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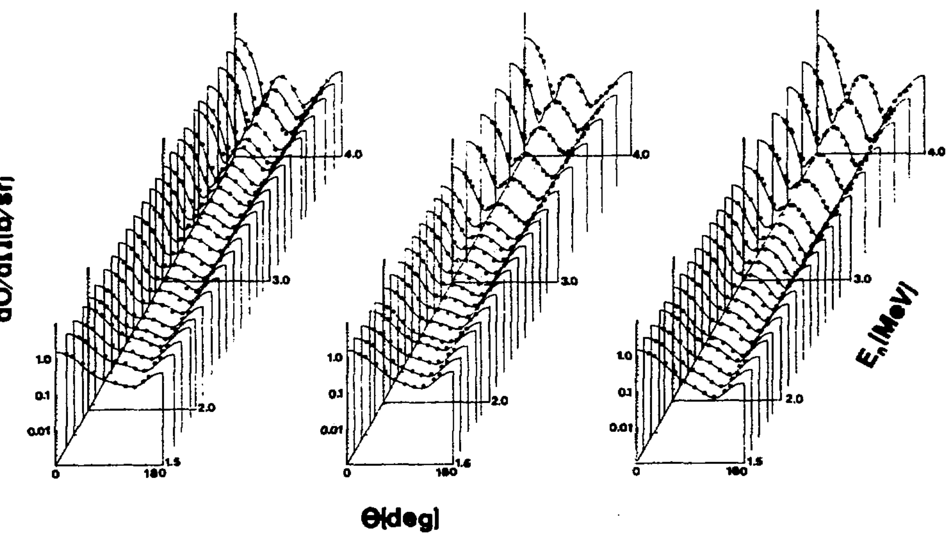
A VECTOR MODEL FOR ERROR PROPAGATION

by

D. L. Smith and L. P. Geraldo

March 1989



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ANL/NDM-110

A VECTOR MODEL FOR ERROR PROPAGATION*

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NUCLEAR DATA UNCERTAINTIES. Random variable transformations. Geometric representation of error. Error propagation. Error vectors. Error correlations. Covariance matrices.

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A VECTOR MODEL FOR ERROR PROPAGATION

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ABSTRACT

A simple vector model for error propagation, which is entirely equivalent to the conventional statistical approach, is discussed. It offers considerable insight into the nature of error propagation while, at the same time, readily demonstrating the significance of uncertainty correlations. This model is well suited to the analysis of errors for sets of neutron-induced reaction cross sections.

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I. INTRODUCTION

An investigation of uncertainty, or error as it is commonly known, involves consideration of the variances and covariances of those random variables which are employed in providing a mathematical model of the particular process under consideration. Such processes usually involve experimental measurements, but the method can also be applied to purely analytical studies. Error propagation refers to that procedure by which the errors of derived random variables are deduced from those of more basic random variables through an examination of the associated random-variable transformations. The statistical concepts and procedures involved in this endeavor are well established and widely discussed in the literature (e.g., Refs. 1-5). The objective of the present work is to describe a vector model for error propagation which is not only entirely equivalent to the statistical approach, but also provides an intuitive geometric view of the nature of error propagation. Since the law of error propagation is well established theoretically, we are justified in relaxing our concern with mathematical rigor in quest of a better conceptual understanding of this procedure. It is in this spirit that the present model of error is suggested.

In Section II, the statistical theory of error propagation is reviewed and the vector model of error is introduced. Attention is paid to the equivalence of these two error propagation formalisms. General features of the vector model are discussed in Section III, and an example is provided in Section IV to demonstrate this model's utility in practical applications. Emphasis is placed on the relationship between the orientation of the error vectors and the corresponding error correlations for those random variables used to represent the physical problem. Finally, Section V offers a few concluding remarks.

II. FORMALISM

We proceed to review the statistical basis for the law of error propagation before progressing to a discussion of the vector model. Let $\bar{x}$ be an array of n random variables, i.e.,

$$\bar{x} = (x_1, \ldots, x_i, \ldots, x_n).$$

The collection of specific values which $\bar{x}$ may assume forms an event space denoted by X. Associated with X is a joint probability function. For convenience, it is assumed here to be a continuous density function, p_X, with the usual normalization condition,

$$\int_X p_X(\bar{x})d\bar{x} = 1.$$

Knowledge of the probability permits computation of expectation, indicated by the notation <...>. For any function $Q(\bar{x})$, the expectation is calculated according to the rule

$$< Q > = \int_X Q(\bar{x})p_X(\bar{x})d\bar{x},$$

if it exists. Existence is assured if, and only if, the indicated integral is finite and there is absolute convergence, i.e.,

$$\int_X |Q(\bar{x})|p_X(\bar{x})d\bar{x}$$

is also finite. In the present development, existence of the mean values,

$$x_{i0} = < x_i >,$$

and the symmetric covariance matrix, $\bar{V}_x$, is assumed. The elements of $\bar{V}_x$ are denoted by μ_{ij} (in this paper, the range of both i and j is always 1 to n).

