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Simulation of robust resonance parameters using information theory

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Abstract

Due to complex nature of resonance region interactions, significant effort has been devoted to quantify the resonance parameter uncertainty information through covariance matrices. Statistical uncertainties arising from measurements contribute only to the diagonal elements of the covariance matrix, but the off-diagonal contributions arise from multiple sources like systematic errors in cross-section measurement, correlation due to nuclear reaction formalism, etc. All the efforts have so far been devoted to minimize the statistical uncertainty by repeated measurements but systematic uncertainty cannot be reduced by mere repetition. The computer codes like SAMMY and KALMAN so far developed to generate resonance parameter covariance have no provision to improve upon the highly correlated experimental data and hence reduce the systematic uncertainty. We propose a new approach called entropy based information theory to reduce the systematic uncertainty in the covariance matrix element wise so that resonance parameters with minimum systematic uncertainty can be simulated. Our simulation approach will aid both the experimentalists and the evaluators to design the experimental facility with minimum systematic uncertainty and thus improve the quality of measurement and the associated instrumentation. We demonstrate, the utility of our approach in simulating the resonance parameters of Uranium-235 and Plutonium-239 with reduced systematic uncertainty.

1. Introduction

Experimentalists of neutron cross-section measurements and evaluators have been constantly striving to provide quality neutron cross-section data to the Reactor Physics Community with the sole aim to mitigate uncertainties in the neutron cross-section data. Although, the accuracy of nuclear data has significantly improved, little information exists on the various components of uncertainties and their correlation (Leal et al., 2005; Larson et al., 2006). We quantify the reactor parameter uncertainty by the covariance matrix as per international recommendation (Shibata et al., 2002). Correlation between the uncertainties can greatly influence the final uncertainty in the resultant reactor parameters of interest (Fort et al., 2003; Kodeli, 2005). The covariance matrix is symmetric and its diagonal and off-diagonal elements express, respectively, the uncorrelated statistical and the correlated systematic uncertainties. Even though the total uncertainty should include both the correlated and the uncorrelated uncertainties, correlated systematic uncertainties in the past have either been neglected or randomized (Cohen, 1992). According to probability theory and compounded by experience, only the statistical uncertainty decreases as $(\frac{1}{\sqrt{N}})$ if a measurement is repeated N times, where as systematic component forms a hard core of uncertainty that cannot be reduced by mere repetition (Frohner, 2003). It is pertinent to note that systematic uncertainty pervades all types of physical measurement and is affected by errors due to instrumentation, environment and personnel (Coates et al., 1983; Leinweber et al., 2006). It is always recommended, to spend the maximum possible effort on identification and minimization of correlated uncertainties (Massart et al., 1988).

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As regards the resonance region of the neutron cross-section, the code SAMMY developed at ORNL (Oak Ridge National Laboratory) and the code KALMAN developed by Kyushu University have been widely used in the evaluation of the experimental data in the resolved and unresolved resonance region (Larson et al., 2006; Arbanas et al., 2006). SAMMY takes into consideration various sources of uncertainties in the experimental data in the evaluation of capture, fission and total cross-sections. In the process of evaluation, SAMMY generates a set of resonance parameters along with their covariance. Even though SAMMY takes into consideration various sources of experimentally measured uncertainties, there is a dominance of correlated systematic uncertainties in the evaluation of resonance parameters. Similarly, in using the code KALMAN, when ever highly correlated data are visible, artificially, a lower correlation coefficient is proposed without any physical basis in order to avoid mathematical singularity (Kawano et al., 2002a). Thus, both in SAMMY as well as in KALMAN, there is no provision to improve upon the highly correlated experimental data and hence reduce the systematic uncertainty.

In this paper, we propose a new approach called entropy based information theory to reduce the systematic uncertainty so that resonance parameters with minimum systematic uncertainty can be simulated. Our simulation approach will aid both the experimentalists and the evaluators to design the experimental facility with minimum systematic uncertainty and thus improve the quality of measurement and the associated instrumentation. We demonstrate, the utility of our approach in simulating the resonance parameters of Uranium-235 and Plutonium-239 with reduced systematic uncertainty.

