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UNBIASED MINIMUM VARIANCE ESTIMATOR OF A MATRIX EXPONENTIAL FUNCTION. APPLICATION TO BOLTZMANN/BATEMAN COUPLED EQUATIONS SOLVING.

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ABSTRACT

This paper derives an unbiased minimum variance estimator (UMVE) of a matrix exponential function of a normal mean, following reference [1] and [2]. The result is then used to propose a reference scheme to solve Boltzmann/Bateman coupled equations, thanks to Monte Carlo transport codes. The last section will present numerical resulst on a simple example.

Key Words: Monte Carlo, Depletion, Burn up, Unbiased minimum variance, Tripoli4

1. INTRODUCTION

Various Monte Carlo transport codes own burnup capabilities (e.g. Tripoli-4 [3,4,5], MONTEBURNS [6], or ALEPH [7]), allowing the calculation of material burnup properties during transport. These capabilities rely on a coupling between the Monte Carlo code, which computes the flux (or reaction rates) in a given volume, and a depletion code, which computes concentrations for different isotopes in this volume, for a given burning time and a given flux. The common scheme consists in computing a mean flux, with the Monte Carlo transport code, using this mean flux to compute mean concentrations with the depletion code. This last concentration "vector" is then used to reload the transport simulation, etc. If this calculation scheme seems, at first sight, safe, it presents nevertheless a consequent drawback: it is biased. It is thus impossible neither to parallelize it nor to estimate its error bar.
Indeed, let's consider a sample $\{\varphi_i\}$ of I flux estimation (the same considerations held with reaction rates). These estimations come from the different batches (cycles) of a Monte Carlo simulation (that solves the Boltzmann equation) and are the realizations of independent and identically distributed (iid) random variables φ of a normal law $N(\varphi_R, \sigma_R)$. The estimator of the flux that is usually built from these estimations is the mean estimator:

$$\bar{\varphi} = \frac{\sum \varphi_i}{I}$$

Now the concentration N of a given isotope is calculated from the Bateman equation. This equation is a function g of the flux (for one burning step) and if we consider the real concentration N_R, we have:

$$N_R = g(\varphi_R) = \lim_{I\to+\infty}(g(\overline{\varphi}))$$

(because $\lim_{I\to+\infty}\left(\overline{\varphi} = \frac{\sum\varphi_i}{I}\right) = \varphi_R$).

Nevertheless, since this function is non-linear, in the general case the function of the mean flux $g(\overline{\varphi})$ is not an unbiased estimator of the real concentration N_R:

$$N_R = g(\varphi_R) \neq E(g(\overline{\varphi}))$$

since the expected value of $g(\overline{\varphi})$, called $E(g(\overline{\varphi}))$, is the mean of g over all possible realizations $\{\overline{\varphi}_j\}$:

$$E(g(\overline{\varphi})) = \lim_{J\to+\infty}\left(\frac{\sum g(\overline{\varphi}_j)}{J}\right)$$

The fact that $g(\overline{\varphi})$ is biased has three important consequences: first, since one given simulation does not have an infinite number of batches, but only I of them, the result is false (the error being a decreasing function of I). Second, it means that if one performs J independent simulations, the resulting distribution of N does not represent the statistical distribution of N (no "error bars"). Finally, this statistical independence of true Monte Carlo processes is used to perform natural parallelization of such calculations: each node of a cluster computes a value of N and the distribution of N over all nodes is the true statistical distribution. This technique is also referred as "independent" replicas (see [12,13]). In our case it can not be performed neither since our estimator of N is biased.

In the following part of this paper, we will recall recent results in the field of non linear function estimation, and show how they can be applied to solve the coupled Boltzmann/Bateman equations.

2. UMVE OF A NON LINEAR FUNCTION OF A NORMAL MEAN

Following a work initiated by Kolmogorov in 1950 (see [8]) concerning the theory of estimation, recent results allow to estimate a non linear function of a normal mean (those functions are defined on iid random variables distributed according to a normal law), with the help of UMVE. The fact that those estimators are minimum variance is important for our problem, as will be seen in section 4.