These elements correspond to those specific central moments of the joint probability function which are obtained using the formula

$$\mu_{ij} = < (x_i - x_{i0})(x_j - x_{j0}) >.$$

The diagonal elements,

$$\mu_{ii} = \mathrm{var}(x_i),$$

are called the variances, and the corresponding standard deviations are given by the expression

$$\sigma_{xi} = \mu_{ii}^{1/2}.$$

The associated correlation matrix, $\bar{C}_x$, has elements which are defined in terms of those of $\bar{V}_x$, according to the relationship

$$c_{xij} = \mu_{ij}/(\sigma_{xi}\sigma_{xj}).$$

Let $\bar{y}$ denote another array of m random variables ($m \le n$), i.e.,

$$\bar{y} = (y_1, \ldots, y_k, \ldots, y_m).$$

The collection of specific values which $\bar{y}$ may assume forms an event space denoted by Y. A typical variable, y_k, is derived from $\bar{x}$ through the functional relationship

$$y_k = y_k(\bar{x}).$$

This corresponds to

$$\bar{y} = \bar{y}(\bar{x})$$

in matrix notation. The transformation from X to Y is assumed to involve only continuous and differentiable functions. An expression for the elements of the corresponding covariance matrix, $\bar{V}_y$, in terms of those for $\bar{V}_x$, can be derived using statistical methodology. They are denoted by $\nu_{k\ell}$ (in this paper, the range of both k and ℓ is always 1 to m). First, an application of Taylor's Theorem produces the expression

$$y_k = y_{k0} + \sum_{i=1}^{n} (\partial y_k/\partial x_i)_0 (x_i - x_{i0}) + \text{higher-order terms}.$$

The partial derivatives are computed at the mean values and the higher-order terms are neglected because the values observed in sampling the random variables usually do not deviate widely from the mean values. Naturally, this approximation should be tested in all practical applications before utilizing the law of error propagation. If

$$x_{i0} = \langle x_i \rangle$$

is taken to be the mean value of x_i, as indicated above, it easily follows, from consideration of the rules of expectation, that the mean value of y_k is given by

$$\langle y_k \rangle = y_{k0}.$$

Simple algebra and an application of the distributive property of expectation yield the result,

$$\langle (y_k - y_{k0})(y_\ell - y_{\ell 0}) \rangle = \sum_{i=1}^{n} \sum_{j=1}^{n} (\partial y_k/\partial x_i)_0 \langle (x_i - x_{i0})(x_j - x_{j0}) \rangle (\partial y_\ell/\partial x_j)_0.$$

The quantities

$$\langle (y_k - y_{k0})(y_\ell - y_{\ell 0}) \rangle$$

are the elements of the covariance matrix $\bar{V}_y$, namely $\nu_{k\ell}$. Utilization of the notation

$$T_{ik} = (\partial y_k/\partial x_i)_0$$

leads to the expression

$$\nu_{k\ell} = \sum_{i=1}^{n} \sum_{j=1}^{n} T_{ik} \mu_{ij} T_{j\ell}.$$

In matrix notation, this becomes

$$\bar{V}_y = \bar{T}^+ \bar{V}_x \bar{T},$$

which is the most general form of the well-known statistical law of error propagation. The diagonal elements of $\bar{V}_y$,

$$\nu_{kk} = \text{var}(y_k),$$

are the variances, and the corresponding standard deviations are given by

$$\sigma_{yk} = \nu_{kk}^{1/2}.$$

The matrix $\bar{T}$, called the transformation matrix, has the dimension (n x m).

