Variance bias analysis for the Gelbard's batch method

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1. Introduction

When we perform a Monte Carlo estimation, we could get a sample variance as the statistical uncertainty of it. However, this value is smaller than the real variance of it because a sample variance is biased. To reduce this bias, Gelbard devised the method which is called the Gelbard's batch method. It has been certificated that a sample variance get closer to the real variance when the batch method is applied. In other words, the bias get reduced. This fact is well known to everyone in the MC field. However, so far, no one has given the analytical interpretation on it. In this paper, variances and the bias will be derived analytically when the Gelbard's batch method is applied. And then, the real variance estimated from this bias will be compared with the real variance calculated from replicas.

2. Analytical derivations of variances and the bias

In this section the analytical derivations of variances and the bias are described.

2.1. Definition of the batch

The conceptual drawing of batches are described in the Fig. 1. N is the number of cycles. Each cycle is represented as yellow boxes in the Fig. 1. N_B is the number of batches. Each batch is represented as green boxes in the Fig. 1. M_B is the batch size which means how many cycles are included in a batch. The j-th batch is defined as follows.

$$Q_{M_B}^j \equiv \frac{1}{M_B}\sum_{i=(j-1)\times M_B+1}^{j\times M_B} Q_1^i \tag{1}$$

A batch is identical to the average value of M_B cycles. The average value of the tally in the conventional MC method is given as follows.

$$\bar{Q}_1 = \frac{1}{N}\sum_{i=1}^{N} Q_1^i \tag{2}$$

By the same token, the average value of the tally in the batch method is given as follows.

$$\bar{Q}_{M_B} = \frac{1}{N_B}\sum_{j=1}^{N_B} Q_{M_B}^j \tag{3}$$

2.2. Real Variance

The real variance of the tally in the conventional MC method can be shown as follows.

$$\sigma_R^2\left[\bar{Q}_1\right] = E\left[\bar{Q}_1^2\right] - E\left[\bar{Q}_1\right]E\left[\bar{Q}_1\right] \tag{4}$$

In the same way, the real variance of the tally in the batch method can be shown as follows.

$$\sigma_R^2\left[\bar{Q}_{M_B}\right] = E\left[\bar{Q}_{M_B}^2\right] - E\left[\bar{Q}_{M_B}\right]E\left[\bar{Q}_{M_B}\right] \tag{5}$$

These two real variances are identical. It can be shown easily.

$$\bar{Q}_{M_B} = \frac{1}{N_B}\sum_{j=1}^{N_B} Q_{M_B}^j = \frac{1}{N_B}\sum_{j=1}^{N_B}\frac{1}{M_B}\sum_{i=(j-1)\times M_B+1}^{j\times M_B} Q_1^i = \frac{1}{N}\sum_{i=1}^{N} Q_1^i = \bar{Q}_1 \tag{6}$$

According to eq. (6), we can derive eq. (7).

$$\begin{aligned}\sigma_R^2\left[\bar{Q}_{M_B}\right] &= E\left[\bar{Q}_{M_B}^2\right] - E\left[\bar{Q}_{M_B}\right]E\left[\bar{Q}_{M_B}\right] \\ &= E\left[\bar{Q}_1^2\right] - E\left[\bar{Q}_1\right]E\left[\bar{Q}_1\right] \\ &= \sigma_R^2\left[\bar{Q}_1\right]\end{aligned} \tag{7}$$

The real variance of the tally in the conventional MC method can be represented with covariance terms of tallies as follows.

$$\sigma_R^2\left[\bar{Q}_1\right] = \frac{1}{N}\sigma_R^2\left[Q_1^i\right] + \frac{1}{N^2}\sum_{l=1}^{N-1} 2\left(N-l\right)\mathrm{cov}\left[Q_1^i, Q_1^{i+l}\right] \tag{8}$$

By the same token, The real variance of the tally in the batch method can be also represented with covariance terms of tallies as follows.

$$\sigma_R^2\left[\bar{Q}_{M_B}\right] = \frac{1}{N_B}\sigma_R^2\left[Q_{M_B}^i\right] + \frac{1}{N_B^2}\sum_{l=1}^{N_B-1} 2\left(N_B-l\right)\mathrm{cov}\left[Q_{M_B}^i, Q_{M_B}^{i+l}\right] \tag{9}$$

