Methodology Investigations on Uncertainties Propagation in Nuclear Data Evaluation

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ABSTRACT

In this paper, we discuss distinct ways of calculating nuclear cross section variance-covariance matrices issued from the spherical optical model such as the deterministic sensitivity method and Monte Carlo method. We also discuss the selection of uncertain parameters using both the local sensitivity and global sensitivity methods (based on spectral methods using a polynomial decomposition) to determine the importance of the input parameters with respect to the final uncertainty. Finally, we attempt to evaluate the differences between the uncertainties generated by methods like least squares method and bayesian method, both necessitating the use of experimental data. Discussing the results of simulation for the cross section calculations of the major neutron reactions on ⁸⁹Y, our interest was particularly focused on the mathematical rigour and quality of the uncertainties that we obtained.

1 INTRODUCTION

Increasing stringent data accuracy requirements have forced nuclear data researchers to examine closely the methods of uncertainties propagation in nuclear data evaluation. Important objectives are the elimination of bias in nuclear evaluations, and realistic assessments of uncertainties in the data bases. Some of the mathematical tools (least square method, etc.), required to handle this problem, have been available to the nuclear data community for a long time. Recently new methods have been developed, that offer complementary insights into the concepts of data evaluation and error analysis: Monte Carlo methods, Global Sensitivity Analysis and Bayesian optimisations. However this increasing number of methods may provide different results for the calculated nuclear data uncertainties. For classical nuclear data, the validation process occurs through comparison with experimental data. The same process is clearly not applicable for the validation of the calculated uncertainties. Therefore a rigorous mathematical approach is required to discriminate from the different chosen methods. In this paper, we mainly focus on analysis, interpretation and comparison of the differences obtained on the data uncertainties calculated from a phenomenological optical model.
2 THE PHENOMENOLOGICAL OPTICAL MODEL POTENTIAL BELOW 30 MEV

The phenomenological optical model potential is defined as follows:

\[ U(r, E) = -[V_v(r, E) + iW_v(r, E)] - [V_s(r, E) + iW_s(r, E)] + [V_{so}(r, E) + iW_{so}(r, E)] \]  

(1)

where \( V_v, V_s, W_v, W_s, W_{so}, W_{so} \) are the real volume potential, the real surface potential, the imaginary volume, the surface potentials, and the real and imaginary spin-orbit potentials, respectively.

These terms are factorised as the product of an energy-dependent well depth and a radial-dependant geometrical factor:

\[
\begin{align*}
V_v(r, E) &= V_v(E)f(r, R_{v_w}, a_{v_w}) & W_v(r, E) &= W_v(E)f(r, R_{v_w}, a_{v_w}) \\
V_s(r, E) &= V_s(E)g(r, R_{v_w}, a_{v_w}) & W_s(r, E) &= W_s(E)g(r, R_{v_w}, a_{v_w}) \\
V_{so}(r, E) &= C_{so}L \cdot g_{so}(E)\phi(r, R_{v_{so}}, a_{v_{so}}) & W_{so}(r, E) &= C_{so}L \cdot g_{so}(E)\phi(r, R_{v_{so}}, a_{v_{so}})
\end{align*}
\]

The radial form factors \( f(r, a_i, R_i) = (1 + e^{-r/R_i})^{-1} (i = v, s, so) \) are Woods-Saxon types with \( R_i = r_i A^{1/3} \) where \( r_i \) is the reduced radius (fm). The depth \( V \) (MeV) of each of the six potential wells, the reduced radii \( r_i \) and the diffusivities \( a_i \) (fm) may have an energy dependence. \( r_i, a_i \) and \( V \) are the input parameters of the optical model. Consistent sets of parameters are used to calculate physical quantities such as total (\( \sigma_T \)), shape elastic (\( \sigma_E \)) and reaction (\( \sigma_R \)) cross sections. The cross sections calculated with the spherical optical model can be characterised as a function of the model parameters.