The first one, denoted $\tilde{g}^1(\varphi_R)$, was proposed by Gray et al. (see [2]):

$$\tilde{g}^1(\varphi_R) = g(\overline{\varphi}) + \sum_{k=1}^{+\infty}\frac{(-1)^k\Gamma\left\{\frac{I-1}{2}\right\}g^{(2k)}(\overline{\varphi})}{k!\Gamma\left\{\frac{I-1}{2}+k\right\}}\left(\frac{\hat{\sigma}^2}{4}\right)^k \qquad (1)$$

with $\hat{\sigma}$ being the estimated square root of the variance of the sample $\{\varphi_i\}$ ($i = 1...I$).

The second one, denoted $\tilde{g}^2(\varphi_R)$ comes from a work of Stefanski et al. (see [1]):

$$\tilde{g}^2(\varphi_R) = \mathrm{Re}\left\{ g\left(\bar{\varphi} + i\sqrt{\frac{I-1}{I}}\hat{\sigma}\frac{Z_1}{\sqrt{Z_1^2 + Z_2^2 + \ldots + Z_N^2}} \right) \right\} \tag{2}$$

with $(Z_1, \ldots, Z_N)$ being a vector made of N independent and identically distributed $N(0,1)$ components, and $i = \sqrt{-1}$.

Those two formulas are UMVE of N since $N = E(\tilde{g}^1(\varphi_R)) = E(\tilde{g}^2(\varphi_R))$. The first one supposes to be able to calculate all the pair derivatives of g, and the second one admits that one can evaluate the real part of a complex value of g and uses a Monte Carlo procedure to build the imaginary part of the random variable. The advantage of the first estimator compared to the second is that there is no need to deal with complex number, while its main drawback is that it is often approximated since its numerical evaluation requires a truncation for the infinite series to become finite. In our case, as we be shown in the next part, it will be possible to handle complex numbers for our need and we will therefore consider only the second estimator.

3. UMVE OF A MATRIX EXPONENTIAL FUNCTION OF A NORMAL MEAN

As indicated by for example [9], the Bateman equation that gives isotopes depletion can be written:

$$\frac{d\vec{N}(t)}{dt} = \overline{\overline{A}}\,\vec{N}(t) \tag{3}$$

with $\vec{N}(t)$ being a vector made of all isotopes concentrations, and $\overline{\overline{A}}$ being a transition matrix with elements $\left\{\overline{\overline{A}}\right\}_{ij}$ given by:

$$\left\{\overline{\overline{A}}\right\}_{ij} = \lambda_{ij} + \Sigma_{ij}\varphi \tag{4}$$

where λ_{ij} are the decay constants from isotope i to j and Σ_{ij} is the alimentation from i to j due to the flux.

Eq.3 can be integrated and one finds:

$$\vec{N}(t) = \vec{N}(0)\, e^{\overline{\overline{A}}\,t} \tag{5}$$

Thus, if g is the function that gives the concentration N of a given isotope i, one can write:

$$g(\varphi) = \left\{\vec{N}(t)\right\}_i = \left\{ \vec{N}(0)\, e^{\overline{\overline{A}}\,t} \right\}_i \tag{6}$$

If we choose Eq.2 to estimate $\tilde{g}(\varphi_R)$, we can then write:

$$\tilde{g}^2(\varphi_R) = \mathrm{Re}\left\{ \left\{ \vec{N}(0)\, e^{\overline{\overline{A^*}}\,t} \right\}_i \right\} \tag{7}$$

