutron spectrum unfolding; Prior spectrum estimation; Pattern recognition; Particle Swarm Optimization (PSO); Maximum Likelihood Expectation Maximization (MLEM); Bonner Spheres Spectrometer (BSS); Monte Carlo simulation

1. Introduction

Neutron spectrum unfolding technology is indispensable across a wide array of disciplines, including nuclear energy, clinical medicine, materials science, and geological exploration. In critical applications such as radiation protection and neutron-based oncological therapy, the ability to rapidly and accurately characterize neutron spectra is paramount. As a cornerstone of neutron metrology, unfolding methodologies are essential for enhancing measurement precision and resolution. However, the current research landscape faces persistent technical hurdles, primarily stemming from the insufficient accuracy and reliability of existing unfolding techniques. These limitations often compromise the reproducibility and trustworthiness of analytical results. Consequently, advanced research into sophisticated unfolding methodologies is vital to refine experimental data quality and foster the broader adoption of neutron measurement technologies in high-stakes fields such as aerospace and nuclear engineering.

Fundamentally, neutron spectrum unfolding entails solving a set of underdetermined equations.

Early methodologies primarily leveraged the least squares method for spectral estimation. For instance, Perey et al. pioneered a least-squares-based unfolding approach; however, its iterative strategy was prone to biases due to a heavy reliance on prior information [1-2]. To address these instabilities, Engl et al. integrated regularization techniques into the least squares framework, enhancing solution continuity through the application of specific constraints [3]. Similarly, Weise et al. employed the maximum entropy principle to solve least squares problems, demonstrating superior noise resistance compared to traditional techniques [4-5]. Nevertheless, the efficacy of these methods remains contingent upon the accuracy of the prior spectrum, as an erroneous initial guess can severely compromise the unfolding outcome. By the late 20th century, singular value decomposition (SVD) was introduced by Pulpan et al. to stabilize response function matrices, though this often came at the cost of precision due to inherent information loss [6]. Concurrently, artificial intelligence and heuristic algorithms gained prominence. Freeman et al. applied Genetic Algorithms (GA) to the unfolding problem; yet, the stochastic nature of standard GA frequently neglected the physical continuity and non-negativity of neutron spectra, occasionally yielding unphysical results [7-8]. To overcome these limitations, Wang Dong et al. proposed an optimized GA incorporating continuity fitness constraints, which effectively guided the population evolution toward a more stable and physically consistent solution [9].

The Maximum Likelihood Expectation Maximization (MLEM) algorithm, an iterative optimization framework for parameter estimation in probabilistic models with incomplete data, has been extensively utilized in various unfolding applications [10]. Cvachovec et al. derived the fundamental MLEM formulations for neutron spectrum unfolding and quantified the associated uncertainties [11]. Subsequent studies by Pehlivanovic et al. and Molina et al. further demonstrated its efficacy in unfolding simple spectra and multi-foil activation data, provided that sufficient prior information was available [12-13]. Nevertheless, MLEM remains inherently limited by its strong dependence on the prior spectrum and its high susceptibility to local convergence. To circumvent these issues, Particle Swarm Optimization (PSO)—a global optimization heuristic inspired by bird flocking—has gained popularity due to its computational simplicity and ease of implementation [14].

While Shahabinejad et al. applied PSO to neutron unfolding, the algorithm's inherent randomness often led to erratic search trajectories, invalid updates, and iteration stagnation, thereby compromising both efficiency and precision [15]. Later refinements, such as inertia weight adjustments and hybrid frameworks (e.g., combining PSO with MLEM or neural networks), have sought to balance global and local search capabilities, significantly enhancing robustness for unfolding complex radiation fields [16-22].

Despite these advancements, few-channel neutron spectrum analysis still faces a critical trade-off: while traditional least-squares and MLEM methods offer high accuracy, they rely heavily on accurate prior information—a luxury often

unavailable in practical measurements of unknown radiation fields. Conversely, although optimization algorithms offer greater independence from prior knowledge, their results are frequently unstable and lack the requisite precision. This study addresses these challenges of initial value dependency and convergence instability by proposing: 1) An adaptive prior spectrum estimation method based on fuzzy pattern recognition; and 2) A hybrid PSO-MLEM algorithm tailored for multi-sphere neutron measurement systems. Validated through both Monte Carlo simulations and experimental measurements, this research aims to overcome the reliance on prior information and provide a high-precision, robust solution for neutron spectrum analysis in unknown radiation environments.

