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Best Numbers for Active Cycles and Histories per Cycle in Monte Carlo Eigenvalue Calculations

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1. Introduction

With an increasing computing power, Monte Carlo (MC) neutronics codes have been widely used to analyze various nuclear systems. In order to conduct MC eigenvalue calculations for k_{eff} estimations, code users have to specify the numbers of inactive cycles, active cycles and neutron histories per cycle in input files. The number of inactive cycles can be determined after or, in the middle of a running by using recent works on the convergence diagnostics of a fission source distribution (FSD) [1,2]. The purpose of this paper is to investigate the best numbers for active cycles and neutron histories per cycle with a given total number of neutron histories to minimize variance biases of the estimations.

2. Minimization of Variance Bias

2.1 Formulation of a Real Variance

For an MC eigenvalue calculation conducted with N active cycles on M neutron histories per cycle, Q_i means an estimation of a tally denoted by Q at active cycle i.

$$Q_i = \frac{1}{M}\sum_{j=1}^{M} Q_{ij} \tag{1}$$

Q_{ij} is a Q estimation from the j-th neutron history at active cycle i.

Then the tally estimation over the N active cycles, $\overline{Q}$ can be calculated by

$$\overline{Q} = \frac{1}{N}\sum_{i=1}^{N} Q_i \ . \tag{2}$$

From a formulation of the variance bias derived by Ueki et al [3], the real variance of $\overline{Q}$, $\sigma^2\left[\overline{Q}\right]$ can be written as

$$\begin{aligned}\sigma^2\left[\overline{Q}\right] &= \sigma^2\left[\frac{1}{N}\sum_i Q_i\right] \\ &= \frac{1}{N}\sigma^2\left[Q_i\right] + \frac{2}{N(N-1)}\sum_{t=1}^{N-1}(N-t)\operatorname{cov}\left[Q_i, Q_{i+t}\right] \ .\end{aligned} \tag{3}$$

And the inter-cycle covariance between Q_i and Q_{i+t}, $\operatorname{cov}\left[Q_i, Q_{i+t}\right]$ can be expressed with that of FSD's as [4]

$$\operatorname{cov}\left[Q_i, Q_{i+t}\right] = \sum_{m=1}^{N_m}\sum_{m'=1}^{N_m} R_m^Q R_{m'}^Q \operatorname{cov}\left[S_m^i, S_{m'}^{i+t}\right]. \tag{4}$$

S_m^i (m=1, …, N_m) is the FSD of the m-th region at active cycle i, defined by $S_m^i = \int_{V_m} d\mathbf{r} S^i(\mathbf{r})$. R_m^Q denotes the Q contribution from a unit fission source in the m-th region, defined by

$$R_m^Q = \frac{\sum_{j=0}^{\infty}\int dPq(P)\int dP' K_j(P'\to P)\int_{V_m} dP'' T\left(P''\to P'\right)S(P'')}{\int_{V_m} dPS(P)} \tag{5}$$

where

$P \equiv (\mathbf{r}, E, \mathbf{\Omega})$,
$q(P)$ = response function of Q
$K_j(P'\to P) = \int dP_1 \cdots \int dP_{j-1} K(P_{j-1}\to P) \cdots K(P'\to P_1)$,
$K(P'\to P) \equiv C(\mathbf{r}'; E', \mathbf{\Omega}'\to E, \mathbf{\Omega})T(E, \mathbf{\Omega}; \mathbf{r}'\to \mathbf{r})$
= transport kernel,
$C(\mathbf{r}'; E', \mathbf{\Omega}'\to E, \mathbf{\Omega})$ = collision kernel,
$T(E, \mathbf{\Omega}; \mathbf{r}'\to \mathbf{r})$ = free flight kernel,
$S(P)$ = fission source distribution.

Suppose that the active cycle calculation starts after many inactive cycle ones which are enough to make a converged FSD. Then using the cycle-by-cycle error propagation model [5] and the direct posterior estimation method for the stochastic error's covariance [6], $\operatorname{cov}\left[S_m^i, S_{m'}^{i+t}\right]$ in Eq. (4) can be expressed as

$$\begin{aligned}\operatorname{cov}\left[S_m^i, S_{m'}^{i+t}\right] &= \sum_{i'=0}^{\infty}\sum_{n=1}^{N_m}\sum_{n'=1}^{N_m} a_{mn}^{i'} a_{m'n'}^{i'+t} \operatorname{cov}\left[\varepsilon_n, \varepsilon_{n'}\right] \\ &= \frac{1}{M}\sum_{i'=0}^{\infty}\sum_{n=1}^{N_m}\sum_{n'=1}^{N_m} a_{mn}^{i'} a_{m'n'}^{i'+l} \operatorname{cov}\left[\varepsilon_{n,j}, \varepsilon_{n',j}\right],\end{aligned} \tag{6}$$

$$\begin{aligned}&\operatorname{cov}\left[\varepsilon_{n,j}, \varepsilon_{n',j}\right] \\ &= E\left[\left(S_{n,j}^i - E\left[S_n^i \middle| \mathbf{S}^{i-1}\right]\right)\cdot\left(S_{n',j}^i - E\left[S_{n'}^i \middle| \mathbf{S}^{i-1}\right]\right)\right].\end{aligned} \tag{7}$$

a_{mn}^i is the m-th row and n-th column element of the matrix A^i where the matrix A is defined by

$$\mathbf{A} = \frac{1}{k_0}\left(\mathbf{H} - \mathbf{S}_0 \cdot \boldsymbol{\tau}^T\right); \tag{8}$$

$\boldsymbol{\tau}^T$ = N_m dimensional row vector (1,1,...,1).