$\overline{\overline{\Lambda}}^*$ being defined by $\left\{\overline{\overline{\Lambda^*}}\right\}_{ij} = \lambda_{ij} + \Sigma_{ij}\varphi^*$, and:

$$\varphi^* = \bar{\varphi} + i\sqrt{\frac{I-1}{I}}\hat{\sigma}\frac{Z_1}{\sqrt{{Z_1}^2 + {Z_2}^2 + ... + {Z_N}^2}}$$

that we can rewrite $\varphi^* = \bar{\varphi} + i\xi$ for the sake of simplicity. Thanks to this last notation, Eq.4 becomes $\left\{\overline{\overline{\Lambda^*}}\right\}_{ij} = \lambda_{ij} + \Sigma_{ij}\bar{\varphi} + i\Sigma_{ij}\xi$ and Eq.7 can be rewritten:

$$\begin{aligned}
\tilde{g}^2(\varphi_R) &= \mathrm{Re}\left\{\left\{\vec{N}(0)\, e^{\overline{\overline{\Lambda}}t + i\,\overline{\overline{\Sigma}}\,\xi\, t}\right\}_i\right\} \\
\tilde{g}^2(\varphi_R) &= \left\{\mathrm{Re}\left\{\vec{N}(0)\, e^{\overline{\overline{\Lambda}}t}\; e^{i\,\overline{\overline{\Sigma}}\,\xi\, t}\right\}\right\}_i \\
\tilde{g}^2(\varphi_R) &= \left\{\vec{N}(0)\, e^{\overline{\overline{\Lambda}}t}\cos(\,\overline{\overline{\Sigma}}\,\xi\, t\,)\right\}_i
\end{aligned} \tag{8}$$

If we write $\vec{N}_B(t)$ the usual biased expression of the concentration vector, the non-biased estimate of this vector can be written $\vec{N}_{NB}(t)$ and we finally obtain:

$$\vec{N}_{NB}(t) = \vec{N}_B(t)\cos\left(\overline{\overline{\Sigma}}\xi t\right) \tag{9}$$

with $\left\{\overline{\overline{\Sigma}}\right\}_{ij} = \Sigma_{ij}$ and:

$$\xi = \sqrt{\frac{I-1}{I}}\hat{\sigma}\frac{Z_1}{\sqrt{{Z_1}^2 + {Z_2}^2 + ... + {Z_N}^2}}$$

This last expression, as demonstrated in [1], can even be simplified if each mean flux is estimated with only two estimations of φ_i (i.e. I=2):

$$\xi = \frac{\varphi_1 - \varphi_2}{2} \tag{10}$$

Obviously, in pretty much the same way as the matrix exponential is calculated with its limited development:

$$e^{\overline{\overline{\Lambda}}t} = \sum_{k=0}^{+\infty}\frac{\overline{\overline{\Lambda}}^k t^k}{k!}$$

the matrix cosine is calculated via:

$$\cos\left(\overline{\overline{\Sigma}}\xi t\right) = \sum_{k=0}^{+\infty}(-1)^k\frac{\overline{\overline{\Sigma}}^{2k}(\xi t)^{2k}}{(2k)!} \tag{11}$$

4. SOLVING THE COUPLED BOLTZMANN/BATEMAN EQUATION

Since we have derived an UMVE for the matrix exponential function (the Bateman equation) of a normal mean (from the stochastic solving of the Boltzmann equation) we are able to estimate the concentrations after one time step. Now it is legitimate to wonder if the result still held for an arbitrary number of time steps. If we consider the whole process that consists in doing a Monte Carlo transport, calculating a mean flux, then computing thanks to Eq.9 the unbiased value of the concentration vector and to restart the Monte Carlo transport with this new vector, and repeating this n_T times, the question is "is the final estimation unbiased and is it minimum variance?". The answer is yes, by trivial recurrence, and only because the estimator for one time step is minimum variance.
Concerning the implementation of such an unbiased estimator of concentration, two solutions are possible. Either the deterministic depletion solver uses Runge Kutta type methods to solve Eq.3, and then it is possible to linearize the isotope decay chain (this is called the linear decay chain method, see [10]) and then to use Eq.1 (if the chain is linear the pair derivatives of Eq.3 can be formally derived). Or the depletion solver calculates the matrix exponential of Eq.5, and in this case one can just evaluate Eq.9, calculating the matrix cosine of Eq.11 (with a limited development) in exactly the same way as the matrix exponential. Though it is always possible to use Eq.9 which formulation is "ready to use", instead of Eq.1 that requires all the pair derivatives of *g* (or to do an approximation by truncating this series).

