

NUCLEAR DATA AND MEASUREMENTS SERIES

ANL/NDM-104

**Some Thoughts on Positive Definiteness
in the Consideration of Nuclear Data Covariance Matrices**

by

L.P. Geraldo and D.L. Smith

January 1988

**ARGONNE NATIONAL LABORATORY,
ARGONNE, ILLINOIS 60439, U.S.A.**

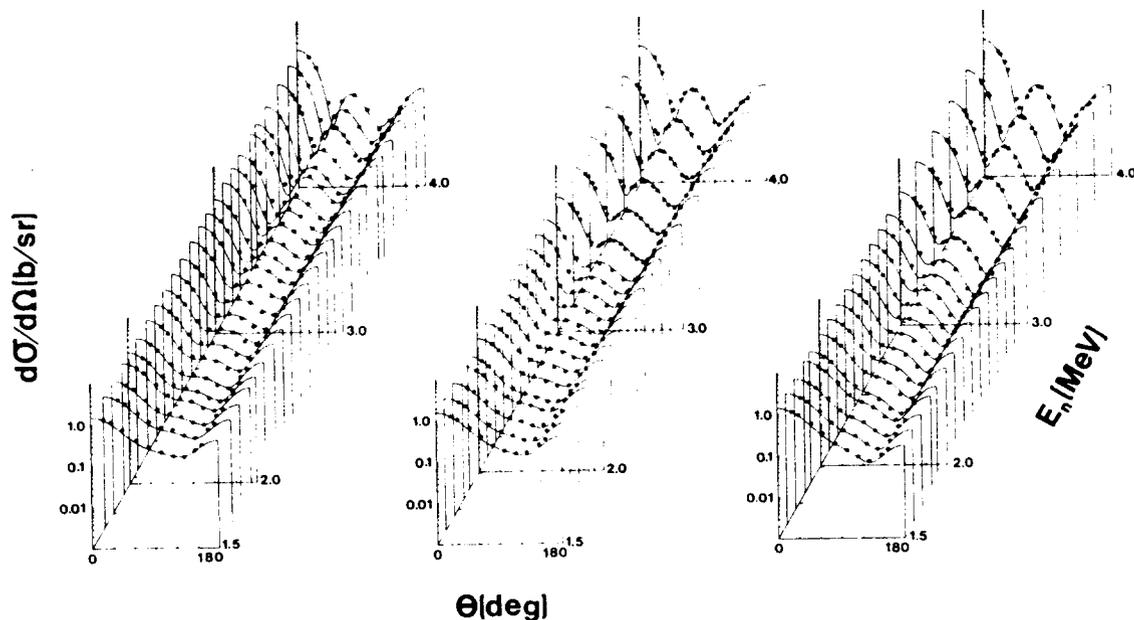
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ARGONNE NATIONAL LABORATORY, ARGONNE, ILLINOIS

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CONSIDERATION OF NUCLEAR DATA COVARIANCE MATRICES*

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NUCLEAR DATA COVARIANCE MATRICES. The nature of positive definiteness. Testing for positive definiteness. Origins of non-positive definite covariance matrices. Generation of positive definite covariance matrices. Covariances for evaluated data files.

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ABSTRACT

Some basic mathematical features of covariance matrices are reviewed, particularly as they relate to the property of positive definiteness. Physical implications of positive definiteness are also discussed. Consideration is given to an examination of the origins of non-positive definite matrices, to procedures which encourage the generation of positive definite matrices and to the testing of covariance matrices for positive definiteness. Attention is also given to certain problems associated with the construction of covariance matrices using information which is obtained from evaluated data files recorded in the ENDF format. Examples are provided to illustrate key points pertaining to each of the topic areas covered.

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I. INTRODUCTION

Covariance matrices have gained an increasingly prominent role in nuclear data research since the 1970's, when Perey (e.g., Per75 and Per78) first undertook to acquaint the community of investigators in this field with the potential usefulness of these matrices, and the various analytical techniques associated with them, for addressing certain important technical issues which were being faced at that time. Since then considerable progress has been made in implementing covariance matrix methods in various aspects of nuclear data research. A great deal has been written about this subject, so an exhaustive compilation of references would be too extensive to include in this report. A few examples will suffice to illustrate the scope of work which has been undertaken during this period. Guides have been prepared to acquaint investigators in the field with the basic concepts (e.g., Per75, Per78, All80, Man81, Smi81). Covariance methodology has been put to work in the important area of nuclear data evaluation (e.g., Sch78, SS80, Poe81, GD81, VT81, Fro86 and M+87). Considerable progress has been made in the area of neutron dosimetry through the use of covariance matrices in spectrum unfolding applications (e.g., Per77, Gre81, Smi82b, Man87), and in reactor sensitivity studies (e.g., Pee82). Covariance methods have also found their way into routine laboratory practice (e.g., Smi82a, L+83 and SS85). Furthermore, it appears that a promising area for the application of covariance methods is in the merging of information from both experimental and theoretical origins (e.g., SG83 and KU87). In recognition of the importance of covariance matrices in various nuclear data applications, recent evaluated data file formats offer the possibility for inclusion of covariance information (e.g., for ENDF/B-V (Kin79 and KM83) this appears in File 33).

It is essential to realize that covariance matrices are introduced when statistical methods are employed in the modeling of physical phenomena (Zeh70)--namely, in the area of uncertainty. For this reason it is important to insure that the mathematical models which are developed conform to physical reality (e.g., Mue79 and C+83). It is intuitively evident that all sets of information with which one deals in practical situations involve at least some random uncertainty (Hol86), and, very likely, sources of systematic uncertainty as well. Realistic covariance matrices should reflect this fact. Covariance matrices must, therefore, be positive definite in order to represent uncertainties which are positive, not vanishing or imaginary. In fact, it is evident that investigators in this field have not always satisfied this important physical requirement in their work with covariance matrices (e.g., FH82, Man82, Nol87, Smi87b and ZN87). This issue is explored in the present report. However, it should be appreciated that this is not a trivial issue, but, rather, one with many ramifications. The intent of this paper is to report upon the results of our investigation into a few of these, and to share with the reader some of our thoughts on the subject. We have appealed more to intuition than to rigor in this

exposition, hoping thereby to encourage the reader to be aware of the general issues while, at the same time, realizing that matters of specific interest must be investigated on a case-by-case basis. We have endeavored to provide some insight and guidance on how to approach the problem of generating covariance matrices which model physical uncertainty in a consistent fashion, and on how to recognize some of the pitfalls which the reader may encounter either in his own work or in dealing with material from the literature.

Section II is devoted to a discussion of some relevant aspects of the basic theory of matrices, but emphasis there is on consideration of examples which demonstrate how covariance matrices can come to be non-positive definite. The issues are examined from a geometrical point of view, an approach which serves to emphasize the physical implications of the formalism. Procedures which, by their very nature, tend to encourage the production of covariance matrices that are positive definite are discussed in Section III, and the importance of pursuing such relatively "safe" analytical practices in nuclear data applications is stressed there. The reader should recognize, however, that we have encountered no foolproof rules to insure that manipulations involving covariance matrices won't lead to non-positive definite behavior. A closely related topic is that of managing covariance information for parameters which are formulated in group structures, particularly as regards the issue of collapsing, expanding, or merging of groups, or the merging of data from group structures with non-compatible limits through the use of union groups. A few comments are made in Section III regarding this issue, but the technical problems are complex and there are ambiguities which, we believe, will require further investigation, since it is clearly a matter of considerable importance to the field of reactor physics. Section IV deals with the matter of testing covariance matrices for positive definiteness, a process which we have discovered to be a very important one, in the light of the preceding comments. Two approaches are presented, and the associated computer programs and demonstrative examples are documented in greater detail in the appendix. Finally, Section V briefly explores the issue of covariance matrices and evaluated data files. Some problems that arise in trying to avoid generating covariance matrices that are non-positive definite from File 33 information in the ENDF/B system (Kin79 and KM83) are discussed in this context.

II. BASIC FORMALISM AND ORIGINS OF NON-POSITIVE DEFINITE MATRICES

A fundamental consideration underlying the requirement that matrices included for applications in nuclear data research be positive definite is that they are intended to represent uncertainties in real physical parameters, and these uncertainties must be positive quantities. Zero errors are pointless in the physical world, as discussed in Section I, and imaginary errors are totally unrealistic.

In this section we focus attention on this issue through the examination of some properties of symmetric quadratic forms. Such quadratic forms are most often encountered in error propagation applications and in least squares analyses. Let F be a scalar function of a collection of n random variables which can be denoted collectively by \bar{x} . Suppose that we have a covariance matrix \bar{V}_x representing the uncertainties associated with these variables and their correlations. We seek the uncertainty in the derived quantity F . In the following development we shall demonstrate how the issue of the positive definiteness of \bar{V}_x arises. There are several ways we can express the uncertainty E_F in the quantity F through utilization of quadratic forms. They are all entirely equivalent, as discussed elsewhere, e.g., in reports by Mannhart (Man81) and Smith (Smi81 and Smi87a). The following error propagation formula summarizes this point

$$[1] \quad Q_F = E_F^2 = (\bar{S} \bar{E}_x)^+ \bar{C}_x (\bar{S} \bar{E}_x) = (\bar{S} \bar{I})^+ \bar{V}_x (\bar{S} \bar{I}) = \bar{T}^+ \bar{V}_x \bar{T}.$$

Matrix multiplication is indicated in this expression, but not by means of an explicit symbol. The symbol "+" is used to denote matrix transposition. \bar{E}_x is the vector of total errors in \bar{x} ; \bar{V}_x is the covariance matrix (as mentioned above); \bar{C}_x is the corresponding correlation matrix; \bar{I} is a vector with all n elements equal to 1; \bar{T} is a vector with typical element equal to $\partial F / \partial x_i$; and \bar{S} is an $n \times n$ matrix with the following form:

$$[2] \quad \bar{S} = \begin{bmatrix} \partial F / \partial x_1 & \dots & 0 \\ 0 & \dots & \partial F / \partial x_n \end{bmatrix}$$

The information content of matrices \bar{S} and \bar{T} is identical. They are commonly referred to as sensitivity matrices. The relationship

$$[3] \quad V_{xij} = C_{xij} E_{xi} E_{xj}$$

between some of these elements is a fundamental one, and it appears often in the following discussion.

The reader is referred to treatises on matrices (e.g., Bro58) or earlier discussions of the properties of nuclear data covariance matrices (e.g., Man81 and Smi81) for tutorial material on the basic mathematics. Some of the concepts of particular importance in the present discussion are repeated here in order to clearly establish the terminology. For example, as concerns the correlation matrix \bar{C}_x values for the elements C_{xij} must fall within the closed interval $[-1,1]$. The significance of the various values of C_{xij} is as follows: = 1, complete positive correlation; = 0, no correlation; = -1, complete negative correlation (anticorrelation); > 0 but not equal to 1, partial correlation in the positive sense; and < 0 but not equal to -1, partial correlation in the negative sense (partial anticorrelation).

Eq. 1 can be rewritten without the use of matrix notation, as follows:

$$[4] \quad Q_F = E_F^2 = \sum_{i=1}^n \sum_{j=1}^n (\partial F / \partial x_i) V_{xij} (\partial F / \partial x_j) \\ = \sum_{i=1}^n \sum_{j=1}^n (\partial F / \partial x_i) E_{xi} C_{xij} E_{xj} (\partial F / \partial x_j).$$

Two other points to remember are that \bar{V}_x and \bar{C}_x are both symmetric (i.e., $V_{xij} = V_{xji}$ and $C_{xij} = C_{xji}$) and that $E_{xi} = (V_{xij})^{1/2}$.

At this point we choose to introduce a vector model which we believe will prove useful to the reader in helping to understand the concepts under consideration. Let us consider a set of vectors \bar{e}_{xi} ($i=1,n$), defined in an abstract space and having the property that their magnitudes $e_{xi} = |\bar{e}_{xi}| = |\partial F / \partial x_i| E_{xi}$. Furthermore, let \bar{E}_F be defined as the sum of these vectors, namely, $\bar{E}_F = \sum_{i=1}^n \bar{e}_{xi}$. We now demonstrate that the familiar quadratic form Q_F can be obtained from the expression

$$[5] \quad Q_F = \bar{E}_F^+ \bar{E}_F = \left(\sum_{i=1}^n \bar{e}_{xi} \right)^+ \left(\sum_{i=1}^n \bar{e}_{xi} \right) = \sum_{i=1}^n \sum_{j=1}^n \bar{e}_{xi}^+ \bar{e}_{xj}.$$

In order to achieve this, we must interpret the expression $\bar{\epsilon}_{x_i}^+ \bar{\epsilon}_{x_j}^-$ as a simple dot product of two vectors. From a rule of vector analysis, it is evident that

$$[6] \quad \bar{\epsilon}_{x_i}^+ \bar{\epsilon}_{x_j}^- = \epsilon_{x_i} \epsilon_{x_j} \cos \alpha_{ij},$$

where α_{ij} represents the "angle" between the two vectors $\bar{\epsilon}_{x_i}^+$ and $\bar{\epsilon}_{x_j}^-$ in the abstract space in which they are defined. The cosine function has the property that $-1 \leq \cos \alpha_{ij} \leq 1$, just as does the correlation coefficient $C_{x_{ij}}$. For this reason it is reasonable to treat them as equivalent, i.e., $C_{x_{ij}} = \cos \alpha_{ij}$, thereby verifying Eq. 5 through a comparison with Eq. 4. In this model, strong correlation between the uncertainties in x_i and x_j implies near colinearity between the two vectors $\bar{\epsilon}_i$ and $\bar{\epsilon}_j$ which contain information concerning the total errors and the sensitivity of the derived function F to the parameters x_i and x_j . Analogously, small correlation implies near orthogonality, while significant anticorrelation is manifested in near anti-colinearity of the vectors in question.

We now turn our attention to determining those conditions where the quadratic form Q_F , discussed above, is positive, zero, or negative. First, we note that each of the different matrix expressions for the symmetric quadratic form considered above can be viewed as a specific manifestation of the general quadratic form

$$[7] \quad Q = \bar{z}^+ \bar{M} \bar{z} = \sum_{i=1}^n \sum_{j=1}^n z_i M_{ij} z_j,$$

where Q is a scalar, \bar{M} is an $n \times n$ symmetric matrix, and \bar{z} is an $n \times 1$ matrix (vector). The determinant $\det(\bar{M}) = |\bar{M}|$ is called the discriminant of the quadratic form. The rank of the matrix \bar{M} is called the rank of the quadratic form. It gives information about the number of independent variables involved.

In general, \bar{M} will not be diagonal, but it is possible to transform Eq. 7 into an equivalent expression, namely,

$$[8] \quad Q = \bar{y}^+ \bar{D} \bar{y} = \sum_{i=1}^n \lambda_i y_i^2.$$

Here, \bar{D} is a diagonal matrix with parameters λ_i along the diagonal. The λ_i are called eigenvalues of the matrix \bar{M} . These parameters represent all the solutions to the equation $\det(\bar{M} - \lambda \bar{U}) = 0$. \bar{U} is the identity or unit matrix (an $n \times n$ matrix with ones along the diagonal and zeros elsewhere). The conversion from \bar{M} to \bar{D} is accomplished by what is known as an orthogonal transformation, using an orthogonal matrix \bar{P} , i.e.,

$$[9] \quad \bar{D} = \bar{P}^+ \bar{M} \bar{P} = \bar{P}^{-1} \bar{M} \bar{P}.$$

Note that, for an orthogonal matrix, the inverse exists and equals the transpose of the matrix. The same matrix \bar{P} defines the transformation between \bar{z} and \bar{y} , i.e., $\bar{z} = \bar{P} \bar{y}$. Summarizing, we see from basic properties of matrices that

$$[10] \quad Q = \bar{z}^+ \bar{M} \bar{z} = (\bar{P} \bar{y})^+ \bar{M} (\bar{P} \bar{y}) = \bar{y}^+ (\bar{P}^+ \bar{M} \bar{P}) \bar{y} = \bar{y}^+ \bar{D} \bar{y}.$$

The orthogonal matrix \bar{P} is formed using the normalized eigenvectors of \bar{M} as column vectors, a procedure which will be demonstrated later in this section. Therefore, to diagonalize a matrix it is enough to know the eigenvalues of that matrix. The Method of Lagrange Reduction (e.g., Ayr62 and Bra63) is often employed for this purpose in computer routines.

