https://doi.org/10.61092/iaea.hqeg-efbt

INDC(NDS)-0750
Distr. J,NM,SD,ST

IAEA
International Atomic Energy Agency

INDC International Nuclear Data Committee

Some Algorithms for Evaluating Nuclear Data and Generating Uncertainty Covariance Matrices

E.V. Gai
Institute of Physics and Power Engineering
State Research Centre of the Russian Federation

English translation from Voprosy Atomnoi Nauki i Tekhniki,
Ser.: Yadernye konstanty 1-2 (2007) 56
Translated by IAEA/NDS

January 2018

IAEA Nuclear Data Section
Vienna International Centre, P.O. Box 100, 1400 Vienna, Austria

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International Atomic Energy Agency
Vienna International Centre
PO Box 100
1400 Vienna
Austria

Printed by the IAEA in Austria
January 2018

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ABSTRACT

Nuclear data is evaluated using a realistic covariance matrix of observable uncertainties in experimental data. This matrix is built on a model of the piecewise constant energy dependence of experimental uncertainties. Using this model least square problems can be solved without inversion of ill-conditioned matrices with a rank equal to the total number of experimental points and with inversion of a matrix with a rank equal to the number of energy zones of the function. Within the least squares approach the problem of the combined processing of already known evaluations and new experimental data is considered. The algorithm for construction of the covariance matrixes of the uncertainties of the different reactions multigroup cross sections, correlated because of the use of the same reference cross sections in the relative measurements, is described.

January 2018

Contents

1. Main steps in the evaluation of nuclear data in a model of piecewise-constant experimental uncertainties

1.1. A brute-force search for rational approximants for an entire set of experimental data (in practice, data were taken from the latest version of EXFOR, throwing out or correcting obvious errors) is used to generate a zero-order approximant of the uncorrelated experimental uncertainties (total declared error at each point is taken to be statistical). When generating a realistic uncertainty covariance matrix for an existing evaluation, a rational approximant of the evaluation is constructed as a zero-order approximation.

1.2. Studies that each have only one or two points are combined into a single composite study. For such studies it is not useful to separate out the systematic and statistical components of the errors because the sample systematic error (for example, the background) is for practical purposes statistical (uncorrelated).

1.3. Based on a visual assessment of the entire experimental data set, the energy range is divided into zones that differ according to the dispersion of the data (in relative terms).

1.4. In the single-zone model and in the multi-zone model, the average values for the relative deviation of the experimental data from the zero-order approximant are calculated for each of the studies with data in the zone in question. These values are treated as observable systematic errors in the respective studies. For each study in each zone, the variance of the experimental points relative to the approximant — shifted by the corresponding systematic error of the study in question — is treated as the variance of the statistical error of these points. If only one point in a given study is included in the zone, its total variance (the square of the deviation from the approximant) is apportioned equally between the variance of the systematic and the statistical errors.

1.5. If in the model of a given zone the observed systematic errors of several studies are close in value, their correlation is dealt with by combining some of them into composite studies and then repeating the procedure for determining the observed errors. This approach is an effective way to deal with correlations between studies without increasing the rank of the matrix of systematic errors.

1.6. For each zone, the variance in the observed systematic uncertainties in all the studies with data in the zone and their mean are estimated. Within each zone, the observed systematic errors of the various studies with data points in that zone are assumed to be independent (sample distribution with estimated variance). The mean is the bias that can be used for generating the estimate for the next approximation.

1.7. Based on analysis of previously observed single-zone systematic uncertainties of individual studies, the cross-zone covariances of the systematic uncertainties are estimated.

1.8. A covariance matrix of the actual observed experimental uncertainties is generated using estimated observed values for the single-zone variability (variances) in the systematic uncertainties (shared by all studies) and statistical uncertainties (separately for each study), and for the cross-zone covariances of the systematic uncertainties.

1.9. The iterative least squares problem is solved using the authors' experimental data sets and the estimated covariance matrix.

1.10. If one wishes to estimate uncertainties in a known evaluation (for example, from a nuclear data library) but it is not known which specific experimental data were used in the evaluation in question, the bias in the systematic errors (see 1.6) is eliminated by selecting the studies based on their observed systematic errors, and no least squares iterations are performed.

1.11. To generate covariance matrices of the uncertainties in estimated parameters, the formalism of the Fisher information matrix is used, and the approximation of the estimates using a rational function allows one to use analytical expressions for the sensitivity coefficients. Then covariance matrices of the pointwise and group-wise uncertainties are generated, again using analytical expressions. The evaluated covariance matrices of the uncertainties generated in this way relate to the selected experimental data, and not to the original complete set.

In the course of solving practical problems it was discovered that some stages of the evaluated calculations can be omitted or simplified. This concerns primarily the iterative generation of the

approximant; when generating the first-order approximant (second iteration), instead of solving the least squares problem taking into account correlations, one can construct a rational approximant of the function yielded by the zero-order approximation by properly taking into account the systematic bias. It is even easier to construct an approximant of the points taken from the experimental points by adding a zone-specific bias. The algorithm for calculating the Fisher matrix requires a rational approximant, even though for the generation of evaluated data files approximants with any bias correction may be used. In practice, one iteration is sufficient, meaning that any further improvement of the approximant can be neglected.

