

**GENERATION OF COVARIANCE DATA AMONG
VALUES FROM A SINGLE SET OF EXPERIMENTS**

DONALD L. SMITH

*Engineering Physics Division, Argonne National Laboratory
9700 South Cass Avenue, Argonne, Illinois 60499, U.S.A.***ABSTRACT**

Modern nuclear data evaluation methods demand detailed uncertainty information for all input results to be considered. It can be shown from basic statistical principles that provision of a covariance matrix for a set of data provides the necessary information for its proper consideration in the context of other included experimental data and/or a priori representations of the physical parameters in question. This paper examines how an experimenter should go about preparing the covariance matrix for any single experimental data set he intends to report. The process involves detailed examination of the experimental procedures; identification of all error sources (both random and systematic), and consideration of any internal discrepancies. Some specific examples are given to illustrate the methods and principles involved.

1. Introduction

A collection of measured physical parameters is of limited value unless some specification is made of the associated errors.¹ However, mere specification of total errors for individual quantities from the collection is generally inadequate because various components of these errors can have origins common to more than one member. This important information must be conveyed. Provision of useful, reliable error information for his experimental results clearly places rather heavy demands upon an experimenter to understand and document the results, thereby revealing the intimate details of his work. Of course, such effort is clearly beneficial to the community of his peers and to posterity which must eventually pass judgment on the work. The objectives of this paper are: i) to indicate the significance of covariance information, ii) to explore the statistical origins of error formalism, iii) to discuss the details of providing such information, iv) to offer some suggestions for simplification of the process, and v) to touch upon some problem areas, e.g., discrepancies.

2. Why Covariance Information is Required

The purpose of providing error information is, quite simply, to quantify the confidence to be accorded to each data point of a set and, thereby, establish how it is to be weighted in various analyses which

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incorporate these data (e.g., in evaluations). If we possess estimates for the mean values and a covariance matrix for a set of physical quantities (i.e., the "results" of an experiment and their "errors"), then a fundamental principle of information theory² tells us that we are justified in proposing a normal (Gaussian) probability distribution to describe our current state of understanding of these physical quantities. This is a convenient result since Gaussians are simple and widely accepted localized distributions for expressing knowledge of physical quantities. Finally, there are philosophical justifications for considering errors: "...if a man will begin with certainties, he shall end in doubts; but if he will be content to begin in doubts, he shall end in certainties..." (Francis Bacon, *Novum Organum*), and "...it is only in the realm of doubt that we engage in the pursuit of truth..." (Mortimer Adler, *Six Great Ideas*).

3. Some Basic Attributes of Measurable Parameters

The entity in question should be sufficiently well defined to be acceptable as worthy of determination (e.g., speed of light, neutron total cross section of ¹²C at 2.75 MeV, monthly income of a governor from one of the 50 U.S. states, height of male U.S. citizens over age 20, etc.). All measurable parameters belong to one or the other of the following two categories: i) the quantity itself has natural variance (e.g., the weight of a Valencia orange, the height of male citizens of Paris, France, with ages exceeding 30 years, etc.) or it is assumed to have a precise and immutable value, except possibly on a cosmic time scale (e.g., mass of the proton, speed of light, reaction cross sections, etc.). The physical parameters with which we are concerned belong almost invariably in the second category. Regardless of the category to which any measurable quantity might belong, the process of measurement introduces dispersion in the outcomes and, therefore, uncertainty in our knowledge of that quantity.

4. Statistical Considerations for a Single Parameter

Let p be a single measurable quantity. We suppose that outcomes from measurements of p are governed by the univariate probability function f ³. Furthermore, we consider f to be normalized, i.e., $\int f(p)dp = 1$. Here, and in all following equations, we assume that integration extends over the range of possible values of the variable(s) of integration. The quantity $\langle p \rangle = \int pf(p)dp$ is the mean value. We assume that the value p_e from a single measurement of p is an approximation to $\langle p \rangle$, thus, $\langle p \rangle \approx p_e$. If f is fairly localized, this is the only reasonable assumption we can make when no other data are available. The variance is given by $\text{var}(p) = \int (p - \langle p \rangle)^2 f(p)dp$. Then, $\sigma_p = [\text{var}(p)]^{1/2}$ is the standard deviation, i.e., the "error" or "uncertainty" we should attribute to our measurement. Since f is generally not known, we need to estimate σ_p too. Let σ_e be that estimate, thus, $\sigma_p \approx \sigma_e$. Based on this available information, p_e and σ_e , we are justified, from information theory, in supposing that $f(p) \approx \exp[-(p - p_e)^2 / (2\sigma_e^2)] / (2\pi\sigma_e^2)^{1/2}$ is our best possible choice for f . Knowledge of f can be refined by acquisition of additional data and applications of Bayes theorem.