In Eq. 8, the number p of positive eigenvalues is called the index of the quadratic form Q . If we denote the rank of \bar{M} by r , then $(n-r)$ of the eigenvalues are zero and $(r-p)$ are negative. The usual classification of quadratic forms is given in Table 1, below (Ayr62):

Table 1

p	r	Classification
n	n	Positive definite
r	$r < n$	Positive
0	n	Negative definite
0	$r < n$	Negative
$< r$	$r \leq n$	Indefinite

It is stated in most textbooks on matrices that a matrix \bar{M} is positive definite if and only if every quadratic form as expressed in Eq. 7 is positive for every non-trivial (non-zero) vector \bar{z} . It is evident from Eq. 8 that Q is indeed positive so long as each eigenvalue $\lambda_i > 0$ ($i=1,n$), since we assume that transformation from a non-trivial \bar{z}

leads to a corresponding non-trivial \bar{y} . In summary, a matrix \bar{M} is positive definite if and only if it has rank equal to n , and all its eigenvalues are positive. In the context of the present discussion, the quadratic form is identified with the square of the error in the derived scalar quantity F . In order that this error be physically reasonable (i.e., non-zero real numbers), the covariance matrix for the set of variables \bar{x} must be positive definite. We noted earlier that this specific quadratic form Q_F can be expressed in various ways. In

particular, referring to Eq. 1, if we let $\bar{\epsilon}_x = \bar{S} \bar{E}_x$, we have

$$[11] Q_F = \bar{\epsilon}_x^+ \bar{C}_x \bar{\epsilon}_x.$$

Since this is a perfectly reasonable expression for this quadratic form, we are led to the conclusion that the correlation matrix must pass the test for positive definiteness as well as the full covariance matrix. The same can be said for the relative covariance matrix (e.g., see Smi81).

We turn next to an example which will demonstrate, in the simplest possible terms, all of the concepts developed above.

Example

Here we examine the error in the scalar quantity formed by summing two cross sections. This example is not entirely a hypothetical one since, in nuclear data research, one is quite often interested in sums of cross sections, e.g., the neutron total cross section is the sum of the partial cross sections associated with all the open interaction channels for a neutron incident upon the nucleus in question.

Suppose that σ_1 and σ_2 are the two available cross sections. For convenience we will denote as σ_T the sum, namely $\sigma_T = \sigma_1 + \sigma_2$. Rather than working with a given covariance matrix \bar{V}_σ for these two cross sections, we choose to actually construct this matrix from more fundamental considerations. Table 2, below, provides the information needed for this purpose. For simplicity we assume here that the error in each cross section arises from two sources. The first is a 1% random error while the second is a 2%, fully-correlated systematic error

affecting both values. The reader should be aware, however, that this is not the most general case one might encounter. Indeed, in practice one is normally forced to examine several sources of random (uncorrelated) and systematic (correlated) error, and treatment of partial correlations for some of these components may be necessary (Smi87a).

Table 2

Parameter	Rand. Error	Syst. Error	Total Error
σ_1	$0.01\sigma_1$	$0.02\sigma_1$	$[(0.01\sigma_1)^2 + (0.02\sigma_1)^2]^{1/2}$
σ_2	$0.01\sigma_2$	$0.02\sigma_2$	$[(0.01\sigma_2)^2 + (0.02\sigma_2)^2]^{1/2}$

We denote the total errors in σ_1 and σ_2 as E_{σ_1} and E_{σ_2} , respectively (they form the vector \bar{E}_σ). Then, according to Eq. 1, the error E_T in σ_T can be obtained, e.g., from the quadratic form $E_T^2 = (\bar{S} \bar{E}_\sigma)^T \bar{C}_\sigma (\bar{S} \bar{E}_\sigma)$, with

$$\bar{C}_\sigma = \begin{bmatrix} 1 & 0.8 \\ 0.8 & 1 \end{bmatrix} \quad \bar{S} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \quad \bar{S} \bar{E}_\sigma = \bar{E}_\sigma = \begin{bmatrix} E_{\sigma_1} \\ E_{\sigma_2} \end{bmatrix}$$

Simple matrix algebra leads to the explicit algebraic expression, $E_T^2 = E_{\sigma_1}^2 + E_{\sigma_2}^2 + 2(0.8)E_{\sigma_1}E_{\sigma_2}$, for the quadratic form, and thereby yields the desired formula for the error in the total cross section. It is instructive to produce the diagonalized version of this quadratic form, i.e., as defined in Eq. 8. To accomplish this we need to solve the equation $\det(\bar{C}_\sigma - \lambda \bar{U}) = 0$ for the roots λ_1 and λ_2 . Note that \bar{U} in this instance is a 2 x 2 unit matrix. In algebraic form the equation becomes $\lambda^2 - 2\lambda + 0.36 = 0$, and it has the roots $\lambda_1 = 0.2$ and $\lambda_2 = 1.8$. These are the eigenvalues of \bar{C}_σ and this matrix is clearly positive definite. We are thus led to the diagonalized version of the quadratic form, $E_T^2 = 0.2y_1^2 + 1.8y_2^2$.

Next we turn to the matter of computing the normalized eigenvectors of \bar{C}_σ , since we have need of them in determining the orthogonal transformation matrix \bar{P} which appears in Eqs. 9 and 10. These eigenvectors are denoted by \bar{a}_1 and \bar{a}_2 for convenience. They are obtained by finding the solutions of the matrix equations $(\bar{C}_\sigma - \lambda_1 \bar{U}) \bar{a}_1 = \bar{0}$ and $(\bar{C}_\sigma - \lambda_2 \bar{U}) \bar{a}_2 = \bar{0}$ for which $\bar{a}_1^+ \bar{a}_1 = 1$ and $\bar{a}_2^+ \bar{a}_2 = 1$, with $\bar{0}$ representing a vector with all elements equal to zero. The results are

$$\bar{a}_1 = \begin{bmatrix} (2)^{-1/2} \\ -(2)^{-1/2} \end{bmatrix} \quad \bar{a}_2 = \begin{bmatrix} (2)^{-1/2} \\ (2)^{-1/2} \end{bmatrix} \quad \bar{P} = \begin{bmatrix} \bar{a}_1 & \bar{a}_2 \end{bmatrix} .$$

From this we conclude that, in the diagonal version of the quadratic form (Eq. 8), $y_1 = (2)^{-1/2}(E_{\sigma 1} - E_{\sigma 2})$ and $y_2 = (2)^{-1/2}(E_{\sigma 1} + E_{\sigma 2})$. This concludes our detailed analysis of this particular problem.

We can obtain some feel for the meaning of eigenvalues which are positive, negative, or zero by appealing to analytic geometry. To simplify matters, we choose to limit the following discussion to three dimensions. The diagonalized quadratic form given in Eq. 8 in this special case becomes

$$[12] \quad Q = \rho^2 = \lambda_1 y_1^2 + \lambda_2 y_2^2 + \lambda_3 y_3^2 .$$

The shape of the surface generated by considering all values of the vector \bar{y} that satisfy Eq. 12 depends upon the nature of the eigenvalues. We examine several possibilities below. First, it should be noted that $Q > 0$ is assumed; otherwise, the surfaces would be degenerate. The parameter ρ serves to define the scale or extent of the surface, so we tacitly assume that $\rho > 0$ as well. For example, if $\lambda_1 = \lambda_2 = \lambda_3 = 1$, the surface is a spherical shell with radius ρ . For convenience, we assume in the following discussion that Q has a particular fixed value. Associated with this particular value of Q is a specific geometric surface. Consideration of the positive definiteness of the matrix in question is, of course, not tied to any particular value of Q (or equivalently, ρ) since any positive number may be considered. A family of surfaces therefore exists corresponding to the entire set of positive real values which Q can assume. The shapes of the surfaces described below depend on the values of Q and the eigenvalues but not on the choice of coordinate system, since the transformation which diagonalized the matrix and led to Eq. 12 is an orthogonal one. It is well known that an orthogonal transformation can be interpreted geometrically as a rotation of coordinates without any further change in the underlying metric of the parameter space.

The first case to be considered is that for which all of the eigenvalues are positive (and the associated matrix is positive definite). In general the surface is an ellipsoid, as shown in Fig. 1. Equal eigenvalues, as indicated above, imply that the solution vectors \bar{y} map out a spherical shell. For such a surface, any observer leaving the origin will not be able to find any way to "escape" the region without penetrating this surface at some point (it is therefore a completely closed surface).

If one root is negative, for instance λ_3 , then the matrix is non-positive definite and the surface represented by Eq. 12 is a hyperboloid with one sheet, as shown in Fig. 2. It is tempting to refer to this shape in contemporary terms as a "cooling tower"! In this case the axis y_3 does not intercept the surface at any real points, i.e., the surface is indefinite in that direction. An observer leaving the origin will be able to escape the region without intercepting the surface so long as he proceeds in any direction falling within the confines of two oppositely oriented elliptic cones, each with its apex at the origin and symmetrically positioned about the y_3 axis (a partially open surface). As a mnemonic device, it is convenient to equate the possibility for escape from the region with non-positive definiteness of the matrix under consideration.

If one eigenvalue is positive, for instance, λ_1 , and the other two are negative, the matrix is non-positive definite and the surface represented by Eq. 12 is a hyperboloid with two sheets, as shown in Fig. 3. The conic sections generated by intercepting planes parallel to the two principal planes y_1-y_2 and y_1-y_3 are hyperbolas, while those parallel to the principal plane y_2-y_3 are ellipses. An observer leaving the origin now has a wide range of opportunities for escaping the region without intercepting the surface; in fact, he will intercept the surface only when his departure is confined to a range of directions defined by two elliptic cones, much as described in the preceding paragraph.

If all three eigenvalues are negative, it is clear that no real vectors \bar{y} exist which can satisfy Eq. 12, so no surface exists for discussion.

If two eigenvalues are positive and the third, for instance, λ_3 , is zero, then the surface generated by Eq. 12 is an elliptic cylinder, as shown in Fig. 4. Again the matrix is non-positive definite, and the observer is able to escape the region without intercepting the surface. However, upon careful inspection it becomes evident that escape is possible only if the observer proceeds exactly along the y_3 axis, either in the positive or negative direction! Progress in any other direction will eventually lead to interception of the surface.