The evaluated covariance matrices of the uncertainties are determined mainly by the covariance matrices of the experimental uncertainties, which are generated by an algorithm that does not take into account bias. In our view, a reasonable accuracy for the determination of evaluated uncertainties would be of the order of several tens per cent. Meanwhile, iterative improvement of the approximant, like the use of different regression functions (see [1]), has an effect on uncertainties that is of the order of several per cent. For this reason, when solving many problems in which the main purpose was to generate evaluated covariance matrices of uncertainties, no iterations were performed.

2. Mathematical apparatus of the model of piecewise-constant experimental uncertainties

2.1. Notation

L – number of parameters in the evaluation (approximant)

I – number of study

N_I – number of points in study

J – total number of studies

$N = \sum_{I=1}^{J} N_I$ – total number of experimental points

K – number of energy zone

X_K – lower limit of energy zone

N_{IK} – number of points from the I-th study in the K-th zone

n_{IK} – fill-in numbers; $n_{IK} = 0$, if $N_{IK} = 0$ and $n_{IK} = 1$, if $N_{IK} > 0$

M – total number of zones (not less than one)

M_I – number of zones that include points from the I-th study

M_K – number of studies that have points in the K-th zone

$Y^I(x_i)$ – experimental value of the I-th study at point x_i

$y(x)$ – dependence to be estimated (approximant)

$\Delta Y^I(x_i) = Y^I(x_c) - y(x_i)$ – absolute discrepancy at point x_i

$\delta Y^I(x_i) = \Delta Y^I(x_i)/y(x_i)$ – relative discrepancy

$\varepsilon^I(x_i)$ – sampled absolute statistical error

$\zeta^I(x_i)$ – sampled relative statistical error, $\varepsilon^I(x_i) = y(x_i)\zeta^I(x_i)$

$\chi^I(x_i)$ – sampled absolute systematic error

$\lambda^I(x_i)$ – sampled relative systematic error, $\chi^I(x_i) = y(x_i)\lambda^I(x_i)$

λ_{IK} – sampled relative systematic error for the I-th study in the K-th zone

μ_{IK}^2 – variance in the relative statistical errors of the I-th study in the K-th zone,

$\gamma_I^2(x_i)$ – variance in the absolute statistical error of the I-th study at point x_i,

$$\gamma_I^2(x_i) = y^2(x_i)\,\mu_{IK}^2,\ X_K \le x_i < X_{K+1}$$

μ_I^2 – variance in the relative statistical errors of points in the I-th study over the entire energy range (single-zone model)

W – covariance matrix of relative systematic experimental errors
R – covariance matrix of experimental uncertainties

2.2. Evaluating systematic and statistical uncertainties in experimental data and their covariance matrices (steps 1.4–1.8)

The sample systematic error for the *I*-th study in each zone that includes points from that study is defined as follows:

$$\lambda_{IK} = \frac{\sum_i \delta Y^I(x_i)}{N_{IK}}, \tag{1}$$

summing over points within the zone. The variance in the statistical uncertainty in these same experimental data is taken to be equal to

$$\mu^2_{IK} = \frac{\sum_i (\delta Y^I(x_i) - \lambda_{IK})^2}{N_{IK} - 1}. \tag{2}$$

Eqs (17)–(18) are used if $N_{IK} > 1$. If $N_{IK} = 1$, then

$$\lambda_{IK} = \frac{\delta Y^I(x_i)}{\sqrt{2}} \tag{3}$$

and

$$\mu^2_{IK} = \frac{(\delta Y^I(x_i))^2}{2} \tag{4}$$

The average systematic uncertainty in a zone is defined as:

for $M_K > 1$ and

$$\overline{\lambda_K} = \frac{\sum_I \lambda_{IK}}{M_K} \tag{5}$$

for $M_K = 1$.

$$\overline{\lambda_K} = 0 \tag{6}$$

The elements of the covariance matrix of systematic uncertainties are evaluated based on estimates of the sample systematic uncertainties:

$$W^E_{K_1K_2} = \frac{\sum_I (\lambda_{IK_1} - \overline{\lambda_{K_1}})(\lambda_{IK_2} - \overline{\lambda_{K_2}})}{(\sum_I n_{IK_1} n_{IK_2})\left(1 - \frac{M_{K_1} + M_{K_2} - \sum_I n_{IK_1} n_{IK_2}}{M_{K_1} M_{K_2}}\right)}. \tag{7}$$

The denominator in (7) is a multiplier for $W^E_{K_1K_2}$ in the expected value of the numerator; if the denominator is zero, then $W^E_{K_1K_2}$ is taken to be zero.