2. Method and Materials

The Bonner Sphere Spectrometer (BSS) is designed to measure neutron spectra across a broad energy range by moderating neutrons within polyethylene spheres of varying diameters, each equipped with a central thermal neutron detector. The underlying measurement principle is governed by the Fredholm integral equation of the first kind. For computational analysis, this integral is discretized into the following matrix form: $(2-1)$ Where N represents the vector of measured count rate, R denotes the known response matrix of the spectrometer, ϕ signifies the unknown neutron fluence rate spectrum vector to be determined, and ϵ accounts for the measurement error.

Typically, the number of energy intervals (m) significantly exceeds the number of spheres (n), resulting in an underdetermined system of equations that necessitates a specialized unfolding algorithm. In this work, the PSO-MLEM unfolding algorithm, as established in our previous study [23], is employed to solve this underdetermined problem.

2.1 Research on Adaptive Prior Spectrum Estimation Method

In neutron spectrum unfolding, the selection of the prior spectrum is critical, as it directly governs the algorithm's convergence and calculation accuracy. This section details an adaptive prior spectrum estimation method based on the principles of fuzzy pattern recognition. By leveraging the robust classification capabilities of fuzzy logic, this study implements a three-stage procedure to identify the optimal prior spectrum:

1. Feature Extraction: A preliminary analysis of the response function equation is performed. By

applying the MLEM algorithm directly to the raw data, an estimated spectrum is generated. This estimate, which preserves the fundamental characteristics of the expected spectrum, serves as the input feature collection for subsequent recognition.

2. Feature Classification: The extracted estimated spectrum is classified against a comprehensive

database of standard neutron spectra using fuzzy pattern recognition. This stage determines the most probable spectrum category for the current response model. 3. Pattern Verification: The identified spectrum pattern is substituted back into the unfolding model for final verification to confirm the optimal prior spectrum.

Given that the shape and distribution of the neutron spectrum are of primary interest, the similarity between the estimated and reference spectra is used as the evaluation metric. This algorithm employs the Pearson correlation coefficient to quantify this similarity. For two sets of variables, $X = \{x_1, x_2, \dots, x_n\}$ and $Y = \{y_1, y_2, \dots, y_n\}$, the Pearson correlation coefficient (r) is defined as: $\rho_{XY} = \frac{\sum_{i=1}^n (x_i - \bar{x})(y_i - \bar{y})}{\sqrt{\sum_{i=1}^n (x_i - \bar{x})^2 \sum_{i=1}^n (y_i - \bar{y})^2}}$. For Eq. (2-2), when $r = 0$, the two variables are uncorrelated, when $r > 0$, there is a positive correlation, when $r < 0$, there is a negative correlation, and the degree of correlation is as follows: very strong correlation (0.8-1.0), strong correlation (0.6-0.8), moderate correlation (0.4-0.6), weak correlation (0.2-0.4), very weak correlation or no correlation (0.0-0.2).

A neutron spectrum is essentially a histogram representing the energy distribution of incident particles, where each channel count corresponds to the cumulative particle counts within a specific energy range over a defined time interval. Reducing the dimensionality of the spectrum through coarser energy binning typically results in the loss of spectral detail. However, by applying a channel-merging algorithm, specific spectral features can be intentionally attenuated to facilitate pattern recognition. Analysis of the neutron response function matrix reveals that each row essentially represents the spectral distribution of incident neutrons detected under a specific moderation thickness.

This inherent property allows both the response matrix and the reference neutron database to undergo dimensionality reduction through channel merging. Leveraging a spectrum mapping algorithm, this study proposes a spectral dimensionality reduction method to achieve feature blurring in both the neutron spectra and the response function matrix.

