Variance Bias
in Monte Carlo Eigenvalue Calculations

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Sample Variance

- In the Monte Carlo eigenvalue calculations, the sample variance of the mean value of a tally denoted by Q can be calculated by

$$\sigma_S^2\left[\overline{Q}\right] = \frac{1}{N(N-1)}\sum_{i=1}^{N}\left(Q^i - \overline{Q}\right)^2, \quad \overline{Q} = \frac{1}{N}\sum_{i=1}^{N} Q^i, \qquad \text{(1)}$$

where

Q = tally variable

Q^i = value estimated by the MC calculations at i-th cycle

= mean value of Q

N = total number of stationary cycles

Central Limit Theorem

- Let X_1, X_2, X_3, ... X_n be a sequence of ***n* independent and identically distributed (i.i.d)** random variables each having finite values of expectation μ and variance $\sigma^2 > 0$.
- The central limit theorem states that as the sample size n increases, the distribution of the sample average of these random variables approaches the normal distribution with a mean μ and variance σ^2 / n irrespective of the shape of the original distribution.

Central Limit Theorem (Contd.)

- Telescopes and sampling errors
  - The mathematician Gauss (1777-1855) was also a keen astronomer. He acquired a new telescope, and decided to use it to produce a more accurate calculation of the diameter of the moon.
  - To his surprise, he discovered that every time he took a measurement, his answer was slightly different.
  - He plotted the results and found that they formed a bell shaped curve, with most results close to the central average but the occasional one quite inaccurate.

- Gauss quickly realized that any measurement he took was a 'sample' prone to error but which could be used as an estimate of the correct answer. The more readings he took, the closer the average would be to the correct reading.
- He established that errors in readings belonged to a famous **bell curve** (or **normal distribution** or **Gaussian distribution**).

Bias of Sample Variance (1/2)

- The sample variance of Q can be calculated by

$$\sigma_S^2[Q] = \frac{1}{N-1}\sum_{i=1}^{N}\left(Q_i - \bar{Q}\right)^2, \quad \bar{Q} = \frac{1}{N}\sum_{i=1}^{N} Q_i \qquad \text{(A.1)}$$

- The expected value of $\sum_{i=1}^{N}\left(Q_i - \bar{Q}\right)^2$ can be written as

$$\begin{aligned}
E\left[\sum_{i=1}^{n}\left(Q_i - \bar{Q}\right)^2\right] &= E\left[\sum_{i=1}^{n} Q_i^2 - n\bar{Q}^2\right] \\
&= \sum_{i=1}^{n} E\left[Q_i^2\right] - nE\left[\bar{Q}^2\right] \\
&= nE\left[Q_i^2\right] - nE\left[\bar{Q}^2\right] \\
&= n\left\{\sigma^2[Q] + \cancel{\left(E[Q]\right)^2}\right\} - n\left\{\sigma^2\left[\bar{Q}\right] + \cancel{\left(E\left[\bar{Q}\right]\right)^2}\right\} \\
&= n\sigma^2[Q] - n\left(\frac{\sigma^2[Q]}{n}\right) \\
&= (n-1)\sigma^2[Q]
\end{aligned} \qquad \text{(A.2)}$$

Bias of Sample Variance (2/2)

- The variance of $\bar{Q}$, $\sigma^2\left[\bar{Q}\right]$ can be written as

$$\sigma^2\left[\bar{Q}\right]=\frac{1}{n^2}\sigma^2\left[Q_1+Q_2+\cdots+Q_n\right]$$
$$=\frac{1}{n^2}\left\{E\left[\left(Q_1+Q_2+\cdots+Q_n\right)^2\right]-n^2\left(E[Q]\right)^2\right\}$$
$$=\frac{1}{n^2}\left\{nE\left[Q_i^2\right]-n\left(E[Q]\right)^2\right\}+\frac{1}{n^2}\sum_i\sum_{i\neq j}\left\{E\left[Q_iQ_j\right]-\left(E[Q]\right)^2\right\}$$
$$=\frac{1}{n}\sigma^2[Q]+\frac{1}{n^2}\sum_i\sum_{i\neq j}\left\{\mathrm{cov}\left[Q_i,Q_j\right]\right\} \qquad \text{(A.3)}$$

- Then the sample are independent each other $(\mathrm{cov}\left[Q_i,Q_j\right]=0)$, $\sigma^2\left[\bar{Q}\right]$ becomes

$$\sigma^2\left[\bar{Q}\right]=\frac{1}{n}\sigma^2[Q] \quad (\text{if } \mathrm{cov}\left[Q_i,Q_j\right]=0) \qquad \text{(A.4)}$$

