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# GENERATION OF THE COVARIANCE MATRIX FOR A SET OF NUCLEAR DATA PRODUCED BY COLLAPSING A LARGER PARENT SET THROUGH THE WEIGHTED AVERAGING OF EQUIVALENT DATA POINTS

D.L. SMITH

*Applied Physics Division, Argonne National Laboratory, Argonne, IL 60439, USA*

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A method is described for generating the covariance matrix of a set of experimental nuclear data which has been collapsed in size by the averaging of equivalent data points belonging to a larger parent data set. It is assumed that the data values and covariance matrix for the parent set are provided. The collapsed set is obtained by a proper weighted-averaging procedure based on the method of least squares. It is then shown by means of the law of error propagation that the elements of the covariance matrix for the collapsed set are linear combinations of elements from the parent set covariance matrix. The coefficients appearing in these combinations are binary products of the same coefficients which appear as weighting factors in the data collapsing procedure. As an example, the procedure is applied to a collection of recently-measured integral neutron-fission cross-section ratios.

## 1. Introduction

In any experiment it is advisable to measure a particular quantity several times whenever possible. These distinct but equivalent measurements ought to be performed under somewhat different conditions, thereby providing an opportunity for identifying possible sources of systematic error. When several distinct quantities are measured, e.g., a nuclear-reaction cross section ratio at several energies, the outcome of the experiment will then be several distinct sets of values, with all the values in any one set being equivalent to each other. A thorough analysis of the uncertainties of the experiment will lead to a covariance matrix applicable to the entire data set (prior to collapsing through the averaging process). For reporting purposes, or for subsequent analyses, it may very well be desirable to appropriately average all equivalent quantities (e.g., all measured cross section values corresponding to a particular energy) and thus summarize the results of the experiment by presenting only a single value for each distinct physical entity. When this is done, it becomes necessary to derive a corresponding covariance matrix for the collapsed data set.

The objective of the present investigation is the development of a method for accomplishing this task. The formalism, which is based on the method of least squares and the law of error propagation [1-5], is discussed in section 2, and an example is provided in section 3 to demonstrate the method.

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## 2. Formalism

Let $x$ and $\mathbf{V}_x$ be the parent experimental data set vector and its corresponding symmetric covariance matrix. The objective is to collapse this data set to one of smaller size by averaging equivalent elements $x_j$ of $x$. This exercise will produce a new data set vector designated as $y$. It is desired to develop a rigorous method for obtaining both $y$ and its corresponding symmetric covariance matrix $\mathbf{V}_y$.

For the present, assume that the relationship between $y$ and $x$ is known. That is, assume that the functional expressions are established and that they can be summarized by the set of equations

$$y = y(x). \tag{1}$$

If the set $x$ has size $n$ and the collapsed set $y$ has size $m$ $(m < n)$, then eq. (1) can be written in the more explicit form

$$y_\alpha = y_\alpha(x_1, x_2, \dots, x_j, \dots, x_n) \quad (\alpha = 1, m). \tag{2}$$

In reality, a particular element $y_\alpha$ of $y$ will probably not depend functionally upon all of the elements of $x$, but rather only on a subset which can be designated by $x_j \in \{\alpha\}$. For present purposes, any particular $x_j$ is assumed to be associated with only one subset $\{\alpha\}$, i.e., with only one element $y_\alpha$ of $y$. Thus, eq. (2) can be more appropriately expressed as

$$y_\alpha = y_\alpha(x_j \in \{\alpha\}) \quad (\alpha = 1, m). \tag{3}$$

The law of error propagation [1–5] states that the relationship between $\mathbf{V}_y$ and $\mathbf{V}_x$ is defined by the general matrix formula

$$\mathbf{V}_y = \mathbf{T}^+ \mathbf{V}_x \mathbf{T}. \tag{4}$$

where $\mathbf{T}$ is called the transformation matrix. The superscript "+" indicates matrix transposition. Since the dimensions of $\mathbf{V}_x$ and $\mathbf{V}_y$ are $(n, n)$ and $(m, m)$, respectively, $\mathbf{T}$ has the dimension $(n, m)$. The elements of $\mathbf{T}$ are partial derivatives, i.e.,

$$(\mathbf{T})_{\alpha j} = (\partial y_\alpha / \partial x_j) \quad (\alpha = 1, m \text{ and } j = 1, n). \tag{5}$$

Eq. (4) is derived using the basic definition of the covariance matrix for a multivariate probability density function and first-order Taylor-series expansions of the functional relationships between the elements of $y$ and those of $x$. If these relationships are nonlinear, then the validity of eq. (4) depends upon the elements of $x$ having small variances. In practice, the variances associated with $x$ will generally be small enough so that this is not an issue. Furthermore, in all cases of interest for present purposes it happens that the functional relationships are actually linear. Consequently, the small-variance condition is irrelevant.