Now we turn to a description of the corresponding vector model of error propagation. Let $\bar{E}_{xi}$ be a vector defined in an abstract space which, for lack of a better expression, will be referred to here as "error space." This vector represents the error in the random variable x_i, and it has the property that its magnitude, $|\bar{E}_{xi}|$, equals the standard deviation, σ_{xi}. Likewise, let $\bar{E}_{yk}$ play the corresponding role for y_k. It is proposed that $\bar{E}_{yk}$ be generated as a linear superposition of n distinct component vectors, with the i^{th} one being proportional to $\bar{E}_{xi}$. The appropriate constant of proportionality is suggested by an examination of the transformation which maps values from X to Y. In particular, since

$$y_k = y_k(\bar{x}),$$

the variation in y_k, $(\Delta y_k)_i$, which results from a small deviation, Δx_i, of x_i relative to its mean value, x_{i0}, with the remaining random variables held constant, can be deduced from the differential sensitivity expression,

$$(\Delta y_k)_i = (\partial y_k/\partial x_i)_0 \Delta x_i.$$

Therefore, it is reasonable to conclude that the contribution to $\bar{E}_{yk}$ which can be attributed to $\bar{E}_{xi}$ should simply be

$$(\partial y_k/\partial x_i)_0 \bar{E}_{xi}.$$

This proposition leads to the expression

$$\bar{E}_{yk} = \sum_{i=1}^{n} (\partial y_k/\partial x_i)_0 \bar{E}_{xi},$$

or, in terms of the elements of $\bar{T}$, to

$$\bar{E}_{yk} = \sum_{i=1}^{n} T_{ik} \bar{E}_{xi}.$$

The collection of vector inner products,

$$\bar{E}_{xi}{}^{+}\bar{E}_{xj},$$

forms a symmetric matrix of dimension (n x n). It is completely equivalent to the covariance matrix, $\bar{V}_x$, if the following line of reasoning is pursued: The elements of $\bar{V}_x$, μ_{ij}, satisfy the relationship

$$\mu_{ij} = \sigma_{xi}\sigma_{xj}C_{xij}.$$

Furthermore, standard vector algebra yields the result

$$\bar{E}_{xi}{}^{+}\bar{E}_{xj} = |\bar{E}_{xi}||\bar{E}_{xj}|\cos\alpha_{ij} = \sigma_{xi}\sigma_{xj}\cos\alpha_{ij},$$

where α_{ij} signifies the angle between the vectors $\bar{E}_{xi}$ and $\bar{E}_{xj}$ in "error space." Complete equivalence between the statistical and the vector models of error for the random-variable set $\bar{x}$ is obtained if it is assumed that

$$\cos\alpha_{ij} = C_{xij}.$$

This assumption is a reasonable one, since it is mathematically consistent with the fundamental requirements

$$-1 \le C_{xij} \le 1 \text{ and } -1 \le \cos\alpha_{ij} \le 1.$$

Continuing this line of reasoning leads us to suspect that the (m x m) matrix formed by considering all the derived-variable error-vector inner products,

$$\bar{E}_{yk}{}^{+}\bar{E}_{y\ell},$$

is equivalent to $\bar{V}_y$. This contention is easily proved by straightforward vector algebra, i.e.,

$$\bar{E}_{yk} \cdot \bar{E}_{y\ell} = \sum_{i=1}^{n} \sum_{j=1}^{n} T_{ik}(\bar{E}_{xi} \cdot \bar{E}_{xj})T_{j\ell} = \sum_{i=1}^{n} \sum_{j=1}^{n} T_{ik}(\sigma_{xi}\sigma_{xj}\cos \alpha_{ij})T_{j\ell}$$

$$= \sum_{i=1}^{n} \sum_{j=1}^{n} T_{ik}\mu_{ij}T_{j\ell} = \nu_{k\ell}.$$

By analogy with the treatment for the primary random variables, $\bar{x}$, we observe that for the derived-variable errors,

$$\bar{E}_{yk} \cdot \bar{E}_{y\ell} = |\bar{E}_{yk}||\bar{E}_{y\ell}|\cos \beta_{k\ell} = \sigma_{yk}\sigma_{y\ell}C_{yk\ell},$$

where $C_{yk\ell}$ represents the elements of the correlation matrix $\bar{C}_y$. This preserves notational symmetry between the primary and derived random variables. The symbol $\beta_{k\ell}$ is used here to denote the angle between the error vectors $\bar{E}_{yk}$ and $\bar{E}_{y\ell}$.

III. DISCUSSION

It should be stressed again that no attempt has been made to rigorously substantiate the vector model of error which is described in the preceding section. It is apparent that the basic assumptions of this model are minimal. Furthermore, the analysis involved in providing an alternate derivation of the law of error propagation is consistent with the well-known laws of vector algebra. Let us focus now on examining the main properties of this model from a geometrical point of view.