Assuming a source spectrum aS needs to be mapped onto a target spectrum different energy-axis calibration, the mapping process requires refining the counts channel of aS into $n\Delta$ sub-channels according to a specific distribution model $i\phi$ must satisfy the following relation: bS with a nN in the n th $i\phi$. The distribution (2-3) Following the energy-axis calibration of spectrum channel i , denoted as iE , is determined. Based on the magnitude of channel of aS are aggregated into the corresponding energy bins of the target spectrum process completes the mapping of spectral data from aS , the energy corresponding to each sub- iE , the counts from the n -th bS . This bS . To ensure the fidelity of this $i\phi$ is categorized into three types based on the fitting aS to transformation, the count distribution model precision required [24]: (1) Uniform Distribution Model The uniform distribution model assumes that the counts are

evenly distributed between $n + \Delta$. (2) Linear Distribution Model The counts are distributed according to the following linear formula:

Here, the three parameters k , a , and b are as follows: a i b (2-4) (2-5) (2-6) (3) Quadratic Distribution Model The quadratic distribution model is described by the following formula:

The four parameters k , a , b , and c are obtained by fitting them to the original spectral $k a i + +$ (2-7) counts $1nN -$, nN , and $1nN + : +$ + (2-8) Building upon the spectrum mapping algorithms described above, this study develops a), the systematic dimensionality reduction method for neutron spectra. Assuming a source spectrum with dimension a is to be reduced to a target spectrum procedure is implemented as follows: bS with dimension b ($[1,]$) (1) Parameter Initialization: Set the refinement factor $\Delta =$. Consequently, the total number In this study, with (2) Sub-channel Distribution: Calculate the distribution function of virtual channels in the intermediate refined spectrum becomes b times that of the original spectrum. $\Delta =$, the quadratic distribution model is employed to ensure high-fidelity abS with dimensions redistribution. This step generates an intermediate high-resolution spectrum $a \times . i\phi$ for each channel count (3) Spectral Rebinning: Perform channel merging on the refined spectrum consecutive channels are aggregated into a single bin, resulting in the final target spectrum the desired dimension b . abS . Every a bS with Fig. 1 [Figure 1: see original paper]. Flowchart of the spectral dimensionality reduction algorithm.

The efficacy of the dimensionality reduction algorithm was validated using a multi-sphere neutron spectrometer equipped with a ^3He thermal neutron detector, developed by the China Institute of Atomic Energy. The response functions of the system, following dimensionality reduction, are illustrated in Fig. 2 [Figure 2: see original paper]. As the dimensionality of the response function matrix is reduced from 207 to 150, 100, and 50, fine spectral details distinct from the main peaks are progressively attenuated, resulting in smoother curves. Crucially, the proposed method effectively attenuates fine spectral details and manages energy-axis transformation while preserving the characteristic peak distribution shape of the original spectral lines.

Fig. 2. Response function curves of the ^3He detector at varying dimensionalities: (a) 207 dimensions, (b) 150 dimensions, (c) 100 dimensions, and (d) 50 dimensions.

A ^{252}Cf source was employed as the incident radiation field. The corresponding simulated count rate induced in the ^3He thermal neutron detector of the multi-sphere spectrometer are listed in Table Table 1. Simulated response count rate of the ^3He detector Detector size (inch) Count rate 2.83E-04 2.22E-04 7.00E-03 2.36E-02 5.02E-02 8.11E-02 1.53E-01 1.84E-01 2.06E-01 1.76E-01 1.19E-01 Utilizing the proposed dimensionality reduction technique, the response function of the detection system (as shown in Fig. 2) was systematically reduced from its original 207 dimensions down to 11 dimensions. This process yielded 197 sets

of response matrices at varying resolutions. The MLEM algorithm was then employed to perform unfolding calculations across this dataset to evaluate the impact of dimensionality on spectral reconstruction.

Using the neutron spectrum dimensionality reduction method proposed in this subsection, the dimensionality of the response function from Figure 2 was gradually reduced from 207 to 11, yielding 197 sets of response function matrices at different dimensionalities. The MLEM algorithm was then used to perform unfolding calculations on these 197 sets of response functions. The results are shown in the figures below:

Fig. 3 [Figure 3: see original paper]. Evaluation of dimensionality reduction on spectral reconstruction: (a) Neutron spectrum unfolding results using response functions with reduced dimensionalities of 150, 100, and 50; (b) Evolution of the Pearson correlation coefficient between the unfolded and reference spectra as a function of dimensionality (from 207 to 11).