From the relation in eq. (7), we can conclude as follows.

$$\begin{aligned}&\frac{1}{N}\sigma_R^2\left[Q_1^i\right] + \frac{1}{N^2}\sum_{l=1}^{N-1} 2\left(N-l\right)\mathrm{cov}\left[Q_1^i, Q_1^{i+l}\right] \\ &= \frac{1}{N_B}\sigma_R^2\left[Q_{M_B}^i\right] + \frac{1}{N_B^2}\sum_{l=1}^{N_B-1} 2\left(N_B-l\right)\mathrm{cov}\left[Q_{M_B}^i, Q_{M_B}^{i+l}\right]\end{aligned} \tag{10}$$

2.3. Sample Variance

The sample variance of the tally in the conventional MC method is given as follows.

$$\sigma_S^2\left[\bar{Q}_1\right] = \frac{1}{N(N-1)}\sum_{i=1}^{N}\left(Q_1^i - \bar{Q}_1\right)^2 \tag{11}$$

Along the same lines, the sample variance of the tally in the in the batch method can be shown as follow.

$$\sigma_S^2\left[\bar{Q}_{M_B}\right] = \frac{1}{N_B(N_B-1)}\sum_{j=1}^{N_B}\left(Q_{M_B}^j - \bar{Q}_{M_B}\right)^2 \tag{12}$$

The j-th batch from eq. (2) and the average value of the tally in the batch method from eq. (6) are substituted into eq. (12). And then each term is reorganized to obtain eq. (13).

$$\begin{aligned}\sigma_S^2\left[\bar{Q}_{M_B}\right] &= \frac{1}{N}\frac{1}{N-M_B}\sum_{i=1}^{N}\left(Q_1^i - \bar{Q}_1\right)^2 \\ &+ \frac{1}{N}\frac{1}{N-M_B}\sum_{j=1}^{N_B}\sum_{i=(j-1)\times M_B+1}^{j\times M_B}\sum_{\substack{k\neq i \\ k=(j-1)\times M_B+1}}^{j\times M_B}\left(Q_1^i - \bar{Q}_1\right)\left(Q_1^k - \bar{Q}_1\right)\end{aligned} \tag{13}$$

2.4. Apparent Variance

The apparent variance is defined as a expected value of a sample variance. According to the definition, we can derive the apparent variance of the tally in the conventional MC method given in eq. (14) and the apparent variance of the tally in the batch method given in eq. (15).

$$\sigma_A^2\left[\bar{Q}_1\right] = E\left[\sigma_S^2\left[\bar{Q}_1\right]\right]$$
$$= \frac{1}{N}\sigma_R^2\left[Q_1^i\right] - \frac{1}{N^2}\frac{1}{(N-1)}\sum_{l=1}^{N-1} 2(N-l)\operatorname{cov}\left[Q_1^i, Q_1^{i+l}\right] \quad (14)$$

$$\sigma_A^2\left[\bar{Q}_{M_B}\right] = E\left[\sigma_S^2\left[\bar{Q}_{M_B}\right]\right]$$
$$= \frac{1}{N}\sigma_R^2\left[Q_1^i\right] - \frac{1}{N^2}\frac{M_B}{N-M_B}\sum_{l=1}^{N-1} 2(N-l)\operatorname{cov}\left[Q_1^i, Q_1^{i+l}\right]$$
$$+ \frac{1}{N}\frac{N_B}{N-M_B}\sum_{l=1}^{M_B-1} 2(M_B-l)\operatorname{cov}\left[Q_1^i, Q_1^{i+l}\right] \quad (15)$$

In the right side of eq. (14) and (15), we can see that first terms are identical and second terms are similar, a little bit different. The remarkable difference is the third term in eq. (15). It comes from covariance terms between tallies in a batch. It makes a notable difference between the apparent variance in the batch method and the apparent variance in the conventional MC Method.