From eqs. (1)–(5), and related definitions in the preceding paragraph, it is evident that the elements of $\mathbf{V}_y$ are given in terms of the elements of $\mathbf{V}_x$ by the expression

$$(\mathbf{V}_y)_{\beta\alpha} = \sum_{x_i \in \{\beta\}} \sum_{x_j \in \{\alpha\}} (\partial y_\beta / \partial x_i)(\mathbf{V}_x)_{ij} (\partial y_\alpha / \partial x_j). \tag{6}$$

For convenience, let the coefficient $B_{\alpha j}$ represent the partial derivative indicated in eq. (5). Obviously the elements of $\mathbf{V}_y$ are linear combinations of the elements of $\mathbf{V}_x$, and the coefficients involved in these combinations are binary products of the coefficients $B_{\alpha j}$. That is,

$$(\mathbf{V}_y)_{\beta\alpha} = \sum_{x_i \in \{\beta\}} \sum_{x_j \in \{\alpha\}} B_{\beta i} B_{\alpha j} (\mathbf{V}_x)_{ij}. \tag{7}$$

Next, attention must be given to the task of developing the appropriate formulas for collapsing the data set $x$ to form the set $y$. In other words, the form of the functional relationship implied by eq. (3) must be established. The method to be used resembles the approach which is commonly employed in converting fine-group structures to coarser-group structures in nuclear-reactor-technology applications, e.g., in the NJOY group-cross-section processing procedures developed by Muir and MacFarlane [6]. In these applications, the collapsing process employs as its principal constraint the conservation of neutron fluence throughout the group-conversion process. Consequently, the collapsed group-cross-section sets which result are found to be weighted by the group parameters of the neutron spectrum that is involved in the analysis. The present situation is somewhat different since the matter of a neutron spectrum (with its attendant constraint of fluence conservation) does not enter into consideration. Nevertheless, in forming the elements of $y$, attention does have to be given to the proper weighting of the elements of $x$ which enter into the analysis. The method of choice here is that of least squares. The justification for this approach is discussed elsewhere [4,7] and will not be pursued further in this paper.

Some notation is now introduced. Let $n_\alpha$ $(n_\alpha > 1)$ represent the number of elements $x_j$ of $x$ (i.e., the set $x_j \in \{\alpha\}$) which are to be averaged to form the element $y_\alpha$ of $y$. Furthermore, let the vector $\boldsymbol{x}_\alpha$ of dimension $(n_\alpha, 1)$ explicitly represent this collection of $x_j$. For convenience, envision grouping the elements of $x$ so that it can be represented as a collection of subvectors, with $\boldsymbol{x}_\alpha$ being a typical member of that collection. The notation $\mathbf{V}_{x\alpha}$ is chosen to designate the covariance matrix for $\boldsymbol{x}_\alpha$. Quite clearly, $\mathbf{V}_{x\alpha}$ is a submatrix of $\mathbf{V}_x$ with dimension $(n_\alpha, n_\alpha)$ which is located along the diagonal. Furthermore, let $\boldsymbol{A}_\alpha$ be a vector of dimension $(n_\alpha, 1)$, all of whose elements are unity. Then, according to ref. [7], the value for $y_\alpha$ which corresponds to the least-squares solution is obtained using the formulas

$$y_\alpha = \mathbf{C}_\alpha \boldsymbol{A}_\alpha^+ \mathbf{V}_{x\alpha}^{-1} \boldsymbol{x}_\alpha, \tag{9}$$

$$\mathbf{C}_\alpha = \left(\boldsymbol{A}_\alpha^+ \mathbf{V}_{x\alpha}^{-1} \boldsymbol{A}_\alpha\right)^{-1}. \tag{10}$$

The superscript "−1"designates matrix inversion. It is evident that $\mathbf{C}_\alpha$ is a matrix with dimension (1, 1), i.e., a constant. In fact, it is just the variance of $y_\alpha$, more commonly designated by var($y_\alpha$). The variance, of course, is the square of the standard deviation.