Bearing in mind the limitations imposed by Peelle's pertinent puzzle and the underestimated uncertainty paradox [2], we redefine this covariance matrix as

$$W^R_{K_1K_2} = \min(W^E_{K_1K_2}, W^E_{K_1K_1}, W^E_{K_2K_2}), \tag{8}$$

and in cases where there are few studies shared between zones, i.e., if $\sum_I n_{IK_1} n_{IK_2}$ is a small number, then the following conservative estimate is used.

$$W^{PP}_{K_1K_2} = \min(W^{E}_{K_1K_1}, W^{E}_{K_2K_2}). \quad (9)$$

Under the adopted model

$$Y^I(x_i)=y(x_i)(1+\zeta^I(x_i)+\lambda^I(x_i)) \quad (10)$$

and the elements of the covariance matrix of experimental uncertainties are determined as follows:

$$R^{I_1I_2}_{ik} = y(x_i)y(x_k) < (\zeta^{I_1}(x_i) + \lambda^{I_1}(x_i))(\zeta^{I_2}(x_k) + \lambda^{I_2}(x_k)) >= y(x_i)y(x_k)\,\delta_{I_1I_2}(\delta_{ik}\mu^2_{I_1K_2} + W_{K_1K_2}), \quad (11)$$

where K_1 and K_2 are the numbers of the energy zones that include the points x_i and x_k, respectively.

The elements of the covariance matrix of systematic uncertainties have the same values for all studies. This means that the observed systematic uncertainty for a individual study in an individual zone is treated as a sample from the distribution characterized by the matrix **W**. However, for each study, only those elements of **W** used are those corresponding to energy zones with non-zero fill-in numbers for the study in question, and the corresponding matrix we denote as $\mathbf{W}^I$. Since the uncertainties in individual studies are assumed to be independent, the evaluated covariance matrix of experimental uncertainties is a block-diagonal matrix and the least squares functional is the sum of the functionals of the individual studies.

2.3. Formulating the least squares problem (steps 1.9, 1.11)

2.3.1. Least squares functional for one study

In the traditional formulation of the problem, the least squares functional for each of the studies has the form

$$S = \frac{1}{2}(\Delta\mathbf{y}^T\mathbf{R}^{-1}\Delta\mathbf{y}) \quad (12)$$

and to solve the least squares problem the covariance matrix of experimental uncertainties **R** must be inverted, which is not always possible when the number of experimental points with correlated uncertainties is large, as it is ill-conditioned. It can be shown [3] that in the model chosen by us this functional is equivalent to the functional

$$S = \frac{1}{2}(\Delta\mathbf{y}^T\mathbf{J}^{-1}\Delta\mathbf{y} - \Delta\mathbf{Z}^T\mathbf{U}^{-1}\Delta\mathbf{Z}), \quad (13)$$

where J is a diagonal matrix with elements

$$J_{ii} = \gamma^2(x_i) = y^2(x_i)\,\mu^2_{IK} \quad (14)$$

for the points from the *I*-th study in the *K*-th zone,

$$\Delta Z_{IK} = \sum_i \frac{\Delta Y^I(x_i)}{\gamma^2_I(x_i)} = \sum_i \frac{\delta Y^I(x_i)}{\mu^2_{IK}}, \quad (15)$$

for the same points, and, finally,

$$\mathbf{U} = \mathbf{W}^{-1} + \mathbf{F}^{-1} \quad (16)$$

where, for each study, $\mathbf{F}^{-1}$ is a diagonal matrix with elements

$$F_{KK}^{-1} = \frac{N_{IK}}{\mu_{IK}^2}. \tag{17}$$

When there is a large number of points with small statistical uncertainties, it turns out that the elements of matrix $\mathbf{F}^{-1}$ are orders of magnitude greater than the elements of matrix $\mathbf{W}^{-1}$, which leads to a loss of information about systematic errors. For this reason, using the matrix identity

$$\mathbf{(A^{-1} + B^{-1})^{-1} = A - A(A + B)^{-1}A}, \tag{18}$$

we transform (13) to the form

$$S = \frac{1}{2}(\Delta \mathbf{y}^T \mathbf{J}^{-1} \Delta \mathbf{y} - \Delta \mathbf{Z}^T \mathbf{F} \Delta \mathbf{Z} + \Delta \mathbf{Z}^T \mathbf{F} (\mathbf{W} + \mathbf{F})^{-1} \mathbf{F} \Delta \mathbf{Z}). \tag{19}$$