Fig. 3(a) presents the unfolding results using response functions at 150, 100, and 50 dimensions, specifically highlighting the performance of direct MLEM inversion in the absence of a preset prior spectrum. Fig. 3(b) illustrates the evolution of the Pearson correlation coefficient between the reconstructed neutron spectrum and the reference spectrum as the dimensionality is reduced from 207 to 11. Analysis of the results reveals that while direct MLEM inversion exhibits inherent deviations from the reference spectra at high resolutions (due to the ill-conditioned nature of the problem), the correlation coefficient between the calculated and reference spectra monotonically increases as the spectral dimensionality is reduced. This trend suggests that dimensionality reduction effectively filters out high-frequency noise and local instabilities. Consequently, the reduced-dimension spectra provide a more robust basis for identifying the macroscopic “pattern” or category of the neutron spectrum.

2.2 Multicollinearity Assessment of the Neutron Database

As the dimensionality of the neutron spectrum is progressively reduced, the correlation between the fuzzy solution derived from the response function system (Eq. 2-1) and the expected physical solution typically improves. However, this dimensionality reduction process has practical limits.

Continuous reduction of the spectrum, while maintaining consistent macroscopic trends, inevitably leads to a steady increase in multicollinearity within the neutron spectrum database. In this context, multicollinearity arises when the correlation coefficients between two or more spectra in the database become excessively high. This results in a database populated with spectra possessing highly similar feature values, which can confuse recognition algorithms and degrade identification accuracy.

Therefore, implementing a rigorous collinearity test after dimensionality reduction is essential to prevent performance deterioration. Although a high correla-

tion coefficient is a sufficient but not strictly necessary condition for collinearity, Pearson correlation analysis remains the simplest and most effective metric for detection. Statistically, variables with a Pearson correlation coefficient exceeding 0.8 are generally considered to exhibit significant collinearity.

Drawing upon these principles, this study establishes a multicollinearity testing protocol for the neutron database. Consider a database D consisting of M neutron spectra. The testing procedure is defined as follows:

First, a pairwise correlation analysis is performed on all spectra within the database to construct the correlation coefficient matrix corR : $\text{corR} : \text{cor} D D \text{cor} D D$ (2-9) Where, Each row m of the matrix represents the correlation profile of spectrum $\text{cor} D D$ denotes the correlation coefficient between the m -th and n -th spectra. mD against the entire database.

Next, for each spectrum, a subset corA is formed containing the spectrum itself and all other spectra with which it has a correlation $\text{cor} D D > 0.6$: (2-10) During the iterative dimensionality reduction process, the database is continuously monitored spectrum using the sets defined above. If, after a reduction step, the correlation coefficient between a reference kD was not previously in the strongly correlated corA —exceeds the critical threshold of 0.8, it indicates that spurious collinearity has emerged due to excessive reduction. At this point, it is concluded that the database has compromised its mD and another spectrum kD —where distinguishing capability, and the dimensionality reduction process must be terminated immediately to preserve identification accuracy.

2.3 Residual Analysis for Pattern Recognition Verification

While the database has undergone multicollinearity testing, intrinsic correlations among certain neutron spectra persist due to similarities in experimental conditions and measurement environments.

Consequently, when employing fuzzy pattern recognition methods for spectrum identification, the algorithm often yields multiple candidate results that satisfy the initial selection thresholds. To address this ambiguity, this section employs residual analysis—derived from regression principles—to further screen the identification results by evaluating the discrepancy between the fitted and observed detector counts.

Assume that the fuzzy pattern recognition process yields k candidate spectra, denoted as $D \dots$. Substituting these candidates into the response matrix equation generates the \dots . The optimal prior spectrum is then corresponding fitted count vectors determined by minimizing the residual, as defined by the following condition: $\delta N N \delta N N \delta N N \delta N N$ (2-11) Where, mD is considered the optimal initial iteration spectrum. Here, R is the response function mN and $\delta N N$ represents the residual between matrix, N is the observed detector count, and the observed count N .

In this study, the Euclidean Distance is utilized to quantify the divergence between the fitted and observed counts. Euclidean Distance measures the absolute geometric distance between two points in a multi-dimensional space and is widely used in machine learning to evaluate model accuracy. Its calculation formula is given by: (2-12)

2.4 Algorithmic Procedure of the Adaptive Prior Spectrum Estimation Method

During the prior spectrum estimation process, the required degree of fuzzification for the input data varies depending on the complexity of the response function. To address this, the adaptive prior spectrum estimation method employs a stepwise iterative dimensionality reduction approach to perform adaptive fuzzification for different response function models. The detailed workflow is illustrated in Fig. 4 [Figure 4: see original paper].