It is convenient to define a vector $\boldsymbol{B}_\alpha$ of dimension $(n, 1)$ according to the formula

$$\boldsymbol{B}_\alpha = \left(\mathbf{C}_\alpha \boldsymbol{A}_\alpha^+ \mathbf{V}_{x\alpha}^{-1}\right)^+. \tag{11}$$

Then, eq. (9) can be written in the form

$$y_\alpha = \boldsymbol{B}_\alpha^+ \boldsymbol{x}_\alpha = \sum_{x_j \in \{\alpha\}} B_{\alpha j} x_j, \tag{12}$$

where the elements of $\boldsymbol{B}_\alpha$ are designated as $B_{\alpha j}$ for simplicity, Thus it is evident that the elements of $y$ and $x$ are linearly related. The analytic procedure for determining $y_\alpha$ which is described here must be repeated for all the other elements of $y$, e.g., for $y_\beta$. In summary, the coefficients $B_{\alpha j}$, which are needed both to determine the elements of the collapsed data vector $y$ and of its covariance matrix $\mathbf{V}_y$ according to eqs. (12) and (7), respectively, are deduced from eq. (11).

In practice, considerable care is required in executing this procedure. In particular, if the values $x_j$ which are averaged to form a particular element $y_\alpha$ are seriously discrepant, i.e., they scatter much more than would be indicated by the covariance submatrix $\mathbf{V}_{x\alpha}$, then the method described here will very likely produce dubious results. A simple numerical test can be applied to determine whether the input data which are averaged are indeed discrepant [4,7]. After the solution $y_\alpha$ has been obtained, the quantity $\chi^2_\alpha$ (called the chi-square) given by the formula

$$\chi^2_\alpha = (x_\alpha - y_\alpha A_\alpha)^+ \mathbf{V}_{x\alpha}^{-1} (x_\alpha - y_\alpha A_\alpha) \tag{13}$$

is calculated. If the input data are consistent, then $\chi^2_\alpha/(n_\alpha - 1) \leq 1$ will be obtained. However, if $\chi^2_\alpha/(n_\alpha - 1) \gg 1$, then the input data are discrepant. Various approaches for dealing with discrepant data have been suggested in the literature, but in the final analysis there appears to be no entirely satisfactory way to deal with such discrepancies other than to identify their origins and thereby eliminate them by the application of suitable corrections (e.g., refs. [4,5,7]). Discussion of this issue is, however, beyond the scope of the present investigation.

## 3. An example

In order to demonstrate the procedure described in section 2, consideration is given here to a set of integral neutron-fission cross-section ratio data measured in this laboratory [8]. In this experiment, the ratios were measured in the neutron spectrum produced by bombarding a thick beryllium-metal target with 7 MeV deuterons. The deposits of fissionable material used in the experiment were evaporated onto thin metal plates, and these were placed back-to-back in a low-mass fission detector for the irradiations. Ultimately, a measured value for every included integral fission cross-section ratio was obtained with the detector positioned at each of two distinct distances from the neutron source. In this example, only four of these measured ratios are treated. One pair of these ratios involves neutron fission of $^{232}$Th and $^{235}$U ($^{232}$Th/$^{235}$U). The other pair involves neutron fission of $^{237}$Np and $^{235}$U ($^{237}$Np/$^{235}$U). The equivalent ratios (measured at the two distinct distances) are averaged to collapse the four-component parent data set to two final values. The properties of the parent data set which are needed for this analysis appear in table 1.