5. Statistical Considerations for Several Parameters

Let \underline{p} be a collection of n measured quantities, with f as the corresponding multivariate probability function governing the measurement process³. Again, assume f is normalized, i.e., $\int f(\underline{p})d\underline{p} = 1$. The quantity $\langle p_i \rangle = \int p_i f(\underline{p})d\underline{p}$, $[i=1,n]$, defines the mean value for the i -th component of \underline{p} . A single experiment yields $\underline{p}_e = (p_{e1}, p_{e2}, \dots, p_{en})$. Thus, $\langle p_i \rangle \approx p_{ei}$ is the only reasonable assumption when no other data are available to consider. We are then led to examine the quantity $\text{var}(p_i) = \langle (p_i - \langle p_i \rangle)^2 \rangle = \int (p_i - \langle p_i \rangle)^2 f(\underline{p})d\underline{p}$, $[i=1,n]$. Then, $\sigma_{p_i} = [\text{var}(p_i)]^{1/2}$, $[i=1,n]$, defines the i -th standard deviation. For the multivariate case, we also have to consider the i, j -th covariance, i.e., $\text{cov}(p_i, p_j) = \langle (p_i - \langle p_i \rangle)(p_j - \langle p_j \rangle) \rangle = \int (p_i - \langle p_i \rangle)(p_j - \langle p_j \rangle) f(\underline{p})d\underline{p}$, $[i, j=1, n; i \neq j]$. Then, the $n \times n$ array of elements, $V_{pij} = \langle (p_i - \langle p_i \rangle)(p_j - \langle p_j \rangle) \rangle$, $[i, j=1, n]$, defines the variance-covariance (or simply covariance) matrix \underline{V}_p . It provides complete "uncertainty" information for \underline{p} . Likewise, the $n \times n$ array of elements, $C_{pij} = V_{pij}/(V_{pii}V_{pjj})^{1/2}$, $[i, j=1, n]$, defines the correlation matrix \underline{C}_p . Note that $C_{pii} = 1$, $[i=1, n]$. Since f is not known, we need to estimate \underline{V}_p corresponding to our single experiment which produced \underline{p}_e . Let \underline{V}_e be that estimate. Correspondingly, one obtains the estimated correlation matrix. Thus, $\underline{V}_p \approx \underline{V}_e$ and $\underline{C}_p \approx \underline{C}_e$. Based on this available information (\underline{p}_e and \underline{V}_e , as best estimates of $\langle \underline{p} \rangle = (\langle p_1 \rangle, \langle p_2 \rangle, \dots, \langle p_n \rangle)$ and \underline{V}_p from one experiment), it is suggested that $f(\underline{p}) \approx (2\pi)^{-n/2} [\det(\underline{V}_e)]^{-1/2} \exp[-(1/2)(\underline{p} - \underline{p}_e)^* \underline{V}_e^{-1}(\underline{p} - \underline{p}_e)]$, directly from information theory ("*" implies matrix transposition). Knowledge of f can be refined by acquisition of additional data sets and applications of Bayes theorem. The emphasis in this paper is on procedures for estimating \underline{V}_e for a single data set. Attention is given primarily to those physical considerations which govern the estimation procedure, but the mathematical principles which must be observed are also indicated.