Derivation of Variance Bias (1/4)

- The real or true variance of $\overline{Q}$ can be written as

$$\begin{aligned}
\sigma_R^2\left[\overline{Q}\right] &= E\left[\overline{Q}^2\right] - E\left[\overline{Q}\right]^2 \\
&= E\left[\left(\frac{1}{NM}\sum_{i=1}^{N}\sum_{j=1}^{M} Q_j^i\right)^2\right] - E\left[\frac{1}{NM}\sum_{i=1}^{N}\sum_{j=1}^{M} Q_j^i\right]^2 \\
&= \frac{NM}{(NM)^2} E\left[\left(Q_j^i\right)^2\right] + \frac{1}{(NM)^2}\sum_{i,j}\sum_{i',j'\neq i,j} E\left[Q_j^i Q_{j'}^{i'}\right] \\
&\quad - \frac{NM}{(NM)^2} E\left[Q_j^i\right]^2 - \frac{1}{(NM)^2}\sum_{i,j}\sum_{i',j'\neq i,j} E\left[Q_j^i\right] E\left[Q_{j'}^{i'}\right] \\
&= \frac{1}{NM}\sigma^2\left[Q_j^i\right] + \frac{1}{(NM)^2}\sum_{i,j}\sum_{i',j'\neq i,j} \operatorname{cov}\left[Q_j^i, Q_{j'}^{i'}\right] \qquad \text{(B.1)}
\end{aligned}$$

- On the other hand, the apparent variance of Q is defined as the expected value of the sample variance

$$\sigma_A^2\left[\overline{Q}\right] = E\left[\sigma_S^2\left[\overline{Q}\right]\right] \qquad \text{(B.2)}$$

Derivation of Variance Bias (2/4)

- In the same way that Ueki el al [1] formulated the variance bias for the multiplication factor k_{eff} from its apparent variance, $\sigma_A^2\left[\overline{Q}\right]$ can be expressed as

$$\sigma_A^2\left[\overline{Q}\right]=E\left[\frac{1}{NM(NM-1)}\sum_{i=1}^{N}\sum_{j=1}^{M}\left(Q_j^i-\overline{Q}\right)^2\right]=\frac{1}{NM-1}\left(E\left[\left(Q_j^i\right)^2\right]-E\left[\overline{Q}^2\right]\right)$$

$$=\frac{1}{NM-1}\left(\sigma^2\left[Q_j^i\right]+E\left[Q_j^i\right]^2-E\left[\overline{Q}^2\right]\right) \qquad \text{(B.3)}$$

[1] T. Ueki, T. Mori, and M. Nakagawa, "Error Estimation and their Biases in Monte Carlo Eigenvalue Calculations," *Nucl. Sci. Eng.*, 125, 1-11 (1997).

- And $E\left[\overline{Q}^2\right]$ in Eq. (B.3) can be expressed as

$$E\left[\overline{Q}^2\right]=E\left[\left(\frac{1}{NM}\sum_{i=1}^{N}\sum_{j=1}^{M}Q_j^i\right)^2\right]=\frac{NM}{(NM)^2}E\left[\left(Q_j^i\right)^2\right]+\frac{1}{(NM)^2}\sum_{i,j}\sum_{i',j'\neq i,j}E\left[Q_j^iQ_{j'}^{i'}\right]$$

$$=\frac{1}{NM}E\left[\left(Q_j^i\right)^2\right]+\frac{NM-1}{NM}E\left[Q_j^i\right]^2+\frac{1}{(NM)^2}\sum_{i,j}\sum_{i',j'\neq i,j}\left(E\left[Q_j^iQ_{j'}^{i'}\right]-E\left[Q_j^i\right]^2\right)$$

$$=\frac{1}{NM}\sigma^2\left[Q_j^i\right]+E\left[Q_j^i\right]^2+\frac{1}{(NM)^2}\sum_{i,j}\sum_{i',j'\neq i,j}\operatorname{cov}\left[Q_j^i,Q_{j'}^{i'}\right]. \qquad \text{(B.4)}$$

Derivation of Variance Bias (3/4)