Since this example involves only the averaging of pairs of values, the expressions used in the calculations are quite simple. It is instructive to present these formulas in explicit detail:

$$y_1 = B_{11}x_1 + B_{12}x_2, \tag{14}$$

$$y_2 = B_{23}x_3 + B_{24}x_4, \tag{15}$$

$$\mathrm{var}(y_1) = (\mathbf{V}_y)_{11} = B_{11}^2 V_{12} + 2B_{11}B_{12}V_{21} + B_{12}^2 V_{22}, \tag{16}$$

Table 1

Properties of the parent data set of measured integral neutron-fission cross-section ratios [a]

| Data point index $i$ | Experimental ratio | Measured value $x_i$ | Standard deviation in $x_i$ (%) |
|---|---|---|---|
| 1 | $^{232}$Th/$^{235}$U | 0.09727 | 2.452 |
| 2 | $^{232}$Th/$^{235}$U | 0.09792 | 2.462 |
| 3 | $^{237}$Np/$^{235}$U | 1.252 | 2.110 |
| 4 | $^{237}$Np/$^{235}$U | 1.261 | 2.617 |

*Correlation matrix*

| | 1 | 2 | 3 | 4 |
|---|---|---|---|---|
| 1 | 1 | | | |
| 2 | 0.8666 | 1 | | |
| 3 | 0.3481 | 0.4005 | 1 | |
| 4 | 0.3242 | 0.3950 | 0.7028 | 1 |

[a] For clarity, the covariance information is presented in terms of standard deviations (in percent) and the correlation matrix.

$$\mathrm{var}(y_2) = (\mathbf{V}_y)_{22} = B_{23}^2 V_{33} + 2B_{23}B_{24}V_{43} + B_{24}^2 V_{44}, \tag{17}$$

$$\mathrm{cov}(y_2, y_1) = (\mathbf{V}_y)_{21} = B_{11}B_{23}V_{31} + B_{11}B_{24}V_{41} + B_{12}B_{23}V_{32} + B_{12}B_{24}V_{42}, \tag{18}$$

$$B_{11} = (V_{22} - V_{21})/(V_{11} + V_{22} - 2V_{21}), \tag{19}$$

$$B_{12} = (V_{11} - V_{21})/(V_{11} + V_{22} - 2V_{21}), \tag{20}$$

$$B_{23} = (V_{44} - V_{43})/(V_{33} + V_{44} - 2V_{43}), \tag{21}$$

$$B_{24} = (V_{33} - V_{43})/(V_{33} + V_{44} - 2V_{43}), \tag{22}$$

Table 2

Properties of the collapsed integral neutron-fission cross-section ratio data set which is derived by the weighted averaging of pairs of equivalent values from the parent set (table 1) [a]

| Data point index $\alpha$ | Experimental ratio | Average value $y_\alpha$ | Standard deviation in $y_\alpha$ (%) |
|---|---|---|---|
| 1 | $^{232}$Th/$^{235}$U | 0.097569 | 2.374 |
| 2 | $^{237}$Np/$^{235}$U | 1.2534 | 2.089 |

*Chi-square values*

$\chi_1^2 = 0.1482$

$\chi_2^2 = 0.1443$

*Correlation matrix*

| | 1 | 2 |
|---|---|---|
| 1 | 1 | |
| 2 | 0.4006 | 1 |

[a] For clarity, the covariance information is presented in terms of standard deviations (in percent) and the correlation matrix.

The notation used in these formulas is consistent with section 2, except that $V_{ij}$ is employed as a convenient representation for the covariance matrix element $(\mathbf{V}_x)_{ij}$.

The numerical results from this analysis appear in table 2. An investigation was made of the consistency of the input data for this example using the chi-square formula (eq. (13)). It was found (see table 2) that the input data are very consistent. In this example the averaging process does not lead to a significant reduction in the ratio errors because the error correlations for the equivalent measured values in the parent set are substantial (see table 1). This implies that the systematic error sources, which cannot be reduced by averaging, are dominant.

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## References

[1] E. Parzen, Modern Probability Theory and Its Applications (Wiley, New York, 1960).
[2] J.E. Freund, Mathematical Statistics (Prentice-Hall, Englewood Cliffs, NJ, 1962).
[3] W. Mendenhall, Introduction to Probability and Statistics (Wadsworth, Belmont, CA, 1967).
[4] D.L. Smith, ANL/NDM-62, Argonne National Laboratory (1981).
[5] W. Mannhart, PTB-FMRB-84, Physikalisch-Technische Bundesanstalt (1981).
[6] D.W. Muir and R.E. MacFarlane, LA-9303-M, Vol. IV, Los Alamos National Laboratory (1985).
[7] B.P. Evain, D.L. Smith and P. Lucchese, ANL/NDM-89, Argonne National Laboratory (1985).
[8] Y. Watanabe, J.W. Meadows and D.L. Smith, to be published.