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INFORMATICS APPROACH TO STATIONARITY DIAGNOSTICS OF THE MONTE CARLO FISSION SOURCE DISTRIBUTION

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INTRODUCTION

Stationarity diagnostics of the Monte Carlo fission source distribution have been proposed which utilize Shannon and relative entropies. [1,2] These diagnostics are motivated by the empirical observation that for some problems the "apparent" convergence of k_{eff} to the neighborhood of its stationary level is much faster than the "real" convergence of the fission source distribution to its stationary distribution. In this article, the Shannon and relative entropies of the fission source distribution are utilized in an integrated manner to give practitioners a workable criterion. Its effectiveness is demonstrated for the PWR fuel storage facility with a checkerboard array of fuel bundles and water lattices, which was recently investigated in OECD/NEA Working Party on Nuclear Criticality Safety, Expert Group on Source Convergence Analysis [3,4].

PRELIMINARIES

Let $S(i)$ and $T(i)$ be the binned source normalized to unity. The Shannon entropy of S is defined as

$$H(S) = -\sum_{i=1}^{B} S(i)\log_2\left(S(i)\right), \qquad (1)$$

where B is the number of bins. Shannon entropy satisfies $0 \le H(S) \le \log_2 B$. The relative entropy of S w.r.t. T is defined as

$$D(S \,\|\, T) = \sum_{i=1}^{B} S(i)\log_2\left(\frac{S(i)}{T(i)}\right). \qquad (2)$$

The relative entropy is non-negative and zero only when $S(i) = T(i)$ for all i. These entropies are required quantities in the instantaneously decodable binary encoding of the particles emerging from bins. Here, the instantaneous decodability states that no codeword is the prefix of any other codeword. Let $l(i)$ be the binary codeword length of the particles emerging from bin i. The descriptive length of the particles born under the law of S is defined as

$$L(S) = \sum_{i=1}^{B} l(i)S(i). \qquad (3)$$

Then, the following inequality holds for Shannon entropy and descriptive length [5]:

$$H(S) \le \min_{\substack{\text{instantaneously decodable}\\ \text{encoding schemes}}} \left(L(S)\right) \le H(S) + 1. \qquad (4)$$

One might think of the minimization over the schemes with a weaker constraint of unique decodability. However, the non-negativity of relative entropy and the Kraft inequality $\sum_{i=1}^{B} 2^{-l(i)} \le 1$ are the only mathematical conditions necessary to derive (4), any uniquely decodable encoding must satisfy the Kraft inequality and there exists an instantaneously decodable encoding for any set of codeword lengths that satisfies the Kraft inequality. [5] In other words, the restriction to the instantaneous decodability does not place any further restriction to minimum descriptive length property. Thus, we proceed with instantaneously decodable binary encoding schemes. Note that (4) is achieved by the Shannon code $l_S(i) = \left\lceil \log_2\left(\frac{1}{S(i)}\right) \right\rceil$, where $\lceil x \rceil$ denotes the smallest integer larger than or equal to x. This implies that the data description by the Shannon code is optimal in terms of shortest binary description with one bit uncertainty. Therefore, we seek to characterize the distribution S by the descriptive length using the Shannon code. But, in reality, we do not know the true distribution that governs the observed data, i.e., bins from which particles are born. To overcome this problem, an assumption is made such that the particle source distribution follows the distribution T. Usually, the distribution T is computed based on observations. For example, T may be computed as the average distribution over the second half of active cycles. Under the assumption of T, the bin i is encoded by

$l_T(i) = \left\lceil \log_2\left(\frac{1}{T(i)}\right)\right\rceil$ and the descriptive length becomes

$$L_T(S) = \sum_{i=1}^{B} l_T(i)S(i) . \qquad (5)$$

This descriptive length satisfies the following inequality [5]:

$$\begin{aligned} &H(S) + D(S \,\|\, T) \\ &\le L_T(S) \qquad (6) \\ &\le H(S) + D(S \,\|\, T) + 1. \end{aligned}$$

Comparing (6) with (4), one may interpret $D(S\|T)$ as the penalty incurred by the assumption. In previous work [2], assuming that T is the average binned source over the second half of active cycles and assigning at each cycle the unity-normalized realization of the source to S, the stationarity of the source is diagnosed in a posterior manner by checking whether or not $D(S \,\|\, T)$ crosses the mean level determined from the second half of active cycles. However, it is not clear whether or not this criterion is always conservative. Also, there may be cases where the criterion is too conservative. In the next section, we propose a remedy to overcome these problems.