6. Law of Error Propagation

Let \underline{x} be a collection of q measurable quantities, with a $q \times q$ covariance matrix \underline{V}_x . Then, let \underline{p} be a collection of n derived quantities based on \underline{x} , namely, $p_i = p_i(\underline{x})$, $[i=1, n]$. Finally, let $T_{ki} = \partial p_i / \partial x_k$, $[i=1, n; k=1, q]$. These elements form a $q \times n$ matrix \underline{T} . Then, $\underline{V}_p = \underline{T}^* \underline{V}_x \underline{T}$ yields the covariance matrix for \underline{p} in terms of that for \underline{x} . The elements of \underline{T} are sensitivity coefficients. The expression which relates \underline{V}_p and \underline{V}_x is called the Law of Error Propagation. Actually, This transformation of \underline{V}_x to \underline{V}_p is based upon an assumption that the distribution function for \underline{x} is quite well localized and, thus, that a Taylor series expansion of p_i as a function of \underline{x} can be truncated beyond first order, i.e., that $\delta p_i \approx \sum_{k=1, q} T_{ik} \delta x_k + 0(2)$, with $0(2)$ terms being negligible. It is very important to keep in mind the fact that the relationship between \underline{p} and \underline{x} has been linearized, when considering error propagation. For very large errors, a different approach based on transformation of probability would have to be considered. Such transformations are difficult to do in analytical form for all but the simplest cases, but they can be readily handled by Monte Carlo methods.

7. Derivation of a Basic Formula Used in Constructing Estimates of Covariance Matrices for Sets of Measured Data

Suppose that a particular experiment can be characterized completely by a collection \underline{x} of q measurable quantities (distances, masses, detector yields, calibration parameters, etc.). It is important that these be viewed as the most elementary quantities of the experiment, not higher-level, derived parameters (e.g., cross sections). Let \underline{V}_x be the corresponding covariance matrix. Then, let \underline{p} represent the derived quantities (e.g., cross sections) that are functionally related to \underline{x} , i.e., $p_i = p_i(\underline{x})$, $[i=1,n]$. From error propagation we have that $\underline{V}_p = \underline{T}^* \underline{V}_x \underline{T}$, as described above. Ideally, all the components x_k of \underline{x} would be independent, yielding in a diagonal \underline{V}_x . For practical reasons, this is seldom observed. However, it is frequently the case (either rigorously or to a good approximation) that \underline{x} can be partitioned into w distinct subvectors \underline{x}_r , $[r=1,w]$, such that $\underline{x} = (\underline{x}_1, \underline{x}_2, \dots, \underline{x}_r, \dots, \underline{x}_w)$, and that these \underline{x}_r can be treated as mutually independent⁴. These w subvectors correspond to distinct attributes of the experiment. For example, typical independent attributes of a nuclear experiment are detector calibrations, geometry factors, sample masses, etc. The partitioning of \underline{x} leads to a corresponding partitioning of \underline{V}_x :

$$\underline{V}_x = \begin{bmatrix} \underline{V}_{x1} & & & & 0 \\ & \underline{V}_{x2} & & & \\ & & \dots & & \\ & & & \underline{V}_{xr} & \\ 0 & & & & \dots & \\ & & & & & \underline{V}_{xw} \end{bmatrix}$$

Thus, \underline{V}_x consists of submatrices \underline{V}_{xr} (which are not necessarily diagonal) situated along its diagonal, and zeros elsewhere. Similarly, \underline{T} can be partitioned into submatrices \underline{T}_r , which correspond to the \underline{V}_{xr} , and the remainder which is essentially without influence.

As a consequence of these assumptions, we obtain for \underline{V}_p the expression $\underline{V}_p = \underline{T}^* \underline{V}_x \underline{T} = \sum_{r=1,w} \underline{T}_r^* \underline{V}_{xr} \underline{T}_r$. It follows that the elements of \underline{V}_p are given by $V_{pij} = \sum_{r=1,w} (\underline{T}_r^* \underline{V}_{xr} \underline{T}_r)_{ij}$, $[i,j=1,n]$. Let us denote e_{ir} as the partial error in the derived quantity p_i due to the attribute r , $[i=1,n; r=1,w]$. This error has the same units as p_i . If $p_i \neq 0$, we can express the corresponding fractional error as $f_{ir} = e_{ir}/\text{abs}(p_i)$ and the percent error as $100f_{ir}$. Note that $e_{ir} \geq 0$, always. Furthermore, it is useful to define the parameter $S_{ijr} = (\underline{T}_r^* \underline{V}_{xr} \underline{T}_r)_{ij} / (e_{ir} e_{jr})$, so long as both $e_{ir} > 0$ and $e_{jr} > 0$ (as is usually the case). If either equals zero, assume that $S_{ijr} = \delta_{ij}$ (Kronecker Delta). Clearly, all the S_{ijr} are dimensionless quantities. So, we arrive at the very useful formula $V_{pij} = \sum_{r=1,w} S_{ijr} e_{ir} e_{jr}$ $[i,j=1,n]$. This formula permits us to construct quite readily the covariance matrix, \underline{V}_p , from a table of partial errors e_{ir} which are associated with each derived value p_i , $[i=1,n]$, and correspond to various independent experimental attributes, r , $[r=1,w]$. We are led here to approximate only to the extent that very rarely are complex experiments perfectly resolvable into such distinct attributes. By careful choice of \underline{p} , such approximations can usually be justified.

