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Bias in Monte Carlo Alpha-Eigenvalue Calculations



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The α -Eigenvalue Problem

The α -eigenvalue allows basic analysis of time behavior of a geometry.

First, a separation of variables is performed:

$$\begin{array}{ll} \text{Flux:} & \psi(\mathbf{r}, E, \hat{\Omega}, t) = \psi(\mathbf{r}, E, \hat{\Omega})e^{\alpha t} \\ \text{Precursors:} & C(\mathbf{r}, t) = C(\mathbf{r})e^{\alpha t} \end{array}$$

α then corresponds to the logarithmic time derivative:

$$\frac{1}{\psi} \frac{\partial \psi}{\partial t} = \alpha$$

The α -Eigenvalue Problem

ψ and C are then substituted into the transport equation:

$$\begin{aligned} & \left(\frac{\alpha}{v(E)} + \hat{\Omega} \cdot \nabla + \Sigma_t(\mathbf{r}, E) \right) \psi(\mathbf{r}, E, \hat{\Omega}) \\ &= \frac{\chi_p(E)}{4\pi} \int_0^\infty dE' \nu_p(E') \Sigma_f(\mathbf{r}, E') \phi(\mathbf{r}, E') + \sum_{i=1}^N \frac{\chi_{di}(E)}{4\pi} \lambda_i C_i(\mathbf{r}) \\ &+ \int_{4\pi} d\Omega' \int_0^\infty dE' \nu_s(E') \Sigma_s(\mathbf{r}, E' \rightarrow E, \hat{\Omega}' \rightarrow \hat{\Omega}) \psi(\mathbf{r}, E', \hat{\Omega}') \\ \\ & \alpha C_i(\mathbf{r}) = \int_0^\infty dE' \nu_{di}(E') \Sigma_f(\mathbf{r}, E') \phi(\mathbf{r}, E') - \lambda_i C_i(\mathbf{r}) \end{aligned}$$

$\lambda_i C_i(\mathbf{r})$ can be solved for and substituted into the first eq.

k - α Iteration

Most common Monte Carlo approach to computing α :

- Run normal k -eigenvalue, with a few changes
 - For the $\frac{\alpha}{\nu(E)}$ term:
 - If $\alpha > 0$, add absorption reaction, $\Sigma_\alpha = \frac{\alpha}{\nu(E)}$ (on left hand side)
 - If $\alpha < 0$, add $\left(n, \frac{1+\eta}{\eta}n\right)$ reaction, $\Sigma_\alpha = \frac{\eta|\alpha|}{\nu(E)}$ (we use $\eta = 1$) (on right hand side)
 - Delay precursors: $\nu_{di}(E', \alpha) = \frac{\lambda_j}{\alpha + \lambda_j} \nu_{di}(E')$
- Update α such that $k \rightarrow 1$

Approaches to Updating α

Function of k :

Alpha is given by:

$$\alpha_{n+1} - \alpha_n \propto (k - 1)$$

Function of Tallies:

Solve for the roots of:

$$\alpha \left\langle \frac{1}{v} \right\rangle + \langle \Sigma_t \rangle + [\text{escape}] = \langle \nu_p \Sigma_f \rangle + \sum_{i=1}^N \frac{\lambda_i}{\alpha + \lambda_i} \langle \nu_{di} \Sigma_f \rangle + \langle \nu_s \Sigma_s \rangle$$

Bias

What is bias?

Bias occurs whenever the expected value of the sampled variable $\hat{\theta}$ does not equal the true value θ :

$$E[\hat{\theta}] - \theta \neq 0$$

This is easily induced by taking nonlinear transformations of distributions:

$$E[X \sim \mathcal{N}(\mu, \sigma)^2] \stackrel{?}{=} \mu^2$$

In this example, equality only holds for $\sigma = 0$.

The bias decreases as $\sigma \rightarrow 0$.

Bias in k

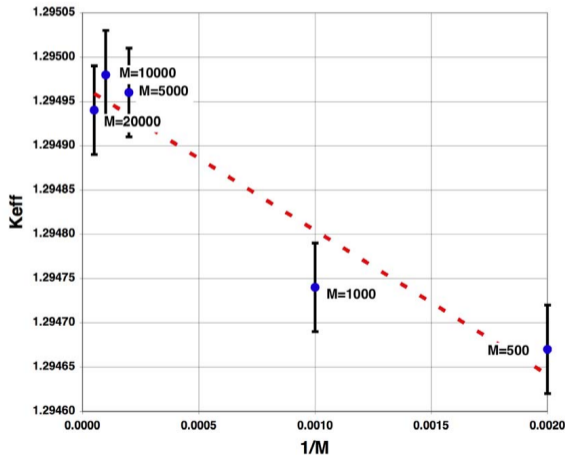
It is well-known from the works of (Brissenden and Garlick, 1986) and (Gelbard and Prael, 1974), that a stochastic k -eigenvalue calculation will be biased:

$$E[\hat{k}] - k \propto \frac{1}{N}$$

where N is the particles per batch.

The source itself is also biased $\propto \frac{1}{N}$, as are the tallies.

Bias in k



As N increases, bias decreases.
10k particles/batch is commonly recommended.