3 DETERMINISTIC APPROACH VS. MONTE CARLO METHOD

3.1 Deterministic approach

First order Taylor’s development. The classical model of prediction of errors is based on the propagation of the covariance of an input random perturbation. The dependence between the covariance matrices of the input parameters and output data can be determined using a Taylor expansion (about the mean value \( \mu_i \)). The Taylor series method approximates \( f_j \) by a linear function. The linearization greatly simplifies error analysis, but at the expense of introducing an approximation error.

\[
Y_j \approx f_j(\mu_1^X, \ldots, \mu_p^X) + \sum_{i=1}^{p} \left( \frac{\partial f_j}{\partial X_i}(\mu_1^X, \ldots, \mu_p^X) \right) (X_i - \mu_i^X) .
\]

(2)

The results are often written in a matrix form as \( \phi = \nabla \phi \nabla \phi^T \) where \( \nabla \phi \) is the parameter covariance matrix and \( \nabla \phi \) the sensitivity matrix.

In order to be coherent with the nonlinear model and the expansion to the second order of Taylor’s development, the uniform distribution \( \mathcal{U}(\alpha, \beta) \) is used for the \( \phi \) calculation, the differentiability of \( f_j \) being assumed. The sensitivities are then estimated by using a centered finite difference approximation.

Calculations have been performed for all the cross sections with the code SCAT2000 [1] for the reaction \( \text{n}^+\text{Y} \). The set of parameters is initialised with the Koning-Dela roche (KD) [2] parameter evaluations. The results are shown on figure 1.

Second order Taylor’s development. The first order Taylor’s expansion is usually employed to obtain an approximate estimation for the output data. This technique is reliable only if several stringent assumptions are satisfied, such as the higher order error terms can safely be omitted in the expansion procedure.
Figure 1: n+\(^{89}\)Y (14 MeV) cross section uncertainties obtained by the first order Taylor’s expansion. On the left: standard deviation. On the right: cross section correlations.

The following paragraph describes how the second order term affects the sensitivity of the results.

\[
Y_j \approx f_j(\mu^X_1, \ldots, \mu^X_p) + \sum_{i=1}^p \left( \frac{\partial f_j}{\partial X_i}(\mu^X_1, \ldots, \mu^X_p) \right) (X_i - \mu^X_i) + \frac{1}{2} \sum_{i=1}^p \sum_{i'=1}^p \left( \frac{\partial^2 f_j}{\partial X_i \partial X_{i'}}(\mu^X_1, \ldots, \mu^X_p) \right) (X_i - \mu^X_i)(X_{i'} - \mu^X_{i'}) \tag{3}
\]

Under the assumptions of independent parameters and continuous uniform distribution, we determine implementable expressions for the covariance matrix elements. In the calculation of the covariances, not only the covariances \(\sigma_{X_{ij}}\) but also the fourth order moment is needed.

Final covariance \(\text{Cov}(Y_j, Y_{j'}) = \sigma_{Y_{jj'}}\) can be written:

\[
\sigma_{Y_{jj'}} = \sum_{i=1}^p \frac{\partial f_j}{\partial X_i} \frac{\partial f_{j'}}{\partial X_i} \sigma_{iX}^X + \frac{1}{4} \sum_{i=1}^p \sum_{i'=1}^p \frac{\partial^2 f_j}{\partial X_i^2} \frac{\partial^2 f_{j'}}{\partial X_i'^2} \left( E \left[ (X_i - \mu^X_i)^4 \right] - (\sigma_{iX}^X)^2 \right) \tag{4}
\]

Introducing the second derivatives and the \(4^{th}\) central moment diagonal matrix, we obtain:

\[
F^2_X = \left( \frac{\partial^2 f_j}{\partial X_i^2} \right)_{1 \leq i \leq g}^{1 \leq j \leq p} \quad Q_X = (Q_{X_{ij}})_{1 \leq i \leq g}^{1 \leq j \leq p} = \begin{cases} 0 & \text{if } i \neq j \\ E \left[ (X_i - \mu^X_i)^4 \right] & \text{if } i = j \end{cases} \tag{5}
\]

The results above can be written in a matrix form as: \(V_X = F_X V_X F_X^T + \frac{1}{4} F_{Q_X}^2 (Q_X - V_X)^2 \) \(F_{Q_X}^2 \) \(F_X^T\).

Using the uniform distribution \(U(\alpha_i, \beta_i)\), in an analogous way one can obtain finite difference approximations to higher order of the derivatives and differential operators. A three point central difference approximation is used to obtain the second derivatives of \(f_j\).