H and $\mathbf{S}_0$ denote the fission matrix and the main mode fission source distribution. k_0 is the main mode eigenvalue. ε_n is the stochastic error at region n.

Using Eqs. (1), (4) and (6), $\sigma^2\left[\overline{Q}\right]$ of Eq. (3) can be written as

$$\sigma^2\left[\overline{Q}\right] = \frac{1}{NM}\sigma^2\left[Q_{ij}\right] + \frac{1}{NM}\cdot B(N)\ ; \qquad (9)$$

$$B(N) = \frac{2}{N-1}\sum_{t=1}^{N-1}(N-t)\cdot C_t^Q, \qquad (10)$$

$$C_t^Q \equiv \text{cov}\left[Q_i, Q_{i+t}\right] = \sum_{m=1}^{N_m}\sum_{m'=1}^{N_m} R_m^Q R_{m'}^Q \left(\sum_{i'=0}^{\infty}\sum_{n=1}^{N_m}\sum_{n'=1}^{N_m} a_{mn}^{i'} a_{m'n'}^{i'+t}\,\text{cov}\left[\varepsilon_{n,j}, \varepsilon_{n',j}\right]\right) \qquad (11)$$

$B(N)/(NM)$ in Eq. (9) is a difference between the real and apparent variance, called the variance bias. *B*(*N*) means the variance bias independent of the total number of neutron histories, *NM*.

2.2 Zero Variance Bias

From Eqs. (9) and (10), we can see that the variance bias depends only on *B*(*N*) when the total number of neutron histories is fixed as *NM* and *B*(*N*) is governed by the number of active cycles, *N*.

When *N*=*n* in Eq. (10), *B*(*n*) can be written as

$$B(n) = 2\sum_{t=1}^{n-1}\frac{n-t}{n-1}\cdot C_t^Q\ . \qquad (12)$$

When *N*=*n*+1, *B*(*n*+1) can be written as

$$B(n+1) = 2\sum_{t=1}^{n}\frac{n+1-t}{n}\cdot C_t^Q\ . \qquad (13)$$

Subtracting Eq. (12) from Eq. (13), *B*(*n*+1) - *B*(*n*) can be written as

$$\begin{aligned} B(n+1) - B(n) &= 2\sum_{t=1}^{n-1}\left(\frac{n+1-t}{n} - \frac{n-t}{n-1}\right)\cdot C_t^Q + \frac{2}{n}\cdot C_n^Q \\ &= 2\sum_{t=1}^{n-1}\left(\frac{t-1}{n(n-1)}\right)\cdot C_t^Q + \frac{2}{n}\cdot C_n^Q\ . \end{aligned} \qquad (14)$$

Assuming that $C_t > 0$ $(t = 1, 2, \ldots)$ because successive Q_i are positively correlated [7], *B*(*n*+1) > *B*(*n*). This means that the greater the number of active cycle is, the larger the variance bias becomes.

Especially when *N*=1, the variance bias becomes zero from Eq. (10). This means that the apparent variance becomes equal to the real variance when the total neutron histories are assigned to a single active cycle and the number of active cycles is set to 1.

2.3 Test Results

Behavior of the variance bias according to the active cycle number was studied for the fuel storage facility problem [8]. Figure 1 shows the $B(N)/\sigma^2\left[Q_{ij}\right]$ calculated by using a fission matrix and power responses for the (1,3) assembly built from an MC eigenvalue calculation with 100,000,000 neutron histories. From Figure 1, we can observe that the amount of variance bias becomes larger as the number of active cycles is increased.

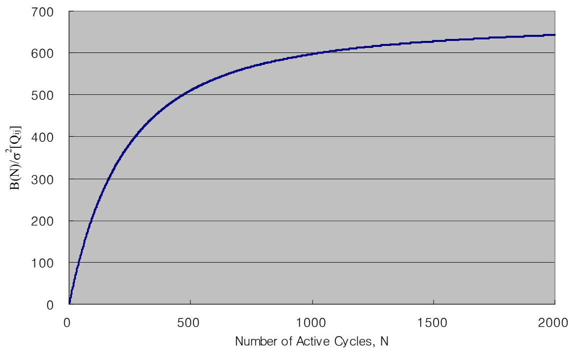

Figure 1. Variance bias according to number of active cycles for fission power tally of the (1,3) assembly

3. Conclusion

A formulation about the relationship between the variance bias and the number of active cycles has been developed from recent works on the estimation of a real variance. From the formulation, we can see that the variance bias becomes zero when the number of active cycles is 1.

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