2.3.2. Complete least squares functional and information matrix

As already indicated, for each study the rank of matrix **W** is determined by the number of energy zones that include points from the study in question, and the same applies to the rank of matrix **F** and the number of dimensions of vector **Z**. From the point of view of software implementation of the algorithm it is more convenient to deal with matrices and vectors that have the same number of dimensions for all studies, and therefore we write the complete functional in the form

$$S = \sum_{I=1}^{J} \frac{1}{2}(\Delta \mathbf{y}^T \mathbf{V}^{-1} \Delta \mathbf{y} - \Delta \mathbf{Z}_I^T \mathbf{F}_I \Delta \mathbf{Z}_I + \Delta \mathbf{Z}_I^T \mathbf{F}_I (\mathbf{W}_I + \mathbf{F}_I)^{-1} \mathbf{F}_I \Delta \mathbf{Z}_I), \tag{20}$$

where the elements of the matrices and vectors are defined as follows:

$$(W_I)_{K,K_2} = W_{K,K_2} n_{IK_1} n_{IK_2} \tag{21}$$

$$(F_I)_{KK} = \frac{N_{IK}}{\mu_{IK}^2} \qquad n_{IK}=1 \tag{22}$$

$$(F_I)_{KK} = \frac{N_I}{\mu_I^2} \qquad n_{IK}=0 \tag{23a}$$

$$\Delta Z_{IK} = \sum_i \frac{\delta Y^I(x_i)}{\mu_{IK}^2} \qquad n_{IK}=1 \tag{23b}$$

$$\Delta Z_{IK} = 0 \qquad n_{IK}=0.$$

The functional (20) can be written in the form

$$S = \sum_{I=1}^{J} \frac{1}{2}(\Delta \mathbf{y}^T \mathbf{J}^{-1} \Delta \mathbf{y} - \sum_{K=1}^{M} \frac{\sum_i \delta Y^I(x_i^K) \sum_k \delta Y^I(x_k^K)}{N_{IK} \mu_{IK}^2} + \sum_{K1=1}^{M} \sum_{K2=1}^{M} \frac{\sum_i \delta Y^I(x_i^{K1}) \sum_k \delta Y^I(x_k^{K2})}{N_{IK1} N_{IK2}} ((\mathbf{W}_I + \mathbf{F}_I)^{-1})_{K1K2}) \tag{24}$$

where $Y^I(x_i^K)$ are the points from the *I*-th study that are in the *K*-th zone.
Functional (20) corresponds to a Fisher information matrix **I** [4] with matrix elements

$$I_{\alpha\beta} = \sum_{I=1}^{J} (\frac{\partial \mathbf{y}^T}{\partial p_\alpha} \mathbf{J}^{-1} \frac{\partial \mathbf{y}}{\partial p_\beta} - \frac{\partial \mathbf{Z}_I^T}{\partial p_\alpha} (\mathbf{F}_I - \mathbf{F}_I (\mathbf{W}_I + \mathbf{F}_I)^{-1} \mathbf{F}_I \frac{\partial \mathbf{Z}_I}{\partial p_\beta}), \tag{25}$$

in which, in place of the discrepancies in the experimental data that appear in functionals (20) and (24), there are the partial derivatives of the evaluation (approximants) with respect to each parameter. We recall that the parameter covariance matrix **P** is related in the following way to the Fisher information matrix:

$$V_{ik} = < \Delta y(x_i) \Delta y(x_k) > = \sum_{\alpha,\beta=1}^{M} \frac{\partial y(x_i)}{\partial p_\alpha} \frac{\partial y(x_k)}{\partial p_\beta} (\mathbf{I}^{-1})_{\alpha\beta} . \tag{26}$$

and for the covariance of the uncertainties in the evaluation at any two points we have

$$V_{ik} = < \Delta y(x_i) \Delta y(x_k) > = \sum_{\alpha,\beta=1}^{M} \frac{\partial y(x_i)}{\partial p_\alpha} \frac{\partial y(x_k)}{\partial p_\beta} (\mathbf{I}^{-1})_{\alpha\beta} . \tag{27}$$

Using (27), it is possible to generate covariance matrices of evaluated uncertainties at any number of points, including on experimental abscissas, and in any multi-group partitioning of the energy range.

3. Global characteristics of uncertainties in experimental data and uncertainties in evaluations

In [1], for any regression functions, the following relationships are obtained between the covariance matrices of experimental uncertainties and the covariance matrices of evaluated uncertainties (summing over all N experimental points):

$$Sp\mathbf{r}^{-1}\mathbf{v} = Sp\mathbf{R}^{-1}\mathbf{V} = \sum_{i,k} R^{-1}_{i,k} V_{k,i} = M \tag{28}$$

where **r** and **v** are relative covariance matrices with matrix elements

$$r_{ik} = \frac{R_{ik}}{y(x_i) y(x_k)}, \qquad v_{i,k} = \frac{V_{i,k}}{y(x_i) y(x_k)}, \tag{29}$$

and

$$\mathbf{v r^{-1} v = v,} \tag{30}$$

$$\mathbf{V R^{-1} V = V.} \tag{31}$$

In addition, for functions in which a constant factor can be distinguished as one of the parameters (for example, for any rational approximant), the following relation holds

$$P_{wr} = \frac{\sum_{i,k,l,m} r^{-1}_{i,k} v_{k,l} r^{-1}_{l,m}}{(\sum_{i,k} r^{-1}_{i,k})^2} = (\sum_{i,k} r^{-1}_{i,k})^{-1}, \tag{32}$$

and for functions with a constant shift parameter (for example, for rational functions in which numerator and denominator are of the same degree), it also holds that

$$P_{wa} = \frac{\sum_{i,k,l,m} R^{-1}_{i,k} V_{k,l} R^{-1}_{l,m}}{(\sum_{i,k} R^{-1}_{i,k})^2} = (\sum_{i.k} R^{-1}_{i,k})^{-1} . \tag{33}$$

All these relations were tested on a large number of practical and model examples.

