Development of spectrum unfolding code for multi-sphere neutron spectrometer using genetic algorithms Postprint

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Abstract

In neutron spectrum measurement using a multi-sphere neutron spectrometer, energy response functions and detector readings are employed for neutron spectrum unfolding. Mathematically, this problem can admit multiple solutions, yet only one actual neutron spectrum exists. Compared with conventional numerical spectrum unfolding methods, genetic algorithms exhibit characteristics of global optimization and probabilistic search. Therefore, they were selected as the spectrum unfolding algorithms for the multi-sphere neutron spectrometer (MNS IL100) developed by Tsinghua University. First, the detector and polyethylene spheres of different sizes in the MNS IL100 were modeled to calculate the energy response functions using Monte Carlo simulation. Then, based on the physical and mathematical properties of the spectrum unfolding problem using genetic algorithms, an effective search space and appropriate fitness function were determined to improve search and iteration efficiency. An elitism replacement scheme was employed to ensure convergence, and a pseudo-parallel strategy was utilized to inhibit premature convergence. Based on the aforementioned algorithms, a spectrum unfolding code was developed and tested with several typical neutron spectra. Finally, the MNS IL100 and the spectrum unfolding code were employed in an actual experiment measuring the 252Cf neutron source spectrum. The experimental results are in good agreement with the standard 252Cf neutron spectrum, thereby verifying the effectiveness and practicality of using genetic algorithms for neutron spectrum unfolding in combination with several processing strategies.

Full Text

Preamble

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Development of Spectrum Unfolding Code for Multi-Sphere Neutron Spectrometer Using Genetic Algorithms

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Abstract:
In neutron spectrum measurement using the multi-sphere neutron spectrometer, energy response functions and detector readings must be applied to neutron spectrum unfolding. Mathematically, multiple solutions may exist for this problem, yet only one actual neutron spectrum exists. Compared with conventional numerical spectrum unfolding methods, genetic algorithms offer global optimization and probabilistic search capabilities. Therefore, they were selected as the spectrum unfolding algorithms for the multi-sphere neutron spectrometer (MNS IL100) developed by Tsinghua University. First, the detector and various-sized polyethylene spheres of MNS IL100 were modeled to calculate the energy response functions via Monte Carlo simulation. Then, based on the physical and mathematical properties of the spectrum unfolding problem, an effective search space and proper fitness function were determined to improve search and iteration efficiency. The elitism replacement scheme was employed to ensure convergence, and a pseudo-parallel strategy was adopted to inhibit premature convergence. Based on these algorithms, a spectrum unfolding code was developed and tested with several typical neutron spectra. Finally, MNS IL100 and the spectrum unfolding code were applied to an actual experiment measuring the ^{252}Cf neutron source spectrum. The experimental result shows good agreement with the standard ^{252}Cf neutron spectrum, verifying the effectiveness and practicality of using genetic algorithms with these combined processing strategies for neutron spectrum unfolding.

Keywords: Multi-sphere neutron spectrometer, Spectrum unfolding, Genetic algorithms, Elitism, Pseudo-parallel
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Introduction

A. Spectrum Unfolding Problem of Multi-Sphere Neutron Spectrometer

The multi-sphere neutron spectrometer, also known as the Bonner sphere neutron spectrometer, was proposed by Bramblett in 1960. Due to its numerous advantages—including wide neutron energy coverage from thermal to high-energy neutrons, simple response functions, near-isotropic response, and high sensitivity—it is widely used in radiation protection applications.

The multi-sphere neutron spectrometer primarily consists of a series of polyethylene spheres with different radii, each containing a thermal neutron detector at its center. Different-sized spheres possess varying neutron moderation capabilities and neutron fluence response functions. As the radius increases, the peaks of the response functions gradually shift to higher energy regions. These response functions can be obtained through Monte Carlo simulation.

For a given multi-sphere neutron spectrometer, the relationship between the neutron spectrum, response functions, and detector readings can be expressed by the following mathematical equation:

$$R_i = \int_0^\infty R_i(E)\Phi(E)dE + \varepsilon_i \quad (i = 1, 2, 3..., n),$$

where $R_i(E)$ represents the response function, $\Phi(E)$ represents the neutron spectrum, N_i represents the detector reading, ε_i represents measurement uncertainty, i represents the detector number, and n represents the number of detectors.

This equation demonstrates the spectrum unfolding principle of the multi-sphere neutron spectrometer. Neglecting ε_i, the spectrum unfolding problem involves solving for the neutron spectrum $\Phi(E)$ given the response functions $R_i(E)$ and detector readings N_i. Mathematically, the response functions $R_i(E)$ are provided in discrete form across many energy groups, making it impossible to obtain a continuous function $\Phi(E)$ directly from $R_i(E)$ and several detector readings. Therefore, $\Phi(E)$ is solved in discrete form by dividing the entire energy range into multiple energy groups matching the response functions $R_i(E)$, with the neutron fluence in each energy group being the unknown quantity. The integral equation is thus rewritten in discrete matrix form as:

$$N_i = \sum_{j=1}^{m} R_{ij}(E)\Phi_j + \varepsilon_i \quad (i = 1, 2, 3..., n),$$

where $R_{ij}(E)$ represents the response matrix, Φ_j represents the neutron spectrum in discrete form, j represents the energy group number, and m represents the number of energy groups.

