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Title:

STATIONARITY DIAGNOSTICS USING SHANNON ENTROPY IN MONTE CARLO CRITICALITY CALCULATIONS I: F TEST

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Stationarity Diagnostics Using Shannon Entropy in Monte Carlo Criticality Calculation I: F test

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I. Introduction

In Monte Carlo (MC) criticality calculations, the source distribution is presumed to converge and settle into stationarity before the tallying of k-effective eigenvalue (Keff) and other quantities of interest begins. To ensure that tallied quantities are generated by particles sampled from the stationary source, MC criticality code users have to specify the number of inactive cycles to discard before tallies begin. Recently, the stationarity detection of a Keff series was discussed based on Brownian bridge [1]. However, a quantity more representative of the state of source distribution than Keff, i.e., the mere integral of source distribution, is desired for stationarity diagnostic purposes. As a step toward that end, this article proposes the two-sample F test [2] of the Shannon entropy [3,4] of source distribution.

II. Example Problem – Keff of the world –

The problem analyzed by Shannon entropy is a one energy group version of the Keff-of-the-world problem [5]: The system consists of a 7×7×7 array of identical cubes with the side length of 6 cm and macroscopic cross sections of $\Sigma_t = 0.31997\, cm^{-1}$, $\Sigma_a = 0.09916\, cm^{-1}$ and $\nu\Sigma_f = 0.22711\, cm^{-1}$, placed at a pitch of 24 cm. The surfaces of the neighboring cubes are faced parallel to each other. The space between the cubes has macroscopic cross sections of $\Sigma_t = 0.05\, cm^{-1}$, $\Sigma_a = 0.001\, cm^{-1}$ and $\nu\Sigma_f = 0\, cm^{-1}$. The space up to 9 cm away from the outermost surfaces of the cubes has the same non-fissile cross sections. Keff of this system is computed to be 0.87609 +– 0.00028. When the center cube is replaced by acube with macroscopic cross sections of $\Sigma_t = 0.56158\, cm^{-1}$, $\Sigma_a = 0.17404\, cm^{-1}$ and $\nu\Sigma_f = 0.3986\, cm^{-1}$ (Keff=1.00785 +– 0.00029 as a bare, isolated unit), the system becomes supercritical and its Keff rises to 1.04527 +– 0.00002. This supercritical problem, which is also analogous to the problem of a supercritical Pu sphere in fissile store [6], is analyzed throughout this article. The confidence interval of the sample mean of Keff's is shown in Fig. 1. Tallying at the early stages of active cycles is observed to be affecting confidence interval estimation when the number of inactive cycles is insufficient. Fig. 2 shows the autocorrelation coefficient estimated for the various combinations of the number of histories per cycle with the numbers of inactive and active cycles. It is observed that autocorrelation estimation is significantly affected by the insufficient number of inactive cycles. This implies that confidence interval estimation from a single replica becomes unreliable under the presence of tallied quantities from nonstationarity. The purpose of stationarity diagnostics is the automatic detection of non-stationary contamination.

III. Posterior Diagnostics of Shannon Entropy

Shannon entropy [4] of the source distribution is defined to be

$$H = -\sum_{i=1}^{B} S_i \ln(S_i), \tag{1}$$

where *i's* stand for spatial bin numbers, B for the total number of spatial bins, S_i's source distribution normalized to unity, ln natural logarithm and $0\ln(0)=0$. H is a measure of the randomness in S_i's associated with a particular spatial binning in the sense that H attains its maximum value ln(B) when $S_i = 1/B$ for all i's and its minimum value 0 when $S_i = 1$ for i and $S_j = 0$ for all $j \neq i$.

A statistical test will be designed for H's evaluated at active cycles. To this end, m and n cycles are selected at equal cycle intervals from the first and second halves of active cycles, respectively. Let the m samples from the first half be $X_i = H_{1+(i\text{-}1)M/(2m)}$, $i = 1,\ldots,m$ and the n samples from the second half $Y_j = H_{M\text{-}(j\text{-}1)M/(2n)}$, $j = 1,\ldots,n$ where M is the number of active cycles. Normality (gaussian) and independence are assumed for these X_i's and Y_j's. The following theorem in two-sample problems is the basis of stationarity diagnostics using Shannon entropy:

