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Improving variance estimation in Monte Carlo eigenvalue simulations ☆

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ABSTRACT

Monte Carlo (MC) methods have been widely used to solve eigenvalue problems in complex nuclear systems. Once a stationary fission source is obtained in MC simulations, the sample mean of many stationary cycles is calculated. Variance or standard deviation of the sample mean is needed to indicate the level of statistical uncertainty of the simulation and to understand the convergence of the sample mean. Current MC codes typically use sample variance to estimate the statistical uncertainty of the simulation and assume that the MC stationary cycles are independent. However, there is a correlation between these cycles, and estimators of the variance that ignore these correlations will systematically underestimate the variance. This paper discusses some statistical properties of the sample mean and the asymptotic variance and introduces two novel estimators based on (a) covariance-adjusted methods and (b) bootstrap methods to reduce the variance underestimation. For three test problems, it has been observed that both new methods can improve the estimation of the standard deviation of the sample mean by more than an order of magnitude. In addition, some interesting patterns were revealed for these estimates over the spatial regions, providing additional insights into MC simulations for nuclear systems. These new methodologies are based on post-processing the tally results and are therefore easy to implement and code agnostic.

1. Introduction

Monte Carlo (MC) algorithms are the most accurate methods for solving the eigenvalue form of the Boltzmann radiation transport equation for performing reactor calculations and criticality safety analyses due to the ability to handle complex geometries and physics. MC eigenvalue calculations must perform iterations (analogous to deterministic power iteration) to compute the source of fission neutrons throughout the system. Therefore, several initial iterations (cycles) are performed to converge the fission neutron distribution within statistical fluctuations (a stationary distribution). These first few cycles, known as inactive cycles, are discarded, and the cycles thereafter are called active cycles. The final tallies are calculated as the average over all the active cycles, and the tally variances are calculated as a sample variance assuming that all the active cycles are independent. However, traditional MC sampling of the fission source introduces correlation among the source points between cycles, which has been shown to result in underprediction of the variance of an MC estimator. As shown in Mervin et al. (2013), the underprediction of the variance may not be an issue for a global tally such as the system multiplication factor (k_{eff}); however, the underprediction is pronounced in local tallies (e.g., axial flux, pin power). The existence of this cycle-to-cycle correlation may also impact the convergence of the sample mean. Additional cycles and particles per cycles may only slightly improve the situation (Miao et al., 2016). As a result, cycle-to-cycle correlation must be considered when using MC where local solutions are important, such as in full core simulations with depletion, as this requires high-fidelity estimation of local tallies, such as reaction rates or pin-wise fluxes.

From the vast literature on MC variance underprediction, the earliest, most significant work was performed by Brissenden and Garlick (1986), who showed that the MC power iteration leads to a bias in the tally because of the source normalization process. Brissenden and Garlick, and also Gelbard (1991), obtained an

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approximate expression for the bias in the eigenvalue estimator due to the source normalization process. The literature on the MC tally variance underprediction can be broadly divided into three categories: (1) literature that proposes various methods without modifying or biasing the MC power iteration and particle transport process, (2) literature that proposes various methods to modify the MC power iteration and particle transport process, and (3) literature that shows that the variance underprediction issue is significant and that simply running more cycles and/or particles per cycle yield negligible improvement. The first category of literature includes an iterative method proposed by Ueki et al. (1997) based on relations between real and lag covariance, fitting methods based on time series methodologies proposed in Demaret et al. (1999) and Jacquet et al. (2000), and many others. Additionally, Ueki (2011) investigated nonoverlapping batch means, overlapping batch means, and standardized time series methods. He studied some interesting relationships between the overlapping batch mean estimator and the classical spectral variance estimator (Bartlett estimator). Both the batch means estimator and the classical Bartlett estimator are especially relevant to the methods proposed in this paper. The second category includes the superhistory method proposed by Brissenden and Garlick (1986), the exponential transform path stretching investigated by Ueki (2002), and many others. The third category includes Mervin et al. (2013), showing the variance underprediction issue for various problems, the review paper by Brown (2009), and a recent paper by Miao et al. (2016) that demonstrates the impact of cycle-to-cycle correlation on the convergence of the sample mean, as well as many others.