8. Micro Correlations and Macro Correlations

The $n \times n$ matrices, \underline{S}_r , consisting of the parameters S_{ijr} , $[i,j=1,n; r=1,w]$, clearly provide all correlations between the partial error components e_{ir} , $[i=1,n; r=1,w]$. For lack of a better term, these have been designated as micro-correlation matrices⁴. The $n \times n$ correlation matrix, \underline{C}_p , derived from \underline{V}_p , describes the correlations between the total errors of the parameter set p . For convenience, this is denoted as the macro-correlation matrix⁴. Given the partial errors, e_{ir} , $[i=1,n; r=1,w]$, and the micro-correlation matrices, \underline{S}_r , $[r=1,w]$, derivation of \underline{V}_p and \underline{C}_p is a straightforward, objective application of the formulas derived earlier. Subjectivity - when it becomes unavoidable - enters only into the estimation of e_{ir} and \underline{S}_r . In general, estimation of the component errors e_{ir} , $[i=1,n; r=1,w]$, is far less difficult than estimation of the correlations appearing in the matrices \underline{S}_r $[r=1,w]$. So, how sensitive are the elements of \underline{V}_p to ambiguities in these \underline{S}_r ? A study of this effect has been reported⁴. It was found that the sensitivity decreases with increasing w according to the factor $w^{-1/2}$, i.e., consistent with the Law of Large Numbers from statistics³.

9. Some Fundamental Constraints on Generation of Covariance Matrices for Data Sets

The method described here aims at providing for an objective determination of \underline{V}_p , based on detailed analysis of partial errors and their correlations. However, no matter how \underline{V}_p is determined, it must end up being a positive definite matrix, e.g., it cannot predict zero total error for any single data point of a set or 100% correlation between the total errors of any two particular data points. Therefore, \underline{V}_p must be tested for positive definiteness after its generation. It follows that when \underline{V}_p is positive definite, then \underline{C}_p is also. However, individual \underline{S}_r need not be positive definite. As an example, consider three data points ($n=3$) corresponding to measurements of a particular neutron activation cross section at three different energies. The activities are all measured by observing the same emitted gamma ray with one detector. Clearly, the detector calibration is the source of a fully correlated error component for these points. Thus, $S_{ijr} = 1$ for this particular r and $[i,j=1,3]$. Such a matrix \underline{S}_r is obviously not positive definite.

10. The Need for a Mathematical Model of an Experiment as a Condition for the Estimation of a Data Covariance Matrix

A mathematical model of the experiment is necessary in order for the experimenter to be able to identify the q -fold collection of characteristic parameters, \underline{x} , even if some of them remain implicit and not directly manipulated. Only if such a model is developed can the distinct, and presumably independent, attributes of the experiment be identified. These attributes are characterized by w subvectors \underline{x}_r . A model is required in order to consider (possibly implicitly) the relationships $p_i = p_i(\underline{x}_1, \underline{x}_2, \dots, \underline{x}_r, \dots, \underline{x}_w)$, $[i=1,n]$. In practice, there is usually a great deal of variability from one attribute to another in

regard to an experimentalist's understanding of the quantitative dependence of each p_i on the individual \underline{x}_r for his measurements. For example, if \underline{x}_1 relates to detector calibration, knowledge of the functional relationship between any p_i and \underline{x}_1 is generally very explicit. However, if \underline{x}_2 relates to neutron multiple scattering, the functional relationship to any p_i will likely be virtually impossible to express. Then, estimation of the partial cross errors e_{i2} , $[i=1,n]$, and the micro-correlation matrix \underline{S}_2 will be far more subjective.