Fig. 4. Flowchart of the adaptive prior spectrum estimation method.

The computational steps are defined as follows: Step 1: Parameter Initialization. Initialize the response function matrix $m \times n$, the observed detector count vector N , and the neutron spectrum database D .

Step 2: Database Preprocessing. Before iteration, the neutron database undergoes two essential preprocessing steps: 1) Energy Calibration Unification: To facilitate synchronized dimensionality transformation between the database spectra and the response function, the spectrum mapping algorithm (Section 2.1) is applied to align the energy-axis calibration of the database with that of the response function. 2) Spectrum Classification: This step serves as a precursor to the multicollinearity test. By analyzing the correlation coefficient matrix, spectra with a correlation coefficient > 0.6 (indicating strong correlation) are grouped together, forming the strongly correlated set $corA$.

Step 3: Iterative Pattern Recognition Initialization. Using the computational model defined by the response matrix R and detector counts N , perform an unfolding calculation using the MLEM algorithm to generate a fuzzy estimated spectrum. Step 4: Database Screening via Fuzzy Recognition. Using the fuzzy spectrum (2-13) f as the input feature and the database D as the pattern set, apply fuzzy pattern recognition to identify the category. If, based on the threshold and proximity principles, f is successfully matched to a specific spectrum or category, the iteration terminates. Proceed to Step 7. Otherwise, proceed to Step 5. f . The recognition threshold is set to $R \cdot f \cdot N$. Step 5: Multicollinearity Assessment. As dimensionality is progressively reduced, spectral details fade, and collinearity within the database increases, creating a risk of local optima. This step tests for multicollinearity. If two spectra $corA$ exhibit a correlation coefficient > 0.8 , it indicates that previously distinct spectra have developed spurious mD (which do not belong to the same set in nD and collinearity due to excessive reduction. In this case, the iteration is stopped immediately to preserve accuracy. Proceed to Step 7.

Step 6: Spectral Dimensionality Reduction. If the multicollinearity test is passed, use the spectrum dimensionality reduction algorithm to reduce the dimensions of both the response function matrix and the database spectra. Update the dimensionality parameter and return to Step 3 for the next round of screening.

Step 7: Final Selection via Residual Analysis. Perform a residual test on the multiple candidate spectra identified within the matching category. The spectrum yielding the smallest back-substitution residual is output as the optimal prior spectrum.

3.1 Effectiveness Analysis of the Prior spectrum Estimation Method

In view of the substantial resource requirements and time investment associated with physical experimentation and software development, this subsection focuses on verifying the feasibility of the proposed prior spectrum estimation algorithm via simulation prior to its full experimental deployment.

To ensure the broad adaptability and robustness of the method, it is imperative to establish a spectrum database containing a diverse array of reference neutron sources. This study draws primarily upon the International Atomic Energy Agency (IAEA) Technical Report Series No. 403, “Compendium of Neutron Spectra and Detector Responses for Radiation Protection Purposes” (2001) [25]. This report provides comprehensive guidance on selecting neutron response matrices and reference sources across various measurement environments, offering 85 corrected reference spectra and numerous experimental spectral lines from major global laboratories. These spectra were compiled to construct the foundational database for the adaptive prior spectrum estimation method.

The multi-sphere neutron measurement system from the GSF National Research Center for Environment and Health, as detailed in the IAEA report, was adopted for the simulation. This system employs LiI detectors embedded within moderator spheres, characterized by a $10\text{\$}\times\text{\$}60$ response function matrix. The detector measurement data simulated for incident Pu-Be and Li-Be reference neutron sources are illustrated in Fig. 5 [Figure 5: see original paper], respectively.

Fig. 5. Simulation models of the multi-sphere neutron measurement system: (a) Response functions of the LiI detectors; (b) Incident neutron reference spectra for Pu-Be and Li-Be sources.

