Information Based Analysis of Fission Source Correlation

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Abstract

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The variances estimated by Monte Carlo codes in k-eigenvalue calculations are underpredicted due to inter-cycle correlation between fission sources. The mutual information serves as a diagnostic to measure the correlation between fission source distributions in different cycles. There is a definite observed relationship between the variance bias and the mutual information of the source distributions. Furthermore, using the mutual information in conjunction with the Wielandt method shows how effective a particular Wielandt shift is at removing variance bias. Finally, the dominance ratio and the mutual information are related to MacMillan’s correction.
Overview

- Fission source correlation
- Mutual Information
- Application to Wielandt Method
- Relationship to Dominance Ratio

MCNP Criticality Calculations

- Power iteration method:

  Initial Guess  | Batch 1 $K_{\text{eff}}^{(1)}$ | Batch 2 $K_{\text{eff}}^{(2)}$ | Batch 3 $K_{\text{eff}}^{(3)}$ | Batch 4 $K_{\text{eff}}^{(4)}$

  - Source particle generation
  - Monte Carlo random walk
  - Neutron
Fission neutrons in following generations tend to be near the source neutron in the previous generations.

- Correlation always positive

- Causes underprediction of variance:

Apparent Variance: \[ \tilde{\sigma}_x^2 = \frac{1}{N} \left[ \frac{1}{N-1} \sum_{i=1}^{N} x_i^2 - \bar{x}^2 \right] \]

Empirical Variance: \[ \sigma_x^2 = \tilde{\sigma}_x^2 + \sum_{i,j} r_{ij} \]
Most Monte Carlo codes give apparent error

Should give empirical error
- MacMillan’s factor (highly conservative)
- Lag coefficients (subject to stochastic noise)
- Brute force method (very time consuming)
  - Average numerous (25-100+) results from calculations with different random number seeds.
Variance Bias

- Small impact on k-effective (5-20%).
- Significant impact on local tallies:

<table>
<thead>
<tr>
<th>Benchmark</th>
<th>Tally $\frac{\sigma}{\bar{\sigma}}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Godiva</td>
<td>1.43</td>
</tr>
<tr>
<td>Two Cylinder</td>
<td>4.56</td>
</tr>
<tr>
<td>B&amp;W Core</td>
<td>3.34</td>
</tr>
<tr>
<td>Checkerboard</td>
<td>3.97</td>
</tr>
</tbody>
</table>

Ergodicity of Fission Source

- Intercycle correlation should decrease with separation distance.
- True if fission source transition is an ergodic Markov chain.
- Ergodic: Loss of memory of initial state after many transitions.
  - Fission matrix for $j$ transitions step measures.
  - Final state independent of initial state.
Ergodicity of Fission Source

Evolution of the Markov Transition Matrix for the Godiva Benchmark

- Information about initial state lost each transition.
- Loss of information implies loss of correlation
  - Final state independent of initial state
- Since correlation leads to variance bias, can some simple measure help estimate this?
Mutual Information

- Measures information gained about an unmeasured result from the measurement of another.

\[ I(X, Y) = H(Y) - H(Y | X) \]

- Measured from fission matrix elements:

\[ I = \sum_i \sum_j F_{ij} \log \left( \frac{F_{ij}}{f_i f_j} \right) \]

Mutual Information

- Measures correlation between fission populations in one generation to the next.

- As separation distance increases to infinity, mutual information goes to zero.

\[ F_{ij} = f_i f_j \]

\[ I = \sum_i \sum_j f_i f_j \log \left( \frac{f_i f_j}{f_i f_j} \right) = 0 \]
Mutual Information Decay

Mutual Information of the Two Cylinder Benchmark w/ Power Iteration Method

Mutual Information Convergence

- Mutual information sensitivity to mesh size for Godiva problem.

<table>
<thead>
<tr>
<th>Mesh Spacing</th>
<th>Mutual Information</th>
</tr>
</thead>
<tbody>
<tr>
<td>3x3x3</td>
<td>0.233</td>
</tr>
<tr>
<td>4x4x4</td>
<td>0.225</td>
</tr>
<tr>
<td>5x5x5</td>
<td>0.217</td>
</tr>
<tr>
<td>6x6x6</td>
<td>0.211</td>
</tr>
</tbody>
</table>
Mutual Information Convergence

- Mutual information sensitivity to batch size for Godiva problem (3x3x3 mesh).

<table>
<thead>
<tr>
<th>Batch Size (histories)</th>
<th>Mutual Information</th>
</tr>
</thead>
<tbody>
<tr>
<td>$10^2$</td>
<td>0.558</td>
</tr>
<tr>
<td>$10^3$</td>
<td>0.327</td>
</tr>
<tr>
<td>$10^4$</td>
<td>0.241</td>
</tr>
<tr>
<td>$10^5$</td>
<td>0.230</td>
</tr>
<tr>
<td>$10^6$</td>
<td>0.229</td>
</tr>
</tbody>
</table>

Wielandt Method

- Stochastically extends the number of generations within a cycle.
Wielandt Method

• **Longer fission chains**
  – Decrease the number of cycles required for convergence (same CPU time).
  – Reduces bias in error estimates.

• **Average chain length:**

\[ L = 1 + \frac{k_0}{\Delta_W} \]

Wielandt Method Results

**Apparent vs. Empirical Error of the Two Cylinder Benchmark**
Wielandt Method Results

Mutual Information of the Two Cylinder Benchmark for Varied Chain Lengths

Mutual Information vs. Average Fission Chain Length

Wielandt Method Results

Apparent vs. Empirical Error of the B&W Core Benchmark

Relative Error vs. Average Fission Chain Length
Wielandt Method Results

Mutual Information of the B&W Core Benchmark for Varied Chain Lengths

Average Fission Chain Length

Mutual Information

2D quarter-core PWR (Nakagawa & Mori model)
+ Explicit fuel pins & rod channels, 17x17
+ 120 M active neutrons for each calculation
+ Tally fission rates in each quarter-assembly

Plot relative error in quarter-assemblies along diagonal
Observations

- Mutual information seems to provide a good measure of variance bias in MOST problems.

- B&W Core benchmark shows disagreement.
  - More investigation needed.

- Variance bias is local in nature.
  - Mutual information is global.
  - No clear relationship to $k$-effective.

Dominance Ratio

- Measures effect of higher order modes.

- Stochastic fluctuations excite higher modes.

- Higher dominance ratio means slower decay, and more correlation.

\[ \rho = \frac{k_1}{k_0} \]
Dominance Ratio vs. Mutual Information

Relation to MacMillan Factor

- MacMillan’s factor:

\[
M = 1 + \frac{2r}{1 - \rho}
\]

- Mutual information curve appears to follow similar asymptotic trend.
  - Suggestive, but more analysis needed.
Conclusions & Future Work

• Mutual information is a useful diagnostic to get general feel of correlation effects.
  – No definitive connection to variance bias.

• Very suggestive for many problems.

• Still issues:
  – Connection to global k-effective estimates
  – B&W core convergence issues
  – Local variations

Questions?