4. Combined handling of several evaluations

Suppose that from the evaluations of several independent sets of experimental data we have the parameters of the regression functions y(x; $\mathbf{p}^k$) (same model for all sets, but different parameter values) $\mathbf{p}^k$ and their information and covariance matrices, respectively,
$\mathbf{I}^k$ and $\mathbf{P}^k = (\mathbf{I}^k)^{-1}$ $(\mathbf{P}^k{}_{\alpha\beta} = \langle \Delta p^k{}_\alpha \Delta p^k{}_\beta \rangle)$.

Then the combined evaluation is obtained by solving the least squares problem with respect to the parameters $p = (p_1,..p_\alpha,...p_L)$ for the following functional:

$$S = \sum_{k=1}^{J_J} \Delta\mathbf{p}^k \mathbf{I}^k (\Delta\mathbf{p}^k)^T , \tag{34}$$

where J_J is the number of sets being considered, the row vector $\Delta\mathbf{p}^k = (\mathbf{p}^k - \mathbf{p})$ describes the discrepancies in the parameters obtained for estimating the *k*-th set of experimental data, with respect to the true values of the parameters, and $(\Delta\mathbf{p}^k)^T$ is the corresponding column vector. The solution of the corresponding (linear!) system of equations has the form:

$$\tilde{\mathbf{p}} = (\sum_{k=1}^{J_J} \mathbf{p}^k \mathbf{I}^k)(\sum_{k=1}^{J_J} \mathbf{I}^k)^{-1} , \tag{35}$$

and the information matrix will simply be the sum of the information matrices for the individual sets:

$$\mathbf{I} = \sum_{k=1}^{J_J} \mathbf{I}^k . \tag{36}$$

The simplest example is one with only one parameter whose uncertainty has a variance equal to one for all sets. Then the combined evaluation is $p = \sum_{k=1}^{J_J} p^k / J_J$, and its mean-square uncertainty is $1/J_J$.

Expressions (34)–(36) can be obtained by writing the least square functional of the combined evaluation of the experimental data as the sum of the functionals of the independent data sets

$$S = \sum_{k=1}^{J_J} \Delta\mathbf{Y}^k (\mathbf{R}^k)^{-1} (\Delta\mathbf{Y}^k)^T , \tag{37}$$

where $\Delta\mathbf{Y}^k$ is the vector of experimental discrepancies for the *k*-th set, and $\mathbf{R}^k$ is the covariance matrix of experimental uncertainties for that set. Representing each of the partial evaluations then in the form

$$y^k = y(x) + \sum_\alpha \frac{\partial y(x)}{\partial p_\alpha} \Delta p_\alpha^k \equiv y(x) + \frac{\partial y(x)}{\partial \mathbf{p}} \Delta\mathbf{p}^k , \tag{38}$$

and the combined evaluation in the form

$$\tilde{y} = y(x) + \sum_\alpha \frac{\partial y(x)}{\partial p_\alpha} \Delta p_\alpha , \tag{39}$$

and differentiating the functional (36) with respect to the components of $\Delta\mathbf{p}$ and using the least square equations for the partial evaluations, for the parameters of the combined evaluation we obtain the equality (35), and for their uncertainties $\Delta\mathbf{p} = \tilde{\mathbf{p}} - \mathbf{p}$, we obtain

$$\Delta\mathbf{p} = \sum_{k=1}^{J_J} \Delta\mathbf{p}^k \mathbf{I}^k \mathbf{I}^{-1} . \tag{40}$$

Bearing in mind the independence of the partial evaluations, for the covariance of uncertainties in the parameters of the partial evaluations and the combined evaluation we obtain

$$\langle (\Delta\mathbf{p})^T \Delta\mathbf{p}^k \rangle = \mathbf{I}^{-1}\mathbf{I}^k \langle (\Delta\mathbf{p}^k)^T \Delta\mathbf{p}^k \rangle = \mathbf{I}^{-1} = \mathbf{P} = \langle (\Delta\mathbf{p})^T \Delta\mathbf{p} \rangle , \tag{41}$$

that is, the covariance matrices of the uncertainties in the parameters of all the partial evaluations coincide with the uncertainties for the full evaluation; the correlation matrices will differ, and the worse the partial evaluation, the lower the correlation with it.