5. APPLICATION TO A SIMPLE EXAMPLE

Let us consider a simple example: the burnup of a material made of one isotope characterized by its cross-section Σ and its time dependent concentration $N(t)$ (for the numerical result we take Σ t=0.5 and $N(0)$ =300). An ad-hoc Monte Carlo simulation was set up to produce estimates of a true flux φ_R. The unbiased result of the concentration after time t is then $g(\varphi_R)$. If we consider i=5000 evaluations (called cycles) of $\overline{\varphi}_i$, each being made of 30 evaluation of φ_R, we obtain the results presented Fig. 1. In this Figure, $\tilde{g}^0(\varphi_R)$ is the biased estimate of φ_R given by $\frac{\sum_i g(\overline{\varphi}_i)}{i}$ while $\tilde{g}^1(\varphi_R)$ and $\tilde{g}^2(\varphi_R)$ are given respectively by Eq.1 and Eq.8 (for Eq.1 an arbitrary truncation at order 10 was used). The unbiased result, $g(\varphi_R)$, is the reference straight line on the plot. As one can see, the use of both Eq.1 and Eq.8 provide excellent result (both estimators are compatible with the correct value within 0.01%), while the biased estimation of the concentration differs from roughly 2%.

6. CONCLUSIONS AND FUTURE WORK

Previous attempts to calculate the error propagation during Monte Carlo burnup calculations were made during the last years (see [11] for example). One way to achieve this consists in finding an unbiased minimum variance estimator of the concentration vector (over all isotopes)

for an arbitrary number of time steps. In this paper, this estimator has been derived thanks to [1] in the case of a matrix exponential function (that represents the depletion operator) and was found to be (we recall Eq.9):

$$\vec{N}_{NB}(t) = \vec{N}_B(t)\cos\left(\overline{\overline{\Sigma}}t\right)$$

Both this unbiased estimator and an other unbiased estimator (given by Eq.1) were applied on a simple example (one burnup step, with one isotope) and were shown to converge to the unbiased result.
This "cosine matrix" method should open new perspectives in the field of Monte Carlo burnup simulations, since the implementation of Eq.9 allows to have an unbiased result, to measure the error bars (from several estimations of this unbiased result) and to fully parallelize the whole code (not only the transport part of it) in the sense of performing "independent replicas".
All this work supposes the flux to be constant in a given volume, and this hypothesis is obviously not valid anymore for strong burnup cases. The more general study of any probability distribution of the flux is currently under investigation by the authors.

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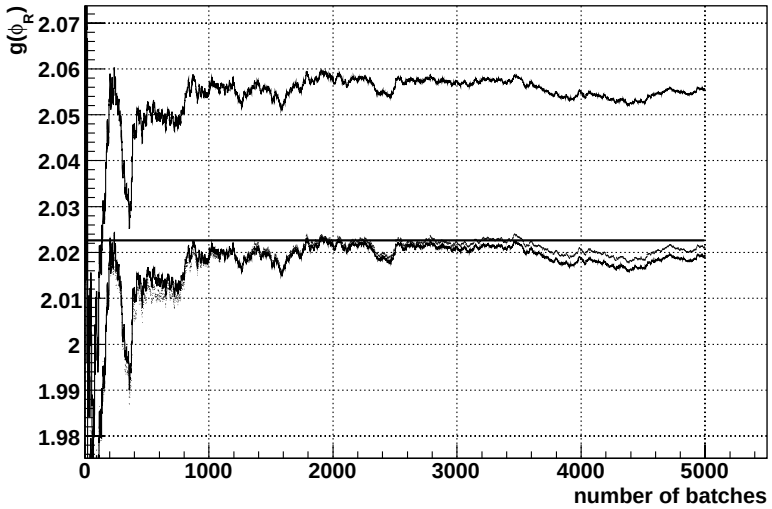

Figure 1: Mean of $\tilde{g}(\phi_R)$ for three different estimators versus batch number (estimator 0 to 2 from top to bottom)