Table 2 . Relative count rate in the LiI detector Bonner Sphere Diameter (inch)
Pu-Be Count rate Li-Be Count rate
The adaptive prior spectrum estimation method was implemented using the Python programming language and the NumPy library, adhering to the workflow defined in Section 2.4. The 85 typical neutron reference spectra served as the pattern set.

The identification results for the Pu-Be incident neutron source are presented in Fig. 6 Figure 6: see original paper. The algorithm converged after 38 iterations, at which point the dimensionality of both the response function and the database spectra was reduced to 22. Through fuzzy pattern recognition, 13 candidate spectral lines were filtered from the database. In contrast, the results for the Li-Be source, shown in Fig. 6(b), required only a single iteration to identify 3 candidate spectra. This rapid convergence is attributed to the relatively simple distribution of the Li-Be incident spectrum, which allowed the algorithm to complete pattern recognition without extensive iterative fuzzification.

Fig. 6. Prior spectrum identification results for different incident sources: (a) Pu-Be source; (b) Li-Be source.

Following fuzzy pattern recognition, residual analysis was performed on the sets of strongly correlated reference spectra identified. Table 3 details the Euclidean distances calculated for the Pu- Be candidates. The spectrum labeled “Pu-Be: At 1 m distance” exhibited the smallest back- substitution residual, and its spectral distribution was consistent with the reference incident spectrum.

Consequently, the algorithm successfully selected it as the optimal prior spectrum (Fig. 7 Figure 7: see original paper). Similarly, based on residual analysis, the optimal prior spectrum for Li-Be was successfully identified, as depicted in Fig. 7(b).

Table 3. Residual analysis results for the Pu-Be incident model Neutron Source 252Cf 252Cfwithout shadow cone C moderated Cf PE moderated Cf Am-Be Am-Be without shadow cone Pu-Be:At 1 m distance Pu-Be:At 2 m distance Pu-Be:At 3 m distance Bare Pu-Be, room scatter H2O moderated Pu-Be Bare Pu metal at 50 cm FLUORIDE Pu at 50 cm Euclidean Distance Fig. 7. Optimal prior spectrum identification results based on residual analysis: (a) Pu-Be source; (b) Li-Be source.

The evolution of multicollinearity within the database during the Pu-Be identification process was monitored by analyzing the correlation coefficient matrix. Fig. 8 [Figure 8: see original paper] display the matrices at the start (60 dimensions) and the termination (22 dimensions) of the iteration, respectively. A comparison reveals that as the dimensionality was reduced to 22, certain neutron spectra—specifically those near coordinate index [45, 85]—transitioned from a state of weak correlation to significant collinearity.

This transition triggered the algorithm’ s termination criterion, prompting it to stop the iteration and output the current recognition results.

Fig. 8. Evolution of the correlation coefficient matrix within the database during dimensionality reduction: (a) 60 dimensions (start of iteration); (b) 22 dimensions (termination of iteration).

3.2 Evaluation of Neutron Spectrum Unfolding Methods

To assess the spectral resolution capabilities and computational stability of the adaptive neutron spectrum unfolding method based on the PSO-MLEM algorithm, a Monte Carlo simulation was conducted. A Bonner Sphere Spectrometer (BSS) equipped with a ^3He proportional counter was modeled to validate the algorithm. The system configuration included 15 moderating spheres of varying diameters. The calculated response function matrix is depicted in Fig. 9 Figure 9: see original paper. Three reference neutron spectra with distinct spectral characteristics were selected as incident sources (Fig. 9(b)) to test the algorithm's versatility: Spectrum (a): "HIGH ENERGY REFERENCE SPECTRA CERN: Fe shield" (Sourced from the database). Spectrum (b): "HIGH ENERGY REFERENCE SPECTRA by CERN, SSRL SPEAR: on the roof" (Unknown spectrum, not in database). Spectrum (c): "FFTP facility" (Unknown spectrum, not in database). The simulated detector counts for these three incident fields are listed in Table 4 .

Fig. 9. Monte Carlo simulation model for the Bonner Sphere Spectrometer (BSS): (a) Response functions of the spectrometer equipped with a ^3He proportional counter; (b) Incident neutron reference spectra used for simulation evaluation.

