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Title: Bias in Monte Carlo Alpha-Eigenvalue Calculations

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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:

$$\text{Flux:} \quad \psi(\boldsymbol{r}, E, \hat{\boldsymbol{\Omega}}, t) = \psi(\boldsymbol{r}, E, \hat{\boldsymbol{\Omega}}) e^{\alpha t}$$

$$\text{Precursors:} \quad C(\boldsymbol{r}, t) = C(\boldsymbol{r}) e^{\alpha t}$$

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:

$$\left(\frac{\alpha}{v(E)} + \hat{\mathbf{\Omega}} \cdot \nabla + \Sigma_t(\boldsymbol{r}, E)\right) \psi(\boldsymbol{r}, E, \hat{\mathbf{\Omega}})$$

$$= \frac{\chi_p(E)}{4\pi} \int_0^\infty dE' \nu_p(E') \Sigma_f(\boldsymbol{r}, E') \phi(\boldsymbol{r}, E') + \sum_{i=1}^{N} \frac{\chi_{di}(E)}{4\pi} \lambda_i C_i(\mathbf{r})$$

$$+ \int_{4\pi} d\Omega' \int_0^\infty dE' \nu_s(E') \Sigma_s(\boldsymbol{r}, E' \rightarrow E, \hat{\mathbf{\Omega}}' \rightarrow \hat{\mathbf{\Omega}}) \psi(\boldsymbol{r}, E', \hat{\mathbf{\Omega}}')$$

$$\alpha C_i(\boldsymbol{r}) = \int_0^\infty dE' \nu_{di}(E') \Sigma_f(\boldsymbol{r}, E') \phi(\boldsymbol{r}, E') - \lambda_i C_i(\boldsymbol{r})$$

$\lambda_i C_i(\boldsymbol{r})$ 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 $\frac{\alpha}{v(E)}$ term:
    - If $\alpha > 0$, add absorption reaction, $\Sigma_\alpha = \frac{\alpha}{v(E)}$ (on left hand side)
    - If $\alpha < 0$, add $\left(n, \frac{1+\eta}{\eta} n\right)$ reaction, $\Sigma_\alpha = \frac{\eta|\alpha|}{v(E)}$ (we use $\eta = 1$) (on right hand side)
  - Delay precursors: $\nu_{di}(E', \alpha) = \frac{\lambda_i}{\alpha + \lambda_i} \nu_{di}(E')$
- 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:

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

This is easily induced by taking nonlinear transformations of distributions:

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

In this example, equality only holds for $\sigma = 0$.
The bias decreases as $\sigma \to 0$.

Bias in k

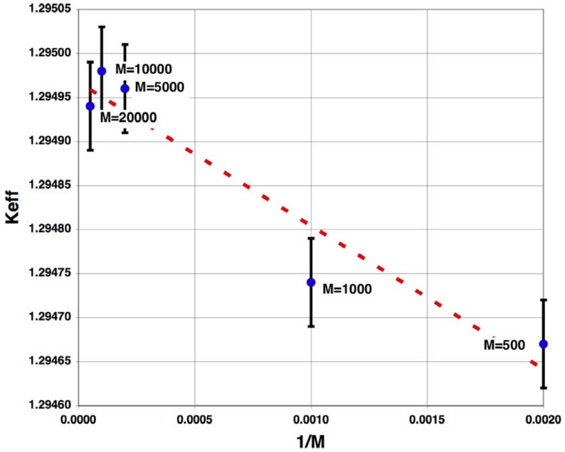
It is well-known from the works of (Brissenden and Garlick, 1986) and (Gelbard and Prael, 1974), that a stochastic k-eigenvalue calculation will be biased:

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

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:

$$\alpha = f(k-1) \qquad f \text{ is some update function}$$
$$\alpha = c(k-1) + \mathcal{O}((k-1)^2) \qquad c \text{ is a constant}$$

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

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

Bias in Prompt α

Considering prompt tally α:

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

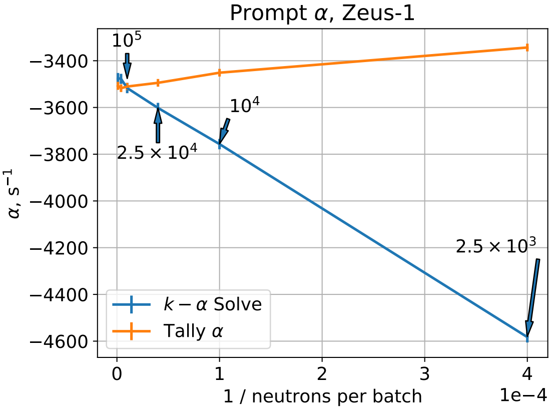
Biases in each individual tally can either cancel out or amplify, complicating analysis.

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.

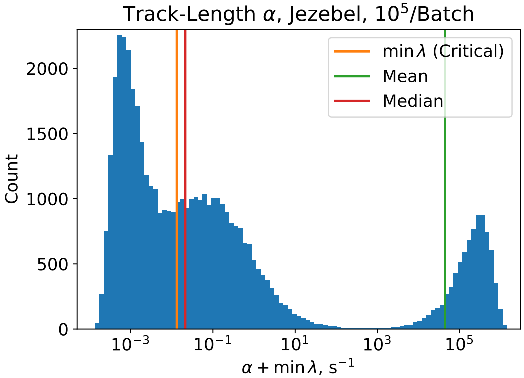
For this near-critical geometry, relative bias is large until 10^5 neutrons.

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:

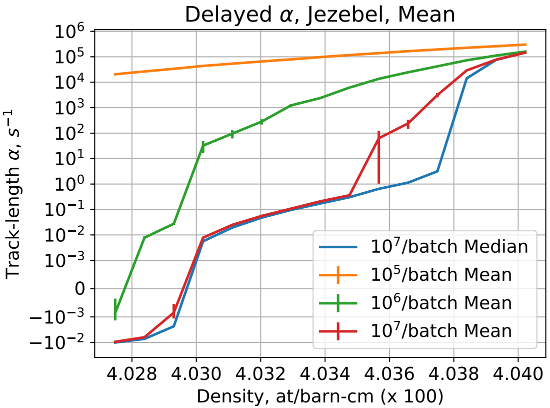


(Batch α, after convergence, one run)

αs above prompt supercritical bias the mean positive.

The median is far less sensitive to outliers.

Testing Delay α - Jezebel

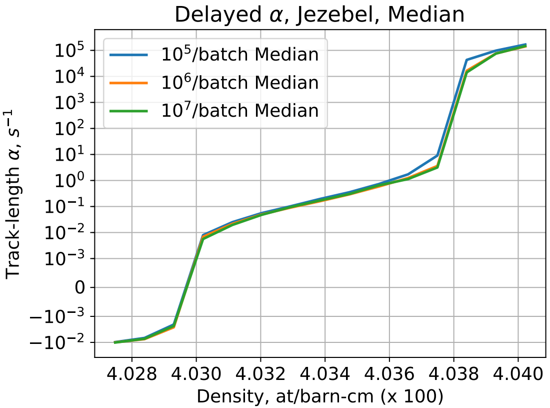


10^5 particles never yields a subcritical result.

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 10^5 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