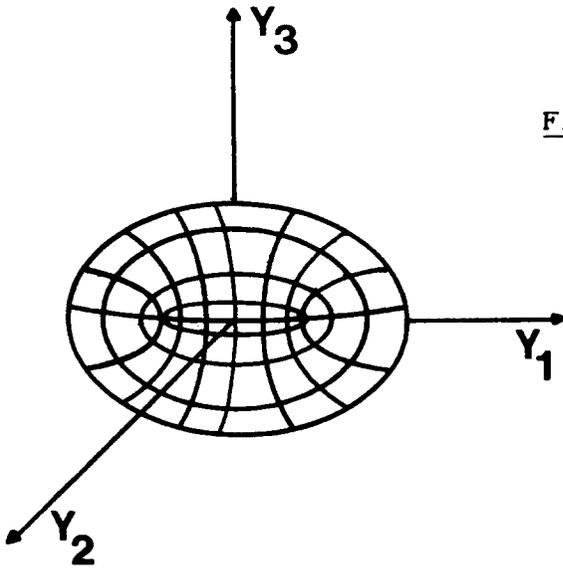


Figure 1: Ellipsoid

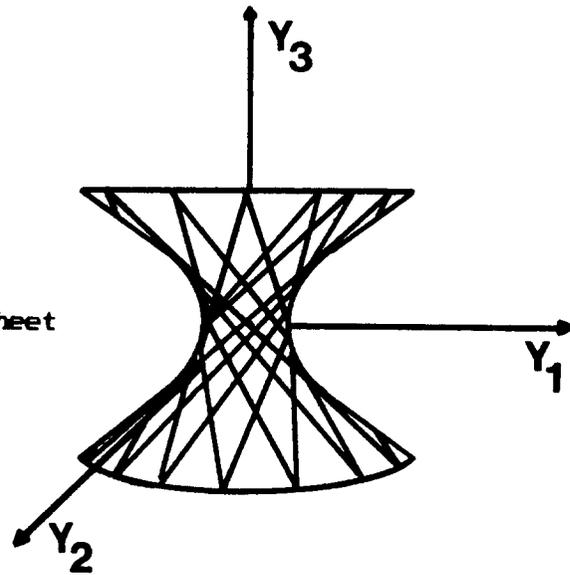


Figure 2: Hyperboloid with one sheet

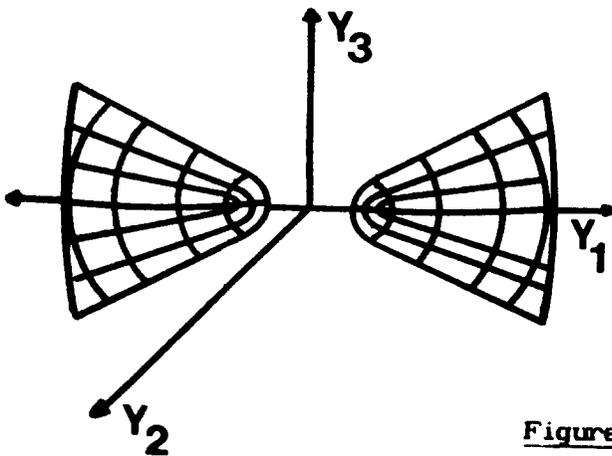


Figure 3: Hyperboloid with two sheets

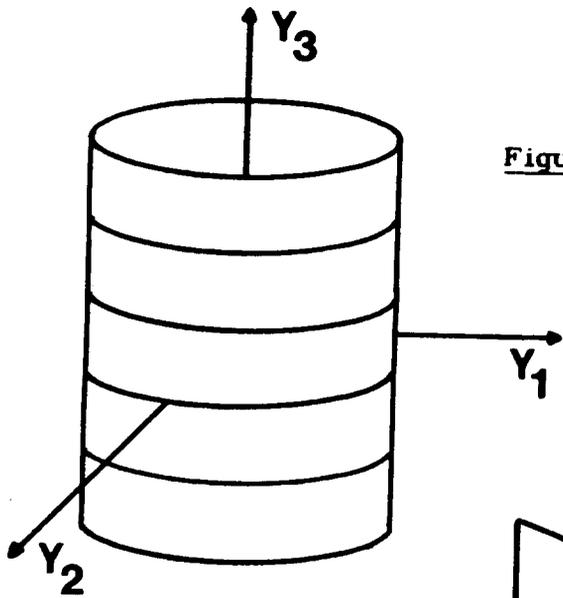


Figure 4: Elliptic cylinder

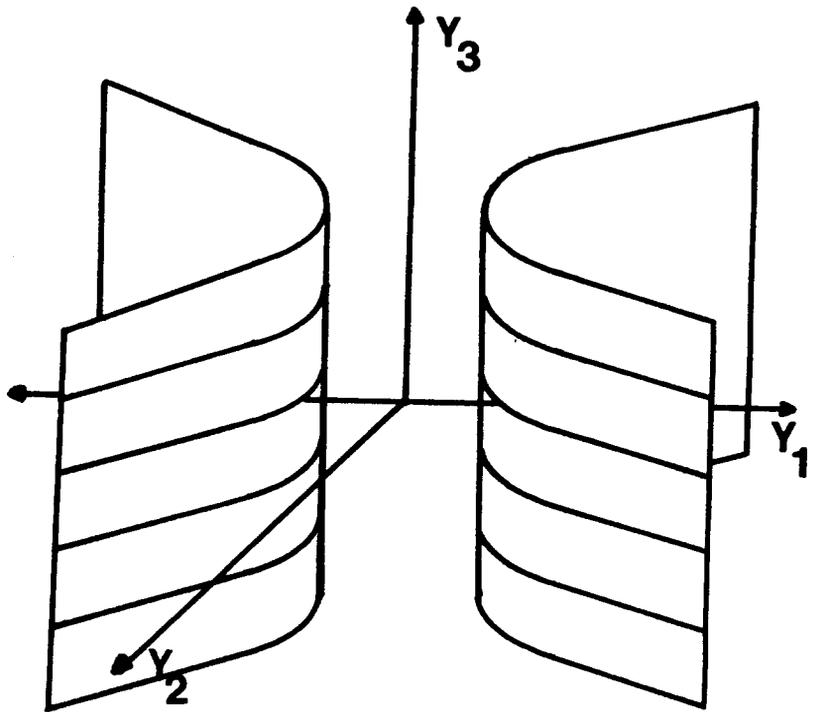


Figure 5: Hyperbolic cylinder

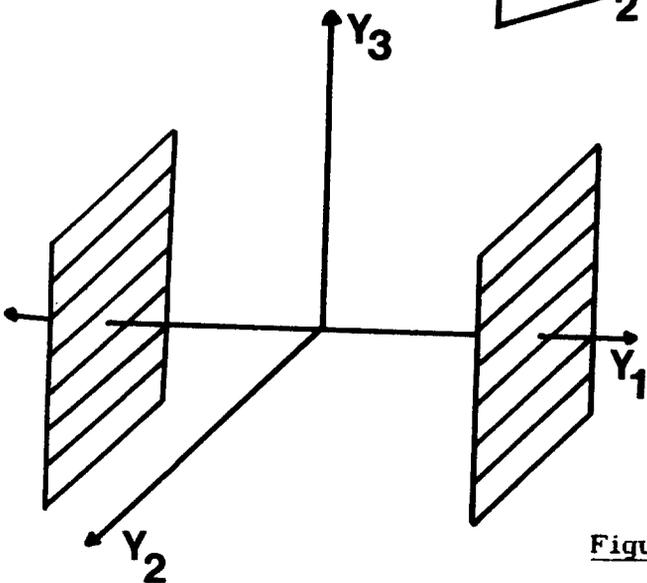


Figure 6: Two parallel planes

If one eigenvalue, for instance, λ_3 , is zero and the other two have opposite signs, e.g. $\lambda_2 < 0$ and $\lambda_1 > 0$, then the matrix is non-positive definite and the surface generated by Eq. 12 is a hyperbolic cylinder, as shown in Fig. 5. Escape from the origin without intercepting this surface must be via directions defined by a solid wedge-shaped region.

Finally, if two eigenvalues are zero and the third, say λ_1 , is positive, then the surface consists of two planes parallel to the principal y_2 - y_3 plane, as shown in Fig. 6. Escape from the origin can be achieved only in directions confined to the y_2 - y_3 plane.

It is evident from the preceding discussion that the nature of the eigenvalues of a matrix uniquely establishes the range of real vectors \bar{y} which are able to satisfy the diagonal quadratic form, as indicated in Eq. 8. If the matrix is positive definite and all the eigenvalues are positive, the family of real solution vectors associated with a particular positive value $\rho > 0$ forms a closed surface and thus is "complete." If one or more of the eigenvalues is zero, no restrictions are placed on the corresponding components of \bar{y} , so the family of solution vectors is "open" or "incomplete". Finally, if negative eigenvalues are present, the family of real vectors \bar{y} which satisfy the quadratic form for a particular $\rho > 0$ maps an open surface and thus is "indefinite". There is also inconsistency since, given certain real values for some of the components of \bar{y} , one must resort to imaginary values for other components corresponding to the negative eigenvalues in order to satisfy Eq. 8.

Example

We now illustrate the preceding discussion through examination of some specific 3 x 3 correlation matrices \bar{C} . In each instance we first derive the eigenvalues and then deal solely with the diagonal quadratic form, i.e., Eq. 12.

The first matrix we consider is

$$\bar{C} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} .$$

There is no need to transform this matrix since it already exists in diagonal form. All three eigenvalues are unity and the matrix is positive definite. Eq. 12 thus takes the form $\rho^2 = y_1^2 + y_2^2 + y_3^2$. For

a specific value of ρ , the solution vectors \bar{y} all lie on the surface of a sphere with radius ρ , a special case of the surface shown in Fig. 1. This matrix provides a generic model for error propagation problems in which a single parameter is derived as a scalar function of three independent random variables.

The second matrix we consider is

$$\bar{C} = \begin{bmatrix} 1 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 1 & 1 \end{bmatrix} .$$

The eigenvalues of this matrix are $\lambda_1 = 3$, $\lambda_2 = \lambda_3 = 0$, so it is non-positive definite. Eq. 12 assumes the form $\rho^2 = 3y_1^2$. The corresponding surface appears as shown in Fig. 6. This matrix represents physical problems where all three random variables are fully correlated, with two out of the three variables providing redundant information. In spite of the presence of three parameters, only one distinct piece of information is available.

The third matrix we consider is

$$\bar{C} = \begin{bmatrix} 1 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 1 \end{bmatrix} .$$

The eigenvalues of this matrix are $\lambda_1 = 2$, $\lambda_2 = 1$ and $\lambda_3 = 0$, so it is non-positive definite. Eq. 12 assumes the form $\rho^2 = 2y_1^2 + y_2^2$. The corresponding surface appears as shown in Fig. 4. This matrix represents physical problems where two out of the three random variables are fully correlated, with one of the variables providing redundant information. In spite of the presence of three parameters, only two distinct pieces of information are available.

Finally, the fourth matrix we consider is

$$\bar{C} = \begin{bmatrix} 1 & 0 & 1 \\ 0 & 1 & 1 \\ 1 & 1 & 1 \end{bmatrix} .$$

The eigenvalues of this matrix are $\lambda_1 = 1$, $\lambda_2 = 2.4142$ and $\lambda_3 = -0.4142$, so it is non-positive definite. Eq. 12 assumes the form $\rho^2 = y_1^2 + 2.4142y_2^2 - 0.4142y_3^2$. The corresponding surface appears as shown in Fig. 2. This matrix cannot represent any real physical situation, since an imaginary error is implied. In fact, a serious inconsistency is indicated. This is quite apparent if we reflect upon the nature of the indicated correlation pattern. It is stated that the first random variable is fully correlated to the third, and the second is fully correlated to the third as well. However, there is no correlation indicated between the first and second variables. It is a clear violation of common sense to suppose that there can exist a strong correlation between two variables and a third but no correlation between the first two. The existence of an imaginary eigenvalue signals that such an inconsistency is present.

The preceding example shows us that matrices can be non-positive definite as a result of either i) redundancy of the information content, ii) inconsistency of the information content, or iii) both of the preceding causes. When a matrix is found to be non-positive definite, it is worthwhile to seek the fundamental source of the problem; computation of the eigenvalues is one of the best ways to accomplish this task.

Another procedure available for the investigation of a covariance matrix is computation of its determinant. It happens that when all the eigenvalues are positive and the matrix is therefore positive definite, the determinant is also positive. It is never possible for the determinant to be negative and the matrix to be positive definite. However, a positive determinant does not necessarily imply that the matrix is indeed positive definite! This important point is made evident in the following discussion. Orthogonal transformations preserve the determinant of a matrix. Since a symmetric covariance matrix can be converted to diagonal form by an orthogonal transformation, the determinant of the matrix always equals the product of its eigenvalues. Thus, a matrix with non-zero eigenvalues can have an even number of negative eigenvalues and still have a positive determinant, though it is certainly non-positive definite. In any event, a negative determinant is a sure signal of inconsistency as well as non-positive definiteness, since then at least one of the eigenvalues has to be negative. When one or more of the eigenvalues is zero, the matrix is not only non-positive definite, it is also singular and some degree of redundancy is indicated. However, the extent of the singularity (number of zero eigenvalues) is not defined by this

consideration. In summary, the determinant of a covariance matrix provides some useful information about the nature of the corresponding random variables, but its computation is not a substitute for more detailed examination of the matrix properties.

Another useful method for determining whether a matrix is positive definite is to examine the principal minors. A matrix can be said to be positive definite if and only if every principal minor is positive. A minor is the determinant of a sub-matrix. A minor is principal if the sub-matrix is formed by deleting certain rows and the corresponding numbered columns. There are $n + 1$ leading principle minors for an $n \times n$ matrix with elements M_{ij} . They are the values $\mu_i = \det(\bar{m}_i)$, where the \bar{m}_i are sub-matrices defined as follows:

$$\bar{m}_0 = 1 \quad \bar{m}_1 = M_{11} \quad \bar{m}_2 = \begin{bmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{bmatrix} \quad \dots \quad \bar{m}_n = \begin{bmatrix} M_{11} & \dots & M_{1n} \\ M_{n1} & \dots & M_{nn} \end{bmatrix}.$$

Without going into further detail, we now state an important theorem of matrices which is very useful in the present context: A real symmetric matrix is positive definite if and only if its rank r equals the dimension n of the matrix and all its leading principal minors are positive. An alternate test for positive definiteness therefore involves computation of all the leading principal minors. The advantage to this method of determining whether a matrix is positive definite or not is that it is generally much faster than alternative approaches. In computer algorithms one begins by calculating all the low-order minors first. If one encounters a zero or negative principal minor, the matrix is automatically non-positive definite and there is no further need for computation. The method also indicates, in a crude way, the point in the matrix where a problem is first encountered. This issue is discussed further in Section IV and in the Appendix. A limitation of this approach is that it does not provide as much detailed information about the matrix as one would usually like to have. This issue is discussed further, below, but first we consider another example.

Example

Table 3 lists neutron cross section values and uncertainties corresponding to a hypothetical experiment performed at six different energies.

Table 3

Cross section (mb)	Systematic error (mb) [*]	Total error (mb)
1) 10.0	0.1	0.1 (1%)
2) 7.5	0.075	0.3 (4%)
3) 10.0	0.1	0.6 (6%)
4) 100.0	1.0	1.0 (1%)
5) 15.0	0.15	1.5 (10%)
6) 20.0	0.2	2.4 (12%)

* 1% fully-correlated systematic error.

From inspection of the table it is clear that the random error is assumed to be zero for the first and fourth data points. The correlation matrix can be readily computed from information in Table 3. The lower triangle of this matrix is

```

1.000
0.250  1.000
0.166  0.041  1.000
1.000  0.250  0.166  1.000
0.100  0.025  0.016  0.100  1.000
0.083  0.021  0.014  0.083  0.008  1.000
    
```

The determinant of this matrix is zero, so it is non-positive definite. This is also readily apparent from an inspection, since column 1 of the matrix equals column 4. If row 2 and row 4 are interchanged as well as column 2 and column 4, the third leading principal minor is zero, which also signals that the matrix is non-positive definite. The procedure of interchanging rows and corresponding columns is justified from physical considerations, since we are always free to relabel any of the data points. Computation of the eigenvalues of this matrix indicates that one of them is zero, also indicating non-positive definiteness. The existence of off-diagonal elements of a correlation matrix equal to ± 1 indicates full correlation (or anti-correlation) and thus redundancy.

with resulting non-positive definiteness. The presence of correlation coefficients with magnitudes exceeding unity is unrealistic, as discussed earlier in the context of a vector model. Nevertheless, such parameters may show up in the matrix as the result of typographical errors. When this happens, negative eigenvalues and negative principal minors will be encountered, thereby signaling not only non-positive definiteness but also inconsistency as well.

There exist two general rules which are very useful in this context. The first rule is called Descartes' Rule of Sign. It states that for a real quadratic form associated with a particular matrix, the index of that form, and thus the number of positive eigenvalues, is exactly equal to the number of variations in sign of the terms of the characteristic equation used to solve for the eigenvalues (as counted from the first through the last term, excluding zero terms, of the characteristic equation when it is written out explicitly). The second rule is called Gundelfinger's Rule. It states that the number of positive eigenvalues of a matrix is precisely the number of permanences (instances in which there is no change) of sign for the sequence of leading principal minors, listed in ascending order. Likewise, the number of negative eigenvalues is precisely the number of variations of sign for this sequence. The following example illustrates the use of these rules.

Example

Consider the following three real symmetric matrices

$$\bar{M}_1 = \begin{bmatrix} -1 & -2 & 1 \\ -2 & 2 & -2 \\ 1 & -2 & -1 \end{bmatrix} \quad \bar{M}_2 = \begin{bmatrix} 5 & -2 & -2 \\ -2 & 2 & -4 \\ -2 & -4 & 2 \end{bmatrix} \quad \bar{M}_3 = \begin{bmatrix} 7 & -2 & 0 \\ -2 & 6 & -2 \\ 0 & -2 & 5 \end{bmatrix}$$

The validity of Descartes' Rule and Gundelfinger's Rule is demonstrated below:

Matrix \bar{M}_1 --

Leading principal minors: $\mu_0 = 1, \mu_1 = -1, \mu_2 = -6, \mu_3 = 16,$
(1 sign permanence and 2 sign variations).

Characteristic equation: $\lambda^3 - 12\lambda - 16 = 0,$
(1 sign variation)

Eigenvalues: $\lambda_1 = 4, \lambda_2 = -2, \lambda_3 = -2,$
(1 positive eigenvalue and 2 negative eigenvalues).

Matrix \bar{M}_2 --

Leading principal minors: $\mu_0 = 1, \mu_1 = 5, \mu_2 = 14, \mu_3 = -108,$
(2 sign permanences and 1 sign variation).

Characteristic equation: $\lambda^3 - 9\lambda^2 + 108 = 0,$
(2 sign variations)

Eigenvalues: $\lambda_1 = 6, \lambda_2 = 6, \lambda_3 = -3,$
(2 positive eigenvalues and 1 negative eigenvalue).

Matrix \bar{M}_3 --

Leading principal minors: $\mu_0 = 1, \mu_1 = 7, \mu_2 = 38, \mu_3 = 162,$
(3 sign permanences and no sign variations).

Characteristic equation: $\lambda^3 - 18\lambda^2 + 99\lambda - 162 = 0,$
(3 sign variations)

Eigenvalues: $\lambda_1 = 3, \lambda_2 = 6, \lambda_3 = 9,$
(3 positive eigenvalues and no negative eigenvalues).

In the preceding discussion it has been stressed that there are two fundamentally distinct manifestations of non-positive definiteness. One has to do with indefiniteness as reflected by the existence of zero eigenvalues, while the other involves inconsistency as reflected by negative eigenvalues. We now examine further the issue of inconsistency. In the following example, it is demonstrated for a 3 x 3 correlation matrix that fixing the values of any two distinct off-diagonal correlation coefficients places limitations on the values which can be assumed by the third, if the matrix is to be positive definite.