STATIONARITY DIAGNOSTICS

Let S_i^B be the binned source normalized to unity at cycle i, where $i = -N+1,\ldots,0,1,\ldots M$ with $i = 1$ being the first active cycle. Let us define $T^B = (2/M)\sum_{i=M/2+1}^{M} S_i^B$ and approximate the Shannon entropy by $H^B = (2/M)\sum_{i=M/2+1}^{M} H(S_i^B)$. The maximum stationary level (*msl*) is defined as

$$msl = f \times \min\left(H^B, 1\right) . \qquad (7)$$

Since (6) is a relation with inherent uncertainty of one bit, the factor f is chosen to be 0.05 so as to not disturb (6). Then, a posterior diagnosis is performed by checking whether or not $D(S_i^B \,\|\, T^B)$ crosses *msl* downward before the active cycle begins $(i \le 0)$. Since $0 \le H^B \le \log_2 B$ where the maximum is attained when all S_i^B are uniform and the minimum is attained when all S_i^B concentrate on the same bin, $msl \cong f$ except when B is a small positive integer or the source has an extremely concentrated mass in one bin. This is indicative of the integrity of the posterior diagnostics criterion against refinement of the mesh for binning. For example:

1) Let B=10, $S_i^B(1) = 0.9$, and $S_i^B(j) = 0.1/9$, $j = 2,\ldots,10$. Then, $H(S_i^B) = 0.79$. If the meshes are refined by uniformly halving the spacing (B=20, $S_i^B(j) = 0.45$, $j = 1$ and 2, and $S_i^B(j) = 0.1/18$, $j = 3,\ldots,20$), $H(S_i^B) = 1.79$.
2) Let B=100, $S_i^B(1) = 0.9$, and $S_i^B(j) = 0.1/99$, $j = 2,\ldots,100$. Then, $H(S_i^B) = 1.13$.

Furthermore, in parallel with 1) ($B^* = 2B$, $S^*(j_1) = S^*(j_2) = 0.5 \times S(j)$, and $T^*(j_1) = T^*(j_2) = 0.5 \times T(j)$), the relative entropy is not affected by uniform halving the mesh spacing:

$$\begin{aligned} D(S^* \,\|\, T^*) &= \sum_{k=1}^{B^*} S^*(k)\log_2\left(\frac{S^*(k)}{T^*(k)}\right) \\ &= \sum_{j=1}^{B}\sum_{i=1}^{2} S^*(j_i)\log_2\left(\frac{S^*(j_i)}{T^*(j_i)}\right) \\ &= \sum_{j=1}^{B}\left[0.5S(j)\log_2\left(\frac{S(j)}{T(j)}\right) + 0.5S(j)\log_2\left(\frac{S(j)}{T(j)}\right)\right] \\ &= D(S \,\|\, T). \end{aligned}$$

In other words, the relative entropy is not sensitive to binning mesh refinement in the limit of sufficiently fine meshes. The posterior diagnosis has integrity against binning mesh refinement.

For progressive diagnostic purposes, $D(S_i^B \,\|\, S_{-N+1}^B)$ is plotted against $i = -N+1,\ldots,M$. Since the penalty against the assumption $T = S_{-N+1}^B$ should increase initially and reach equilibrium, $D(S_i^B \,\|\, S_{-N+1}^B)$ can be utilized as a visual diagnosis. To overcome the singularity that may arise from the bins at $i = -N+1$ with a zero score, the following sum of relative entropies is plotted in practical analyses:

$$D\left(S_i^B \parallel 0.5\times(S_{-N+1}^B + S_i^B)\right) + D\left(S_{-N+1}^B \parallel 0.5\times(S_{-N+1}^B + S_i^B)\right)$$