The principal feature of this model is the assumption that the standard deviations of the primary random variables can be represented by vectors in an "error space," and that these errors are propagated to generate corresponding error vectors for the derived variables through the process of vector addition, in accordance with the fundamental principle of linear superposition. It is evident, from an examination of the conventional statistical treatment of errors, that errors add as scaler quantities only for the special case of full correlation. It is also well known that at the other extreme, namely, in the absence of correlation (e.g., for independent random variables), errors add in quadrature. Both of these fundamental properties of error propagation are clearly reproduced in the vector model. Representation of errors by vectors quite naturally leads to the interpretation of an error correlation as the cosine of the angle between the corresponding vectors. For example, the combination of two independent errors is achieved by the addition of two orthogonal vectors (i.e., $\alpha = \pi/2$, so $\cos \alpha = 0$). In purely geometrical terms, this amounts to determination of the length of the hypotenuse of a right triangle from the other two legs via addition in quadrature. While these aspects of the vector model are intuitively quite familiar, the notion of equating the collection of inner products of these error vectors to the covariance matrix is relatively novel.

The other important feature of this model is the notion that primary-variable error vectors ought to be scaled by appropriate transformation matrix elements before they are added to form error vectors for the derived variables. A plausible argument for this is presented above, but the principal motivation for this assumption is a pragmatic one: It is a necessity in order to be able to interpret the elements of $\bar{V}_y$ as inner products of the derived-variable error vectors, consistent with the procedure employed for $\tilde{V}_x$, while at the same time yielding results in agreement with those obtained from the statistical treatment of error propagation.

IV. AN EXAMPLE

A simple example is provided here to demonstrate how the vector model of error can be used in a practical situation. Let space X represent a collection of pairs of random variables,

$$\bar{x} = (x_1, x_2).$$

Assume that the corresponding mean values and standard deviations are as follows:

$$x_{10} = < x_1 > = 2,$$

$$\sigma_{x1} = 0.1 \text{ (5\% error)},$$

$$x_{20} = < x_2 > = 1,$$

$$\sigma_{x2} = 0.07 \text{ (7\% error)}.$$

Furthermore, assume that a transformation from space X to a space Y of pairs of random variables,

$$\bar{y} = (y_1, y_2),$$

is effected by the linear expressions

$$y_1 = x_1 + 2x_2 \text{ and } y_2 = 3x_1 - 4x_2$$

The transformation need not be linear, but it is taken as such in this example for the sake of simplicity. It is evident that the mean values for the derived variables are given by

$$y_{10} = < y_1 > = 4 \text{ and } y_{20} = < y_2 > = 2,$$

and the elements of the transformation matrix, $\bar{T}$, have the following values:

$$T_{11} = 1,\ T_{12} = 3,\ T_{21} = 2 \text{ and } T_{22} = -4.$$

Finally, it is assumed that the errors in x_1 and x_2 are uncorrelated. Thus,

$$C_{x12} = \cos \alpha_{12} = 0,$$

which implies that

$$\alpha_{12} = \pi/2.$$

These primary-variable errors can therefore be represented by the vectors

$$\bar{E}_{x1} = \sigma_{x1}\bar{u}_1 = 0.1\bar{u}_1 \text{ and } \bar{E}_{x2} = \sigma_{x2}\bar{u}_2 = 0.07\bar{u}_2,$$

where $\bar{u}_1$ and $\bar{u}_2$ are orthogonal unit vectors in a two-dimensional "error space," i.e.,

$$\bar{u}_1^{+}\bar{u}_1 = \bar{u}_2^{+}\bar{u}_2 = 1 \text{ and } \bar{u}_1^{+}\bar{u}_2 = 0.$$

It then follows from the formalism presented above that

$$\bar{E}_{y1} = T_{11}\bar{E}_{x1} + T_{21}\bar{E}_{x2} = T_{11}\sigma_{x1}\bar{u}_1 + T_{21}\sigma_{x2}\bar{u}_2 = 0.1\bar{u}_1 + 0.14\bar{u}_2,$$

$$\bar{E}_{y2} = T_{12}\bar{E}_{x1} + T_{22}\bar{E}_{x2} = T_{12}\sigma_{x1}\bar{u}_1 + T_{22}\sigma_{x2}\bar{u}_2 = 0.3\bar{u}_1 - 0.28\bar{u}_2.$$