Example

Let \bar{C} be a 3 x 3 correlation matrix. The form of the matrix is

$$\bar{C} = \begin{bmatrix} 1 & c_{12} & c_{13} \\ c_{12} & 1 & c_{23} \\ c_{13} & c_{23} & 1 \end{bmatrix} .$$

C_{12} , C_{13} and C_{23} are the only distinct off-diagonal coefficients, owing to the inherent symmetry of correlation matrices. The determinant of \bar{C} is given by $\det(\bar{C}) = 1 + 2C_{12}C_{13}C_{23} - C_{12}^2 - C_{13}^2 - C_{23}^2$. One can now study the behavior of any one correlation coefficient, say $x = C_{23}$, as a function of the remaining two. The requirement for positive definiteness is that $\det(\bar{C}) > 0$. Thus, those values of x for which $x^2 - (2C_{12}C_{13})x + (C_{12}^2 + C_{13}^2 - 1) \geq 0$ lead to non-positive definite matrices. In Table 4, below, the range of unacceptable values of x is indicated for several choices of the remaining two coefficients.

Table 4

C_{12}	C_{13}	$x = C_{23}^*$
0.9	0.9	$-1 \leq x \leq 0.62$ and $x = 1$
0.1	0.9	$0.524 \leq x \leq 1$ and $-1 \leq x \leq -0.344$
0.1	0.1	$-1 \leq x \leq -0.98$ and $x = 1$
0.5	0.5	$-1 \leq x \leq -0.5$ and $x = 1$
0.3	0.5	$0.97 \leq x \leq 1$ and $-1 \leq x \leq -0.676$
0.9	0.8	$0.981 \leq x \leq 1$ and $-1 \leq x \leq 0.458$

* Values of $x = C_{23}$ which lead to a non-positive definite matrix.

It is evident that whenever any two correlation coefficients are relatively large, there is only a very limited range allowed for the third coefficient if the matrix is to be positive definite.

We examine this point further by considering a 3 x 3 correlation matrix which is formed in the following special way. Suppose we have three random variables. Each is affected by random error and a single source of fully correlated error. The correlated errors are e_1 , e_2 , and e_3 , respectively, while the corresponding total errors are E_1 , E_2 , and E_3 . The correlation coefficients are given by the formulas $C_{12} = xy$, $C_{13} = xz$ and $C_{23} = yz$, where $x = e_1/E_1$, $y = e_2/E_2$ and $z = e_3/E_3$. The following example demonstrates how an inconsistency can be detected by examining these formulas

Example

Suppose that one assumes, for example, that $C_{12} = 0.9$ and $C_{13} = 0.9$. Is $C_{23} = 0.4$ an acceptable correlation? Not according to Table 4! In fact, if we substitute these values into the consistency equations, above, that involve the ratios x , y , and z , we are led to the result $x = 1.423$ and $y = z = 0.6324$. The value of $x > 1$ is unrealistic. It is not possible for the systematic error to exceed the total error unless the random error is taken to be imaginary.

The next example demonstrates the effect of an inconsistency which is introduced by a typographical error.

Example

Consider the following correlation matrix (only the lower triangle is shown):

1.0000					
0.2475	1.0000				
0.1650	0.0416	1.0000			
0.9800	<u>0.2475</u>	0.1650	1.0000		
0.0990	0.0250	0.0166	0.0990	1.0000	
0.0825	0.0208	0.0139	0.0825	0.0083	1.0000

This matrix is positive definite. Suppose, however, that due to a typographical error, the underlined coefficient is set equal to 0.8475. The matrix now has a negative leading principal minor and therefore is non-positive definite. How do we go about tracing the origins of this problem once we know that the whole matrix is non-positive definite? The process of computing leading principal minors from the smallest to the largest leads us in a straightforward way to conclude that there is a problem on row 4 of this matrix. Further examination produces the result that the 3 x 3 correlation sub-matrix involving only the first, second, and fourth random variables is also a non-positive definite matrix. We therefore reach the conclusion that the inconsistency is being caused by either the first or second coefficient (or both) in the fourth row. We have found that the process of examining the positive definiteness of 3 x 3 correlation sub-matrices is a very useful one for dealing with this type of problem.

We have observed that inconsistencies involving the correlation coefficients for covariance matrices of multigroup cross sections are quite common in the literature. For example, the correlation matrix for the $^{23}\text{Na}(n,\gamma)$ reaction cross section reported by Noltenius (Nol87) is not only non-positive definite, but it also exhibits a number of inconsistencies of the nature described above. The same can be said for the matrices provided by Mannhart (Man82) and by van der Borg et al (B+80) for the $^{58}\text{Ni}(n,p)$ reaction. On the other hand, the covariance matrix for the 27-group cross section set provided by Gerstl et al (G+77) for the $^{58}\text{Ni}(n,p)$ reaction does appear to be positive definite and thus free of inconsistencies.

One of the conclusions from the REAL-84 exercise (ZN87) is that the presence of non-positive definite covariance matrices, and the existence of inconsistencies leading to negative eigenvalues, are among the more serious problems encountered in this interlaboratory investigation into the methodologies of neutron dosimetry in reactors. Such deficiencies appear to be traceable to shortcomings in the evaluated files as well as to the widespread use of mathematically inconsistent methods in the analysis of dosimetry data.

III. METHODS TO ENCOURAGE GENERATION OF POSITIVE DEFINITE MATRICES

As a rule, the various situations in which one is confronted with the generation of covariance matrices tend to fall into four broad categories: i) postulation of a priori matrices which are intended to serve as a basis for subsequent analyses of a Bayesian nature, ii) development of covariance matrices for sets of experimental parameters which are deduced from measurements in the laboratory, iii) development of covariance matrices for sets of parameters derived via functional transformations from primary sets of parameters for which covariance information exists (e.g., error propagation), and iv) the generation of covariance information as the product of least-squares analyses. These broad categories will serve as the framework for the following discussion. In our experience, certain analytical practices involving covariance matrices appear more often than not to result in the development of matrices which are positive definite. In this section we discuss some of those procedures which appear to be proper and relatively "safe" as regards the generation and manipulation of covariance matrices. Much of this material has been documented elsewhere, so emphasis here is on summarizing the main ideas and providing some examples.

The development of a covariance matrix intended to provide a mathematical representation of assumed uncertainty for an a priori set of information (i.e., a summary of what is known prior to the conduct of a particular investigation) quite often involves considerable subjectivity. Documentation of uncertainties in the literature has been notoriously deficient prior to recent times and still leaves much to be desired in most instances. There appears to be a fixation on the reporting of total errors, with little concern for component errors or correlations. Whenever it becomes necessary to generate a covariance matrix for a set of parameters from existing information in the literature, we have found that it is essential that an attempt be made to break down the total errors into distinct components, subsequently examining the possible correlations at the component-error level (micro-correlations), as discussed in some detail by Smith (Smi87a), rather than attempting to estimate correlations between the total errors directly (macro-correlations). Covariance matrices derived in this manner are far more likely to be positive definite. The same consideration arises when an investigator examines his own data in order to develop a covariance matrix representing the significant uncertainties in his work. The situation ought to be better in this instance, however, because in principle an experimenter is better equipped to examine and summarize the sources of error in his work than any other individual. Nevertheless, anyone who is not prepared to implement the requisite methodology would serve the interests of the community best by merely listing the component errors and providing some information from which others who are more experienced in statistical analysis can base estimates of the correlations and thereby produce the desired covariance matrix.

Covariance matrices which are generated through the explicit consideration of a collection of parameters whose uncertainties are to be represented, as discussed in the preceding paragraph, should only be created after carefully reviewing all the distinct factors which contribute to the overall uncertainty, determining the magnitudes of the partial errors, estimating in a reasonable way their correlations, and then combining this information to form the covariance matrix as briefly outlined below. Ideally, one ought to be able to describe any complex process in terms of a collection of mutually independent parameters (canonical parameters), but in practice this is rarely possible nor does it turn out that it is necessary. This issue has been discussed in some detail in the literature (Smi87a), so it will not be pursued here in any depth. Summarizing briefly, we suppose that there are L distinct sources of error which determine the overall uncertainties for a collection of n quantities $\bar{x} = (x_1, x_2, \dots, x_n)$. Let e_{il} represent the partial error in x_i corresponding to attribute l, and let \bar{C}_l be the correlation matrix corresponding to these partial errors (C_{lij} is a typical element) as they apply to all the components of \bar{x} . Then, the covariance matrix which is applicable to this set of quantities is formed of elements V_{ij} calculated using the expression

$$[13] V_{ij} = \sum_{l=1}^L e_{il} e_{jl} C_{lij}$$

Covariance matrices generated in this fashion tend to be positive definite so long as the partial errors and their assumed correlations are physically reasonable. Generally, several distinct sources of error need to be considered ($L \gg 1$), so even the presence of strong correlations (up to 100%) in some of the partial errors will probably not lead to matrices which are non-positive definite. As mentioned in Section I, no values among any set of parameters can ever be assumed to be entirely free of random error, nor should the approximation be made that the random error is negligible in the presence of much larger systematic error components. To do so is to invite the development of a non-positive definite matrix. The following example will serve to illustrate this point.

Example

Suppose that we have two cross section values in a set. For simplicity, we assume that they are affected by only two sources of error, namely a small random error and a much larger common systematic error (perhaps due to a common detector calibration) which is 100%-correlated. This systematic error is assumed to be 10%, while the

random errors are only 0.5% and 0.3% for the first and second values, respectively. The total errors to six significant figures are thus 10.0125% and 10.0045% for the first and second points, respectively. The relative covariance matrix for this data set is therefore

$$\begin{bmatrix} 0.010025 & 0.01 \\ 0.01 & 0.010009 \end{bmatrix} .$$

This matrix is positive definite. Suppose, however, that we had decided that the random errors are so small in comparison to the systematic error that they could be neglected in considering the total error. From all external appearances, nothing would seem to be significantly affected by assuming a total error of 10% for each point with 100% correlation. When this assumption is implemented, the relative covariance matrix becomes

$$\begin{bmatrix} 0.01 & 0.01 \\ 0.01 & 0.01 \end{bmatrix} .$$

This matrix is obviously non-positive definite. Clearly, inclusion of the small random errors is necessary to preserve the physical integrity of the matrix representation of uncertainty.

Another broad category of problems in which covariance matrices arise is in the transformation of variables. Suppose that we possess a set of variables \bar{x} and a positive definite covariance matrix \bar{V}_x which represents the corresponding uncertainties. We wish to transform to another set of variables \bar{y} and to obtain the appropriate covariance matrix \bar{V}_y for this set. The procedure is straightforward and is widely documented (e.g., Smi87c). Very briefly, the transformation is accomplished with a matrix \bar{T} called the transformation matrix, as discussed in Section II for the case of a scalar function, in accordance with the expression $\bar{V}_y = \bar{T}^+ \bar{V}_x \bar{T}$ (the law of error propagation). This process tends to lead to the generation of a positive definite matrix \bar{V}_y , so long as the transformation does not introduce redundancy.

If the dimension of \bar{x} is n , we have rank n for the primary available information. If the dimension of the set \bar{y} exceeds n then the matrix \bar{V}_y will be non-positive definite, since the rank of the matrix, which reflects the true scope of the available distinct information, cannot exceed n . If the dimension of \bar{y} is less than or equal to n , most transformations of practical interest result in \bar{V}_y being positive

definite, but it should always be tested, e.g., as described in Section IV. The following very simple example will serve to illustrate this concept.

Example

Let (x_1, x_2) be a pair of values with a 5% common systematic error (100% correlated) and 2% and 3% random errors, respectively. For convenience, assume that both x_1 and x_2 are equal to 1. The covariance matrix and relative covariance matrix are therefore both equal to

$$\begin{bmatrix} 0.0029 & 0.0025 \\ 0.0025 & 0.0034 \end{bmatrix} ,$$

and this matrix is clearly positive definite. First, consider the transformation $y_1 = x_1 + 0.1x_2$ and $y_2 = x_1 - 0.1x_2$. Thus $y_1 = 1.1$ and $y_2 = 0.9$. Following the law of error propagation, we obtain for \bar{V}_y the matrix

$$\begin{bmatrix} 0.0113 & -0.00005 \\ -0.00005 & 0.000013 \end{bmatrix} .$$

This matrix is positive definite. Suppose, however, that we had made the assumption that $y_1 = y_2 = x_1 + x_2$; then both of these derived values equal 2. Following the same procedure, we obtain for \bar{V}_y the matrix

$$\begin{bmatrix} 0.0113 & 0.0113 \\ 0.0113 & 0.0113 \end{bmatrix} .$$

This matrix is clearly non-positive definite. The information contained in \bar{y} in this instance is redundant.

The first practical application of random-variable transformation to be discussed here is that of averaging experimental data. Suppose that an experiment has been performed to measure the differential cross section for a neutron-induced reaction at several incident energies. Any cautious experimenter will probably perform several measurements at each of these energies, varying the experimental procedure somewhat on

each occasion to search for possible sources of systematic error. When reporting the final results, however, it is very likely that the investigator will wish to average corresponding quantities in order to obtain a single value to report at each energy. Development of covariance information should begin with consideration of all the primary experimental values. A primary covariance matrix ought to be constructed at this level. However, for reporting purposes, what is desired is a secondary covariance matrix corresponding to the final set of values, namely one cross section for each energy. A procedure for performing this "collapsing" exercise has been developed by Smith (Smi87c) and it was subsequently employed by Watanabe et al (W+87) in the analysis of data from a neutron-fission cross-section-ratio experiment. The reader is referred to the work of Smith (Smi87c) for an example of the procedure. The covariance matrices described in Section 3 of that paper, namely, the primary matrix of 4 x 4 and the collapsed secondary matrix of dimension 2 x 2, are both positive definite.

Another very important type of transformation problem arises routinely in reactor physics. It concerns the transformation required to change the representation of a cross section from a particular group structure to another. Mannhart (Man82) has discussed this problem, and it is dealt with in greater detail by Muir and MacFarlane (MM85) in their documentation for the ERRORR and COVR modules of the NJOY nuclear data processing system. Their procedures are equivalent, and they assume that all of the uncertainty is concentrated in the cross section set. The fundamental requirement is that any group cross section formulation derived from a point representation, or any transformation from one formulation to another, must preserve the integral response, namely, the quantity $\int \sigma(E)\phi(E)dE$, where $\sigma(E)$ is the energy-dependent cross section and $\phi(E)$ is the energy-dependent neutron spectrum. It is shown in both of the above-mentioned references that, given one set of group cross sections, those group cross sections which result from a transformation required to adapt to a new group structure are linear combinations of the original cross sections. The weighting factors are in fact group fluxes. Furthermore, the coefficients of the transformation are also simple functions of the various group fluxes. The formulas are derived by application of the law of error propagation as described above. We can demonstrate this process through the following simple example.

Example

Consider a three group (very coarse) representation of a continuous cross section $\sigma(E)$ and neutron spectrum $\phi(E)$. The group quantities are denoted by $(\sigma_1, \sigma_2, \sigma_3)$ and (ϕ_1, ϕ_2, ϕ_3) . We wish to collapse this three-group structure to a two-group structure. It is assumed that the

group intervals are compatible in the sense that one of the existing groups is preserved while the other two are combined to form a single group. Let $\phi_1 = \phi_1 + \phi_2$ and $\phi_2 = \phi_3$ represent the group fluxes for the collapsed structure while Σ_1 and Σ_2 are the revised group cross sections. Integral response is preserved provided that $\Sigma_1 = (\phi_1 \sigma_1 + \phi_2 \sigma_2) / \phi_1$ and $\Sigma_2 = \sigma_3$. It can be readily shown that the elements of the transformation matrix are $T_{11} = \phi_1 / \phi_1$, $T_{12} = 0$, $T_{21} = \phi_2 / \phi_1$, $T_{22} = 0$, $T_{31} = 0$ and $T_{32} = 1$. For convenience, let us assume that the initial group fluxes and group cross sections are all unity. The total uncertainties in the group cross sections are taken to be 5%, 6%, and 7%, respectively, for the three initial groups. We assume that the correlations between groups amount to 0.5. The covariance matrix \bar{V}_σ for this set is as follows

$$\begin{bmatrix} 0.0025 & 0.0015 & 0.00175 \\ 0.0015 & 0.0036 & 0.0021 \\ 0.00175 & 0.0021 & 0.0049 \end{bmatrix} .$$

This matrix is positive definite.