Using (41) and assuming that all evaluations are close to the true function and therefore

$$\frac{\partial y(x)}{\partial p_\beta} = \frac{\partial y^K(x)}{\partial p_\beta}$$

(this condition was already used to derive the relations (35) and (40)), we obtain for the covariance matrix of the uncertainties in the evaluations:

$$\begin{aligned} &< \Delta y(x_i)\Delta y(x_k) >= \sum_{\alpha,\beta} \frac{\partial y(x_i)}{\partial p_\alpha}\frac{\partial y(x_k)}{\partial p_\beta} < \Delta p_\alpha \Delta p_\beta >= \\ &= \sum_{\alpha,\beta} \frac{\partial y(x_i)}{\partial p_\alpha}\frac{\partial y(x_k)}{\partial p_\beta} < \Delta p_\alpha \Delta p_\beta^K >=< \Delta y(x_i)\Delta y^K(x_k) > \end{aligned} \tag{42}$$

Thus, when dealing with independent partial evaluation, the conclusion regarding the coincidence of the covariance matrix of the complete and partial uncertainties in the evaluated parameters with the covariance matrix of the complete uncertainties carries over to the uncertainties in the evaluations themselves.

If evaluations for some sets of experimental data are to be considered together with new experimental data, it is simplest first to separately evaluate the new experimental data and then use the least squares functional (34). It is also possible to solve the least squares problem for the sum of functional (34) (only for the past evaluations) and the usual functional for the discrepancies in the new experimental data with respect to the regression function *y(x; **p**)*. The information matrix for the parameters of the combined evaluations will be the sum of the information matrices of these functionals. Since the enumeration method cannot be used for such a functional, the least squares problem, if possible, is solved in a linear approximation and the parameters of the combined evaluation **q** are expressed as follows in terms of the parameters of the old evaluation **p**, the new experimental data **Y**, the new covariance matrix of the experimental uncertainties **S**

and the new information matrix: $\mathbf{I}^{new} = \frac{\partial \mathbf{y}(\mathbf{p})}{\partial \mathbf{p}} \mathbf{S}^{-1} \frac{\partial \mathbf{y}(\mathbf{p})^T}{\partial \mathbf{p}}$

$$\mathbf{q} = \mathbf{p} + (\mathbf{Y} - \mathbf{y}(\mathbf{p}))\mathbf{S}^{-1} \frac{\partial \mathbf{y}(\mathbf{p})}{\partial \mathbf{p}} (\mathbf{I} + \mathbf{I}^{new})^{-1} . \tag{43}$$

If the evaluations of different sets are correlated (for example, through a common standard), it is necessary first to construct the covariance matrices of the parameters of the partial evaluations $\mathbf{P}^{k_1 k_2}$ Then, when constructing the covariances for the full and partial evaluations, replace Eqs (34) and (39) by

$$\tilde{\mathbf{p}} = \sum_{k_1,k_2=1}^{J_J} \mathbf{p}^{k_1} (\mathbf{P}^{k_1 k_2})^{-1} \Big(\sum_{k_3,k_4=1}^{J_J} (\mathbf{P}^{k_3 k_4})^{-1} \Big)^{-1}, \tag{44}$$

$$\Delta\tilde{\mathbf{p}} = \sum_{k_1,k_2=1}^{J_J} \Delta\mathbf{p}^{k_1} (\mathbf{P}^{k_1 k_2})^{-1} \Big(\sum_{k_3,k_4=1}^{J_J} (\mathbf{P}^{k_3 k_4})^{-1} \Big)^{-1} . \tag{45}$$

In this case, of course, relations (41) and (42) are no longer satisfied.

5. Generating covariance matrices of uncertainties in evaluated cross sections for various reactions

Let Δy^R be the absolute error, based on relative measurements, in the estimate of the absolute value of the cross section, Δy^r the absolute error in the relative measurements, Δy^s the absolute error in the standard, $f(x)$, $g(x)$, $h(x)$ the values of the respective evaluations, $f(x) = g(x)h(x)$, and $\delta y^R = \Delta y^R/f$, $\delta y = \Delta y^r/g$, and $\delta y^s = \Delta y^s/h$ the respective relative errors. If the errors in the relative measurements are not related in any way to the errors in the standard, then for the absolute errors we get

$$\Delta y^R = h\Delta y^r + g\Delta y^s = f\delta y^R = hg\delta y^r + gh\delta y^s \tag{46}$$

and the relative errors are simply added,

$$\delta y^R = \delta y^r + \delta y^s. \tag{47}$$

In this case, we have for the elements of the covariance matrices of the absolute uncertainties

$$\begin{aligned} &< \Delta y^R(x_i)\Delta y^s(x_k) >= g < \Delta y^s(x_i)\Delta y^s(x_k) >, \\ &< \Delta y^R(x_i)\Delta y^R(x_k) >= h^2 < \Delta y^r(x_i)\Delta y^r(x_k) > + g^2 < \Delta y^s(x_i)\Delta y^s(x_k) > \end{aligned} \tag{48}$$

and for the relative uncertainties

$$\begin{aligned} &< \delta y^R(x_i)\delta y^s(x_k) >=< \delta y^s(x_i)\delta y^s(x_k) >, \\ &< \delta y^R(x_i)\delta y^R(x_k) >=< \delta y^r(x_i)\delta y^r(x_k) > + < \delta y^s(x_i)\delta y^s(x_k) > \end{aligned} \tag{49}$$