Table 4. Simulated detector count rate results for the three reference spectra

Detector Moderator Thickness (inch)	Reference Spectrum a	Reference Spectrum b	Reference Spectrum c
8.38E-03	3.97E-01	8.53E-01	1.35E+00
1.79E+00	2.11E+00	2.28E+00	2.28E+00
1.97E+00	1.56E+00	9.92E-01	8.40E-01
4.15E-01	1.47E-01	6.24E-02	4.05E-01
9.48E-01	1.16E+00	1.36E+00	1.52E+00
1.64E+00	1.70E+00	1.68E+00	1.53E+00
1.32E+00	9.84E-01	8.84E-01	5.64E-01
2.88E-01	1.57E-01	6.81E-02	3.36E-01
5.79E-01	8.57E-01	1.13E+00	1.36E+00
1.53E+00	1.70E+00	1.68E+00	1.56E+00
1.29E+00	1.20E+00	8.83E-01	5.67E-01
3.88E-01			

The adaptive prior spectrum estimation method was applied to identify the optimal prior spectra for the three datasets. As shown in Fig. 10 Figure 10: see original paper, even with a $\pm 10\%$ random error introduced to the simulated counts, the algorithm successfully identified the target spectrum from the database, demonstrating robust stability. For the unknown spectra (b) and (c), the identification results (Fig. 10(b) and Fig. 10(c)) show that although deviations in neutron fluence exist in certain energy intervals, the peak distribution trends remain fundamentally consistent with the reference spectra. The correlation coefficients (Table 5) exceed 0.8, confirming a strong shape correlation and the reliability of the estimation algorithm for unknown fields.

Fig. 10. Identification results of the prior spectrum estimation algorithm for reference spectra (a), (b), and (c).

Table 5. Similarity analysis (Correlation Coefficient) between reference spectra and algorithm identification results

Reference Spectrum	Correlation Coefficient
Using the identified optimal initial spectra, the PSO-MLEM, PSO, and MLEM algorithms were employed to unfold the neutron spectra, with the iteration	

count set to 200 for all methods. The unfolding results and convergence trends are presented in Fig. 11 [Figure 11: see original paper]. Table 6 provides a quantitative comparison using correlation coefficients and Euclidean distances.

Fig. 11. Comparison of unfolding results: (a, c, e) Unfolded spectra using PSO-MLEM, MLEM, and PSO; (b, d, f) Fitness value convergence curves for PSO-MLEM and PSO.

Table 6. Performance comparison (Correlation Coefficient and Euclidean Distance) of PSO-MLEM, MLEM, and PSO Reference Spectra PSO-MLEM algorithms.

Correlation Coefficient Euclidean Distance For Spectrum (a) (Fig. 11(a)): Since the prior spectrum closely matches the incident field, all three algorithms achieved high accuracy, with correlation coefficients exceeding 0.99 and minimal Euclidean distances. For Spectrum (b) (Fig. 11(c)): This spectrum features two well-separated peaks. With an imperfect prior spectrum, the MLEM results were systematically low, and the PSO results exhibited significant oscillatory artifacts despite matching the overall shape. In contrast, the PSO-MLEM algorithm demonstrated superior unfolding performance, accurately reconstructing the spectral features despite the initial fluence discrepancies.

For Spectrum (c) (Fig. 11(e)): This spectrum is characterized by complex overlapping peaks.

Under conditions of a significantly deviated prior spectrum, PSO showed the worst accuracy with severe distortion in the 0.1–100 MeV range. MLEM fell into a local optimum, underestimating the spectrum above 1 MeV. The PSO-MLEM algorithm, however, successfully reconstructed the overlapping peak distribution, proving its ability to escape local optima.

Figs. 11(b), (d), and (f) illustrate the fitness evolution of the global optimal solution. A comparison indicates that PSO-MLEM achieves significantly faster convergence than standard PSO.

Moreover, the final fitness values for PSO-MLEM are consistently lower, confirming that the hybrid approach effectively enhances both the convergence efficiency and the quality of the final solution.

3.3 Experimental System

Conventional Bonner Sphere Spectrometers (BSS) typically require more than ten moderating spheres, which limits portability and operational efficiency. To address these constraints, developing integrated single-sphere systems has become a key research focus. This study utilizes a single-moderator diamond detector spectrometer developed by the China Institute of Atomic Energy (Fig. 12 [Figure 12: see original paper]). This novel system integrates multiple diamond detectors at specific depths within a single polyethylene block. Neutrons enter from the front face and pass through varying thicknesses of moderator

before detection. This design minimizes the physical footprint and enables simultaneous measurement of responses at multiple depths, significantly reducing measurement time.