Clearly, the transformation matrix \bar{T} has the form

$$\begin{bmatrix} 0.5 & 0 \\ 0.5 & 0 \\ 0 & 1 \end{bmatrix} .$$

The transformation yields the solution values $\Sigma_1 = \Sigma_2 = 1$, $\phi_1 = 2$, $\phi_2 = 1$ and a covariance matrix \bar{V}_Σ equal to

$$\begin{bmatrix} 0.002275 & 0.001925 \\ 0.001925 & 0.0049 \end{bmatrix} .$$

This matrix is positive definite.

It is intuitively clear that with care it is quite possible to preserve positive definiteness through the process of collapsing group cross sections. It is quite another story for the expansion of group representations. Redundancy enters unavoidably through such procedures and the matrices obtained will not be positive definite! It has been

suggested by some authors (e.g., Pee82 and ZN87) that no serious harm can come in practice from manipulations involving covariance matrices which possess only a few non-positive eigenvalues/ provided that the magnitude of the largest negative eigenvalues are significantly smaller than those of the dominant positive eigenvalues of the matrix. The arguments appear to be based upon an assumption that the impact upon the magnitude of the quadratic form will be small. It is our opinion that the results to be expected from performing analyses involving non-positive definite covariance matrices which originate due to manipulations such as those indicated above merit further study. However, owing to the general complexity of the computational procedures routinely employed in reactor physics, this would be a difficult task which is beyond the scope of the present work. We suggest that workers in the field should at least be aware that the issue exists and ought to realize that, unless they take suitable precautions, they will often be working with non-positive definite matrices as a consequence of transformations of this nature.

It is apparent that most of the problems associated with the preservation of positive definiteness in random variable transformations are generally not attributable to the process of error propagation itself, but are deeply rooted in the nature of the transformations. For this reason, whenever a transformation of variables is performed, the resulting covariance matrix should be tested for positive definiteness. If the matrix is non-positive definite, the problem most probably can be uncovered from an inspection of the transformation unless a numerical mistake has been made. Non-positive definiteness is a signal that the transformation has introduced either redundancy or some other inconsistency into the analytical process.

Last on our list for discussion is the matter of the positive definiteness of covariance matrices generated by the method of least squares. This topic has been reviewed by several authors (e.g., Man81, Pee82, and Fro86). It is a complex issue which we also choose not to pursue with any depth in this report. We merely add as an observation that, in our experience, those analytic procedures involving the method of least squares generally lead to positive definite matrices so long as the covariance matrices for the input parameters are positive definite and the data being analyzed are reasonably consistent. We have found that the generalized least-squares method offers valuable procedures for combining information from diverse sources (e.g., prior representations, nuclear model calculations, differential data, and integral data) in a consistent way, just as long as one does not demand more from the aggregate of information than is there to provide. Put another way, the method of least squares as an information combination procedure appears in practice to generate solution covariance matrices which are positive definite (given physically consistent input) if the dimension of the solution parameter set which is sought does not exceed the rank (number of distinct pieces of information) of the input parameter set.

IV. PROCEDURES TO TEST FOR POSITIVE DEFINITENESS OF MATRICES

Two FORTRAN computer programs, MATXTST and MATXTST1, have been developed to test symmetric matrices for positive definiteness. They have been implemented on an IBM personal computer, but the routines are written in a sufficiently general fashion to be useful on a variety of machines, with only minor changes anticipated for the I/O formats. The mathematical procedures employed in these routines are described in Section II. The present chapter focuses on a general description of these programs and the manner in which they should be employed. Details on the computational procedures and the I/O formats are described in the Appendix.

As indicated in Section II, the mathematical tools available for the investigation of positive definiteness include the computation of matrix determinants, evaluation of leading principal minors, determination of matrix eigenvalues, and consistency tests for correlations (for matrices with $n > 3$ this essentially involves examination of the internal consistency of various 3×3 sub-matrices). While the two programs utilize the same input, the calculational procedures employed are somewhat different and their functions are complementary, as is described below and in the Appendix. The available input options include: i) the full covariance matrix, ii) the basic variables plus the relative covariance matrix, or iii) uncertainties in the basic variables plus the correlation matrix.

Algorithms in FORTRAN from LINPACK (D+79) and a collection of low-level subroutines called Basic Linear Algebra Subprograms [BLAS] (L+79) have been employed in the development of MATXTST and MATXTST1. The main differences in these programs are indicated below:

MATXTST

This program tests all leading principal minors to see whether they are positive. If so, then the main matrix is declared to be positive definite. Computation of the determinant of the main matrix and its inverse is performed as an option if requested. However, if one principal minor is found to be zero or negative, the code identifies the principal minor, declares the matrix to be non-positive definite, and prompts the user for an optional correlation test. If this option is selected, then (for matrices with $n > 3$) the code tests all 3×3 sub-matrices that can be formed from the matrix associated with the anomalous leading principal minor to determine whether or not they are positive definite. In this fashion the user is provided with useful information concerning the origin of non-positive definiteness in the main matrix. The process of purging a large matrix of sources of non-positive definiteness is by necessity an iterative one, since MATXTST halts as soon as the first non-positive principal minor is encountered.

MATXTST1

This program first tests the whole matrix for singularity. If the matrix is found to be singular (to within the numerical precision of the code), it is declared as such and the analysis stops. However, if the matrix is non-singular, then the matrix determinant, the inverse matrix and the number of positive and negative eigenvalues, is determined.

If the user needs only to determine whether a matrix is positive definite or not, then use of the basic routine in MATXTST is the method of choice. On the other hand, if the matrix is found to be non-positive definite and further details are required to uncover the source of the problem, then the optional features of MATXTST and the algorithms of MATXTST1 are found to be useful.

Examples of the application of these codes are provided in the Appendix along with a listing of the FORTRAN sources statements.

V. COVARIANCE MATRICES AND EVALUATED DATA FILES

A very important issue for consideration is that of the manner in which covariance information is recorded in and extracted from evaluated data files. The formats employed in the ENDF system (KM83) are the most widely emulated around the world, so it forms the basis for the present discussion. Covariance information in this system is recorded specifically in File 33. The details of the various allowed formats for that file are rather complicated, so they will not be dealt with here. In general, these formats allow for covariance information which is self-contained within a specific reaction, and they also provide for cross-referencing between reactions. They allow for the possibility of constructing a covariance matrix by superimposing contributions containing information recorded using various types of numerical structures, thereby providing a capability for simulating relatively complicated correlation patterns. However, there is one common feature to all of these structures which is problematic in the present context, and that is that they all rely upon the use of energy-interval formats. While cross section values in File 3 of the ENDF system are compiled in energy-grid fashion, with prescriptions provided for numerically interpolating between grid values to obtain specific cross section values, in File 33 energy intervals are established and covariance information applicable to a particular interval is assumed to be invariant within that interval and, consequently, applies uniformly to cross section values deduced at any energy falling within that interval.

It is not difficult to see how matrices which are non-positive definite can result from drawing covariance information out of files containing information recorded in energy-interval fashion. Let us suppose that the essential information contained in a positive definite matrix is transformed into a File 33 structure. The original matrix presumably represents the uncertainties for a well-defined collection of cross section values corresponding either to a specific group structure or to a specific grid structure. Suppose, however, that it is subsequently desired to deduce the total uncertainties and correlations for evaluated cross sections at two particular energies which happen to fall within the same corresponding energy intervals for each of the provided components of the covariance matrix representation found in File 33. The resulting correlation pattern which will then be deduced in this instance is 100%. Consequently, the derived covariance matrix will be non-positive definite. This is a very real problem in practical applications because, as a general rule, the energy-interval structures encountered in ENDF representations of covariance information for evaluated files, e.g., ENDF/B-V (Kin79), tend to be rather coarse in order to minimize the volume of numerical material which has to be stored in these files. On the other hand, in reactor physics applications, e.g., it is very common to use rather fine group structures (often several hundred energy intervals) to represent the cross section information over a wide energy range with sufficient precision for applications such as those encountered in neutron

shielding computations. The consequence of these conflicting requirements is that the processing codes which are used to produce group covariance matrices from ENDF files, e.g., the NJOY code (MM85), commonly generate matrices which are non-positive definite. An example of this can be seen by referring to Table 6 of the recent report by Noltenius (Nol87).

There do not appear to be any convenient methods for dealing with this problem within the limitations of the existing ENDF File 33 formats. What is needed is to introduce into the system the means to denote a truly random (zero-range) error component. The magnitude of the random error could be allowed to vary with energy, perhaps using a grid-point method with interpolation, or even an energy-interval structure in which a constant random error over a particular energy interval is indicated. The method by which this is accomplished is not of particular importance. What is crucial, however, is that when processing covariance information in evaluated data systems such as ENDF, in order to generate covariance matrices for specific applications, random error ought to always be introduced in such a way that the resulting matrix will be positive definite. This could be accomplished by merely adding to each File 33 entry an additional component which, when manipulated by processing codes, leads to the addition of a random error component to each of the diagonal covariance matrix elements for the particular application in question. By using this approach, most other aspects of the existing File 33 format structure could be preserved. Symbolically, we could represent the covariance matrices generated through this procedure by the expression $V_{ij} = \sum_k V_{kij} + \delta_{ij} V_R(E)$, where the sum over k represents addition of all of the individual components V_{kij} (short-range, long-range, etc.) normally encountered in the ENDF system (as currently formulated), while V_R is the suggested additional random (zero-range) component. The quantity δ_{ij} is the Kronecker Delta Function. The additional term signifies that insofar as the evaluation is concerned, the cross section value at energy E possesses a random error component with a magnitude as indicated by the added term. If this approach were used, care would have to be taken in error propagation analyses to insure that this random error is either averaged down or left unaltered, as indicated by the physical circumstances. Attention to such details would have to be the responsibility of the user of this information.

We are cognizant of the serious implications of any suggestions to alter existing ENDF formats. In particular, we recognize that a large number of complex computer codes exist which employ data recorded in the contemporary ENDF formats as input, and any changes in these formats would probably necessitate some revision of these codes. In any event, we believe that this proposition warrants serious study within the community, and that any alterations to the existing ENDF formats which might be entertained should be very carefully considered from the point of view of their impact upon major user codes, as well as from purely physical and mathematical considerations.

VI. CONCLUSIONS

Nuclear data covariance matrices ought to be positive definite so that a physically reasonable representation of uncertainties is provided. Non-positive definiteness in these covariance matrices can always be traced to the presence of redundant and/or inconsistent information. Certain analytical practices are shown to lead, more often than not, to the generation of consistent, positive definite matrices, e.g., adherence to rigorous procedures in the propagation of error, in the transformation of information from one group representation to another, and in the use of statistical procedures such as the least-squares method in the adjustment of data. Furthermore, it is evident that random error should always be included in the representation of real physical uncertainties. Covariance matrices should always be tested for positive definiteness and for consistency. Routines for accomplishing this task and for identifying specific problem sources are described in this report, and they have proved to be very useful in practice. It has been concluded that certain deficiencies in the covariance content of existing evaluated nuclear data files, and some inadequacies in the contemporary ENDF procedures for representing covariance information, have led to the generation of non-positive definite matrices in several applications reported in the literature. A suggestion is offered for dealing with this important problem.

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APPENDIX

The FORTRAN programs MATXTST and MATXTST1 provide the user with selectable options that enable the following operations to be carried out for a covariance matrix:

- i) Test for singularity.
- ii) Test for positive definiteness.
- iii) Compute the inverse if the matrix is non-singular.
- iv) Compute the determinant.
- v) Determine the inertia, i.e., the number of positive, negative and zero eigenvalues.
- vi) Examine all possible 3 x 3 cross correlations within a sub-matrix corresponding to a leading principal minor which is non-positive definite (if the dimension of the sub-matrix equals or exceeds 3).

The user of these codes should be aware that the specific conclusions reached concerning singularity, positive definiteness, or the existence of zero eigenvalues will depend to a considerable extent upon the attainable numerical precision of the computer being used in the analysis. Thus, one should preface all such conclusions by the remark: "to within working precision."

The computational procedures employed in these codes are described next.

MATXTST

This code employs two LINPACK (D+79) subroutines called SPOFA and SPODI in the analyses used to test for positive definiteness and to perform further optional calculation. Subroutine SPOFA factors a symmetric matrix \bar{M} using the Cholesky algorithm to determine the elements of a matrix \bar{R} which satisfies the relation $\bar{M} = \bar{R}^+ \bar{R}$. During the process of factorization, each leading principal minor of \bar{M} is tested and the first one found which is not positive definite triggers a return of control to the main program, thereby abandoning the process of factorization. Within the main program, a declaration is made that the entire matrix is non-positive definite and the offending leading principal minor is identified. The program then offers the user the option of either quitting or examining all the 3 x 3 cross correlations between elements in the corresponding submatrix (if its dimension equals or exceeds 3). On the other hand, if the entire matrix is found to be positive definite, it is declared as such and the user has the option of either quitting or calculating the determinant and inverse of the matrix. The latter computation is performed using subroutine SPODI.

MATXTST1

The matrix computations and classifications in this code are performed using the LINPACK (D+79) subroutines SSICO, SSIFA, and SSIDI. Subroutine SSICO is used to estimate whether the matrix \bar{M} is near to singularity or not, and to perform the matrix diagonalization process, i.e., the transformation from \bar{M} to \bar{D} that is indicated in Eq. 9. The test for singularity is accomplished through estimation of the parameter $RCOND = 1/[\det(\bar{M})\det(\bar{M}^{-1})]$. If RCOND is so small that within the range of the floating point arithmetic of the computer it is negligible compared to unity, i.e., if the computer finds that $(1.0 + RCOND).EQ.1.0$ is satisfied, then the matrix \bar{M} is considered to be singular to working precision. In this case the program declares \bar{M} to be singular and the computation is terminated. If the matrix is found to be non-singular, then it is diagonalized by the subroutine SSIFA. The algorithm used is a generalization of the Method of Lagrange Reduction. Next, subroutine SSIDI is used to compute the determinant and inertia of the matrix. A matrix of order n is classified according to the number of positive, INERT(1), negative, INERT(2), and zero, INERT(3), eigenvalues found. Since this procedure is not executed if subroutine SSICO has determined that the matrix is singular, one might ask how zero eigenvalues could occur. This apparent contradiction arises because of limits in numerical precision. It is possible for a matrix to pass the SSICO test for non-singularity and still have eigenvalues so close to zero that subroutine SSIDI classifies them as equivalent to zero for purposes of establishing the inertia of the matrix. The corresponding matrix classification scheme is as follows:

Table A.1

Eigenvalues	Matrix Classification
INERT(1) = n	Positive definite
INERT(2) = n	Negative definite
INERT(1) + INERT(3) = n	Positive
INERT(2) + INERT(3) = n	Negative
INERT(1) + INERT(2) + INERT(3) = n	Indefinite

It is important to emphasize that underflows and overflows may be encountered in the computation of determinants, owing to computer limitations. The manner in which this situation is handled depends, of

course, upon the nature of the computer used and the manner in which the operating system handles the computer's inherent limitations. Underflows (very small values) are often treated as zero by operating systems (except in division), thereby allowing computations to proceed essentially unaffected. Overflows are far more problematic, and the user will be forced to deal individually with such situations.

Next we turn to details of the operation of these codes. As indicated in Section IV, the input structure for both codes is identical. Listings of each of these codes are included at the end of this Appendix, as well as some sample problems. Input is from a file, while output is both to the screen and to a file, depending upon the options selected.