2. Generation of covariance matrix

Let $p_1, p_2, \ldots p_n$ be the resonance parameters and the reaction cross-section can be written as

$$\sigma = \sigma(p_1, p_2, \ldots p_n) \tag{1}$$

We wish to estimate the uncertainty $\Delta\sigma$ in σ due to uncertainty Δp of p_i. Using the first order perturbation theory, the change in σ due to change in dp of p_i can be expressed as

$$\mathrm{d}\sigma \cong \sum_i \left(\frac{\partial\sigma}{\partial p_i}\right) \mathrm{d}p_i \tag{2}$$

Using the notation $\delta\sigma = (\frac{\mathrm{d}\sigma}{\sigma})$, the relative variance–covariance in σ is usually obtained as the expectation value, i.e. $\langle\delta\sigma\delta\sigma^{\mathrm{T}}\rangle$ and hence can be expressed using Eq. (2) as

$$\langle\delta\sigma\delta\sigma^{\mathrm{T}}\rangle = B_\sigma\langle\delta p_i\delta p_j\rangle B_\sigma^{\mathrm{T}} \tag{3}$$

where $B_\sigma = \frac{\partial\sigma}{\partial p}\frac{p}{\sigma}$ is called relative sensitivity matrix.

In Eq. (3) the expectation value of the product of input data uncertainties, i.e. $\langle\delta p_i\delta p_j\rangle$ is the basic definition of the covariance matrix M_p. Eq. (3) can be rewritten as

$M_\sigma = B_\sigma M_p B_\sigma^{\mathrm{T}}$ where $M_\sigma = \langle\delta\sigma\delta\sigma^{\mathrm{T}}\rangle$ is the relative variance–covariance matrix for σ and M_p is the relative variance–covariance matrix for the resonance parameter p_i and B_σ^{T} is the transpose of B_σ.

The correlation coefficient K_{ij} is defined as

$$K_{ij} = [\mathrm{Cov}(p_i, p_j)/\{\mathrm{Var.}(p_i)\}^{0.5}\{\mathrm{Var.}(p_j)\}^{0.5}]. \tag{4}$$

and it varies between +1 and −1. K_{ij} is a measure of linear association between the resonance parameters and this linear association vanishes and hence the resonance parameters become independent when $K_{ij} = 0$.

3. Mutual information as a measure of discrimination

According to the information theory (Cover and Thomas, 1991) the mutual information I between the output vector σ and the input vector p for a system is expressed as

$$I(\sigma, p) = H(\sigma) + H(p) - H(\sigma, p) \tag{5}$$

where $H(\sigma)$ and $H(p)$ are the entropies of σ and p, respectively and $H(\sigma,p)$ is the joint entropy and

$$\begin{aligned} I(\sigma, p) &= \mathrm{Cons\ tan}\, t \ln(\mathrm{Det}\cdot M_p \text{ or } \mathrm{Det}\cdot K_p) \\ &= \mathrm{Cons\ tan}\, t \cdot \ln G \end{aligned} \tag{6}$$

where $G = \mathrm{Det}\cdot M_p$ or $\mathrm{Det}\cdot K_p$ and it is a $(n \times n)$ determinant with elements of M or K, respectively. Thus, the value of the mutual information depends on the value of the determinant of the covariance matrix M or the correlation matrix K and the value of mutual information is maximum only when the determinant of either of them is maximum (Te, 1998).