We call this progressive relative entropy.
We have implemented the proposed stationarity diagnostics in the MCNP5 code [6] and analyzed a PWR fuel storage facility consisting of a checkerboard array of the fuel bundles and water lattices [3,4]. This problem is one of the benchmark problems in OECD/NEA Working Party in Nuclear Criticality Safety, and the details of the problem specification can be found in the participants' reports, for example, Ref. [7]. Brief problem description is as follows: The PWR fuel storage area consists of a 24 by 3 checkerboard array. For the first column, fresh fuel bundles are placed at (1,1) and (1,3), and (1,2) is occupied by water. For the second column, the fuel bundle is placed at (2,2), and (2,1) and (2,3) are occupied by water. These placements are repeated alternately through 24 columns. The entire placement is surrounded by concrete on three vertical sides and by water on one vertical side. The lower exterior vertical side of (1,1) through (24,1) is faced with water. Since concrete is a superior reflector to water, the fission source has a strong peak at (1,3). Thus, computations from two initial fission source distributions are analyzed; one is uniform over all the fuel bundles, and other concentrates on the fuel bundle at (1,3). Figure 1 shows the cyclewise k_{eff} for computations with 50000 histories per cycle. Upon inspection, both the computations appear to be stationary after the 500th cycle. Figure 2 shows 95% confidence intervals assuming 500 inactive and 500 active cycles. It is observed that the result from a uniform initial source is far away from the separately computed reference result. Figure 3 shows the progressive relative entropy, where each fuel bundle is assigned equally spaced five vertical bins (total number of bins = $(24\times3/2)\times5$). One can clearly observe that the computation from a uniform initial source does not converge even at the 700th cycle, while the computation from a source concentrating on (1,3) lattice does converge at around 200th cycle. Figure 4 shows the posterior relative entropy diagnosis with $msl(f=0.05)$. One can again observe that 500 inactive cycles are not enough for the computation from a uniform initial source, while 300 inactive cycles are enough for the computation from a source concentrating on (1,3) lattice.

CONCLUSION

We have shown that relative entropy is useful to both the progressive and posterior diagnosis of Monte Carlo fission source. Furthermore, the posterior relative entropy diagnosis can be performed in an integrated manner with a maximum stationary level determined by Shannon entropy.

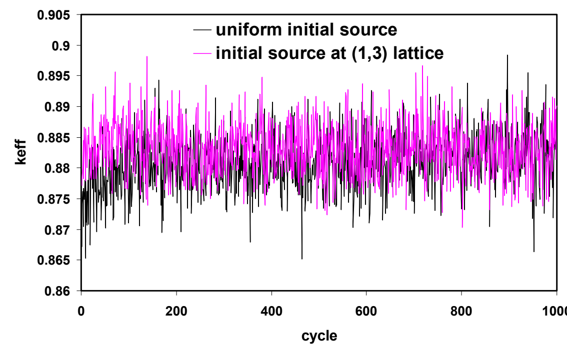

Fig. 1 A realization of cyclewise k_{eff} for two different initial fission source distributions

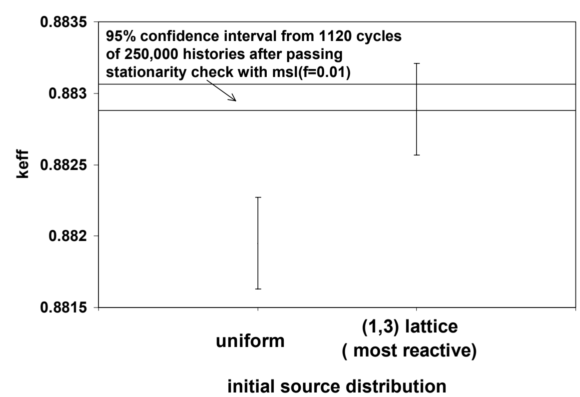

Fig. 2 Confidence intervals (95%) assuming 500 inactive and 500 active cycles

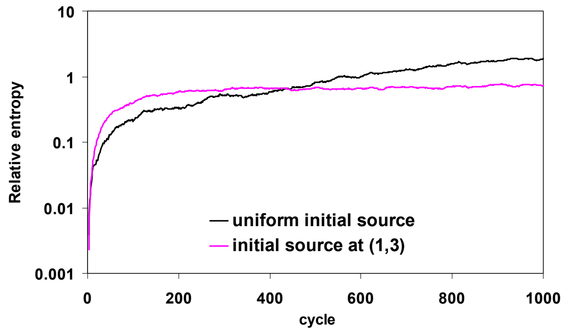

Fig. 3 Progressive relative entropy for two different initial fission source distributions

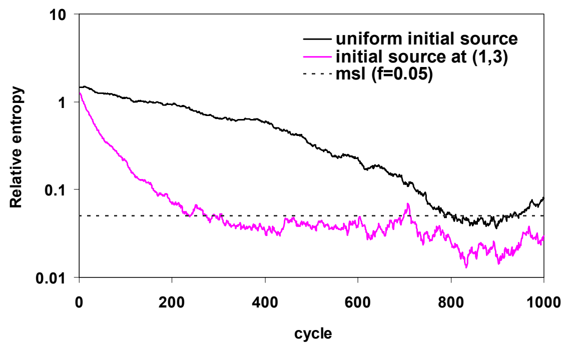

Fig. 4 Posterior relative entropy assuming 500 inactive and 500 active cycles

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