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On random sampling of correlated resonance parameters with large uncertainties

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ABSTRACT

Three different methods for multivariate random sampling of correlated resonance parameters are proposed: the diagonalization method, the Metropolis method, and the correlated sampling method. For small relative uncertainties (typical for *s*-wave resonances) and weak correlations all methods are equivalent. Differences arise under difficult conditions: large relative uncertainties of inherently positive parameters (typical for widths of higher-*l*-wave resonances) and/or strong correlations between a large number of parameters. The methods are tested on realistic examples; advantages and disadvantages of each method are pointed out. The correlated sampling method is the only method which produces consistent samples under any conditions. In the field of reactor physics, these methods are mostly used for the sampling of nuclear data, however, they may be used for any data with given uncertainties and correlations.

1. Introduction

Following the constant fast computer development, the use of nuclear data uncertainty information for applications in nuclear science is becoming more and more frequent. Opposite to deterministic sensitivity analysis, Monte Carlo based methods like Unified Monte Carlo (UMC) [1] and Total Monte Carlo (TMC) [2] have been developed in recent years. These methods enable to asses both statistical uncertainty (by generating more particle histories) and uncertainty due to inaccurate nuclear data (by generating more evaluated nuclear data samples from covariance data) of any integral parameter. Even more important is the fact that UMC deals better with non-linearities than the traditional generalized least-squares method.

As a part of nuclear data, resonance parameters are of utmost importance especially when dealing with large resonance self-shielding effects [3–5]. In general, the resonance parameters of stronger *s*-waves have smaller relative uncertainties, while the weaker higher-*l*-waves usually feature larger uncertainties because of worse signal-to-background ratio in the transmission or reaction yield measurements. The improvement of measurement techniques will decrease the uncertainties in the parameters of the existing resonances, while on the other hand this will inevitably lead to discovery of new, weaker resonances with even larger relative uncertainties.

The main objective of this paper is to find optimal sampling procedure for resonance parameters considering possible large relative uncertainties (i.e. reducing or completely avoiding negative values for inherently positive parameters, e.g. resonance widths) and strong correlations. Sampling in diagonal space, sampling by Metropolis algorithm [6], and the so-called correlated sampling method [7] are considered. In Section 2, these methods with several variations are briefly reviewed. A more detailed description of the methods can be found in the Appendices.

The two main issues arising at different conditions will be addressed in this paper. First, strong correlations between the parameters may require a large increase in numerical effort which may limit the applicability of some of the methods especially when the set of coupled parameters is increasingly large. And second, large uncertainties lead to negative values of inherently positive parameters [8], e.g. resonance widths or reaction cross-sections. This may be avoided in different ways: by zero cutoff, by using positive distribution functions like the log-normal distribution, etc. However, the former is on shaky physical grounds and increasingly decreases the standard deviation of the sampled parameters when uncertainties become larger, where the latter leads to substantial biases in the mean value and standard deviation of the sampled parameters. If the uncertainties are extremely large (above 100%), the correspondence of the

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parameter mean value and standard deviation to its best value and uncertainties is invalid and may be treated merely as abstract parameters of the distribution function [9]. In these cases, parameters should be given in the form of median value and confidence intervals rather than mean value and standard deviation [9]. These cases will be avoided in further discussion, which is focused on data interpretation and sampling rather than their representation.

In this paper, the use of the methods is described on cases with sampling of resonance parameters for nuclear data applications, even though the methods are general and can be applied to any correlated parameters with uncertainties. The sampling methods have been tested and compared on two different ^{55}Mn resolved resonance parameters evaluations: either ORNL[1] with small relative uncertainties and strong correlations, or NRG (TENDL-2010 nuclear data library) [10] with large uncertainties but sparse correlation matrix.

The results of the numerical comparison of the sampling methods' performances on the chosen ^{55}Mn evaluations are presented in Section 3.

2. Overview of the Monte Carlo sampling methods

A sampling method, that is efficient, stable, and, most importantly, consistent in a wide range of conditions, is sought. In this discussion, three different methods with several variations are proposed:

1. *Diagonalization method*: The method is a linear approximation and is based on diagonalization of the covariance matrix and individual sampling of uncorrelated linear combinations of correlated parameters in diagonal space. A more detailed description of the method is given in Appendix A.
2. *Metropolis method*: The method is based on generation of a stochastic Markov chain of states, from which random samples can be produced. In principle, any distribution may be used for sampling with Metropolis algorithm.
3. *Correlated sampling method*: The method can be used for random sampling of correlated parameters according to the multivariate normal or log-normal distribution. A more detailed description of the method is given in Appendix B.