11. Relative Covariance Matrix

Let \underline{V}_p be a covariance matrix for the data set p . Suppose that all $p_i > 0$, $[i=1,n]$. Then, we can define the relative covariance matrix, \underline{R}_p , by the formula $V_{pij} = p_i p_j R_{pij}$, $[i,j=1,n]$. From the basic expression for deriving V_{pij} , we have that $R_{pij} = \sum_{r=1,w} S_{ijr} (e_{ir}/p_i)(e_{jr}/p_j)$. The quantity $f_{ir} = e_{ir}/p_i$ is the fractional error in p_i . We could also work with percent errors, namely, $100f_{ir}$. Clearly, \underline{C}_p can be derived directly from \underline{R}_p . Thus, $C_{pij} = V_{pij}/(V_{pii}V_{pjj})^{1/2} = R_{pij}/(R_{pii}R_{pjj})^{1/2}$, since the factors p_i and p_j cancel. There is a very important reason why it is preferable to work with \underline{R}_p and \underline{C}_p rather than \underline{V}_p and \underline{C}_p . It has to do with an issue that has acquired the label "Peelle's Pertinent Puzzle (PPP)"⁵. It will be mentioned briefly in Section 18 of this paper.

12. Requirements for the Tabulation of Errors and Techniques for Reducing the Volume of Error Information to be Recorded

It is suggested that what ought to be required of an experimenter who reports an individual data set is that he provide a table of estimated error components (preferably fractional), as follows:

$$\begin{array}{cccccc}
 f_{11} & f_{12} & \dots & f_{1r} & \dots & f_{1w}, \\
 f_{21} & f_{22} & \dots & f_{2r} & \dots & f_{2w}, \\
 & & & \cdot & & \\
 f_{i1} & f_{i2} & \dots & f_{ir} & \dots & f_{iw}, \\
 & & & \cdot & & \\
 f_{n1} & f_{n2} & \dots & f_{nr} & \dots & f_{nw},
 \end{array}$$

plus a set of w estimated micro-correlation matrices, i.e.,

$$\underline{S}_r = \begin{pmatrix} S_{11r} & S_{12r} & \dots & S_{1jr} & \dots & S_{1nr} \\ S_{21r} & S_{22r} & \dots & S_{2jr} & \dots & S_{2nr} \\ & & & \cdot & & \\ S_{i1r} & S_{i2r} & \dots & S_{ijr} & \dots & S_{inr} \\ & & & \cdot & & \\ S_{n1r} & S_{n2r} & \dots & S_{njr} & \dots & S_{nnr} \end{pmatrix}, \quad [r=1,w].$$

Given this information, \underline{R}_p and \underline{C}_p can always be derived when needed and, if demanded, also \underline{V}_p through knowledge of p . There are opportunities to reduce the number of values f_{ij} , $[i,j=1,n]$, and S_{ijr} , $[i,j=1,n; r=1,w]$, that need to be reported. These should be exploited. Let us consider two brief examples. First, Suppose $n=10$ and $w=5$. Also, suppose that for $r=3$, f_{i3} represents a detector calibration error of 5%, regardless of the

data point, $[i=1,10]$. Then, $f_{i3} = 0.05, [i=1,10]$. One can simply express this fact. Actually, explicit tabulation of each f_{ir} , for fixed r , $[i=1,10]$, is necessary only when these errors are distinct for each i . Certain blocks of data points might have equal errors; e.g., $f_{i2} = 0.04, [i=1,3]$; $f_{i2} = 0.05, [i=4,6]$; $f_{i2} = 0.08, [i=7,10]$. Next, consider the situation above where $f_{i3} = 0.05, [i=1,10]$. Suppose this error source is attributable to a common origin which afflicts each data point in a 100%-correlated manner. Then, $S_{ij3} = 1, [i,j=1,10]$. Obviously, there is no need to write down an explicit matrix consisting entirely of "ones"! A similar approach is sometimes used to represent components of covariance matrices in the widely applied ENDF formats⁶.