In this paper, two novel estimators are introduced based on post-processing the tally results over the active cycles. These estimators are applied to three test problems to estimate the variance of the mesh-based energy integrated flux tallies. These estimators are shown to improve the variance estimation by an order of magnitude when compared to the estimator based on sample variance that is used by most current production MC codes. The first estimator is based on the estimation of the autocorrelation coefficient using the tally mean values over the active cycles. In contrast with other similar estimators such as the classical spectral estimator (see Ueki, 2011), one of the proposed estimators is data adaptive. At different locations of a Monte Carlo simulation, we allow the use of different numbers of sample auto-covariances in the calculation of the data adaptive variance estimates. With a very simple data adaptive rule, the improvement is significant and the results are stable for different situations. The second estimator also uses tally mean values over the active cycles and applies a statistical technique known as bootstrap (Efron, 1979). Although bootstrap has been widely used in statistical science (Davison and Hinkley, 1997), its application in nuclear engineering is limited. Both of these estimators require that the tally mean values calculated by the MC code be stored or written to disk in each active cycle for post-processing. Alternatively, underestimation of the variance could be avoided by simply performing multiple independent simulations with different initial random seeds. While this yields excellent variance estimates, it requires a large amount of additional computer time and resources, since each independent simulation must converge the fission source before starting the active cycles (Miao et al., 2016). The objective of this work is to bootstrap MC simulations by using the data generated during the MC simulation to improve the MC tally variance estimations.

Block bootstrap methods provide a new framework for variance estimation. The methods try to mimic the calculation of the reference variance estimation using multiple independent simulations by generating multiple bootstrap samples. From a probabilistic point of view, a sample of an independent MC simulation is a random sample from the unknown joint distribution of the underlying random process. Bootstrap samples can be considered as independent samples from the data or equivalently from the empirical joint distribution of the underlying process. A bootstrap sample consisting of multiple blocks is analogous to a sample from an independent MC simulation. Though a single block within block bootstrap is similar to a batch in the batch-based methods, the use of a block in block bootstrap is to maintain the dependency structure between different cycles, while that in the batch methods attempts to generate uncorrelated means of different batches. Note that, while the batch mean methods use the batch mean (partial sample mean) of each batch, bootstrap uses the mean of a bootstrap sample, which is in essence an independent MC simulation.

This paper is organized as follows: Section 2 introduces the notation used throughout this paper, as well as the traditional variance estimate of the sample mean, and two new estimators. Section 3 introduces the performance metrics used to evaluate the variance estimators, the MC code used to produce the numerical results, and results for three test problems. Additionally, Section 3 includes a performance comparison between the estimators introduced in this paper and the non-overlapping and overlapping batch means methods proposed by Ueki (2011). Finally, concluding remarks are provided in Section 4.

2. Theory

We begin by considering a geometry of M tally regions in a MC neutron transport eigenvalue simulation of T active cycles with N_p particle histories per cycle. For the purposes of this discussion, we assume that a sufficient number of inactive cycles have been performed to allow the fission source to reach a stationary distribution. Two approaches are commonly employed for variance estimation. With the first approach, history-based statistics, every particle history is treated as an independent sample. In this case the total number of samples over which the variance is computed is $T \times N_p$. With cycle-based statistics, the mean value for each cycle is first computed, and the variance is then taken over the T individual cycle means. It should be noted that history- and cycle-based statistics will compute the same mean value for all tallies; only the variance estimation will differ. Although both history- and cycle-based statistics are commonly used, the following discussion is focused primarily on cycle-based statistics because the application of advanced approaches for variance estimation is more straightforward in this case.

Let $\boldsymbol{x}_t = (x_{t,1}, x_{t,2}, \ldots, x_{t,M})^{\mathrm{T}}$ be an $M \times 1$ vector to denote the tally values over all M tally regions at the t-th cycle. We assume that $x_{t,m}$, for $m = 1, \ldots, M$ are weakly stationary random processes, meaning that both the mean and autocovariances are close to constant over the T cycles. Let

$$\gamma_{h,m} \equiv \mathrm{cov}(x_{t,m}, x_{t+h,m}) = E(x_{t,m}, x_{t+h,m}) - E(x_{t,m})E(x_{t+h,m}) \tag{1}$$

be the h-th autocovariance of the process at the m-th tally region. The autocovariance $\gamma_{h,m}$ measures how strongly cycle t is correlated with cycle $t \pm h$. In general, MC simulations exhibit the short memory property. This means that the total of all the absolute values of true autocorrelations of the underlying process is finite. The Hurst exponent (Beran, 1992) is a measure of long memory. The long memory models were used for the simulated data; however, the Hurst parameters for MC data are not significant. Thus, the autocorrelation between cycles t and $t \pm h$ decays to zero quickly as h becomes large. Without this property, the ratio between the true variance and the simple variance estimate (without information of the correlation structure) tends to infinity as the number of cycles grows large (Beran, 1992).

Due to the complexity of the inter-cycle dependence, estimating the unknown mean μ_m of the m-th process and the correspond-