Entropy may be seen as the average amount of information required in selecting observations by categories like different input data p_i. A novel property of entropy is that categories may be permuted without changing its value. Thus, entropy is content free and does not make assumptions about the distribution of data thereby belonging to the non-parametric family of statistics. When σ and p are independent, the mutual information is zero. Thus mutual information is a measure of statistical correlation between the variables σ and p (Deco and Obradovic, 1996). As an illustration, let us consider the simple case of just two resonance parameters. The entropy of either the input $H(p)$ or the output $H(\sigma)$ and the joint entropy are respectively, (Ronen, 1984),

$$H(p) \text{ or } H(\sigma) = 1/2\log[(2\pi\mathrm{e})^2\mathrm{Det}(M)]$$

and $H(\sigma,p) = \log(2\pi\mathrm{e})$. Substituting these values in Eq. (5) the mutual information

$I(\sigma,p) = \log(\mathrm{Det}\cdot M)$ or $\log(G)$. For, $n = 2$, the elements of the covariance matrix,

$$M_p = \mathrm{Cov}(p_1, p_2) = \begin{pmatrix} p_{11} & p_{12} \\ p_{21} & p_{22} \end{pmatrix}$$

The elements of the covariance matrix can be written as the variance of p_1 and p_2,

$p_{11} = S_1^2$, $p_{22} = S_2^2$, $p_{12} = p_{21} = S_1\ S_2\ K_{12}$, where K_{12} is the correlation coefficient between p_1 and p_2. The determinant of the covariance matrix is then

$$G = \mathrm{Det} \cdot M_p = S_1^2 S_2^2 (1 - K_{12}^2). \quad (7)$$

or when $G = \mathrm{Det} \cdot K = (1 - K_{12}^2)$.

Thus apart from S_1 and S_2 the value of G depends upon K_{12} and G can be either maximized or minimized by finding the upper and lower bounds of K_{12}. As mutual information is a measure of statistical correlation between the variables σ and p, maximizing G by the knowledge of the bounds for the correlated elements of K leads to minimization of the linear association or the correlated information. Minimization of the correlated information leads to variables being heterogeneous (Massart et al., 1988). Hence, an index of discrimination between the correlated inputs is the maximization of the mutual information by the estimation of upper and lower bounds for the correlated elements of K. The algorithm to estimate the upper and lower bounds for the correlated elements of the correlation matrix based on the technique of determinant inequalities has been described in detail in (Krishna Kumar, 2007).

The correlation matrix for the averaged Uranium-235 unresolved resonance parameters like the averaged level spacing D, the averaged neutron width Γ_n, neutron inelastic scattering width Γ_{in}, the radiative capture width Γ_γ and fission width Γ_f and the strength functions S_0 and S_1 are depicted in Table 1 (Kawano et al., 2002a) and the upper and lower bounds for some of the non-diagonal elements are obtained using (Krishna Kumar, 2007) are tabulated in Table 2. Similarly, the correlation matrix for the Pu-239 resolved resonance parameters at 0.2956 eV (Kawano and Shibata, 2002b) is depicted in Table 3 and the upper and lower bounds for the third row are tabulated in Table 4. The bounds for the other non-diagonal elements can also be obtained by using the similar procedure.

Table 1
Correlation matrix for U-235 resonance parameters

Resonance parameter	Error (%)	D	S_0	S_1	Γ_γ	Γ_f
D	2.39	1.0				
S_0	0.69	0.274	1.0			
S_1	2.16	0.529	0.325	1.0		
Γ_γ	4.81	0.254	−0.266	−0.361	1.0	
Γ_f	7.06	0.143	−0.095	−0.329	0.951	1.0

Table 2
Upper and lower bounds for the correlation coefficients for some of the non-diagonal elements of Table 1 and the value of the respective determinant

Value of K_{ij} from Table 1	Upper bound of K_{ij}	Lower bound of K_{ij}	G with K_{ij} as in Table 1	G with upper bound of K_{ij}	G with lower bound of K_{ij}
$K_{31} = 0.529$	0.6527	−0.5556			
$K_{32} = 0.325$	0.8774	0.1307			
$K_{43} = -0.361$	0.404	0.1401	0.0085	−0.4818	0.2028
$K_{53} = -0.329$	−0.2753	−0.5409			
$K_{54} = 0.951$	0.9616	−0.3163			

$G = \mathrm{Det}\, K_{ij}$.