Let us discuss a somewhat more detailed example to illustrate the present approach. We shall consider providing errors associated with a Ge photon detector calibration procedure⁷. The calibration is carried out using standard point gamma-ray sources situated at a distance $d \approx 20$ cm from the Ge detector. The formulas (model) used in this analysis are $C = AB\epsilon$ and $A = A_0 \exp(-\lambda t)$, where C is the gamma-ray peak count, B is the branching factor, ϵ is detector efficiency, A is the source activity at the time of the count, A_0 is the same activity at the time of source calibration, λ is the decay constant and t is the time elapsed between the source calibration and the detector calibration. The sources employed and their activities are: ^{60}Co [$3.193 \times 10^5 (\pm 0.9\%)$ on 1 February 1984], ^{137}Cs [$1.565 \times 10^5 (\pm 1.5\%)$ on 1 January 1985], and ^{152}Eu [$4.208 \times 10^5 (\pm 1.5\%)$ on 20 April 1979]. Twelve gamma-ray lines were measured and analyzed from these sources, each identified by a line number (LN). Here are the specifics:

Source	LN	Gamma-ray Energy (keV)	Gamma-ray Branch (%)
^{60}Co	1	1173	100.0
	2	1333	100.0
^{137}Cs	3	662	85.0
^{152}Eu	4	245	7.42
	5	344	26.4
	6	444	3.08
	7	779	13.0
	8	867	4.16
	9	964	14.5
	10	1086	11.8
	11	1112	13.6
	12	1408	20.7

Using this information and the observed yields of the full-energy peaks it is possible to deduce the efficiency of the detector at each of the indicated energies. The following table provides the various errors needed for a complete analysis. Associated with each data point is the line number (LN), efficiency multiplied by 10^4 (Eff), four error components ($r = 1$ to $r = 4$), and total error (Tot Err). These errors are

given in percent:

LN	Eff	r = 1	r = 2	r = 3	r = 4	Tot Err
1	3.089	0.4	0.0	0.9	0.0	1.0
2	2.783	0.4	0.0	0.9	0.0	1.0
3	5.016	0.3	0.0	1.5	0.6	1.6
4	12.69	0.2	0.1	1.5	2.1	2.6
5	9.278	0.1	0.1	1.5	1.5	2.1
6	7.337	0.4	0.1	1.5	1.6	2.2
7	4.315	0.3	0.1	1.5	1.7	2.3
8	4.031	0.4	0.1	1.5	1.3	2.0
9	3.681	0.2	0.1	1.5	1.6	2.2
10	3.320	0.3	0.1	1.5	2.2	2.7
11	3.284	0.2	0.1	1.5	1.5	2.1
12	2.683	0.2	0.1	1.5	1.3	2.0

The correlations involved can be expressed as follows: the statistical error in C is uncorrelated ($r = 1$), the half-life uncertainty is 100% correlated for all lines from the same source and uncorrelated otherwise ($r = 2$), the uncertainty in A_0 is 100% correlated for all lines from the same source and is uncorrelated otherwise ($r = 3$), and the uncertainty in B is uncorrelated for all lines from different sources and is effectively uncorrelated for ^{152}Eu lines because the errors are largely due to peak yields and, thus, are mainly statistical ($r = 4$). Combining this information according to the standard prescription given in Section 7 leads to the following macrocorrelation matrix:

	1	2	3	4	5	6	7	8	9	10	11	12
1	1											
2	.84	1										
3	0	0	1									
4	0	0	0	1								
5	0	0	0	.41	1							
6	0	0	0	.39	.48	1						
7	0	0	0	.38	.46	.44	1					
8	0	0	0	.43	.52	.50	.49	1				
9	0	0	0	.40	.48	.46	.45	.51	1			
10	0	0	0	.33	.40	.38	.37	.42	.38	1		
11	0	0	0	.41	.50	.47	.46	.52	.48	.40	1	
12	0	0	0	.44	.53	.51	.49	.56	.51	.42	.53	1

13. Objective Estimation of Errors and Correlations

Suppose we choose to fit an empirical curve to the set of detector efficiency values, with associated errors and correlations, as given in Section 12 above. The least-squares fitting process will generate a covariance matrix for the fitted parameters³. Through error propagation,

errors and their correlations for derived values at arbitrary energy points along the curve can be deduced objectively. For example, if we decide to fit the formula $\ln \epsilon = a_1 + a_2 \ln E_g$ (where ϵ is the efficiency and E_g is photon energy) to the calibration data given in Section 12, and derive efficiency (Eff) from the fitted curve at $E_g = 300, 500, 700, 900, 1100$ and 1300 keV, we obtain the following results:

ID	E_g (keV)	Eff ($\times 10^4$)	Total Error (%)
1	300	10.28	1.3
2	500	6.552	1.0
3	700	4.870	0.8
4	900	3.902	0.7
5	1100	3.270	0.7
6	1300	2.822	0.8

Associated with this solution is the error correlation matrix:

	1	2	3	4	5	6
1	1					
2	.96	1				
3	.84	.96	1			
4	.65	.83	.96	1		
5	.44	.67	.86	.97	1	
6	.26	.51	.74	.90	.98	1

Clearly this approach offers a relatively objective means for estimating errors and correlations for these derived physical results.