### 3.2 Monte Carlo method

The Monte Carlo method is used to determine how random variations of the parameter values affect the sensitivity of the system that is being modeled. Monte Carlo simulation inputs are randomly generated from probability distributions. So, we determine a distribution for the input parameters that most closely matches the parameters we already have.
Uniform distribution  In the context of a comparison between both methods, we used a uniform distribution $U(\alpha_i, \beta_i)$ as the parameter probability distribution function (pdf) to be coherent with the sensitivity approach. The pdf of the parameter vector $X$ is the product of the marginal distributions $f_{X_i}$ of each parameter $X_i$: \[ f_X = \prod_{i=1}^{P} f_{X_i}. \] The results are plotted on figure 2.

Figure 2: $n^+^{89}Y$ (14 MeV) cross section uncertainties calculated from the $n$ simulated parameter games using the Monte Carlo method. On the left: standard deviation. On the right: cross section correlations.

3.3 Comparisons

$\sigma$ symbolizes the derived physical quantities generated by optical model calculations. Figure 3 shows the evolution of the cross section correlations $\text{Cor}(\sigma_\xi(E_i), \sigma_\xi'(E_j))$, $((\xi, \xi') \in \{\text{total, elastic, reaction}\} \times \{\text{total, elastic, reaction}\})$ obtained respectively by the sensitivity method (left) and the Monte Carlo method (right). Using the second order Taylor’s development (fig. 3), we notice a better agreement for the results obtained by the two methods.

Figure 3: $n^+^{89}Y$: comparisons of the reaction cross section correlations calculated by the Monte Carlo Method (MMC) and by the Sensitivity Method (first order Taylor’s development (MS) on the left - Second order Taylor’s development (MS2) on the right. Up: correlation superposition, Down: absolute correlation differences).

Though the Monte Carlo method seems well suited, it leaves too much degrees of freedom for non verified assumptions (choices of pdf parameters and random interval widths).
4 LOCAL SENSITIVITY ANALYSIS & GLOBAL SENSITIVITY ANALYSIS

The aim of sensitivity analysis is to estimate the rate of change in the model output with respect to changes in model inputs. Such a knowledge is important to determine parameters for which more accurate values are required, and to understand the behavior of the system being modeled.

4.1 Local Sensitivity Analysis

The method involves expansion of model outputs in terms of small random perturbations of model parameters. Different \( \delta x_i \) were tested in \([0, \alpha_{X_i} = \pm 5\%]\) (see figure 4).

![Figure 4: relative sensitivities of the total cross section of \(^{89}\)Y due to optical parameter perturbations as a function of energy.](image)

The main limitation is the requirement that the perturbation terms be small. Furthermore, these methods are in general difficult to apply in conjunction with the modeling of complex, nonlinear systems. In this study, we use the normalized gradient \( \frac{\partial f}{\partial X_i} \frac{\mu^X}{f_j} \).

4.2 Global Sensitivity Analysis

Global Sensitivity Analysis (GSA) allows to quantify the importance of model parameters and their interactions with respect to model output.

**Sobol decomposition** Let us assume the model function \( y = f(x_1, x_2, \ldots, x_p) \), where \( x_1, x_2, \ldots, x_p \) are independent input factors. Whenever \( y = f(x_1, x_2, \ldots, x_p) \) is integrable over \([0, 1]^p\), \( y \) can be decomposed \([3]\) as:

\[
f(x_1, x_2, \ldots, x_p) = f_0 + \sum_{i=1}^{p} f_i(x_i) + \sum_{1 \leq i \leq j \leq p} f_{ij}(x_i, x_j) + \ldots + f_{1,2,\ldots,p}(x_1, x_2, \ldots, x_p)
\]

with the classical orthogonality property. Considering that the input parameters are independent random variables, the joint pdf of the input factors is \( P(X_1, X_2, \ldots, X_p) = \prod_{i=1}^{p} p(X_i) \). and using Sobol decomposition (eq. 6), the output variance is univocally decomposed in orthogonal terms of increasing dimensionality.

\[
V[Y] = \int_{[0,1]^p} f^2(X_1, X_2, \ldots, X_p) \prod_{i=1}^{p} p(X_i) dX_i - f_0^2 = \sum_{i=1}^{p} D_i + \sum_{1 \leq i \leq j \leq p} D_{ij} + \ldots D_{1\ldots p}
\]