Choosing the reference ordinates as parameters and considering the covariance of the errors for reference values on the abscissa, using (48)–(49) we can show that for any parametrization

$$\begin{aligned} &< \delta p_\alpha^R \delta p_\beta^s >=< \delta p_\alpha^s \delta p_\beta^s >, \\ &< \delta p_\alpha^R \delta p_\beta^R >=< \delta p_\alpha^r \delta p_\beta^r > + < \delta p_\alpha^s \delta p_\beta^s > \end{aligned} \tag{50}$$

Henceforth, covariance matrices of relative uncertainties shall be donated by **Q** with the relevant indices: *A* for an estimate based on absolute measurements, *C* for a combined estimate based on relative and absolute measurements, and other indices as introduced above. Since the errors in the standard are correlated only with the errors in the estimate based on systematic measurements, using (40) and (47) we get:

$$\mathbf{Q}^{Cs} =< (\delta\mathbf{p}^C)^T \delta\mathbf{p}^s >= \mathbf{I}^{-1}\mathbf{I}^R < (\delta\mathbf{p}^R)^T \delta\mathbf{p}^s >= \mathbf{V}(\mathbf{V}^R)^{-1}\mathbf{Q}^{ss}, \tag{51}$$

that is, a representation of the covariance matrix of the relative uncertainties in the parameters of the complete estimate and the uncertainties in the parameters of the standard, in terms of the covariance matrices of the uncertainties in the parameters of the complete estimate, in the parameters of the estimate based on relative measurements, and in the parameters of the standard. The covariances of the corresponding uncertainties at any points have the following form:

$$< \Delta y(x_i)\Delta y^s(x_k) >= \sum_{\alpha,\beta} \frac{\partial y(x_i)}{\partial p_\alpha} \frac{\partial y(x_k)}{\partial p_\beta} < \Delta p_\alpha \Delta p_\beta^s >= \sum_{\alpha,\beta} \frac{\partial y(x_i)}{\partial p_\alpha} \frac{\partial y(x_k)}{\partial p_\beta} p_\alpha p_\beta Q_{\alpha,\beta}^{Cs}. \tag{52}$$

Expressions (51) and (52) are strong, but to use them one must know the covariance matrices of the parameters.

The group average cross sections are defined as follows:

$$\bar{y}_K = \int_{x_K}^{x_{K+1}} y(x)dx \,. \tag{53}$$

The evaluation error of a group average cross section in the first-approximation based on the errors in the parameters can be written in the form

$$\Delta\bar{y}_K = \sum_{\alpha=1}^{M} \int_{x_K}^{x_{K+1}} \frac{\partial y(x)}{\partial p_\alpha} dx \Delta p_\alpha \,, \tag{54}$$

and therefore, the covariance matrix of the uncertainties in the group average cross sections has the form

$$\Delta\bar{y}_{K1}\Delta\bar{y}_{K2} = \sum_{\alpha,\beta=1}^{M} F_\alpha^{K1} F_\beta^{K2} < \Delta p_\alpha \Delta p_\beta > \,, \tag{55}$$

where

$$F_\alpha^K = \frac{1}{x_{K+1} - x_K} \int_{x_K}^{x_{K+1}} \frac{\partial y(x)}{\partial p_\alpha} dx \,. \tag{56}$$

The dimension of the covariance matrix of the uncertainties of the group average cross sections is equal to the number of groups but its rank cannot exceed the number of parameters, since, according to expression (54), the errors in the estimates of the group average cross sections are linear combinations of the parameter errors. If the number of groups and the number of parameters of the approximant coincide, then the group average cross sections are one of the possible parametrizations of the approximant and therefore the covariance matrices of their uncertainties obey relations (49) and (50).

If the number of groups is smaller than the number of parameters, we partition one of the groups into subgroups so that the strong relations (51) and (52) can be used. Next, one must move on to the original number of groups. Aggregation of a group entails summing the factors (56) and averaging the corresponding matrix elements; we will illustrate this by combining two groups (x_1,x_2) and (x_2,x_3) into one (x_1,x_3), with the condition that $x_3 - x_2 = x_2 - x_1$,

$$< \Delta\bar{y}^2 >= \sum_{\alpha,\beta=1}^{M} (F_\alpha^1 + F_\alpha^2)(F_\beta^1 + F_\beta^2) < \Delta p_\alpha \Delta p_\beta > / 4 = \frac{< \Delta\bar{y}_1^2 + \Delta\bar{y}_2^2 + 2\Delta\bar{y}_1 \Delta\bar{y}_2 >}{4} \,. \tag{57}$$

It can be shown that if the cross section in at least one of the original groups is nearly constant, its partitioning and subsequent approximate aggregation leads to relations of the form (51) and (50) for the covariance matrices of the uncertainties in the group average cross sections even in the case where the number of groups is smaller than the number of parameters of the approximant.