14. Subjective Estimation of Errors and Correlations

Often, errors and their correlations can be estimated only on rather subjective grounds. Experience is an important consideration here. Let us consider the fairly common situation where we encounter a number of small error components of complex origin. Then, it may suffice to assign as the correlations one or more of the following values, based on qualitative considerations:

S_{ijr}^*	Strength
± 1.00	Full correlation
± 0.75	Strong correlation
± 0.50	Moderate correlation
± 0.25	Weak correlation
0	Negligible correlation

* Negative values imply anti-correlation.

Another frequently observed occurrence can be illustrated by the following example. Let us suppose that a set of neutron activation cross sections has been measured in the range $E = 2-10$ MeV. Each data point has an uncertainty due to multiple scattering of $\sim 3\%$. It is reasonable to assume that the error correlation is strong for neighboring points (in neutron energy) and progressively weaker if the energy separation is large. It is not unrealistic to assume that $S_{ijr} \approx \text{abs}(E_i - E_j)/(10-2)$. This ad hoc assumption can be defended only in that it is "plausible" under the circumstances.

15. Some Typical Attributes of Neutron Nuclear Data Experiments

It was pointed out earlier that one needs to consider for each experiment the various independent or nearly independent attributes which contribute error to the results. In the case of nuclear data experiments, the following are commonly considered: i) event statistics, ii) background corrections, iii) event determination procedures, iv) event determination calibration standards, v) sample assay parameters, vi) decay activity half lives, vii) decay activity branching parameters, viii) elemental isotopic abundances, ix) geometry factors, x) neutron source parameters, xi) absolute or relative neutron fluences, xii) neutron absorption, xiii) neutron scattering, xiv) absorption and scattering of secondary radiations, and xv) standard cross sections (for ratio measurements). There are many other factors, often quite specific to particular measurement techniques, which might have to be considered in individual experiments. It is up to the responsible experimenter, who ought to be well informed about all the details of his measurement procedures, to insure that each "significant" attribute of his experiment is considered in the modeling and error analysis.

16. The Virtues of Redundancy and Data Averaging

Whenever possible, it is worthwhile incorporating as much redundancy into an experiment as time and circumstances allow. For example, the cross section at a particular energy might be measured several times, perhaps with some variations of the experimental details (sample size, geometry, etc.) in order to test for reproducibility, to uncover systematic error sources and improve statistical accuracy. Multiple values for a single physical quantity generally ought to be averaged to produce a single "best" number for reporting purposes. A procedure for doing this, with full consideration of data covariances, has been developed and reported⁸. The method involves transformation from data vector \underline{x} to a "collapsed" vector \underline{y} by least squares, and application of the law of error propagation, $\underline{V}_y = \underline{T}^+ \underline{V}_x \underline{T}$.

The process of data averaging can be thwarted by unresolved discrepancies. Actually, this procedure forces upon the experimenter the necessary discipline to face up to and, ultimately, either resolve the discrepancies, increase the errors or reject certain values. This issue is discussed in the next section.

17. Data Discrepancies

Discrepancies in data are the nemesis of all research endeavors. Evaluators must deal routinely with discrepant data from diverse experiments. For all the concern, there are no foolproof techniques for handling discrepant data. Here, we are involved with discrepancies amongst data from a single experiment. Discrepancies cannot arise in an individual experiment unless enough data are acquired to signal the presence of a systematic deviation of some result(s) from what was anticipated. For example, repeated measurements of a particular quantity under fixed conditions may lead to a flyer. Another possibility is that measurements of a physical parameter with systematic changes of a variable, e.g., cross section versus energy, may suddenly produce anomalous departure from a smooth curve trend. Discrepancies arise from two basic origins: i) systematic experimental errors or blunders, or ii) a real, but previously unanticipated physical phenomenon (e.g., discovery of an unexpected resonance). It is hard to identify the real cause in any single instance. Further investigation is usually required.

