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K-effective Confidence Intervals

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Autoregressive Fitting for Monte Carlo
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I. Introduction

For Monte Carlo eigenvalue calculations, it is well-known that the correlation of fission cycles (generations) can introduce significant negative bias into the estimated confidence interval for k-effective [1]. That is, the "apparent" confidence interval for k-effective computed under the assumption of independent cycles will underestimate the true confidence interval which accounts for inter-cycle correlation. We have investigated the use of autoregressive (AR) fitting [2] to improve the estimation of confidence intervals for k-effective.

Stationary stochastic processes with bounded auto(lag)-covariance are called covariance stationary processes. It has been known for decades that the confidence interval of mean quantities of interest from covariance stationary processes can be reliably estimated by autoregressive (AR) fitting [2]. Jacquet et al recently showed that AR fitting performed well for the confidence interval estimation for Monte Carlo k-effective calculations [3]. This summary compares AR fitting with conventional batching methods [1] for a physical system with highly correlated fission sources and proposes a statistical feedback method as an option for improving AR fitting.

II. Theory

The feasibility of AR fitting is discussed in terms of the integral formulation of particle transport as follows. Let $H(\vec{r}' \to \vec{r})$ be the expected number of the first generation descendant particles per unit volume at $\vec{r}$ resulting from a particle born at $\vec{r}'$ with a position independent energy spectrum. The stationary source distribution (S) and effective multiplication factor (k-eigenvalue) satisfy

$$S(\vec{r}) = \frac{1}{k} \int S(\vec{r}') H(\vec{r}' \to \vec{r}) dr . \tag{1}$$

Under the normalization condition $\int S(\vec{r}) dr = k$, a realization of the source distribution after simulating the m-th stationary cycle may be written as

$$\hat{S}^{(m)}(\vec{r}) = NS(\vec{r}) + \sqrt{N} \hat{e}^{(m)}(\vec{r}) , \tag{2}$$

where $\hat{e}^{(m)}(\vec{r})$ is the fluctuating component of the source distribution, N is the number of particle histories per cycle, and the hats indicate a realization of stochastic quantities. The random noise component $\hat{\varepsilon}^{(m)}(\vec{r})$ resulting from the starter selection and subsequent simulation for the particle histories at the m-th stationary cycle can then be introduced as

$$\sqrt{N}\hat{\varepsilon}^{(m)}(\vec{r}) = \hat{S}^{(m)}(\vec{r}) - \frac{N\int H(\vec{r}' \to \vec{r})\hat{S}^{(m-1)}(\vec{r}')dr'}{\int \hat{S}^{(m-1)}(\vec{r}'')dr''} \qquad (3)$$

It can be shown [4] that $\hat{\varepsilon}^{(m)}$, $\hat{e}^{(m)}$ and $\hat{e}^{(m-1)}$ satisfy

$$\hat{e}^{(m)}(\vec{r}) = \int A(\vec{r}' \to \vec{r})\hat{e}^{(m-1)}(\vec{r}')dr + \hat{\varepsilon}^{(m)}(\vec{r}) + O(N^{-1/2}) \qquad (4)$$

where O is the order notation defined as $\lim_{x \to 0} O(x)/x = $ constant with respect to x, and A is defined as

$$A(\vec{r}' \to \vec{r}) = \frac{1}{k}\left[H(\vec{r}' \to \vec{r}) - S(\vec{r})\right]. \qquad (5)$$

If the $\hat{\varepsilon}^{(m)}$'s are independent, then the $\hat{e}^{(m)}$'s approximately follow a functional version of an AR process with order one. If not, one may decompose $\hat{\varepsilon}^{(m)}$ into the linear combination of uncorrelated random functions $\hat{\eta}^{(j)}$:

$$\hat{e}^{(m)}(\vec{r}) = \int A(\vec{r}' \to \vec{r})\hat{e}^{(m-1)}(\vec{r}')dr + \hat{\eta}^{(m)}(\vec{r}) - \sum_{j=1}^{\infty}\theta_j\hat{\eta}^{(m-j)}(\vec{r}) + O(N^{-1/2}). \qquad (6)$$