- Insertion of Eq. (B.4) into Eq. (B.3) leads to

$$\sigma_A^2\left[\overline{Q}\right]=\frac{1}{NM-1}\left\{\sigma^2\left[Q_j^i\right]+\cancel{E\left[Q_j^i\right]^2}-\frac{1}{NM}\sigma^2\left[Q_j^i\right]-\cancel{E\left[Q_j^i\right]^2}-\frac{1}{(NM)^2}\sum_{i,j}\sum_{i',j'\neq i,j}\operatorname{cov}\left[Q_j^i,Q_{j'}^{i'}\right]\right\}$$

$$=\frac{1}{NM-1}\cdot\frac{NM-1}{NM}\sigma^2\left[Q_j^i\right]-\frac{1}{NM-1}\cdot\frac{1}{(NM)^2}\sum_{i,j}\sum_{i',j'\neq i,j}\operatorname{cov}\left[Q_j^i,Q_{j'}^{i'}\right]$$

$$=\frac{1}{NM}\sigma^2\left[Q_j^i\right]-\frac{1}{NM-1}\cdot\frac{1}{(NM)^2}\sum_{i,j}\sum_{i',j'\neq i,j}\operatorname{cov}\left[Q_j^i,Q_{j'}^{i'}\right]. \qquad \text{(B.5)}$$

- From Eqs. (B.1) and (B.5), the variance bias defined by the difference between the real and apparent variance can be written as

$$\sigma_R^2\left[\overline{Q}\right]-\sigma_A^2\left[\overline{Q}\right]=\cancel{\frac{1}{NM}\sigma^2\left[Q_j^i\right]}+\frac{1}{(NM)^2}\sum_{i,j}\sum_{i',j'\neq i,j}\operatorname{cov}\left[Q_j^i,Q_{j'}^{i'}\right]$$

$$-\cancel{\frac{1}{NM}\sigma^2\left[Q_j^i\right]}+\frac{1}{NM-1}\cdot\frac{1}{(NM)^2}\sum_{i,j}\sum_{i',j'\neq i,j}\operatorname{cov}\left[Q_j^i,Q_{j'}^{i'}\right]$$

$$=\frac{1}{NM(NM-1)}\sum_{i,j}\sum_{i',j'\neq i,j}\operatorname{cov}\left[Q_j^i,Q_{j'}^{i'}\right]. \qquad \text{(B.6)}$$

Derivation of Variance Bias (4/4)

- Because there is no inter-cycle correlation between the histories except when $j' \neq j$, the following condition is satisfied

$$\mathrm{cov}\left[Q_j^i, Q_{j'}^{i'}\right] = 0 \;\; (j \neq j') \qquad \text{(B.7)}$$

- Using Eq. (B.7), the variance bias of Eq. (B.6) can be expressed as

$$\sigma_R^2\left[\overline{Q}\right] - \sigma_A^2\left[\overline{Q}\right] = \frac{1}{N\left(NM-1\right)} \sum_i \sum_{i' \neq i} \mathrm{cov}\left[Q_j^i, Q_j^{i'}\right] \qquad \text{(B.8)}$$

- Because $\mathrm{cov}\left[Q_j^i, Q_j^{i'}\right] = \frac{1}{M}\mathrm{cov}\left[Q^i, Q^{i'}\right]$, Eq. (B.8) can be written as

$$\sigma_R^2\left[\overline{Q}\right] - \sigma_A^2\left[\overline{Q}\right] = \frac{1}{N\left(N-1/M\right)} \sum_i \sum_{i' \neq i} \mathrm{cov}\left[Q^i, Q^{i'}\right] \qquad \text{(B.9)}$$

- Assuming that $\mathrm{cov}\left[Q^i, Q^{i'}\right]$ depends only on the cycle difference from the equilibrium property, the variance bias of Eq. (B.9) can be expressed as

$$\sigma_R^2\left[\overline{Q}\right] - \sigma_A^2\left[\overline{Q}\right] = \frac{2}{N\left(N-1/M\right)} \sum_{l=1}^{N-1} (N-l) \cdot \mathrm{cov}\left[Q^i, Q^{i+l}\right] \qquad \text{(B.10)}$$

$$\sigma_R^2\left[\overline{k}\right] - \sigma_A^2\left[\overline{k}\right] = \frac{2}{N\left(N-1\right)} \sum_{l=1}^{N-1} (N-l) \cdot \mathrm{cov}\left[k^i, k^{i+l}\right]$$

Bias of the Sample Variance in MC Eigenvalue Calculations

- As Ueki et al derived[1] the relation between the real variance, σ_R^2 and the expected value of the sample variance, $E\left[\sigma_S^2\right]$ of the eigenvalue k, the bias of the sample variance of $\overline{Q}$ can be expressed by

$$\sigma_R^2\left[\overline{Q}\right]-E\left[\sigma_S^2\left[\overline{Q}\right]\right]=\frac{1}{N(N-1)}\sum_{i=1}^{N}\sum_{\substack{j=1\\ j\neq i}}^{N}\mathrm{cov}\left[Q^i,Q^j\right]. \qquad \text{(2)}$$

