Nuclear Instruments and Methods in Physics Research A 807 (2016) 137–149

Contents lists available at ScienceDirect

Nuclear Instruments and Methods in Physics Research A

journal homepage: www.elsevier.com/locate/nima

Sampling of systematic errors to estimate likelihood weights in nuclear data uncertainty propagation

P. Helgesson [a,b,*], H. Sjöstrand [a], A.J. Koning [b,a], J. Rydén [c], D. Rochman [d], E. Alhassan [a], S. Pomp [a]

[a] Department of Physics and Astronomy, Uppsala University, Box 516, 751 20 Uppsala, Sweden
[b] Nuclear Research and Consultancy Group NRG, Petten, The Netherlands
[c] Department of Mathematics, Uppsala University, Uppsala, Sweden
[d] Paul Scherrer Institute PSI, Villigen, Switzerland

ARTICLE INFO

Article history:
Received 3 June 2015
Received in revised form
5 October 2015
Accepted 8 October 2015
Available online 30 October 2015

Keywords:
Nuclear data
Uncertainty propagation
Experimental correlations
Systematic uncertainty
Total Monte Carlo

ABSTRACT

In methodologies for nuclear data (ND) uncertainty assessment and propagation based on random sampling, likelihood weights can be used to infer experimental information into the distributions for the ND. As the included number of correlated experimental points grows large, the computational time for the matrix inversion involved in obtaining the likelihood can become a practical problem. There are also other problems related to the conventional computation of the likelihood, *e.g.*, the assumption that all experimental uncertainties are Gaussian.

In this study, a way to estimate the likelihood which avoids matrix inversion is investigated; instead, the experimental correlations are included by sampling of systematic errors. It is shown that the model underlying the sampling methodology (using univariate normal distributions for random and systematic errors) implies a multivariate Gaussian for the experimental points (*i.e.*, the conventional model). It is also shown that the likelihood estimates obtained through sampling of systematic errors approach the likelihood obtained with matrix inversion as the sample size for the systematic errors grows large.

In studied practical cases, it is seen that the estimates for the likelihood weights converge impractically slowly with the sample size, compared to matrix inversion. The computational time is estimated to be greater than for matrix inversion in cases with more experimental points, too. Hence, the sampling of systematic errors has little potential to compete with matrix inversion in cases where the latter is applicable.

Nevertheless, the underlying model and the likelihood estimates can be easier to intuitively interpret than the conventional model and the likelihood function involving the inverted covariance matrix. Therefore, this work can both have pedagogical value and be used to help motivating the conventional assumption of a multivariate Gaussian for experimental data. The sampling of systematic errors could also be used in cases where the experimental uncertainties are not Gaussian, and for other purposes than to compute the likelihood, *e.g.*, to produce random experimental data sets for a more direct use in ND evaluation.

1. Introduction

In nuclear data (ND) uncertainty assessment and propagation, it is common to use Bayes' theorem to update the distributions for the ND with experimental information, see *e.g.* Refs. [1–8]. In methodologies based on random sampling of the nuclear data, such as Total Monte Carlo (TMC) [9,10], such an updating procedure involves computing the likelihood function for any sampled set of ND.

The errors in the experimental points are correlated due to systematic uncertainties that different experimental points have in common, such as uncertainties of the thickness or nuclide density of a particular target, detector efficiencies or (not the least) normalizing cross-sections. Because of this correlation, the computation of the likelihood function typically involves the computation of the generalized χ^2. This, in turn, involves the inversion of the experimental covariance matrix $\mathbf{C}_E$, with non-zero off-diagonal elements.

* Corresponding author.
E-mail address: petter.helgesson@physics.uu.se (P. Helgesson).