Input Format

N (I2)

This integer is the order (size) of the symmetric matrix

IOP (I2)

This integer selects the input option. Three input options are permitted for defining the covariance matrix, namely,

IOP = 1: Input errors in appropriate units and the correlation matrix,

IOP = 2: Input covariance matrix directly,

IOP = 3: Input relative covariance matrix and the fundamental variables in appropriate units (e.g., cross sections).

IND (I2)

This integer parameter selects the options for execution of the programs. The execution options available for the two programs are as follows:

IND	MATXTST	MATXTST1
00	Stop	Only inertia
10	Only determinant	Determinant and inertia
01	Only inverse matrix	Inertia and inverse matrix
11	Determinant and inverse matrix	Determinant, inertia and inverse matrix

The floating point parameters which serve to specify the matrix are entered in a form consistent with the selected input option (IOP). Since we are only interested in symmetric matrices, only the lower triangle of the matrix is provided in the input. Specific format details are evident from the program source listing. All such input is in 6E12.6 format.

In each program the correlation matrix is first tested to determine if any of its elements exceed unity in value. If any do, program execution ceases. The output is self-explanatory, as is evident from the examples provided in this appendix.

MATXTEST - CDC - L.P.GERALDO - AP 314
 TESTS A SYMMETRIC MATRIX FOR POSITIVE DEFINITENESS.
 THIS PROGRAM ALSO COMPUTATES THE DETERMINANT AND
 INVERSE MATRIX

OPTIONS FOR MATRIX INPUT (IOP)

OPTION 1 - INPUT ERRORS AND CORRELATION MATRIX
 OPTION 2 - INPUT COVARIANCE MATRIX
 OPTION 3 - INPUT CROSS SECTIONS AND RELATIVE COVARIANCE MATRIX

OPTIONS FOR MATRIX INFORMATION OUTPUT (IND)
 TOGETHER WITH POSITIVE DEFINITENESS TEST.

OPTION - 00 = STOP
 OPTION - 10 = ONLY DETERMINANT
 OPTION - 01 = ONLY INVERSE MATRIX
 OPTION - 11 = BOTH DETERMINANT AND INVERSE MATRIX

REAL A(50,50),C(50,50),F(50,50),E(50),X(50),DET(3),T,D
 REAL V(50,50),W(3,3),TS,XS,YS,ZS

DATA LDA/50/
 DATA LD/3/
 DATA IN/'N '
 WRITE(*,5)

5 FORMAT(1X,'DATA INPUT: ')
 OPEN(3,FILE=' ',STATUS='OLD ')
 READ(3,10)N
 10 FORMAT(I2)
 READ(3,10)IOP
 READ(3,10)IND
 15 FORMAT(6E12.6)
 GO TO (20,40,50) IOP
 20 CONTINUE
 READ(3,15) (E(I), I=1,N)
 DO 25 I=1,N
 25 READ(3,15) (C(I,J), J=1,I)
 DO 30 I=1,N
 DO 30 J=1,I
 30 C(J,I)=C(I,J)
 DO 35 I=1,N
 DO 35 J=1,N
 35 A(I,J) = E(I)*E(J)*C(I,J)
 DO 36 I=1,N
 DO 36 J=1,N
 36 V(I,J)=A(I,J)
 GO TO 70
 40 CONTINUE
 DO 45 I=1,N
 45 READ(3,15) (A(I,J), J=1,I)
 DO 46 I=1,N
 DO 46 J=1,N
 46 A(I,J)=A(J,I)
 DO 47 I=1,N
 DO 47 J=1,N
 47 C(I,J)=A(I,J)/(A(I,I)*A(J,J)**0.5

DO 48 I=1,N
 DO 48 J=1,N
 48 V(I,J)=A(I,J)
 GO TO 70
 50 CONTINUE
 READ(3,15) (X(I), I=1,N)
 DO 55 I=1,N
 55 READ(3,15) (F(I,J), J=1,I)
 DO 60 I=1,N
 DO 60 J=1,N
 60 F(I,J)=F(J,I)
 DO 65 I=1,N
 DO 65 J=1,N
 65 A(I,J)=X(I)*X(J)*F(I,J)
 DO 67 I=1,N
 DO 67 J=1,N
 67 C(I,J)=A(I,J)/(A(I,I)*A(J,J)**0.5
 DO 68 I=1,N
 DO 68 J=1,N
 68 V(I,J)=A(I,J)
 70 CONTINUE

CORRELATION MATRIX TEST

DO 73 I=1,N
 DO 73 J=1,I
 IF(I .EQ. J) GO TO 73
 IF(ABS(C(I,J)) .LE. 1) GO TO 73
 WRITE(*,71)
 71 FORMAT(1X,'... I J C(I,J) ... ')
 WRITE(*,72)I,J,C(I,J)
 72 FORMAT(1X,I5,I10,F18.6)
 73 CONTINUE
 DO 74 I=1,N
 DO 74 J=1,I
 IF(I .EQ. J) GO TO 74
 IF(ABS(C(I,J)) .GT. 1) GO TO 240
 74 CONTINUE

POSITIVE DEFINITENESS TEST

CALL SPOFA(A,LDA,N,INFO)
 IF (INFO .NE. 0) GO TO 125

OUTPUT DATA

WRITE(*,80)
 80 FORMAT(1X,' THIS MATRIX IS POSITIVE DEFINITE ')
 IF (IND .EQ. 0) GO TO 120

DETERMINANT AND INVERSE MATRIX COMPUTATION

CALL SPODI(A,LDA,N,DET,IND)

IF (IND .EQ. 11) GO TO 85
 IF (IND .EQ. 1) GO TO 85
 85 DT=DET(1)*10.0**DET(2)

```

WRITE(*,90) DT
90 FORMAT(1X, 'DET= ',E12.6)
IF (IND .EQ. 10) GO TO 120
91 WRITE(*,92)
92 FORMAT(1X, 'Do you want to save the inverse matrix?Y/N ')
READ(*,143,ERR=91) IOP
IF(IOP .EQ. IN) GO TO 95
WRITE(*,93)
93 FORMAT(1X, 'Please type the output file name ')
OPEN(5,FILE=' ',STATUS='NEW ')
WRITE(5,94)
94 FORMAT(1X, 'XXXXXXXXXXXX INVERSE MATRIX XXXXXXXXXXXX ')
DO 941 I=1,N
DO 941 J=1,N
941 A(J,I)=A(I,J)
DO 942 J=1,N
942 WRITE(5,115) (A(J,I), I=1,J)
GO TO 120
C
95 WRITE(*,100)
100 FORMAT(1X, 'XXXXXXXXXXXX INVERSE MATRIX XXXXXXXXXXXX ')
DO 105 I=1,N
DO 105 J=1,N
105 A(J,I)=A(I,J)
DO 110 J=1,N
110 WRITE(*,115) (A(J,I), I=1,J)
115 FORMAT(1X,SOE12.6)
120 STOP
125 WRITE(*,130)
130 FORMAT(1X, 'THIS MATRIX IS NOT POSITIVE DEFINITE ')
WRITE(*,135)
135 FORMAT(1X, 'VERIFY THE FOLLOWING MATRIX LINE: ')
I=INFO
WRITE(*,140) I
140 FORMAT(1X, 'LINE I= ', I2)
WRITE(*,115) (A(I,J), J=1, I)
141 WRITE(*,142)
142 FORMAT(1X, 'Do you want to test all the cross correlations inside t
this leading principal minor?Y/N ')
READ(*,143,ERR=141) IOP
143 FORMAT(A1)
IF(IOP .EQ. IN) GO TO 235
WRITE(*,145)
145 FORMAT(1X, 'Test of the cross correlation consistency ')
N=INFO
IF(N .LT. 3) GO TO 238
150 I1=1
160 J1=I1+1
170 K1=J1+1
178 W(1,1)=V(I1,I1)
W(2,2)=V(J1,J1)
W(3,3)=V(K1,K1)
W(1,2)=V(I1,J1)
W(1,3)=V(I1,K1)
W(2,3)=V(J1,K1)
M=3
CALL SPOFA(W,LD,M,INF)
IF(INF .EQ. 0) GO TO 188

```

42

```

WRITE(*,185)
185 FORMAT(1X, 'This cross correlation is not positive definite. ')
WRITE(*,187) I1, J1, K1
187 FORMAT(1X, 'The correspondent parameters are: ', 3I4)
188 IF(K1 .EQ. N) GO TO 200
K1=K1+1
GO TO 178
200 IF(J1 .EQ. N-1) GO TO 210
J1=J1+1
GO TO 170
210 IF(I1 .EQ. N-2) GO TO 220
I1=I1+1
GO TO 160
220 CONTINUE
WRITE(*,230)
230 FORMAT(1X, 'All 3x3 principal minors were tested ')
235 STOP
238 WRITE(*,239)
239 FORMAT(1X, 'The matrix order is lower than 3. ')
STOP
240 WRITE(*,245)
245 FORMAT(1X, 'This matrix is unreal because the correlation coefficie
ints above are higher than 1 ')
STOP
END
C
C
C
SUBROUTINE SPOFA(A,LDA,N,INFO)
SPOFA TESTS IF THE MATRIX IS POSITIVE DEFINITE AND
FACTORS A REAL SYMMETRIC POSITIVE DEFINITE MATRIX
C
C
C
INTEGER LDA,N,INFO
REAL A(LDA,1)
REAL SDOT,T
REAL S
INTEGER J,JM1,K
BEGIN BLOCK WITH...EXITS TO 40
C
C
DO 30 J = 1, N
INFO = J
S = 0.0E0
JM1 = J - 1
IF (JM1 .LT. 1) GO TO 20
DO 10 K = 1, JM1
T = A(K,J) - SDOT(K-1,A(1,K),1,A(1,J),1)
T = T/A(K,K)
A(K,J) = T
S = S + T*T
10 CONTINUE
20 CONTINUE
S = A(J,J) - S
EXIT
IF (S .LE. 0.0E0) GO TO 40
A(J,J) = SQRT(S)
30 CONTINUE

```

```

INFO = 0
40 CONTINUE
RETURN
END

```

```

SUBROUTINE SPODI(A,LDA,N,DET,JOB)
SPODI COMPUTES THE DETERMINANT AND INVERSE OF A CERTAIN
REAL SYMMETRIC POSITIVE DEFINITE MATRIX.

```

```

INTEGER LDA,N,JOB
REAL A(LDA,1)
REAL DET(2)
INTERNAL VARIABLES
REAL T
REAL S
INTEGER I,J,JM1,K,KP1

```

```

COMPUTE DETERMINANT

```

```

IF (JOB/10 .EQ. 0) GO TO 70
DET(1) = 1.0E0
DET(2) = 0.0E0
S = 10.0E0
DO 50 I = 1,N
  DET(1) = A(I,I)**2*DET(1)
  ...EXIT
  IF (DET(1) .EQ. 0.0E0) GO TO 60
10  IF (DET(1) .GE. 1.0E0) GO TO 20
    DET(1) = S*DET(1)
    DET(2) = DET(2) - 1.0E0
    GO TO 10
20  CONTINUE
30  IF (DET(1) .LT. S) GO TO 40
    DET(1) = DET(1)/S
    DET(2) = DET(2) + 1.0E0
    GO TO 30
40  CONTINUE
50 CONTINUE
60 CONTINUE
70 CONTINUE

```

```

COMPUTE INVERSE(R)

```

```

IF (MOD(JOB,10) .EQ. 0) GO TO 140
DO 100 K = 1, N
  A(K,K) = 1.0E0/A(K,K)
  T = -A(K,K)
  CALL SSCAL(K-1,T,A(1,K),1)
  KP1 = K + 1
  IF (N .LT. KP1) GO TO 90
  DO 80 J = KP1, N
    T = A(K,J)
    A(K,J) = 0.0E0
    CALL SAXPY(K,T,A(1,K),1,A(1,J),1)
80  CONTINUE

```

```

90 CONTINUE
100 CONTINUE

```

```

FORM INVERSE(R) * TRANS(INVERSE(R))

```

```

DO 130 J = 1, N
  JM1 = J - 1
  IF (JM1 .LT. 1) GO TO 120
  DO 110 K = 1, JM1
    T = A(K,J)
    CALL SAXPY(K,T,A(1,J),1,A(1,K),1)
110 CONTINUE
120 CONTINUE
    T = A(J,J)
    CALL SSCAL(J,T,A(1,J),1)
130 CONTINUE
140 CONTINUE
RETURN
END

```

```

SUBROUTINE SSCAL(N,SA,SX,INCX)

```

```

SSCAL SCALES A VECTOR BY A CONSTANT

```

```

REAL SA,SX(1)
INTEGER I,INCX,M,MP1,N,NINCX

```

```

M=MOD(N,5)
IF(M .EQ. 0) GO TO 40
DO 30 I=1,M
  SX(I)=SA*SX(I)
30 CONTINUE
IF(N .LT. 5) RETURN
40 MP1=M+1
DO 50 I=MP1,N,5
  SX(I)=SA*SX(I)
  SX(I+1)=SA*SX(I+1)
  SX(I+2)=SA*SX(I+2)
  SX(I+3)=SA*SX(I+3)
  SX(I+4)=SA*SX(I+4)
50 CONTINUE
RETURN
END

```

```

SUBROUTINE SAXPY(N,SA,SX,INCX,SY,INCY)

```

```

SAXPY COMPUTES THE OPERATION: CONSTANT TIMES A VECTOR
PLUS A VECTOR.