The first-order term quantifies the effect of each single factor \( (S_i) \). The second-order terms \( (S_{ij}) \) display the effect due to the interaction between a given pair of factors that is different from the...
linear combination of the effects due to each of them on the others. Higher orders terms \( S_{ijk} \) give mixed influence of parameters.

\[
S_i = \frac{D_i}{D} = \frac{V(E[Y|X_i])}{V(Y)}, \quad S_{ij} = \frac{D_{ij}}{D} = \frac{V(E[Y|X_i, X_j]) - V(E[Y|X_i]) - V(E[Y|X_j])}{V(Y)}, \quad S_{ijk} = \frac{D_{ijk}}{D}.
\]

Polynomial Chaos (PC) Theory

The chaos expansion expresses the random process through a complete orthogonal basis in terms of random variables: 

\[
f(X) = \sum_{k=0}^{\infty} f_k \Psi_k(\{\xi_i(\omega)\}_{i=1}^{\infty}).
\]

\( \Psi_k \) are orthogonal polynomials from which the Legendre and Hermite polynomials are a subset and \( \{\xi_i(\omega)\}_{i=1}^{\infty} \) independent random variables.

It is possible to represent the random response of a system as a PC expansion. Polynomial chaos is restricted to second-order stochastic processes (i.e. processes with finite second-order moments). The combination of a random vector and polynomials is carefully selected from the distribution of the random input \([4]\). Generalized polynomial chaos (the Wiener-Askey Polynomial Chaos) forms a complete orthonormal basis of the Hilbert space with the inner product which satisfy the orthogonality relation.

In practical computations, the stochastic space must be truncated. The total number of expansion terms \( M + 1 \) is determined by \( N \) \( \{\xi_i(\omega)\}_{i=1}^{N} \) and \( P \), which is the highest degree of the orthogonal polynomials: 

\[
f(X) = \sum_{k=0}^{M} f_k \Psi_k(\xi(\omega)), \quad M + 1 = (N + P),
\]

Due to the orthogonality of the basis, we can calculate the expansion coefficients \([5]\):

\[
< f(X) \Psi_k(X) >= \frac{1}{f_k} \Psi_k(X) = \frac{1}{\Psi_k(X)}
\]

The expansion coefficients \( f_k \) are known as spectral modes. The partial variances can be obtained from the spectral mode calculations:

\[
V[f(X_{i_1},...,X_{i_s})] = E \left[ \sum_{k \in \Gamma_{i_1},...,i_s} f_k \Psi_k(X) \right]^2 = \sum_{k \in \Gamma_{i_1},...,i_s} f_k^2 E[\Psi_k^2(X)]
\]

with \( \Gamma_{i_1,...,i_s} = \{ k \in N \} \Psi_k(X) = \Psi_k(X_{i_1},...,X_{i_s}) \} \).

We can link the spectral modes to the Sobol decomposition and from the PC representation we can reach the full list of Sobol indices \([6]\):

\[
S_{i_1,...,i_s} = \frac{\sum_{k \in \Gamma_{i_1},...,i_s} f_k^2 E[\Psi_k^2(X)]}{\sum_{k=1}^{\infty} f_k^2 E[\Psi_k^2(X)]}.
\]

Application to \( n + 89Y \): Reference values have been computed using Quasi Monte Carlo Method.

<table>
<thead>
<tr>
<th>Table 1: Nuclear Optical Model Random Parameters (KD)</th>
</tr>
</thead>
<tbody>
<tr>
<td>( r1 = r_{v_0} \in [1.206, 1.230] )</td>
</tr>
<tr>
<td>( a3 = a_{v_0} \in [0.6593, 0.6727] )</td>
</tr>
<tr>
<td>( pot1 = V_v \in [50.8, 51.82] )</td>
</tr>
</tbody>
</table>

We first consider the effects of the variation of the input parameter values. The array in figure 5 shows the partial variances. \( Vr1 \), first-order index, must be understood as the contribution of the input parameter \( r1 \) on the total variance; \( Vr1r3 \), a second-order index, is a good descriptor of the sensitivity of the model due to the couple of input parameters \( (r1, r3) \). The figure 5 gives an example of the convergence estimation depending of the Van der Corput quasi-random sequences.
Parameter Sensitivities