Correlation betw. Samples

- If Q^i and Q^j ($i \neq j$) are uncorrelated ($\mathrm{cov}\left[Q^i, Q^j\right] = 0$), the sample variance becomes unbiased.

$$E\left[\sigma_S^2\left[\overline{Q}\right]\right] = \sigma_R^2\left[\overline{Q}\right]$$

- If Q^i and Q^j ($i \neq j$) are correlated ($\mathrm{cov}\left[Q^i, Q^j\right] \neq 0$), the sample variance is biased as much as $\dfrac{1}{N(N-1)} \sum_{i=1}^{N} \sum_{\substack{j=1 \\ j \neq i}}^{N} \mathrm{cov}\left[Q^i, Q^j\right]$.

- **Why are Q^i and Q^j ($i \neq j$) correlated in the MC eigenvalue calculations?**

Correlation betw. Fission Source Distributions

- In the Monte Carlo power method, the fission source distribution (FSD) at cycle t is calculated from the FSD of the previous cycle by

$$S^t(\mathbf{r}) = \frac{1}{k^{t-1}} \int H(\mathbf{r}' \to \mathbf{r}) S^{t-1}(\mathbf{r}) d\mathbf{r} + \varepsilon^t(\mathbf{r}), \qquad (3)$$

where

$S^t(\mathbf{r})$ = fission source distribution at cycle t,

k^t = eigenvalue estimated at cycle t ,

$H(\mathbf{r}' \to \mathbf{r})$ = expected number of first-generation fission neutrons born per unit volume about $\mathbf{r}$, due to a parent neutron born at $\mathbf{r}'$,

ε^t = stochastic error generated at cycle t.

- **The FSD at *t*-th cycle gets correlated with the FSDs of the previous cycles by Eq. (3).**

Relation betw. FSD and Tally

- The tally Q is defined by a detector response in the MC simulation as follows:

$$Q=\int_{\chi} dPg(P)\Psi(P)$$

$$=\sum_{j=0}^{\infty}\int_{\chi} dPg(P)\int dP'K_j(P'\to P)\int dP''T\left(P''\to P'\right)S(P''), \qquad (4)$$

where

$$P\equiv(\mathbf{r},E,\mathbf{\Omega}),$$

$$\Psi(P)=\text{collision density},$$

$$g(P)=\text{response function for the tally } Q \text{ at } P,$$

$$K_0(P'\to P)=\delta(P'-P),$$

$$K_j(P'\to P)=\int dP_1\cdots\int dP_{j-1}K(P_{j-1}\to P)\cdots K(P'\to P_1),$$

$$K(P'\to P)\equiv C(\mathbf{r}';E',\mathbf{\Omega}'\to E,\mathbf{\Omega})T(E,\mathbf{\Omega};\mathbf{r}'\to\mathbf{r})=\text{transport kernel}$$

$$S(P)=\text{fission source distribution.}$$

- **The tally Q is related to the FSD by Eq. (4).**

Mechanism of Variance Bias in MC Eigenvalue Cal.

Correlation betw. FSDs by the MC power method:

$$S^t(\mathbf{r}) = \frac{1}{k^{t-1}} \int H(\mathbf{r}' \to \mathbf{r}) S^{t-1}(\mathbf{r}) d\mathbf{r} + \varepsilon^t(\mathbf{r}) \quad \text{(3)}$$

$$\Downarrow \quad \mathrm{cov}\left[S^t, S^{t'}\right] \neq 0, \ (t \neq t')$$

Relation betw. tally and FSD:

$$Q = \sum_{j=0}^{\infty} \int_{\chi} dP g(P) \int dP' K_j(P' \to P) \int dP'' T\left(P'' \to P'\right) S(P'') \quad \text{(4)}$$

$$\Downarrow \quad \mathrm{cov}\left[Q^i, Q^j\right] \neq 0, \ (i \neq j)$$

Bias of the sample variance:

$$\sigma_R^2\left[\overline{Q}\right] - E\left[\sigma_S^2\left[\overline{Q}\right]\right] = \frac{1}{N(N-1)} \sum_{i=1}^{N} \sum_{\substack{j=1 \\ j \neq i}}^{N} \mathrm{cov}\left[Q^i, Q^j\right]$$