Theorem. Let $U_1,\ldots,U_m \sim N(\mu_U,\sigma)$ and $W_1,\ldots,W_n \sim N(\mu_W,\sigma)$, and let U's and W's be independent. The distribution function of the ratio of the sample variances is $F_{m-1,n-1}$, the F distribution with m-1 and n-1 degrees of freedom, i.e., $v_U^2 / v_W^2 \sim F_{m-1,n-1}$ where

$$v_U^2 = 1/(m-1)\sum_{i=1}^{m}(U_i - \bar{U})^2 \text{ and } v_W^2 = 1/(n-1)\sum_{j=1}^{n}(W_j - \bar{W})^2.$$

The theorem can easily be checked by $(m-1)v_U/\sigma^2 \sim \chi^2_{m-1}$, $(n-1)v_W/\sigma^2 \sim \chi^2_{n-1}$ and $F_{m-1,n-1} \sim \left[\chi^2_{m-1}/(m-1)\right]/\left[\chi^2_{n-1}/(n-1)\right]$ where χ^2 denotes the chi square distribution with degree of freedom being its subscript [2]. When the X's are contaminated by nonstationarity, the fitting of them to normal distribution will yield large variance. This speculation leads to the following two-sample F test:

F test. Assume $X_1,\ldots,X_m \sim N(\mu_X,\sigma_X)$ and $Y_1,\ldots,Y_n \sim N(\mu_Y,\sigma_Y)$. Let the null hypothesis be "$\sigma_X = \sigma_Y$" and alternative hypothesis "$\sigma_X > \sigma_Y$". Reject the null hypothesis at the α level significance if $v_X^2 / v_Y^2 \geq F_{1-\alpha,m-1,n-1} = F^{-1}_{m-1,n-1}(1-\alpha)$. v_X^2 / v_Y^2 is called the F statistic.

The F test was applied to the supercritical problem in Sec. II by setting m=n=10. Here, m was chosen to be equal to n because the F test in analysis of variance, which is similar to the F test above, is relatively insensitive to violations of independence and normality assumptions, but only when the sample sizes are equal [7]. One spatial bin was assigned to each cube. Fig. 3 shows the F statistic for various numbers of inactive cycles and seven different initial random number seeds that were chosen so as to avoid the overlapping of the striding of the random number generator. The F statistic is observed to be rapidly decreasing toward its stationary level.

IV. Summary and future work

It has been shown that the application of the two-sample F test to the Shannon entropy of the source distribution would be an effective stationarity diagnostic. The numerical results show the power of rejecting the null hypothesis when the null hypothesis is false. However, the F test is merely a test for checking the equality of variances, which is a prerequisite for the two-sample t test for checking the equality of means. [2] Thus, the t test should be investigated. Future work will include the exploration of the violation of independence assumption using randomization test techniques.

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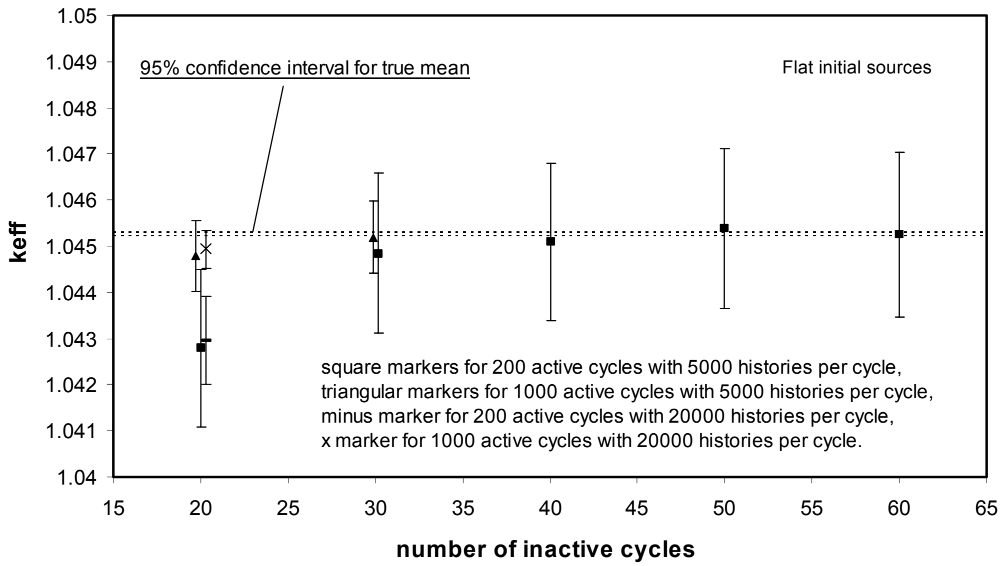