Bias in Prompt α

Propagating only the effect of k :

$$\alpha = f(k - 1)$$

f is some update function

$$\alpha = c(k - 1) + \mathcal{O}((k - 1)^2)$$

c is a constant

$$\begin{aligned} \frac{\alpha_{\text{bias}} - \alpha_{\text{true}}}{\alpha_{\text{true}}} &\approx \frac{c \left(k_{\text{true}} + \frac{k_b}{N} - 1 \right) - c (k_{\text{true}} - 1)}{c (k_{\text{true}} - 1)} \\ &\approx \frac{\frac{k_b}{N}}{(k_{\text{true}} - 1)} \end{aligned}$$

Relative bias increases when $k \approx 1$ (as expected). Absolute bias is roughly constant.

Bias in Prompt α

Considering prompt tally α :

$$\alpha = \frac{\langle \nu_p \Sigma_f \rangle + \langle \nu_s \Sigma_s \rangle - \langle \Sigma_t \rangle - [\text{escape}]}{\langle \frac{1}{v} \rangle}$$

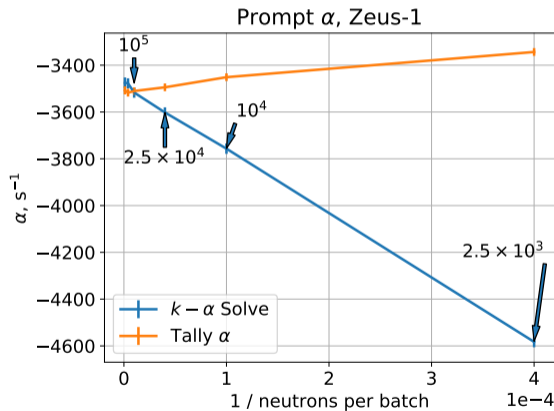
Biases in each individual tally can either cancel out or amplify, complicating analysis.

During testing, biases often canceled out.

Testing Prompt α - Zeus

- Used HEU-MET-INTER-006 Case 1 from ICSBEP
- ENDF/B-VII.1, 293.6K
- 5×10^8 active neutrons in each simulation
- Geometry ν scaled to precisely delay critical
- Simulation run without delay neutrons

Testing Prompt α - Zeus



Convergence of bias is $1/N$ as expected.

The tally α has a much lower bias than the k -eigenvalue estimator.

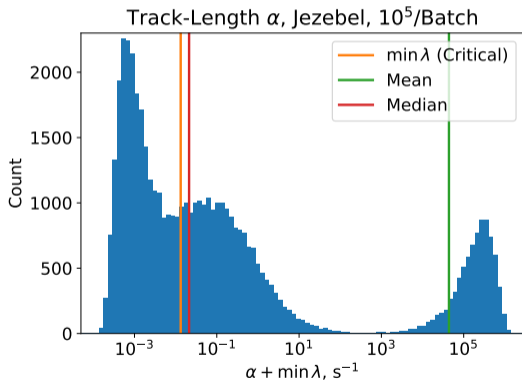
For this near-critical geometry, relative bias is large until 10^5 neutrons.

Testing Delay α - Jezebel

- Used PU-MET-FAST-001 from ICSBEP
- ENDF/B-VII.1, 293.6K
- 5×10^9 active neutrons in each simulation
- Density scaled from subcritical to prompt supercritical
- Only tally α considered

Testing Delay α - Jezebel

α with delayed neutron precursors has a particular bias problem:

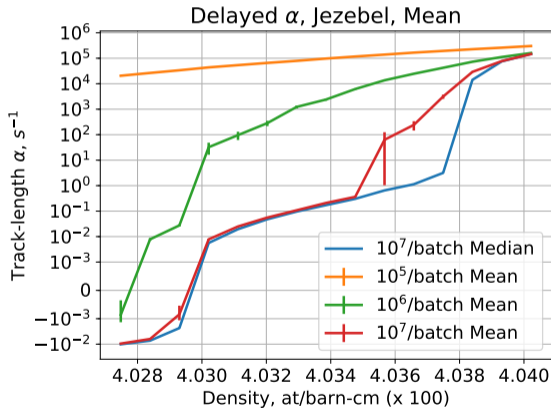


(Batch α , after convergence, one run)

α s above prompt supercritical bias the mean positive.

The median is far less sensitive to outliers.

Testing Delay α - Jezebel

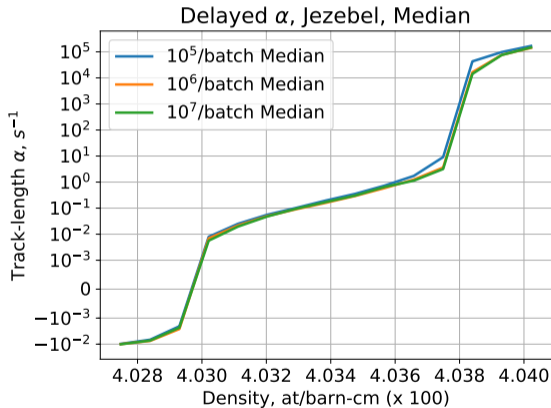


10^5 particles never yields a subcritical result.

10^6 particles does go subcritical, but is often > 4 orders of magnitude off.

10^7 is closer, but it still falls apart near the transition.

Testing Delay α - Jezebel



Median results are much closer.

Maximum bias of a factor of 3
seen for 10⁵ particles/batch.

Summary

Care must be taken in α -eigenvalue calculations.

As $\alpha \rightarrow 0$, small biases can dominate the solution.

With delayed neutrons, nonlinearities can lead to significant positive bias.

Care should be taken to detect the effects of bias:

- Compare the mean α to the median
- Examine the distribution of α
- Run convergence studies if at all possible