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Use of probability tables for propagating uncertainties in neutronics

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ABSTRACT

Probability tables are a generic tool that allows representing any random variable whose probability density function is known. In the field of nuclear reactor physics, this tool is currently used to represent the variation of cross-sections versus energy (neutron transport codes TRIPOLI4®, MCNP, APOLLO2, APOLLO3®, ECCO/ERANOS...). In the present article we show how we can propagate uncertainties, thanks to a probability table representation, through two simple physical problems: an eigenvalue problem (neutron multiplication factor) and a depletion problem.

1. Introduction

A random variable ξ, defined on a domain (D), whose probability density function (pdf) $p(\xi)$ is known, can be represented by a moment-based probability table of order $N\{(p_i, \xi_i),\ i = 1, N\}$ where the probabilities p_i and the steps (or bands) ξ_i are calculated in order to preserve $2N$ moments:

$$M_n = \int_{(D)} \xi^n p(\xi) d\xi = \sum_{i=1}^{N} p_i \xi_i^n \quad n = L, \ldots, 2N + L - 1 \tag{1}$$

where L is the order (positive or negative) of the first moment to be preserved. To ensure probability normalization and mean value preservation, we need to exactly perform zero-order and one-order moments. That leads to $2 - 2N \leqslant L \leqslant 0$.

In the neutronics field, when dealing with nuclear reaction cross-sections, the most accurate probability tables are obtained by preserving negative and positive moments (the value $L = 1 - N$ is the one recommended by P. Ribon (Ribon and Maillard, 1986), positive moments giving a good representation of cross-section peaks and negative moments a good representation of cross-section depressions. But, in the present work, in order to calculate the moments of any random variable, we chose to preserve only positive moments ($L = 0$). As a matter of fact, negative moments of a Gaussian law do not exist (Piegorsch and Casella, 1982).

The physical interpretation of such a probability table is that it provides a set of values ξ_i "attained" by the random variable and the associated probabilities.

Consequently, any random variable can be sampled:

- either by a Monte Carlo technique using the exact probability density function,
- or by a multiband technique using the bands and the probabilities of the probability table.

Physical data, such as nuclear reaction cross-sections or radioactive decay constants are given in nuclear data bases by their mean values and their standard deviations. We generally make the assumption that their associated probability density functions follow a Gaussian law. When such "uncertain data" are the input of a physical equation $\mathcal{E}$ (slowing-down equation or depletion equation for instance), they induce a distribution on the output of equation $\mathcal{E}$. Classical perturbation methods give the mean value and the standard deviation of the output of $\mathcal{E}$ but not the probability distribution of $\mathcal{E}$ itself. In this paper, we show how such a distribution can be carried out using probability tables. Section 2 describes the moment-based probability table calculation and their mathematics properties. Sections 3 and 4 deal with uncertainty propagation in the context of neutronics field, respectively for an eigenvalue and a depletion problem.

This work is a continuation of a previous work done by the authors (Diop et al., 2012). It extends the concept of using probability tables for propagating uncertainties established for a fixed particle source problem to more general problems: eigenvalue and depletion problems.

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2. Moment-based probability table

2.1. Calculation

To compute the moment-based probability tables, we use a Padé approximant technique (Ribon and Maillard, 1986). It can be summarized in the following algorithm. Let us consider the function:

$$I(z) = \int_{(D)} \frac{p(\xi)}{1 - z\xi} d\xi$$

in the neighborhood of $z = 0$. We can give two expressions of $I(z)$. On one hand, using relations (1):

$$\begin{aligned} I(z) &= \int_{(D)} \frac{p(\xi)}{1 - z\xi} d\xi = \sum_{n=0}^{2N-1} M_n z^n + O(z^{2N}) \\ &= \sum_{n=0}^{2N-1} \sum_{i=1}^{N} p_i (z\xi_i)^n + O(z^{2N}) \\ &= \sum_{i=1}^{N} p_i \sum_{n=0}^{2N-1} (z\xi_i)^n + O(z^{2N}) \\ &= \sum_{i=1}^{N} p_i \frac{1}{1 - z\xi_i} + O(z^{2N}) \end{aligned} \tag{2}$$

and on another hand, using a $[N-1/N]$ Padé approximant:

$$\begin{aligned} I(z) &= \int_{(D)} \frac{p(\xi)}{1 - z\xi} d\xi = \sum_{n=0}^{2N-1} M_n z^n + O(z^{2N}) \\ &= \underbrace{\frac{P_{N-1}(z)}{Q_N(z)}}_{[N-1/N]} + O(z^{2N}) \end{aligned} \tag{3}$$