At this point, the spectrum unfolding problem is abstracted to solving a system of linear equations. There are n equations but m unknowns. Unfortunately, the number of detectors n is typically far less than the number of energy groups m required for accuracy—for example, often no more than 10 detectors but 100 energy groups. With fewer equations than unknowns, this linear system mathematically has many solutions, yet only one actual neutron spectrum exists. Therefore, this problem is difficult to solve using conventional numerical methods.

B. Spectrum Unfolding Using Genetic Algorithms

Genetic algorithms simulate natural biological evolution processes, operating on the principle of survival of the fittest and employing population search techniques to find the global optimal solution. Genetic algorithms are highly suitable for optimization problems, featuring global optimization and probabilistic search capabilities that ensure the search space evolves toward states containing or approaching the optimal solution. For a specific problem, a search space generation t is created. Based on fitness evaluations, some solutions are selected while others are eliminated, followed by code space genetic operators such as crossover and mutation that simulate chromosome genetic manipulations. Finally, search space generation $t + 1$ is produced, and the process repeats until the optimal solution is obtained. The genetic algorithm process is illustrated in [Figure 1: see original paper].

Genetic algorithms are particularly suitable for problems seeking optimal solutions without sufficient known conditions. Consequently, they were selected for neutron spectrum unfolding. Freeman developed the genetic algorithm unfolding code UMRGA using multi-seed averaging and monoenergetic peak reward techniques, testing it with data provided by EURADOS containing 8 different radius spheres and 47 energy groups. Mukherjee developed BONDI-97, a genetic algorithm spectrum unfolding tool operating on Microsoft EXCEL. This paper presents a new spectrum unfolding code using genetic algorithms combined with several processing strategies, including proper fitness function selection, elitism, and pseudo-parallelism. The unfolding code, verified through typical spectrum tests and actual experiments, has been successfully applied to the multi-sphere neutron spectrometer MNS IL100, which contains 9 different radius spheres and 100 energy groups.

Methods

A. Coding and Decoding

Binary codes are used to represent solutions, with each binary code representing one solution. Since genetic algorithms execute in a search space containing many solutions, multiple binary codes are needed to represent the entire search space.

If the maximum and minimum possible values are defined as V_{max} and V_{min}, and the precision is P, then the binary code length L can be determined by:

$$\frac{V_{max} - V_{min}}{2^L - 1}$$

The binary codes can be translated to real solution values using:

$$x = V_{min} + \left(\sum_{i=1}^{L} b_i \cdot 2^{i-1} \right) \cdot \frac{V_{max} - V_{min}}{2^L - 1}$$

It is known that the minimum possible neutron flux value is zero. Determining the maximum possible value is crucial because it affects the precision and code length, which in turn determines computational workload and solving efficiency.

For each energy group and detector pair, assuming the detector reading is generated solely from that energy group, the maximum possible value for that group is determined by:

$$\Phi_{jmax}(E) = \frac{N_i}{R_{ij}(E)}$$

With n detectors, n maximum possible values for each group can be calculated. However, the actual maximum possible value for each group is the minimum of these n values:

$$\Phi_{jmax}(E) = MIN \left(\frac{N_i}{R_{ij}(E)} \right)$$

This is because if any solution value exceeds the minimum of these n values, the detector readings calculated by Eq. 2 will exceed the actual detector readings.

Binary codes can be generated randomly for the initial search space only, meaning the algorithms do not require a preset spectrum. The coding and decoding process is illustrated in [Figure 2: see original paper].

B. Fitness Functions, Selection, Crossover and Mutation

The following two equations are used as fitness functions to evaluate solutions:

$$F_1(x) = \frac{\sum_{i=1}^{n} (N_i - N_i')^2}{N_i^2}$$

$$F_2(x) = C - \sum \frac{(N_i - N_i')^2}{N_i^2}$$

where $C = MAX \left(\sum (N_i - N_i')^2 / N_i^2 \right) \cdot 2$.

First, the expected detector readings N_i' are calculated using the solution values and Eq. 2, then the function values $F_1(x)$ and $F_2(x)$ can be determined. Obviously, if a solution is closer to the optimal solution, its function value will be larger, and its probability of being selected will be higher. Roulette wheel parent selection is used here to determine which solutions advance to the next generation based on normalized probability calculated from all solution function values. A larger probability means a greater chance of selection, though not certainty.

Code space genetic operators crossover and mutation, which simulate chromosome genetic manipulations (chiasmata and variation), are methods for generating new solutions. One-point crossover and bit mutation are employed here.

C. Elitism Replacement Scheme

Elitism replacement scheme is used to ensure convergence. After completing the evolution process of the current generation, the best solution of the next generation is compared with the best solution of the current generation. If the best solution of the next generation is superior, the elitism replacement scheme is skipped; otherwise, the best solution of the current generation is forcibly preserved into the next generation to replace its worst solution. This scheme prevents the best solution from being eliminated through selection operations, significantly improving genetic algorithm performance.

D. Pseudo-Parallel Strategy

Pseudo-parallel strategy is employed to inhibit premature convergence, which occurs when the solution process converges to a local optimum instead of the global optimum prematurely.

In parallel genetic algorithms, the search space is divided into multiple subsearch spaces where basic genetic algorithms execute independently. After each sub-search space completes one generation evolution, information is exchanged between them to preserve population diversity and inhibit premature convergence. "Pseudo-parallel" means the algorithm is logically parallel but physically serial, with parallel algorithms implemented in a serial manner. The island model is applied here for information exchange. For each sub-search space, one swap-in and one swap-out sub-search space are selected randomly. The worst solution of the swap-in sub-search space is replaced by the best solution of the current sub-search space, and the worst solution of the current sub-search space is replaced by the best solution of the swap-out sub-search space.

Results

Based on the algorithms described above, a spectrum unfolding code was developed with different strategies and fitness functions. Verification and validation relied on the multi-sphere neutron spectrometer MNS IL100 developed by Ts-

inghua University. First, the energy response functions were calculated. The entire energy range was divided into 100 energy groups on a logarithmic scale. MCNP-4C was used to calculate the response functions for 9 spheres with radii of 0, 2, 5, 6, 7, 8, 10, 12, and 15 cm. These 9 energy response function curves are shown in [Figure 3: see original paper].

Simulation Tests

[Figure 4: see original paper] shows three typical neutron spectra used in simulation tests, which are combinations of several differential fluence spectra mentioned in reference [6]:

1. ^{252}Cf spontaneous fast fission spectrum
2. Combination of thermal Maxwellian spectrum, monoenergetic neutron beams spectrum, and uniform distribution spectrum
3. Combination of thermal Maxwellian spectrum and ^{252}Cf spontaneous fast fission spectrum

Four genetic algorithm variants were tested and compared:

1. **Simple Genetic Algorithm (SGA):** Neither elitism replacement scheme nor pseudo-parallel strategy is applied
2. **Simple Genetic Algorithm with Elitism (ESGA):** Elitism replacement scheme is added to SGA
3. **Pseudo-Parallel Genetic Algorithm with Elitism (EPPGA):** Pseudo-parallel strategy is added to ESGA. Subpopulation size is 100 with 20 subpopulations, maintaining total population size consistent with ESGA
4. **Pseudo-Parallel Genetic Algorithm with Elitism and Different Fitness Functions (EPPGA2):** Eq. 8 is used as the fitness function instead of Eq. 7 in EPPGA

Equation 2 was used to calculate detector readings from these spectra, which were then input into the spectrum unfolding code. The following two functions evaluated algorithm performance, where N' and Φ'_j represent calculated detector readings and neutron spectrum in discrete form. Lower F_N and F_Φ values indicate better performance:

$$F_N = MIN\left(\frac{(N_i - N'_i)^2}{N_i^2}\right)$$

$$F_\Phi = MIN\left(\frac{(\Phi_j - \Phi'_j)^2}{\Phi_j^2}\right)$$

[Figure 5: see original paper] shows calculation results for different genetic algorithms with spectrum 1, demonstrating that EPPGA produces the best results, though the advantages are not immediately obvious. However, performance

comparison through convergence curves of F_N and F_Φ for spectrum 1, shown in [Figure 6: see original paper], proves that EPPGA' s convergence rate and precision are significantly superior to the other three algorithms.

Due to large-scale fluctuations in the original results, the initial 100 values across 100 energy groups were averaged to 25 values across 25 energy groups. The averaged results for the three typical neutron spectra using EPPGA are shown in [Figure 7: see original paper].

Actual ^{252}Cf Spectrum Measurement

MNS IL100 and the spectrum unfolding code were used in an actual experiment measuring the ^{252}Cf neutron source spectrum. [Figure 8: see original paper] shows both the standard ^{252}Cf spectrum function curve [11] and the original 100-value calculation result using EPPGA.

The results demonstrate good agreement between the calculation result and the standard ^{252}Cf neutron spectrum from 0.1 MeV to 10.0 MeV. However, some distributions appear in the low-energy region that are not present in the standard spectrum. These represent thermal neutrons generated from original neutrons that were slowed down through wall scattering effects.

Conclusions

The EPPGA calculation results from simulation tests with several typical neutron spectra match expected outcomes, and the EPPGA calculation result from the actual experiment shows good agreement with the standard ^{252}Cf neutron spectrum. This verifies that by determining an effective search space and proper fitness function, and by employing the elitism replacement scheme and pseudo-parallel strategy, genetic algorithms can be successfully applied to spectrum unfolding problems. However, the simulation test results exhibit large-scale fluctuations because the algorithm' s search direction depends on fitness evaluations. Despite smooth iteration results, the fitness function used here focuses only on the degree of closeness between calculated and optimal results, leading to non-smooth outcomes. Adding a smoothness-ensuring component to the fitness function is under consideration, though no theoretical reference exists for determining its form and weight. Future work will focus on constructing this smoothness-ensuring component.

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Note: Figure translations are in progress. See original paper for figures.