The variances in y_1 and y_2 can then be computed from a knowledge of these error vectors, i.e., to three significant figures,

$$\sigma_{y1} \approx 0.172 \text{ (4.3\% error) and } \sigma_{y2} = 0.410 \text{ (20.5\% error)}.$$

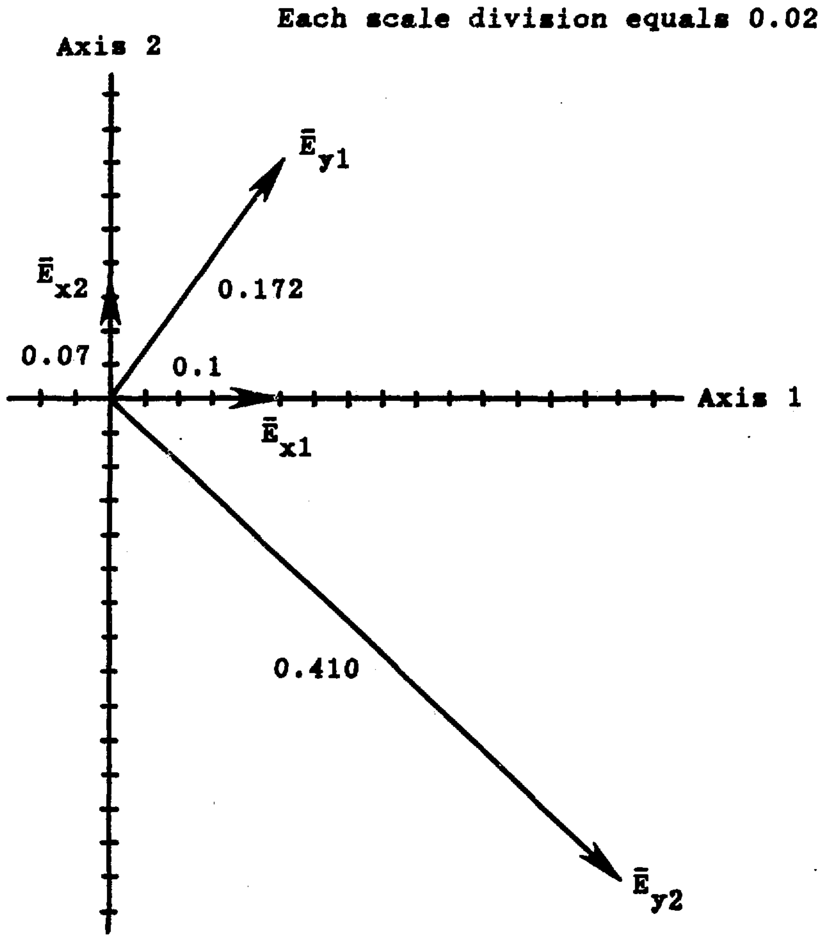
Furthermore, the derived correlation parameter is given, to three significant figures, by

$$C_{y12} = -0.130.$$

This corresponds to an angle of 97.5 degrees between the error vectors $\bar{E}_{y1}$ and $\bar{E}_{y2}$, indicating graphically that these errors are rather weakly anti-correlated. The results of this simple exercise are illustrated in Fig. 1.

V. CONCLUDING REMARKS

It is apparent that the vector model of error described in this report is well suited to the analysis of errors for experimentally determined neutron-induced reaction cross sections (e.g., Refs. 6 and 7). In practice, cross-section values for a particular neutron-induced reaction are often measured for a range of experimental conditions, e.g., at several different



Angle between $\bar{E}_{y1}$ and $\bar{E}_{y2}$ is 97.5 degrees

Angle between $\bar{E}_{x1}$ and $\bar{E}_{x2}$ is 90 degrees

Fig. 1. Error vectors for the example provided in Section IV.

neutron energies. These cross sections are derived parameters, in the sense that they are functions of such measured primary variables as neutron fluence, standard-cross-section values, detector efficiencies, radioactive-decay half-lives, branching factors, etc. Other practical uses for the vector model of error are currently being explored as part of this laboratory's on-going investigation into the nature of nuclear data uncertainties and their applications (e.g., Ref. 7).

In conclusion, we find that the vector model of error provides a convenient method for visualizing the process of propagating errors from primary random variables to derived random variables. In particular, error propagation is conveniently represented in terms of the addition of primary random-variable error vectors that are scaled by the sensitivity parameters which constitute the elements of a transformation matrix, $\tilde{T}$. Error correlations between random variables (both primary and derived) are seen to be equivalent to the cosines of angles between the corresponding error vectors in "error space".

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