The decomposition could be established by Wold decomposition [5] because the expected value of $\hat{\varepsilon}^{(m)}$ is identically zero on function space and the uncorrelatedness of such functions is equivalent to orthogonality. $\hat{e}^{(m)}(\vec{r})$'s are therefore approximated by a functional version of Auto Regressive Moving Average (ARMA) processes. Since $\int\hat{e}^{(m)}(\vec{r})dr$ can be interpreted as the difference of the observed and expected values of the k-eigenvalue collision estimator at the m-th stationary cycle, the fitting of cycle k-eigenvalues to ARMA models is feasible. In this work, the independence of the $\hat{\varepsilon}^{(j)}$'s is assumed. The AR fitting coefficients of cycle k-eigenvalues are computed by the least squares method and the autocovariances of lag-i ($c(i)$) are then computed to estimate the variance (σ^2) of the sample mean [6]:

$$\sigma^2 = \frac{1}{M}\left[c(0) + 2\sum_{i=1}^{M-1}\left(1 - \frac{i}{M}\right)c(i)\right], \qquad (7)$$

where M is the number of stationary cycles simulated.

III. Numerical Results

An example problem is a fissionable system with a sharp, localized peak [7]. The spatial domain is an infinite square column with sides of 24 cm, which is filled with material having isotropic scattering and energy-independent macroscopic cross sections of $\Sigma_t = 1.0\ cm^{-1}$, $\Sigma_a = 0.3\ cm^{-1}$, and $\nu\Sigma_f = 0.24\ cm^{-1}$ except for the central region. The central region is an infinite square column with sides of 3 cm, filled with a material having $\Sigma_t = 1.0\ cm^{-1}$, $\Sigma_a = 0.3\ cm^{-1}$, and $\nu\Sigma_f = 0.39\ cm^{-1}$. The problem is an extreme mock up of a control rod drop accident at the cold standby condition of a boiling water nuclear reactor. We applied AR fitting to the cycle k-eigenvalues $\hat{k}^{(m)}$, $m = 1,\ldots,M$. In addition, the effect of the following statistical feedback was studied:

$$\hat{K}^{(m)} = \hat{k}^{(m)} - c_1(\hat{k}^{(m-1)} - \hat{k}^{(m-2)}) - c_2(\hat{k}^{(m-2)} - \hat{k}^{(m-3)}), \, m = 3,\dots,M . \quad (8)$$

Using the first and second order AR(2) fitting coefficients of $\hat{k}^{(m)}$ (ϕ_1 and ϕ_2), c_1 and c_2 are determined to be: $c_1 = \phi_1, c_2 = \phi_2 + c_1$. Note that c_1 and c_2 are intended to offset the correlation effects of the most recent two cycles. AR fitting is again applied to $\hat{K}^{(m)}$ to compute the standard deviation. Figure 1 shows the observed confidence levels for the two AR fitting schemes and the conventional batching method with batch groupings of 1, 5, 10, and 20 cycles. The 300 cycle simulation of 2000 histories per cycle (with the first 100 settling cycles discarded) was replicated 4000 times and the sample mean of the sample means from the 4000 replicas is taken to be the reference value of the true mean. We checked whether or not the reference value is included in each of the 4000 one-sigma confidence intervals formed by the mean and standard deviation at each replica. The observed confidence level in the vertical axis of Figure 1 is the ratio of the inclusion of the reference value. For ideal, uncorrelated calculations, the confidence level of the standard deviation (one-sigma) should be 68%; negative bias from correlation effects will reduce the confidence levels of the computed standard deviations.

The results in Figure 1 indicate that the batching method and the AR fitting of the original $\hat{k}^{(m)}$'s appear to perform comparably, with each of them reducing the negative bias in computing standard deviations (i.e, increasing the observed confidence levels toward the 68% level). However, AR fitting is desirable because the number of active samples is larger. That is, for AR fitting of order n, the sample size is reduced by n; batching with groupings of m cycles/batch will reduce the sample size by a <u>factor</u> of $1/m$. The beneficial effect of feedback is clearly observed in Figure 1.

IV. Conclusions

We have investigated the use of AR and batching methods to provide improved Monte Carlo estimates of the confidence interval for k-effective. Numerical testing on a highly correlated k-effective problem has demonstrated that both are effective in reducing the negative bias caused by inter-cycle correlation, with AR fitting having the advantage of larger sample size. In addition, the use of feedback, with AR fitting of the k-effective estimator given by Eq. (8), appears to raise one-sigma confidence level toward the correct level (68 %). This favorable result indicates that AR fitting with appropriate techniques in process adjustment and control is worth investigating in terms of the standard deviation computation taking account of correlation effects in Monte Carlo eigenvalue calculations. Future work will include the criteria for determining what order of AR fitting is most effective.

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Figure 1: Observed One-Sigma Confidence Level, based on 4000 replicas of 200 active cycles with 100 inactive cycles.