Figure 1: Expected 68% confidence interval of the Keff mean over active cycles
(Keff values at markers and standard deviation computed from 500 replicas)

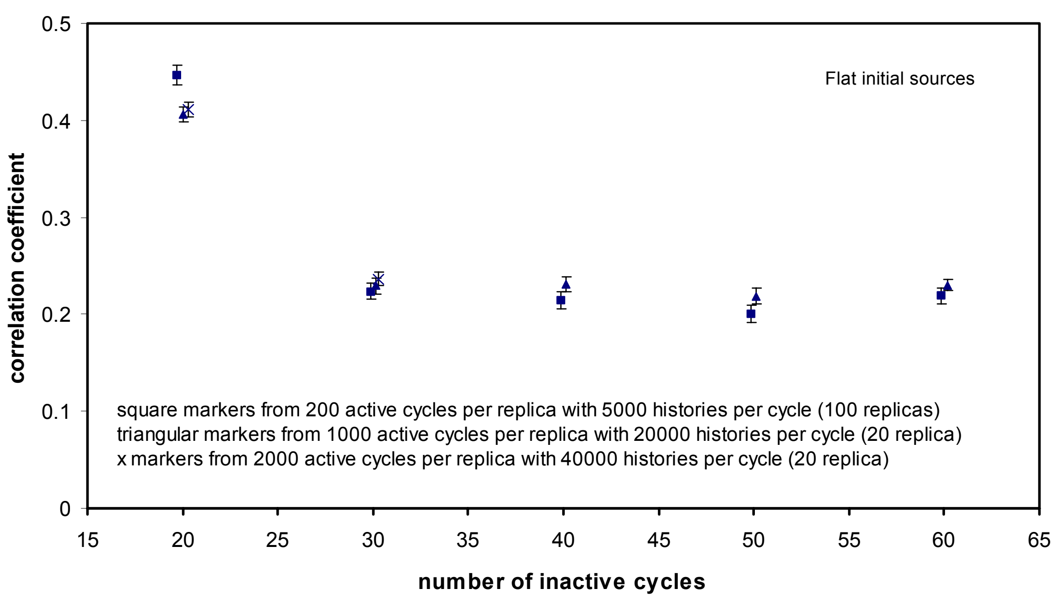

Figure 2: Autocorrelation coefficient of active cycle Keff's
(averaged over replicas, error bars showing 68% confidence interval)

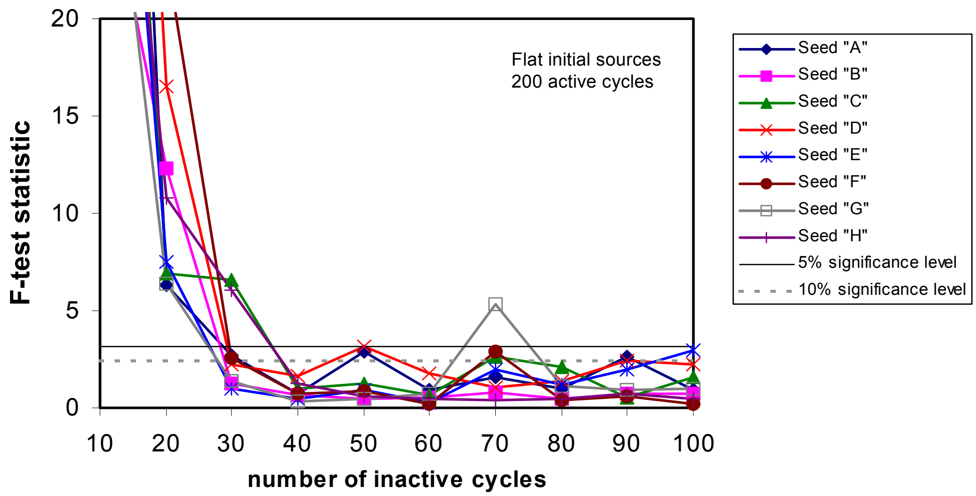

Figure 3: F statistic of Shannon entropy