Fig. 12. Schematic of the diamond detector neutron measurement system.

The detection system was modeled using the GEANT4 simulation toolkit (Fig. 13 [Figure 13: see original paper]) [26]. The simulation generated response functions for both thermal (Fig. 14 Figure 14: see original paper) and epithermal (Fig. 14(b)) neutrons, establishing the necessary response matrix for unfolding.

Fig. 13. Simulated detector model.: (a) Front incident surface; (b) Rear view.

Fig. 14. Simulated response functions of the single-moderator diamond detector system: (a) Thermal neutron response; (b) Epithermal neutron response.

Experimental measurements were conducted using a thermal and epithermal neutron irradiator.

The count recorded by each diamond detector channel are displayed in Fig. 15 [Figure 15: see original paper]. Subsequently, the adaptive estimation and PSO-MLEM algorithms were applied to unfold the spectra.

Fig. 15. Measured counts for thermal and epithermal neutrons across detector channels.

Fig. 16 [Figure 16: see original paper]. Experimental spectrum identification and unfolding results using the diamond detector system: (a) Prior spectrum identification for thermal neutrons; (b) Prior spectrum identification for epithermal neutrons; (c) Final unfolded thermal neutron spectrum; (d) Final unfolded epithermal neutron spectrum.

Table 7 . Quantitative analysis of experimental reconstruction results for thermal and epithermal neutrons.

Analysis Metric	Correlation Coefficient	Euclidean Distance	Thermal Neutron Unfolding Result	Epithermal Neutron Unfolding Result
The prior spectrum estimation algorithm successfully identified appropriate thermal and epithermal reference spectra from the database (Figs. 16(a) and 16(b)). The final unfolded spectra are compared with reference spectra in Figs. 16(c) and 16(d).				

The unfolding results for thermal and epithermal neutrons confirm the efficacy of the automated program in practical experimental settings. Specifically, the PSO-MLEM algorithm accurately reconstructed the simple peak distribution of incident thermal neutrons. For epithermal neutrons, although minor deviations occurred in the 10-5-10-1 MeV range due to system measurement errors and overlapping peak structures, the overall spectral curve remained highly consistent with the reference distribution, achieving a correlation coefficient greater than 0.99 (as shown in Table 7).

4. Conclusion

To overcome the challenge of accurately specifying the prior spectrum in unknown radiation fields—a critical factor for iterative unfolding—this paper proposes an adaptive prior spectrum estimation method leveraging fuzzy pattern recognition principles. By applying spectral channel merging to reduce dimensionality, the method achieves feature fuzzification, enabling the automatic identification and estimation of the prior spectrum. Validation results indicate that the algorithm allows for a tolerance of $\pm 10\%$ random error in detector counts while still accurately identifying reference spectra. Even for unknown spectra, the identified prior estimates maintain a correlation coefficient above 0.8 with the true spectrum, thereby ensuring the convergence and accuracy of subsequent unfolding.

Comprehensive validation was performed using both Monte Carlo simulations of a BSS and experimental measurements with a diamond detector system. Simulation results demonstrate that the proposed PSO-MLEM hybrid algorithm significantly outperforms traditional MLEM and PSO algorithms in terms of computational accuracy, stability, and convergence speed, particularly when the prior spectrum deviates from the truth. Experimental verification with thermal and epithermal neutron sources further confirmed the system's practical applicability. The program successfully identified reference spectra and reconstructed the incident energy distributions with high fidelity. In conclusion, the proposed methodology provides a robust, high-precision solution for neutron spectrum analysis in complex and unknown radiation environments.

Author contributions All authors contributed to the study conception and design. Material preparation, data collection and analysis were performed by Hong-Fei Xiao, Qing-Xian Zhang, Rui Yang, Biao Jiang, Zi-Yang Wang, Bin Shi, Jun Chen, Zhi-Qiang Cheng and Jian Zhang. The first draft of the manuscript was written by Hong-Fei Xiao, Qing-Xian Zhang and all authors commented on previous versions of the manuscript. All authors read and approved the final manuscript.

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