We obtain the same result if we represent the evaluation as a step function whose parameters (step heights) are the group average cross sections. Under this approach, using (36) for the covariance matrix of the relative uncertainties in the combined evaluations, we get:

$$\mathbf{Q}^{CC} = ((\mathbf{Q}^{AA})^{-1} + (\mathbf{Q}^{RR})^{-1})^{-1}, \tag{58}$$

and using (49), we can write

$$\mathbf{Q}^{Rs} = \mathbf{Q}^{ss} \tag{59}$$

$$\mathbf{Q}^{RR} = \mathbf{Q}^{rr} + \mathbf{Q}^{ss}. \tag{60}$$

The covariance matrix of the uncertainties in the complete evaluation of the group average cross sections and the uncertainties in the standard is given by expression (49), in which the role of the covariance matrices of uncertainties in the parameters is played by the corresponding matrices for the group average cross sections, i.e. $\mathbf{V} = \mathbf{Q}^{CC}$, $\mathbf{V}^R = \mathbf{Q}^{RR}$. Using (51), (58) and (60) and the familiar relation (18) from matrix algebra, we finally get

$$\mathbf{Q}^{CC} = \mathbf{Q}^{rr} + \mathbf{Q}^{ss} - (\mathbf{Q}^{rr} + \mathbf{Q}^{ss})(\mathbf{Q}^{AA} + \mathbf{Q}^{rr} + \mathbf{Q}^{ss})^{-1}(\mathbf{Q}^{rr} + \mathbf{Q}^{ss}) \tag{61}$$

$$\mathbf{Q}^{Cs} = \mathbf{Q}^{ss} - (\mathbf{Q}^{rr} + \mathbf{Q}^{ss})(\mathbf{Q}^{AA} + \mathbf{Q}^{rr} + \mathbf{Q}^{ss})^{-1}\mathbf{Q}^{ss}. \tag{62}$$

If the evaluations of the cross sections of two nuclides are obtained using the same standard, then their uncertainties are correlated. Using (36), for the covariance matrix for these evaluations, we get

$$\begin{aligned}\mathbf{Q}^{C_1C_2} &= <(\delta\mathbf{p}^{C_1})^T \delta\mathbf{p}^{C_2}> = \mathbf{I}_1^{-1}\mathbf{I}_1^R <(\delta\mathbf{p}^R)^T \delta\mathbf{p}^s> \mathbf{I}_2^R\mathbf{I}_2^1 = \mathbf{V}_1(\mathbf{V}_1^R)^{-1}\mathbf{Q}^{ss}(\mathbf{V}_2^R)^{-1}\mathbf{V}_2 = \\ &= \mathbf{Q}^{ss} - (\mathbf{Q}^{r_1r_1} + \mathbf{Q}^{ss})(\mathbf{Q}^{A_1A_1} + \mathbf{Q}^{r_1r_1} + \mathbf{Q}^{ss})^{-1}\mathbf{Q}^{ss} - \mathbf{Q}^{ss}(\mathbf{Q}^{A_2A_2} + \mathbf{Q}^{r_2r_2} + \mathbf{Q}^{ss})^{-1}(\mathbf{Q}^{r_2r_2} + \mathbf{Q}^{ss}\} + \\ &+ (\mathbf{Q}^{r_1r_1} + \mathbf{Q}^{ss})(\mathbf{Q}^{A_1A_1} + \mathbf{Q}^{r_1r_1} + \mathbf{Q}^{ss})^{-1}\mathbf{Q}^{ss}(\mathbf{Q}^{A_2A_2} + \mathbf{Q}^{r_2r_2} + \mathbf{Q}^{ss})^{-1}(\mathbf{Q}^{r_2r_2} + \mathbf{Q}^{ss}\}\end{aligned} \tag{63}$$

6. Conclusion

The mathematical apparatus described above has been coded and tested on model problems and is successfully being used in the evaluation of nuclear data. In practice, the maximum number of parameters of the regression function was 40, the maximum number of experimental studies was 75, and the maximum number of experimental points in the least squares functional was 4000 (in some cases, following preliminary processing of studies with many thousands of points). The evaluations of nuclear data and the covariance matrices of their uncertainties are stable with respect to changes, within reasonable limits, in the number of parameters, with respect to the number of energy zones and with respect to the choice of a conservative or realistic version of the covariance matrix of the observed experimental uncertainties, despite the fact that when the approximant has a large number of parameters some of them can only be determined with very large uncertainty.

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Nuclear Data Section
International Atomic Energy Agency
Vienna International Centre, P.O. Box 100
A-1400 Vienna, Austria

E-mail: nds.contact-point@iaea.org
Fax: (43-1) 26007
Telephone: (43-1) 2600 21725
Web: http://www-nds.iaea.org