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Sensitivity</th>
</tr>
</thead>
<tbody>
<tr>
<td>$V_{r1}$</td>
<td>76.3%</td>
</tr>
<tr>
<td>$V_{a1}$</td>
<td>2.9%</td>
</tr>
<tr>
<td>$V_{r3}$</td>
<td>&lt;0.001%</td>
</tr>
<tr>
<td>$V_{a3}$</td>
<td>0.003%</td>
</tr>
<tr>
<td>$V_{r4}$</td>
<td>7.4%</td>
</tr>
<tr>
<td>$V_{a4}$</td>
<td>0.7%</td>
</tr>
<tr>
<td>$V_{pot1}$</td>
<td>12.6%</td>
</tr>
<tr>
<td>$V_{pot3}$</td>
<td>0.004%</td>
</tr>
<tr>
<td>$V_{pot4}$</td>
<td>0.01%</td>
</tr>
<tr>
<td>$V_{r1r3}$</td>
<td>&lt;0.001%</td>
</tr>
<tr>
<td>$V_{r1a1}$</td>
<td>0.001%</td>
</tr>
</tbody>
</table>

Figure 5: Numerical values of variances and partial variances obtained with the non intrusive method with 9 random parameters - degree of PC expansion $p = 4$ for an incident neutron energy $E_n = 14$ MeV (on the left). Estimation of the convergence of the variance and partial variance values (on the right).

5 LEAST SQUARE OPTIMISATION & BAYESIAN OPTIMISATION

In order to estimate the uncertainty on the calculated cross section, one needs an algorithm to estimate the uncertainty on the parameters ($V_X$) which appears in the multi-variate pdf. The most probable distribution of the unknown theoretical parameter distribution is the multinormal Gaussian distribution. Since the covariance matrix of the estimated parameters is symmetric and positive definite, it can be diagonalised by $V_X = PDP^T$. To obtain $V_X$, we have to determine parameter values that minimize the difference between the experimental observations and the chosen model. We consider the whole model-fitting process described in terms of the minimization of an error function. This nonlinear least squares problem can be solved with the Levenberg-Marquardt minimization algorithm. However, it must be initialized by estimates close to the solution for unknown parameters. Figure 6 gives an example of optimisation using a set of parameters initialised with the Koning-Delaroche [2] global parameter evaluations.

Figure 6: $n^+$ total cross section - On the left, parameters optimisation obtained with the Levenberg-Marquardt minimization algorithm. On the right, comparisons of the standard error obtained by least square optimisations in green and Bayesian optimisations (in brown: random parameter interval ± 1%, in yellow: random parameter interval ± 0.05%).
The Bayesian inferential approach compares the standard deviation obtained with the least squares and the bayesian methods (see figure 6). By using an initial prior based on a uniform distribution of the parameters, we assign the KD parameter values (see table 1) to the prior mean. The Bayesian process of updating the inference from prior to posterior gives the standard deviations. All Bayesian inferential conclusions are made conditional to the observed data.

6 CONCLUSION

The objective of the present paper was to investigate the use of different error propagation techniques applied to the estimation of covariance matrices for nuclear cross sections obtained from optical model calculations. The sensitivity method is straightforward. Yet the main problem is that the method yields inherently approximate results. Therefore it is not always possible to determine whether the approximations made are utterly acceptable. The Monte Carlo method does not suffer from this limitation and, as a rule, it can reach an arbitrary level of accuracy. Moreover this method will probably prevail when used for the study of error propagation with a complex nuclear reaction code such as TALYS, according to its easy implementation and generality. However, the main problem with the Monte Carlo method is that error propagation calculation necessitates the prior knowledge of the input errors of the model parameters and their probability distribution function. However, since most of the problems encountered in nuclear physics are non-linear, they call for a non-linear global sensitivity analysis independent of nuclear model structure. Sobol sensitivity measures offer the possibility to cope with this situation. They allow for the computation of total effect indices permitting to rank quantitatively the parameters with respect to their influence on the output. For that purpose, polynomial chaos expansions were used to determine a method that estimates the sensitivity of the optical model output to a random variation of the input parameters of the model. Rigorous simulation of uncertainty propagation requires the knowledge of the variance-covariance matrix of the parameters. Generally this matrix is obtained through a minimization process which necessitates the utilization of experimental data. Since comparison between regression method and Bayesian method put into evidence a strong dependence to experimental data, in order to have a better understanding of these phenomena, we propose next to investigate the field of the spectral intrusive methods.

REFERENCES