Table 3
Correlation matrix for Pu-239 resonance parameters

Resonance parameter	Error (%)	Γ_n	Γ_γ	Γ_f
Γ_n	5.48	1.0		
Γ_γ	5.99	0.184	1.0	
Γ_f	5.08	0.949	0.422	1.0

Table 4
Upper and lower bounds for the correlation coefficients for the non-diagonal elements (third row) of Table 3 and the value of the respective determinant

Value of K_{ij} from Table 3	Upper bound of K_{ij}	Lower bound of K_{ij}	G with K_{ij} as in Table 1	G with upper bound of K_{ij}	G with lower bound of K_{ij}
$K_{31} = 0.949$	0.968	−0.813	0.034	− 0.032	0.327
$K_{32} = 0.422$	0.484	−0.135			

$G = \mathrm{Det}\, K_{ij}$.

4. Results and discussions

In order to simulate resonance parameters with reduced systematic uncertainty, we choose all those correlated non-diagonal elements having correlation coefficient more than 30%. Hence, in Table 1 the elements of the correlation matrix having more that 30% are K_{31}, K_{32}, K_{43}, K_{53} and K_{54} for the U-235 and K_{31}, K_{32} in Table 3 for Pu-239. The corresponding values of the upper and lower bounds are depicted in Tables 2 and 4, respectively.

According to Hadamard's inequality, the maximum value of the determinant is the product of the diagonal elements and its value is 1 in both Table 1 and in Table 3. Hence, any value of the determinant closer to 1 is equivalent to minimizing the correlation among the resonance parameters. The values of the determinant with the above chosen non-diagonal elements of Tables 1 and 3 replaced by the respective lower bound values is 0.2028 and 0.327, respectively. On comparing these values with the values of the determinant with the existing elements, we find the determinant of the lower bound values to be higher. We have thus provided a unique approach using information theory where by we can simulate robust resonance parameters with minimized systematic uncertainty by using the lower bound values of the respective correlated elements.

5. Critical analysis of usefulness of mutual information

Common errors are the main cause of correlations between experimental results. Correlation between the uncertainties can greatly influence the final uncertainty in the resultant parameters of interest. All the earlier attempts

on minimization of uncertainty relied on the minimization of standard deviation (Ronen, 1984) or estimation of only the upper bound values (Ronen, 1985). Minimization of only the uncorrelated uncertainty component due to marvelous counting statistics will cause problems due to shape inconsistencies with other data sets (Tagesan, 1993). Even the chi-square test does not discriminate between statistical and systematic uncertainties and predict only the quality of the covariance matrix as a whole from the ratio of chi-squared divided by the degrees of freedom (Geraldo and Smith, 1990). Thus one cannot improve the quality of each element of the covariance matrix by the chi-squared test.

The determination of only the upper bound has the disadvantage that one does not know how far one is from the real value. Further, the knowledge of the upper bound alone does not minimize the correlated systematic uncertainty as evident from the determinant of the correlation matrix with the above chosen non-diagonal elements replaced by their respective upper bound values. The value of the determinant with upper bound values as depicted in Tables 2 and 4 are −0.4818 and −0.0328, respectively. These negative values suggest the dominance of the non-diagonal correlated components over the diagonal uncorrelated components. We can thus choose the lower bound values to simulate resonance parameters with reduced systematic uncertainty. The knowledge of lower bounds will help the experimentalist to reduce the systematic uncertainty by improving the quality of measurement and associated instrumentation. The method of determinant inequalities is conceptually elegant and computationally easier to implement to minimize the correlated component element by element of the correlation matrix. But such element wise processing is not feasible by principal component analysis (PCA) or by the chi-squared test. Further, compared to PCA and other related methods whose prime objective is only decorrelation, mutual information takes into account the whole structure of the correlation matrix and thus minimizes the effect of correlation rather than merely decorrelation. Further our algorithm can process correlation matrices of large dimension and hence errors due to collapsing of correlation matrices do not arise (Smith, 1987).

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