There are several ways to deal with a discrepancy. In order of descending preference they are as follows: Method 1: Identify and eliminate the source of the discrepancy. Method 2: Increase the error of the afflicted data point if the origin of discrepancy is elusive. Method 3: Average a collection of comparable values if several are available - including the discrepant value - and increase the error of the average accordingly. This effectively "dilutes" the effect of the discrepancy. Method 4: Discard the discrepant value outright. The hazard of this method is that the "discrepancy" could be indicative of new knowledge (e.g., a previously unsuspected resonance). Method 5: Keep the discrepant value and live with the full consequences without dilution.

The best way to search for the source of discrepancy (if there is one) is to examine all of the measured or standard parameters which enter into the derivation of a result, in the context of the model which is employed to compute this result and/or estimate its error. This approach will eliminate many possibilities and focus attention on a few critical areas of the experiment. The "detective" work just described may narrow the problem to a single aspect of the experiment, yet still not resolve the issue. Nevertheless, the experimenter will be in a better position to judge which of the Methods 2-5 might best be invoked in order to deal with the problem.

When a discrepancy is not outrageous, and there are several comparable data values available, then Method 3 (averaging the results and enhancing the error) is probably the best practical approach, whenever the origin of the discrepancy cannot be identified. For example, suppose there are five comparable measurements of count yield (with statistical error) as follows: Count 1 - 10250 ± 101.2 ; Count 2 - 10138 ± 100.7 , Count 3 - 9987 ± 99.9 , Count 4 - 10649 ± 103.2 ; Count 5 - 10069 ± 100.3 . Count No. 4 looks discrepant in this data collection. Let

us average the results using two methods. Method 3: $\langle N \rangle = 10213 \pm 45.2$ (0.4%), $(\chi^2/f) = 6.43$ ($f=4$), "enhanced" error = 114.6 (1.1%); Method 4: $\langle N \rangle = 10110 \pm 50.3$ (0.5%), $(\chi^2/f) = 1.22 \approx 1$ ($f=3$), "enhanced" error = 55.6 ($\sim 0.5\%$). Here, $\langle N \rangle$ signifies average counts and (χ^2/f) is the chi square per degree of freedom, a test of statistical significance. Both results are consistent with the errors of the majority of the data points. However, Method 3 is the most most conservative approach.

18. The Issue of "Peelle's Pertinent Puzzle"

Under certain conditions, covariance matrices generated directly from experimental data lead to anomalous results when employed in analyses involving the least squares method. A symptom of the problem is the emergence of values that are "too low" in evaluations of such data. The problem is particularly acute when there are seriously discrepant data but, in fact, is present to some degree under any circumstances.

For practical reasons, there is a great advantage in expressing the uncertainties for a set of experimental data in terms of a relative covariance matrix. This provides an evaluator or other user of such information with possibilities for adjusting input values (to account for revisions in the experimental data for objective reasons as well as subjective ones) in order to circumvent discrepancies. With relative covariance matrices, this can be done without altering the fundamental uncertainty information content provided by the author of the data set.

One empirical approach which has been suggested to deal with the "Peelle Puzzle" issue is to alter p and, thus, V_p , but not R_p . This may be required if there are hidden variables involved in a transformation of the raw data to derived parameters (with loss of information)⁵.

19. Summary

The formalism needed to generate the covariance matrix for an experimental data set follows from general statistical principles and application of the Law of Error Propagation. In practice, it is essential to develop a mathematical model for the experiment and identify the essentially independent attributes of the measurement process. Certain aspects of every experiment can be analyzed quite rigorously (statistics, calibration standards, etc.) while others can be approached only with considerable subjectivity (radiation absorption and scattering, etc.). One separates the various attributes of the experiment and does the best one can to attend to each distinct issue. There are certain advantages to dealing with relative covariance matrices, R_p , rather than the explicit covariance matrices, V_p , in this context. Discrepancies are the nemesis of both producers and users of nuclear data. When they occur, it is best to try to identify and eliminate them. If this is not possible, then there are some compromise approaches that can be used to dilute the negative impact.

20. References

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