```

```

REAL SX(1),SY(1),SA
INTEGER I,INCX,INCY,IX,IY,M,MP1,N

```

```

M=MOD(N,4)
IF(M .EQ. 0) GO TO 40
DO 30 I=1,M

```

```

        SY(I)=SY(I)+SA*SX(I)
30 CONTINUE
    IF(N .LT. 4) RETURN
40 MP1=M+1
    DO 50 I=MP1,N,4
        SY(I)=SY(I)+SA*SX(I)
        SY(I+1)=SY(I+1)+SA*SX(I+1)
        SY(I+2)=SY(I+2)+SA*SX(I+2)
        SY(I+3)=SY(I+3)+SA*SX(I+3)
50 CONTINUE
    RETURN
    END

```

C
C
C
C
C
C

```

REAL FUNCTION SDOT(N,SX,INCX,SY,INCY)

```

```

SDOT FORMS THE DOT PRODUCT OF TWO VECTORS

```

```

REAL SX(1),SY(1),STEMP
INTEGER I,INCX,INCY,IX,IY,M,MP1,N

```

```

STEMP=0.0E0
SDOT=0.0E0
IF(N .LE. 0)RETURN
20 M=MOD(N,5)
IF(M .EQ. 0) GO TO 40
DO 30 I=1,M
    STEMP=STEMP+SX(I)*SY(I)
30 CONTINUE
IF(N .LT. 5) GO TO 60
40 MP1=M+1
    DO 50 I=MP1,N,5
        STEMP=STEMP+SX(I)*SY(I)+SX(I+1)*SY(I+1)+SX(I+2)*SY(I+2)+
        * SX(I+3)*SY(I+3)+SX(I+4)*SY(I+4)
50 CONTINUE
60 SDOT=STEMP
    RETURN
    END

```



```

117 FORMAT(1X,'XXXXXXXXXX INVERSE MATRIX XXXXXXXXXXXX ')
    DO 118 I=1,N
      DO 118 J=1,N
118 A(J,I)=A(I,J)
      DO 119 J=1,N
119 WRITE(5,128) (A(J,I), I=1,J)
    GO TO 130
120 WRITE(*,122)
122 FORMAT(1X,'XXXXXXXXXX INVERSE MATRIX XXXXXXXXXXXX ')
    DO 124 I=1,N
      DO 124 J=1,N
124 A(J,I)=A(I,J)
      DO 126 J=1,N
126 WRITE(*,128) (A(I,J),I=1,J)
128 FORMAT(1X,50E12.6)
    IF (INP .NE. 111) GO TO 154
130 CONTINUE
140 DT=DET(1)*10.0**DET(2)
149 WRITE(*,150) DT
150 FORMAT(1X,'DET= ',E12.6)
154 WRITE(*,155)
155 FORMAT(1X,'XXXXX INERTIA=Number of Eigenvalues XXXXX ')
    WRITE(*,160) (INERT(L),L=1,3)
160 FORMAT(1X,'Positive= ',I2,' Negative= ',I2,' Zero= ',I2)
    IF (INERT(1) .EQ. N) GO TO 162
    IF (INERT(2) .EQ. N) GO TO 164
    IF (INERT(1)+INERT(3) .EQ. N) GO TO 166
    IF (INERT(2)+INERT(3) .EQ. N) GO TO 168
    IF (INERT(1)+INERT(2)+INERT(3) .EQ. N) GO TO 170
162 WRITE(*,163)
163 FORMAT(1X,'This matrix is Positive Definite')
    STOP
164 WRITE(*,165)
165 FORMAT(1X,'This matrix is Negative Definite')
    STOP
166 WRITE(*,167)
167 FORMAT(1X,'This matrix is Positive ')
    STOP
168 WRITE(*,169)
169 FORMAT(1X,'This matrix is Negative ')
    STOP
170 WRITE(*,171)
171 FORMAT(1X,'This matrix is Indefinite ')
    STOP
180 WRITE(*,185)
185 FORMAT(1X,'This matrix is unreal because the correlation coefficie
    ints above are higher than 1')
    STOP
    END
    SUBROUTINE SSICO(A,LDA,N,KPVT,RCOND,Z)
    INTEGER LDA,N,KPVT(1)
    REAL A(LDA,1),Z(1)
    REAL RCOND

```

```

C
C SSICO FACTORS A REAL SYMMETRIC MATRIX BY ELIMINATION WITH
C SYMMETRIC PIVOTING AND ESTIMATES THE CONDITION OF THE MATRIX
C
C INTERNAL VARIABLES

```

```

C
REAL AK,AKM1,BK,BKM1,SDOT,DENOM,EK,T
REAL ANORM,S,SASUM,YNORM
INTEGER I,INFO,J,JM1,K,KP,KPS,KS
C
DO 30 J=1,N
  Z(J)=SASUM(J,A(1,J),1)
  JM1=J-1
  IF(JM1 .LT. 1) GO TO 20
  DO 10 I=1,JM1
    Z(I)=Z(I)+ABS(A(I,J))
10 CONTINUE
20 CONTINUE
30 CONTINUE
  ANORM=0.0EO
  DO 40 J=1,N
    ANORM=AMAX1(ANORM,Z(J))
40 CONTINUE
  CALL SSIFA(A,LDA,N,KPVT,INFO)
  EK=1.0EO
  DO 50 J=1,N
    Z(J)=0.0EO
50 CONTINUE
  K=N
60 IF(K .EQ. 0) GO TO 120
  KS=1
  IF(KPVT(K) .LT. 0) KS=2
  KP=IABS(KPVT(K))
  KPS=K+1-KS
  IF(KP .EQ. KPS) GO TO 70
  T=Z(KPS)
  Z(KPS)=Z(KP)
  Z(KP)=T
70 CONTINUE
  IF(Z(K) .NE. 0.0EO) EK=SIGN(EK,Z(K))
  Z(K)=Z(K)+EK
  CALL SAXPY(K-KS,Z(K),A(1,K),1,Z(1),1)
  IF(KS .EQ. 1) GO TO 80
  IF(Z(K-1) .NE. 0.0EO) EK=SIGN(EK,Z(K-1))
  Z(K-1)=Z(K-1)+EK
  CALL SAXPY(K-KS,Z(K-1),A(1,K-1),1,Z(1),1)
80 CONTINUE
  IF(KS .EQ. 2) GO TO 100
  IF(ABS(Z(K)) .LE. ABS(A(K,K))) GO TO 90
  S=ABS(A(K,K))/ABS(Z(K))
  CALL SSCAL(N,S,Z,1)
  EK=S*EK
90 CONTINUE
  IF(A(K,K) .NE. 0.0EO) Z(K)=Z(K)/A(K,K)
  IF(A(K,K) .EQ. 0.0EO) Z(K)=1.0EO
  GO TO 110
100 CONTINUE
  AK=A(K,K)/A(K-1,K)
  AKM1=A(K-1,K-1)/A(K-1,K)
  BK=Z(K)/A(K-1,K)
  BKM1=Z(K-1)/A(K-1,K)
  DENOM=AK*AKM1-1.0EO
  Z(K)=(AKM1*BK-BKM1)/DENOM

```

```

110 CONTINUE
    K=K-KS
    GO TO 60
120 CONTINUE
    S=1.0EO/SASUM(N,Z,1)
    CALL SSCAL(N,S,Z,1)
    K=1
130 IF(K .GT. N) GO TO 160
    KS=1
    IF(KPVT(K) .LT. 0) KS=2
    IF(K .EQ. 1) GO TO 150
    Z(K)=Z(K)+SDOT(K-1,A(1,K),1,Z(1),1)
    IF(KS .EQ. 2)
      * Z(K+1)=Z(K+1)+SDOT(K-1,A(1,K+1),1,Z(1),1)
    KP=IABS(KPVT(K))
    IF(KP .EQ. K) GO TO 140
    T=Z(K)
    Z(K)=Z(KP)
    Z(KP)=T
140 CONTINUE
150 CONTINUE
    K=K+KS
    GO TO 130
160 CONTINUE
    S=1.0EO/SASUM(N,Z,1)
    CALL SSCAL(N,S,Z,1)
    YNORM=1.0EO
    K=N
170 IF(K .EQ. 0) GO TO 230
    KS=1
    IF(KPVT(K) .LT. 0) KS=2
    IF(K .EQ. KS) GO TO 190
    KP=IABS(KPVT(K))
    KPS=K+1-KS
    IF(KP .EQ. KPS) GO TO 180
    T=Z(KPS)
    Z(KPS)=Z(KP)
    Z(KP)=T
180 CONTINUE
    CALL SAXPY(K-KS,Z(K),A(1,K),1,Z(1),1)
    IF(KS .EQ. 2) CALL SAXPY(K-KS,Z(K-1),A(1,K-1),1,Z(1),1)
190 CONTINUE
    IF(KS .EQ. 2) GO TO 210
    IF(ABS(Z(K)) .LE. ABS(A(K,K))) GO TO 200
    S=ABS(A(K,K))/ABS(Z(K))
    CALL SSCAL(N,S,Z,1)
    YNORM=S*YNORM
200 CONTINUE
    IF(A(K,K) .NE. 0.0EO) Z(K)=Z(K)/A(K,K)
    IF(A(K,K) .EQ. 0.0EO) Z(K)=1.0EO
    GO TO 220
210 CONTINUE
    AK=A(K,K)/A(K-1,K)
    AKM1=A(K-1,K-1)/A(K-1,K)
    BK=Z(K)/A(K-1,K)
    BKM1=Z(K-1)/A(K-1,K)
    DENOM=AK*AKM1-1.0EO
    Z(K)=(AKM1*BK-BKM1)/DENOM

```

```

    Z(K-1)=(AK*BKM1-BK)/DENOM
220 CONTINUE
    K=K-KS
    GO TO 170
230 CONTINUE
    S=1.0EO/SASUM(N,Z,1)
    CALL SSCAL(N,S,Z,1)
    YNORM=S*YNORM
    K=1
240 IF(K .GT. N) GO TO 270
    KS=1
    IF(KPVT(K) .LT. 0) KS=2
    IF(K .EQ. 1) GO TO 260
    Z(K)=Z(K)+SDOT(K-1,A(1,K),1,Z(1),1)
    IF(KS .EQ. 2)
      * Z(K+1)=Z(K+1)+SDOT(K-1,A(1,K+1),1,Z(1),1)
    KP=IABS(KPVT(K))
    IF(KP .EQ. K) GO TO 250
    T=Z(K)
    Z(K)=Z(KP)
    Z(KP)=T
250 CONTINUE
260 CONTINUE
    K=K+KS
    GO TO 240
270 CONTINUE
    S=1.0EO/SASUM(N,Z,1)
    CALL SSCAL(N,S,Z,1)
    YNORM=S*YNORM
    IF(ANORM .NE. 0.0EO) RCOND=YNORM/ANORM
    IF(ANORM .EQ. 0.0EO) RCOND=0.0EO
    RETURN
    END

```

C
C
C
C
C
C
C

SUBROUTINE SSIFA(A,LDA,N,KPVT,INFO)
 SSIFA FACTORS A REAL SYMMETRIC MATRIX BY ELIMINATION
 WITH SYMMETRIC PIVOTING

INTEGER LDA,N,KPVT(1),INFO
 REAL A(LDA,1)
 REAL AK,AKM1,BK,BKM1,DENOM,MULK,MULKM1,T
 REAL ABSAKK,ALPHA,COLMAX,ROWMAX
 INTEGER IMAX,IMAXP1,J,JJ,JMAX,K,KM1,KM2,KSTEP,ISAMAX
 LOGICAL SWAP

ALPHA = (1.0EO + SQRT(17.0EO))/8.0EO
 INFO = 0
 K=N

10 CONTINUE
 IF(K .EQ. 0) GO TO 200
 IF(K .GT. 1) GO TO 20
 KPVT(1) = 1
 IF (A(1,1) .EQ. 0.0EO) INFO = 1
 GO TO 200
 20 CONTINUE
 KM1 = K - 1

```

ABSACK = ABS(A(K,K))
IMAX = ISAMAX(K-1,A(1,K),1)
COLMAX = ABS(A(IMAX,K))
IF (ABSACK .LT. ALPHA*COLMAX) GO TO 30
  KSTEP = 1
  SWAP = .FALSE.
GO TO 90
30 CONTINUE
ROWMAX = 0.0E0
IMAXP1 = IMAX + 1
DO 40 J = IMAXP1, K
  ROWMAX = AMAX1(ROWMAX,ABS(A(IMAX,J)))
40 CONTINUE
IF (IMAX .EQ. 1) GO TO 50
JMAX = ISAMAX(IMAX-1,A(1,IMAX),1)
ROWMAX = AMAX1(ROWMAX,ABS(A(JMAX,IMAX)))
50 CONTINUE
IF (ABS(A(IMAX,IMAX)) .LT. ALPHA*ROWMAX) GO TO 60
  KSTEP = 1
  SWAP = .TRUE.
GO TO 80
60 CONTINUE
IF (ABSACK .LT. ALPHA*COLMAX*(COLMAX/ROWMAX)) GO TO 70
  KSTEP = 1
  SWAP = .FALSE.
GO TO 80
70 CONTINUE
KSTEP = 2
SWAP = IMAX .NE. KM1
80 CONTINUE
90 CONTINUE
IF (AMAX1(ABSACK,COLMAX) .NE. 0.0E0) GO TO 100
  KPVT(K) = K
  INFO = K
  GO TO 190
100 CONTINUE
IF (KSTEP .EQ. 2) GO TO 140
IF (.NOT.SWAP) GO TO 120
CALL SSWAP(IMAX,A(1,IMAX),1,A(1,K),1)
DO 110 JJ = IMAX, K
  J = K + IMAX - JJ
  T = A(J,K)
  A(J,K) = A(IMAX,J)
  A(IMAX,J) = T
110 CONTINUE
120 CONTINUE
DO 130 JJ = 1, KM1
  J = K - JJ
  MULK = -A(J,K)/A(K,K)
  T = MULK
  CALL SAXPY(J,T,A(1,K),1,A(1,J),1)
  A(J,K) = MULK
130 CONTINUE
  KPVT(K) = K
  IF (SWAP) KPVT(K) = IMAX
  GO TO 190
140 CONTINUE
IF (.NOT.SWAP) GO TO 160

```

```

CALL SSWAP(IMAX,A(1,IMAX),1,A(1,K-1),1)
DO 150 JJ = IMAX, KM1
  J = KM1 + IMAX - JJ
  T = A(J,K-1)
  A(J,K-1) = A(IMAX,J)
  A(IMAX,J) = T
150 CONTINUE
T = A(K-1,K)
A(K-1,K) = A(IMAX,K)
A(IMAX,K) = T
160 CONTINUE
KM2 = K - 2
IF (KM2 .EQ. 0) GO TO 180
AK = A(K,K)/A(K-1,K)
AKM1 = A(K-1,K-1)/A(K-1,K)
DENOM = 1.0E0 - AK*AKM1
DO 170 JJ = 1, KM2
  J = KM1 - JJ
  BK = A(J,K)/A(K-1,K)
  BKM1 = A(J,K-1)/A(K-1,K)
  MULK = (AKM1*BK - BKM1)/DENOM
  MULKM1 = (AK*BKM1 - BK)/DENOM
  T = MULK
  CALL SAXPY(J,T,A(1,K),1,A(1,J),1)
  T = MULKM1
  CALL SAXPY(J,T,A(1,K-1),1,A(1,J),1)
  A(J,K) = MULK
  A(J,K-1) = MULKM1
170 CONTINUE
180 CONTINUE
KPVT(K) = 1 - K
IF (SWAP) KPVT(K) = -IMAX
KPVT(K-1) = KPVT(K)
190 CONTINUE
K = K - KSTEP
GO TO 10
200 CONTINUE
RETURN
END

```

C
C
C
C
C

SUBROUTINE SSIDI(A,LDA,N,KPVT,DET,INERT,WORK,JOB)

SSIDI COMPUTES THE DETERMINANT, INERTIA AND INVERSE OF A REAL SYMMETRIC MATRIX USING THE FACTORS FROM SSIFA.