http://dx.doi.org/10.1016/j.nima.2015.10.024
0168-9002/

Nomenclature

β	power in expression for computational complexity $T_{\text{needed}} \propto m^{\beta}$
$\mathbf{C}_{\text{E}}$	experimental covariance matrix
χ^2_k	generalized χ^2 for k'th random file
$\chi^2_{k,\text{no corr.}}$	χ^2_k assuming no experimental correlations
δ_{ij}	Kronecker delta
$\mathcal{E}_\ell$	random variable describing ℓ'th systematic contribution
$\boldsymbol{\mathcal{E}}$	the random vector $(\mathcal{E}_1, \mathcal{E}_2, \ldots, \mathcal{E}_\nu)^{\text{T}}$
$\boldsymbol{\varepsilon}$	possible observation of $\boldsymbol{\mathcal{E}}$
$\boldsymbol{\varepsilon}^{(s)}$	s'th sample from $\boldsymbol{\mathcal{E}}$
$\langle \cdot \rangle$	expected value
$f_{\mathbf{W}}$	probability density function for random variable/vector $\mathbf{W}$
$\mathbf{G}$	matrix used for numerical evaluation of determinant ratio
$\mathbf{I}$	identity matrix
k	random file number
$L(\mathbf{p}^{(k)};\mathbf{x})$	likelihood function for $\mathbf{p}^{(k)}$ under $\mathbf{x}$
$L(\mathbf{p}^{(k)};\mathbf{x}\|\boldsymbol{\mathcal{E}}=\boldsymbol{\varepsilon})$	likelihood for $\mathbf{p}^{(k)}$ and $\mathbf{x}$ given $\boldsymbol{\mathcal{E}}=\boldsymbol{\varepsilon}$
m	# of experimental points
m_{max}	greatest m for which reasonable convergence is observed
$\boldsymbol{\mu}$	true values corresponding to $\mathbf{x}$
μ_{i}	true value corresponding to x_i (element of $\boldsymbol{\mu}$)
N	length of $\mathbf{p}$
n	# of random files in TMC
ν	# of systematic contributions
$\mathbf{p}$	vector with nuclear model parameters
p_j	j'th element of $\mathbf{p}$
$\mathbf{p}^{(k)}$	nuclear model parameters used for k'th random file
$Q_k(S)$	ratio of likelihood estimate with sample size S and likelihood from matrix inversion
S	sample size for sampling systematic errors
σ_{i}	random uncertainty in i'th experimental point
$\sigma_{i\ell}$	uncertainty in the i'th experimental point due to the ℓ'th systematic contribution
S_{needed}	S needed to obtain V_{goal}
$.^{\text{T}}$	transpose of matrix or vector
$\boldsymbol{\tau}^{(k)}$	vector with model values corresponding to $\mathbf{x}$ in k'th random file
T_{needed}	computational complexity to obtain V_{goal}
$V(\cdot)$	variance
V_{goal}	desired $\hat{V}(Q_k(S))$
$\hat{V}(Q_k(S))$	estimated variance of $Q_k(S)$
w_k	weight for k'th random file
$\mathbf{X}$	random vector describing the experimental points
$\mathbf{x}$	vector with experimental results
X_i	random variable describing i'th experimental point (i'th element of $\mathbf{X}$)
x_i	i'th element of $\mathbf{x}$ (i'th experimental point)
$\xi_k{}^2$	"conditioned χ^2" for k'th random file
$X_i\|(\boldsymbol{\mathcal{E}}=\boldsymbol{\varepsilon})$	X_i given $\boldsymbol{\mathcal{E}}=\boldsymbol{\varepsilon}$
Y_i	random variable for i'th experimental point without systematic uncertainty
$\mathbf{0}$	zero vector

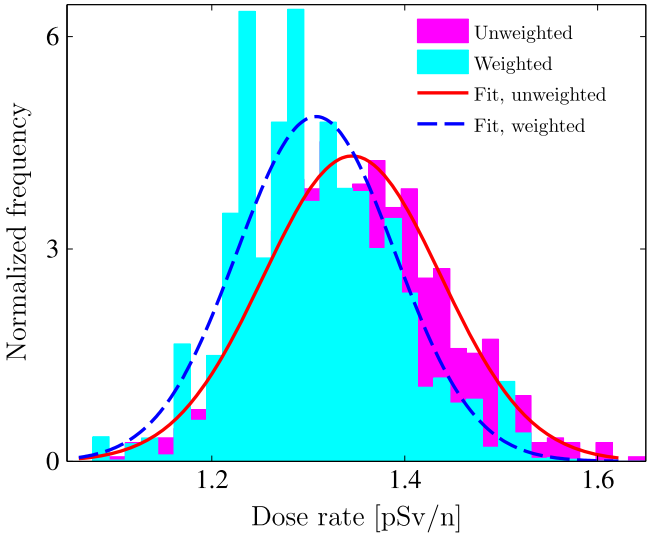

Fig. 1. The unweighted and weighted distributions for the dose rate from a neutron source shielded by iron-rich concrete, varying ^{56}Fe data (from Ref. [2]).

To enable the inclusion of cross-nuclide experimental correlations in such a methodology, it is necessary to construct an experimental covariance matrix that spans over experiments for several nuclides. As more nuclides get included in the same matrix, the size of $\mathbf{C}_{\text{E}}$ increases, and since the computational complexity of the inversion of a general $m \times m$ matrix is proportional to approximately $m^{2.8}$ (using Strassen's algorithm [11,12]) the computational time needed for matrix inversion can become a practical problem. As an example of this, the deterministic evaluation code of the GANDR project [13], which has the capability of a simultaneous evaluation of 130 important materials, is currently limited to 3600 correlated experimental points [13]. Further, the computation of the generalized χ^2 can be hard to intuitively interpret due to the matrix inversion. The use of the generalized χ^2 also relies on the assumption that all experimental uncertainties are normally distributed.

For these reasons, this work presents and investigates an alternative approach to compute the likelihood weights, based on simulating the correlated experimental errors instead of constructing an experimental covariance matrix. This novel way of computing the likelihood is compared to the conventional way, *i.e.*, making use of matrix inversion.

In Section 2, the reader is introduced to TMC, the ND uncertainty propagation methodology which is used as a practical starting point in this paper. Then, a brief description of the file weighting is given, followed by a description of the two discussed methods to compute the likelihood: matrix inversion and sampling of systematic errors. Section 2 is closed by some details on how the two methods are compared numerically. In Section 3, the results from applying the methodology to a set of test cases are found, with focus on the rate of convergence. The paper ends with discussion and conclusions in Sections 4 and 5, respectively.

2. Methodology

2.1. Total Monte Carlo (TMC)

The idea of the Total Monte Carlo methodology (TMC) [9,10] is to