All the methods discussed in this paper are in principle completely stochastic. Generally speaking, in some cases a combination of deterministic and probabilistic approach might be more efficient. A possible way to introduce deterministic elements into a random sampling method is to divide the domains of the sampled variables into subdomains with predetermined numbers of random samples in each subdomain, such as in the Latin hypercube sampling method [11]. The Latin hypercube sampling might be useful for multivariate sampling problems with a only few variables. Since the total number of subdomains exponentially increases with dimension of the sampled parameter vector, this method is extremely impractical when dealing with a large number of correlated variables like in the studied case. It has been found out that the use of the Latin hypercube sampling is beneficial for distributions with extremely high "tails" like the log-normal distribution with extremely large relative uncertainty, however, with only a very limited number of correlated variables [12].

In the field of reactor physics, the random sampling methods are mostly used for the sampling of nuclear data, however, in principle their applicability is much more general since they may be used for any data with given uncertainties. All calculations in this paper were performed using home-made codes, programmed in Mathematica,[2] as a proof-of-principle of the sampling methods described below. Further implementation in FORTRAN for production runs is planned. All methods can be used with same input/output as the existing nuclear data processing or reactor calculation codes, e.g. fitted resonances with covariance matrices derived by SAMMY [13] or REFIT [14] can be used as input and the sampling aimed at producing representative samples of the resonances.

2.1. Challenges of large relative uncertainties

When the mean value $\langle x\rangle$ and the standard deviation σ_x (which correspond to the best estimate and uncertainty for parameters with small relative uncertainty [9]) provide the only available information about a physical quantity, the *normal distribution* with mean value and standard deviation as its parameters

$$p(x)=\frac{1}{\sqrt{2\pi\sigma_x^2}}\exp\left(-\frac{(x-\langle x\rangle)^2}{2\sigma_x^2}\right) \tag{1}$$

is the best possible assumption for the parameter probability distribution function (PDF) according to the maximum entropy principle [15].

Some physical quantities, like the resonance widths, are inherently positive. Therefore, when large relative standard deviations are present (above ~0.5), a significant fraction of negative samples of inherently positive parameters is produced if sampled according to the normal distribution, which is unphysical. Samples with negative values may be ignored, but this affects the mean and the standard deviation of the parameter. If the *uniform* instead of the normal *distribution* is used

$$p(x)=\begin{cases}(2\sqrt{3}\sigma_x)^{-1}, & x\in[\langle x\rangle-\sqrt{3}\sigma_x,\langle x\rangle+\sqrt{3}\sigma_x]\\ 0 & \text{otherwise}\end{cases} \tag{2}$$

this reduces the number of cases with negative parameters but on the other hand, when the relative standard deviation exceeds $1/\sqrt{3}\approx 0.58$, negative values are not excluded. Furthermore, when the relative standard deviation exceeds ≈0.666 (see Fig. 1), the fraction of negative samples becomes larger than for the normal distribution. Therefore, the applicability of uniform sampling is limited to a narrow interval of relative uncertainties. Also, since the uniform distribution has no tails, sampling may give very different results in integral calculations if the observable happens to be highly sensitive to parameter values sampled from the distribution tails. Finally, the recommendation made in Ref. [16] should also be noted: *the use of the uniform distribution by evaluators should be discouraged because of the potential complications involved*.

For inherently positive parameters with known mean value and standard deviation, the *log-normal* instead of the normal *distribution* should in principle be employed [8] since the maximum entropy principle is applied in the logarithmic rather than the linear space. The form of the PDF is

$$p(x)=\frac{1}{\sqrt{2\pi\sigma^2x^2}}\exp\left(-\frac{(\ln x-\mu)^2}{2\sigma^2}\right),\quad x>0 \tag{3}$$

where

$$\sigma=\sqrt{\ln\left(1+\frac{\sigma_x^2}{\langle x\rangle^2}\right)} \tag{4}$$

[1] Luiz Leal, private communication, October 2010.

[2] Copyright, Wolfram Research, http://www.wolfram.com/.