INTEGER LDA,N,JOB
REAL A(LDA,1),WORK(1),DET(2)
INTEGER KPVT(1),INERT(3)
REAL AKK1,SDOT,TEMP
REAL TEN,D,T,AK,AKP1
INTEGER J,JB,K,KM1,KS,KSTEP
LOGICAL NOINV,NODET,NOERT

C

NOINV = MOD(JOB,10) .EQ. 0
NODET = MOD(JOB,100)/10 .EQ. 0
NOERT = MOD(JOB,1000)/100 .EQ. 0
IF (NODET .AND. NOERT) GO TO 140

```

IF (NOERT) GO TO 10
INERT(1) = 0
INERT(2) = 0
INERT(3) = 0
10 CONTINUE
IF (NODET) GO TO 20
DET(1) = 1.0EO
DET(2) = 0.0EO
TEN = 10.0EO
20 CONTINUE
T = 0.0EO
DO 130 K = 1, N
  D = A(K,K)
  IF (KPVT(K) .GT. 0) GO TO 50
  IF (T .NE. 0.0EO) GO TO 30
  T = ABS(A(K,K+1))
  D = (D/T)*A(K+1,K+1) - T
  GO TO 40
30 CONTINUE
  D = T
  T = 0.0EO
40 CONTINUE
50 CONTINUE
  IF (NOERT) GO TO 60
  IF (D .GT. 0.0EO) INERT(1) = INERT(1) + 1
  IF (D .LT. 0.0EO) INERT(2) = INERT(2) + 1
  IF (D .EQ. 0.0EO) INERT(3) = INERT(3) + 1
60 CONTINUE
  IF (NODET) GO TO 120
  DET(1) = D*DET(1)
  IF (DET(1) .EQ. 0.0EO) GO TO 110
  IF (ABS(DET(1)) .GE. 1.0EO) GO TO 80
  DET(1) = TEN*DET(1)
  DET(2) = DET(2) - 1.0EO
  GO TO 70
70 CONTINUE
80 CONTINUE
  IF (ABS(DET(1)) .LT. TEN) GO TO 100
  DET(1) = DET(1)/TEN
  DET(2) = DET(2) + 1.0EO
  GO TO 90
90 CONTINUE
100 CONTINUE
110 CONTINUE
120 CONTINUE
130 CONTINUE
140 CONTINUE
  IF (NOINV) GO TO 270
  K = 1
150 IF (K .GT. N) GO TO 260
  KM1 = K - 1
  IF (KPVT(K) .LT. 0) GO TO 180
  A(K,K) = 1.0EO/A(K,K)
  IF (KM1 .LT. 1) GO TO 170
  CALL SCOPY(KM1,A(1,K),1,WORK,1)
  DO 160 J=1, KM1
    A(J,K) = SDOT(J,A(1,J),1,WORK,1)
    CALL SAXPY(J-1,WORK(J),A(1,J),1,A(1,K),1)
160 CONTINUE
  A(K,K) = A(K,K) + SDOT(KM1,WORK,1,A(1,K),1)

```

```

170 CONTINUE
  KSTEP = 1
  GO TO 220
180 CONTINUE
  T = ABS(A(K,K+1))
  AK = -A(K,K)/T
  AKP1 = A(K+1,K+1)/T
  AKKP1 = A(K,K+1)/T
  D = T*(AK*AKP1 - 1.0EO)
  A(K,K) = AKP1/D
  A(K+1,K+1) = AK/D
  A(K,K+1) = -AKKP1/D
  IF (KM1 .LT. 1) GO TO 210
  CALL SCOPY(KM1,A(1,K+1),1,WORK,1)
  DO 190 J = 1, KM1
    A(J,K+1) = SDOT(J,A(1,J),1,WORK,1)
    CALL SAXPY(J-1,WORK(J),A(1,J),1,A(1,K+1),1)
190 CONTINUE
  A(K+1,K+1) = A(K+1,K+1) + SDOT(KM1,WORK,1,A(1,K+1),1)
  A(K,K+1) = A(K,K+1) + SDOT(KM1,A(1,K),1,A(1,K+1),1)
  CALL SCOPY(KM1,A(1,K),1,WORK,1)
  DO 200 J = 1, KM1
    A(J,K) = SDOT(J,A(1,J),1,WORK,1)
    CALL SAXPY(J-1,WORK(J),A(1,J),1,A(1,K),1)
200 CONTINUE
  A(K,K) = A(K,K) + SDOT(KM1,WORK,1,A(1,K),1)
210 CONTINUE
  KSTEP = 2
220 CONTINUE
  KS = IABS(KPVT(K))
  IF (KS .EQ. K) GO TO 250
  CALL SSWAP(KS,A(1,KS),1,A(1,K),1)
  DO 230 JB = KS, K
    J = K + KS - JB
    TEMP = A(J,K)
    A(J,K) = A(KS,J)
    A(KS,J) = TEMP
230 CONTINUE
  IF (KSTEP .EQ. 1) GO TO 240
  TEMP = A(KS,K+1)
  A(KS,K+1) = A(K,K+1)
  A(K,K+1) = TEMP
240 CONTINUE
250 CONTINUE
  K = K + KSTEP
  GO TO 150
260 CONTINUE
270 CONTINUE
  RETURN
  END

```

```

C
C
C
C
C
C
SUBROUTINE SSWAP(N,SX,INCX,SY,INCY)
SSWAP INTERCHANGES TWO VECTORS
REAL SX(1),SY(1),STEMP

```

```

      INTEGER I, INCX, INCY, IX, IY, M, MP1, N
      IF (N .LE. 0) RETURN
      M = MOD(N, 3)
      IF (M .EQ. 0) GO TO 40
      DO 30 I = 1, M
         STEMP = SX(I)
         SX(I) = SY(I)
         SY(I) = STEMP
30 CONTINUE
      IF (N .LT. 3) RETURN
40 MP1 = M+1
      DO 50 I = MP1, N, 3
         STEMP = SX(I)
         SX(I) = SY(I)
         SY(I) = STEMP
         STEMP = SX(I + 1)
         SX(I + 1) = SY(I + 1)
         SY(I + 1) = STEMP
         STEMP = SX(I + 2)
         SX(I + 2) = SY(I + 2)
         SY(I + 2) = STEMP
50 CONTINUE
      RETURN
      END

C
C
C
C
      SUBROUTINE SAXPY(N, SA, SX, INCX, SY, INCY)
C
C
C
C
      SAXPY COMPUTES THE OPERATION: CONSTANT TIMES A VECTOR
      PLUS A VECTOR.

      REAL SX(1), SY(1), SA
      INTEGER I, INCX, INCY, IX, IY, M, MP1, N

      IF (N .LE. 0) RETURN
      IF (SA .EQ. 0.0) RETURN
      M = MOD(N, 4)
      IF (M .EQ. 0) GO TO 40
      DO 30 I = 1, M
         SY(I) = SY(I) + SA * SX(I)
30 CONTINUE
      IF (N .LT. 4) RETURN
40 MP1 = M + 1
      DO 50 I = MP1, N, 4
         SY(I) = SY(I) + SA * SX(I)
         SY(I+1) = SY(I+1) + SA * SX(I+1)
         SY(I+2) = SY(I+2) + SA * SX(I+2)
         SY(I+3) = SY(I+3) + SA * SX(I+3)
50 CONTINUE
      RETURN
      END

C
C
C
      REAL FUNCTION SDOT(N, SX, INCX, SY, INCY)

```

```

C
C
      SDOT FORMS THE DOT PRODUCT OF TWO VECTORS
C
      REAL SX(1), SY(1), STEMP
      INTEGER I, INCX, INCY, IX, IY, M, MP1, N

C
      STEMP = 0.0E0
      SDOT = 0.0E0
      IF (N .LE. 0) RETURN
20 M = MOD(N, 5)
      IF (M .EQ. 0) GO TO 40
      DO 30 I = 1, M
         STEMP = STEMP + SX(I) * SY(I)
30 CONTINUE
      IF (N .LT. 5) GO TO 60
40 MP1 = M + 1
      DO 50 I = MP1, N, 5
         STEMP = STEMP + SX(I) * SY(I) + SX(I+1) * SY(I+1) + SX(I+2) * SY(I+2) +
         * SX(I+3) * SY(I+3) + SX(I+4) * SY(I+4)
50 CONTINUE
60 SDOT = STEMP
      RETURN
      END

C
C
      INTEGER FUNCTION ISAMAX(N, SX, INCX)
C
C
C
      ISAMAX FINDS THE INDEX OF ELEMENT HAVING MAX. ABSOLUTE VALUE

      REAL SX(1), SMAX
      INTEGER I, INCX, IX, N

C
      ISAMAX = 0
      IF (N .LT. 1) RETURN
      ISAMAX = 1
      IF (N .EQ. 1) RETURN
      SMAX = ABS(SX(1))
      DO 30 I = 2, N
         IF (ABS(SX(I)) .LE. SMAX) GO TO 30
         ISAMAX = I
         SMAX = ABS(SX(I))
30 CONTINUE
      RETURN
      END

C
C
C
      SUBROUTINE SCOPY(N, SX, INCX, SY, INCY)
C
C
C
      SCOPY COPIES A VECTOR X TO A VECTOR Y

      REAL SX(1), SY(1)
      INTEGER I, INCX, INCY, IX, IY, M, MP1, N

C
      IF (N .LE. 0) RETURN
      M = MOD(N, 7)
      IF (M .EQ. 0) GO TO 40
      DO 30 I = 1, M
         SY(I) = SX(I)

```

```

30 CONTINUE
  IF(N .LT. 7) RETURN
40 MP1 = M+1
  DO 50 I = MP1,N,7
    SY(I)=SX(I)
    SY(I+1)=SX(I+1)
    SY(I+2)=SX(I+2)
    SY(I+3)=SX(I+3)
    SY(I+4)=SX(I+4)
    SY(I+5)=SX(I+5)
    SY(I+6)=SX(I+6)
50 CONTINUE
  RETURN
  END

```

```

DO 50 I=MP1,N,5
  SX(I)=SA*SX(I)
  SX(I+1)=SA*SX(I+1)
  SX(I+2)=SA*SX(I+2)
  SX(I+3)=SA*SX(I+3)
  SX(I+4)=SA*SX(I+4)
50 CONTINUE
  RETURN
  END

```

C
C
C
C
C

```

REAL FUNCTION SASUM(N,SX,INCX)
SASUM TAKES THE SUM OF THE ABSOLUTE VALUES.

```

```

REAL SX(1),STEMP
INTEGER I,INCX,M,MP1,N,NINCX

SASUM=0.0E0
STEMP=0.0E0
IF(N .LE. 0) RETURN
20 M=MOD(N,6)
  IF(M .EQ. 0) GO TO 40
  DO 30 I=1,M
    STEMP=STEMP+ABS(SX(I))
30 CONTINUE
  IF(N .LT. 6) GO TO 60
40 MP1=M+1
  DO 50 I=MP1,N,6
    STEMP=STEMP+ABS(SX(I))+ABS(SX(I+1))+ABS(SX(I+2))+
    * ABS(SX(I+3))+ABS(SX(I+4))+ABS(SX(I+5))
50 CONTINUE
60 SASUM=STEMP
  RETURN
  END

```

C
C
C
C
C

```

SUBROUTINE SSCAL(N,SA,SX,INCX)
SSCAL SCALES A VECTOR BY A CONSTANT.

```

```

REAL SA,SX(1)
INTEGER I,INCX,M,MP1,N,NINCX

IF(N .LE. 0) RETURN
20 M=MOD(N,5)
  IF(M .EQ. 0) GO TO 40
  DO 30 I=1,M
    SX(I)=SA*SX(I)
30 CONTINUE
  IF(N .LT. 5) RETURN
40 MP1=M+1

```

Test Problem 1

```
C:\MATXTST>
C:\MATXTST>
C:\MATXTST>MATXTST
DATA INPUT: File name missing or blank - Please enter name

UNIT 3? C:\MATXTST\MATXTST.INP
THIS MATRIX IS POSITIVE DEFINITE
DET= .879280E-06
Do you want to save the inverse matrix?Y/N
N
XXXXXXXXXXXX INVERSE MATRIX XXXXXXXXXXXX
.141991E+04
-.454736E+03 .946593E+03
Stop - Program terminated.

C:\MATXTST>MATXTST1
DATA INPUT: File name missing or blank - Please enter name

UNIT 3? C:\MATXTST\MATXTST.INP
RCOND= .362802E+00
Do you want to save the inverse matrix?Y/N
N
XXXXXXXXXXXX INVERSE MATRIX XXXXXXXXXXXX
.141991E+04
-.454736E+03 .946593E+03
DET= .879280E-06
XXXXX INERTIA=Number of Eigenvalues XXXXX
Positive= 2 Negative= 0 Zero= 0
This matrix is Positive Definite
Stop - Program terminated.

C:\MATXTST>TYPE MATXTST.INP
 2
 2
11
0.00083232
0.00039984 0.0012485
```

Test Problem 2

```
C:\MATXTST>
C:\MATXTST>MATXTST
DATA INPUT: File name missing or blank - Please enter name

UNIT 3? C:\MATXTST\MATXTST.INP
... I ..... J ..... C(I,J) ...
 3      1      2.500000
This matrix is unreal because the correlation coefficients above are higher than
1
Stop - Program terminated.

C:\MATXTST>MATXTST1
DATA INPUT: File name missing or blank - Please enter name

UNIT 3? C:\MATXTST\MATXTST.INP
... I ..... J ..... C(I,J) ...
 3      1      2.500000
This matrix is unreal because the correlation coefficients above are higher than
1
Stop - Program terminated.

C:\MATXTST>TYPE MATXTST.INP
 3
 2
11
2.0
1.0      3.0
5.0      2.0      2.0
```

Test Problem 3

```
C:\MATXTST>MATXTST
DATA INPUT: File name missing or blank - Please enter name

UNIT 3? C:\MATXTST\MATXTST.INP
THIS MATRIX IS NOT POSITIVE DEFINITE
VERIFY THE FOLLOWING MATRIX LINE:
LINE I= 4
.980000E-01 .254250E+00 .990000E-01 .100000E+01
Do you want to test all the cross correlations inside this leading principal min
or?Y/N
Y
Test of the cross correlation consistency
This cross correlation is not positive definite.
The correspondent parameters are: 1 2 4
All 3x3 principal minors were tested
Stop - Program terminated.

C:\MATXTST>MATXTST1
DATA INPUT: File name missing or blank - Please enter name

UNIT 3? C:\MATXTST\MATXTST.INP
RCOND= .132216E-02
Do you want to save the inverse matrix?Y/N
N
XXXXXXXXXX INVERSE MATRIX XXXXXXXXXXXX
-.808684E+02
-.590545E+02-.133759E+01
-.293525E+01-.341399E-01 .285546E+01
.234041E+02 .613283E+01 .137344E-01-.285504E+01
-.691406E+00-.803655E-02-.320508E-03 .318789E-02 .448840E+00
-.359202E+00-.417788E-02-.214484E-03 .168075E-02-.392230E-04 .174800E+00
DET= -.132085E-02
XXXXX INERTIA=Number of Eigenvalues XXXXX
Positive= 5 Negative= 1 Zero= 0
This matrix is Indefinite
Stop - Program terminated.

C:\MATXTST>TYPE C:\MATXTST\MATXTST.INP
6
1
11
0.10      0.30      0.60      1.0      1.5      2.4
1.0
0.2475    1.0
0.1650    0.0416    1.0
0.9800    0.8475    0.1650    1.0
0.0990    0.0250    0.0166    0.0990    1.0
0.0825    0.0208    0.0139    0.0825    0.0083    1.0
```

Test Problem 4

```
MATXTST
DATA INPUT: File name missing or blank - Please enter name

UNIT 3? C:\MATXTST\MATXTST.INP
THIS MATRIX IS POSITIVE DEFINITE
DET= .149169E-03
Do you want to save the inverse matrix?Y/N
N
XXXXXXXXXX INVERSE MATRIX XXXXXXXXXXXX
.252806E+04
-.443971E+01 .118440E+02
-.142717E+01-.213098E-02 .285633E+01
-.247194E+03-.443971E+00-.142717E+00 .252806E+02
-.336370E+00-.598013E-03-.115278E-03-.336371E-01 .448889E+00
-.174651E+00-.260780E-03-.107803E-03-.174650E-01-.141072E-04 .174813E+00
Stop - Program terminated.
```

```
C:\MATXTST>MATXTST1
DATA INPUT: File name missing or blank - Please enter name

UNIT 3? C:\MATXTST\MATXTST.INP
RCOND= .649482E-04
Do you want to save the inverse matrix?Y/N
N
XXXXXXXXXX INVERSE MATRIX XXXXXXXXXXXX
.252806E+04
-.443970E+01 .118440E+02
-.142717E+01-.213099E-02 .285633E+01
-.247195E+03-.443972E+00-.142717E+00 .252806E+02
-.336370E+00-.598011E-03-.115278E-03-.336369E-01 .448888E+00
-.174652E+00-.260781E-03-.107803E-03-.174650E-01-.141127E-04 .174813E+00
DET= .149169E-03
XXXXX INERTIA=Number of Eigenvalues XXXXX
Positive= 6 Negative= 0 Zero= 0
This matrix is Positive Definite
Stop - Program terminated.
```

```
C:\MATXTST>TYPE MATXTST.INP
6
1
11
0.10      0.30      0.60      1.0      1.5      2.4
1.0
0.2475    1.0
0.1650    0.0416    1.0
0.9800    0.2475    0.1650    1.0
0.0990    0.0250    0.0166    0.0990    1.0
0.0825    0.0208    0.0139    0.0825    0.0825    1.0
```

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