2.5. Bias

The bias is defined as the difference between the real variance and the apparent variance. According to the definition, we can derive the bias. The bias in the conventional MC method is given as follows.

$$B\left[\bar{Q}_1\right] = \sigma_R^2\left[\bar{Q}_1\right] - \sigma_A^2\left[\bar{Q}_1\right]$$
$$= \frac{1}{(N-1)}\frac{1}{N}\sum_{l=1}^{N-1} 2(N-l)\operatorname{cov}\left[Q_1^i, Q_1^{i+l}\right] \quad (16)$$

The bias in the conventional MC method is given as follows.

$$B\left[\bar{Q}_{M_B}\right] = \sigma_R^2\left[\bar{Q}_{M_B}\right] - \sigma_A^2\left[\bar{Q}_{M_B}\right]$$
$$= \frac{1}{N}\frac{1}{N-M_B}\sum_{l=1}^{N-1} 2(N-l)\operatorname{cov}\left[Q_1^i, Q_1^{i+l}\right]$$
$$- \frac{1}{N}\frac{N_B}{N-M_B}\sum_{l=1}^{M_B-1} 2(M_B-l)\operatorname{cov}\left[Q_1^i, Q_1^{i+l}\right] \quad (17)$$

In the right side of eq. (16) and (17), we can see that first terms are a little bit different. The remarkable difference is the second term in eq. (17). Covariance terms between tallies in a batch are fallen apart from the bias. For this reason, the bias in the batch method is less than the bias in the conventional MC method.

3. Real variance estimation in the batch method

It is necessary to examine the validation of the apparent variance and the bias which were derived in the previous section. In this paper, it is performed with the 2 by 2 fission matrix problem[3]. In this problem, the fission matrix is defined as follows.

$$\mathbf{H} = \begin{pmatrix} \alpha & k_0-\alpha \\ k_0-\alpha & \alpha \end{pmatrix} \quad (18)$$

We can calculate $\operatorname{cov}\left[Q_1^i, Q_1^{i+l}\right]$ terms in eq.(14) ~ eq.(17) directly from tallies. However, This approach could cause a problem as shown in Fig. 1. We can expect that the covariance of tallies decreases in proportion to the dominance ratio of the fission matrix as the cycle length increases. It can be shown analytically. However, its behavior gets out from this tendency. For this reason, the error propagation model[2] was adopted to calculate $\operatorname{cov}\left[Q_1^i, Q_1^{i+l}\right]$ terms.

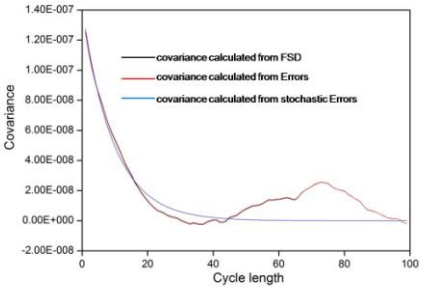

Fig. 1. Covariance behavior vs. Cycle length

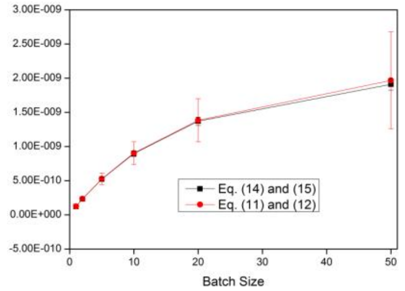

Fig. 2. Apparent and sample variance comparison

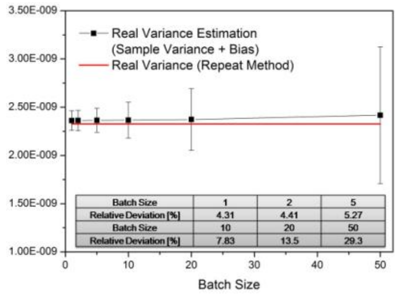

Fig. 3. Real variance estimation

4. Conclusions

Variance and the bias were derived analytically when the batch method was applied. If the batch method was applied to calculate the sample variance, covariance terms between tallies which exist in the batch were eliminated from the bias.

With the 2 by 2 fission matrix problem, we could calculate real variance regardless of whether or not the batch method was applied. However as batch size got larger, standard deviation of real variance was increased.

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