where:

$$P_{N-1}(z) = \sum_{j=0}^{N-1} a_j z^j \tag{4}$$

and:

$$Q_N(z) = \sum_{j=0}^{N} b_j z^j \tag{5}$$

Eq. (3) shows that the k-order monomials for $0 \leqslant k \leqslant 2N-1$ must be equal in the expressions:

$$B = \left(\sum_{n=0}^{2N-1} M_n z^n \right) \left(\sum_{j=0}^{N} b_j z^j \right) \tag{6}$$

and

$$A = \sum_{j=0}^{N-1} a_j z^j \tag{7}$$

The coefficients b_j of the denominator of the Padé approximant $[N-1/N]$ are obtained by identifying the k-order monomials for $N \leqslant k \leqslant 2N-1$. All these monomials must be equal to zero. That leads to the system of N equations, $(N+1)$ unknowns:

$$\sum_{j=0}^{N} b_j M_{k-j} = 0 \quad N \leqslant k \leqslant 2N-1 \tag{8}$$

Once the coefficients b_j are known, the coefficients a_j of the numerator of the Padé approximant $[N-1/N]$ are obtained by identifying the k-order monomials for $0 \leqslant k \leqslant N-1$. That leads to the system of N equations, N unknowns:

$$\sum_{j=0}^{k} b_j M_{k-j} = a_k \quad 0 \leqslant k \leqslant N-1 \tag{9}$$

System (9) shows that:

$$b_0 = 0 \Rightarrow a_0 = 0$$

and more generally:

$$\{b_l = 0, \quad 0 \leqslant l \leqslant k\} \Rightarrow \{a_l = 0, \quad 0 \leqslant l \leqslant k\}$$

Consequently, if zero is a k -order root of $Q_N(z)$, zero is also a k -order root of $P_{N-1}(z)$. By supposing that the Padé approximant is reduced (no zero roots), we can always choose:

$$b_0 = 1$$

System (8) can be rewritten as a system of N equations, N unknowns:

$$\sum_{j=1}^{N} b_j M_{k-j} = -M_k \quad N \leqslant k \leqslant 2N-1 \tag{10}$$

Once system (10) is solved, system (9) can be solved and the exact orders of $P_{N-1}(z)$ and $Q_N(z)$ are found. Let us denote L_P and L_Q the respective orders of $P_{N-1}(z)$ and $Q_N(z)$.

When $L_Q = N$, which is the general case, the Padé approximant can be decomposed into:

$$\frac{P_{N-1}(z)}{Q_N(z)} = \sum_{l=1}^{N} \frac{\alpha_l}{1 - z\beta_l} \tag{11}$$

When $L_Q = N-1$ and $L_P = N-1$, which happens for symmetric distributions in a domain (D) centered in zero when N takes odd values (cf. Appendix A), the Padé approximant can be decomposed into:

$$\frac{P_{N-1}(z)}{Q_N(z)} = \alpha_N + \sum_{l=1}^{N-1} \frac{\alpha_l}{1 - z\beta_l} \tag{12}$$

In formulas (11) and (12), β_l are the inverses of $Q_N(z)$ roots. These roots are simple because they are the roots of orthogonal polynomials as shown in the continuation of this paper.

By considering the equality obtained by comparing formulas (2) and (3):

$$\sum_{i=1}^{N} p_i \frac{1}{1 - z\xi_i} + O(z^{2N}) = \frac{P_{N-1}(z)}{Q_N(z)} + O(z^{2N}) \tag{13}$$

and by substituting the Padé approximant by its decomposition given either by Eq. (11) or by Eq. (12), we can take:

- when $L_Q = N$

$$\begin{cases} \xi_i = \beta_i, \\ p_i = \alpha_i \end{cases}, \quad i = 1, \ldots, N \tag{14}$$

- when $L_Q = N-1$ and $L_P = N-1$,

$$\begin{cases} \xi_i = \beta_i, \\ p_i = \alpha_i \end{cases}, \quad i = 1, \ldots, N-1 \tag{15}$$

and

$$\begin{cases} \xi_N = 0, \\ p_N = \alpha_N \end{cases} \tag{16}$$

Some very efficient algorithms exist for calculating the roots of a polynomial, and then, the bands of the probability tables are calculated by Eqs. (14) or (15) and (16). But for the probability calculation, we prefer solving the linear system, once the bands are known: