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Contributions to Few-Channel Spectrum Unfolding

F. G. Perey

OAK RIDGE NATIONAL LABORATORY
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F. G. Perey

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ABSTRACT

In this report are two papers dealing with the subject of spectrum unfolding. These papers are closely related and will appear in the proceedings of two different conferences. Although they deal with analysis of dosimetry data, the method presented in these two papers is very general and applicable to any few-channel unfolding problem.

INTRODUCTION

As Chairman of the Data Covariance Subcommittee of the Cross Section Evaluation Working Group (CSEWG) I was invited to present a paper at the Second Euratom Symposium on Reactor Dosimetry to discuss how the data covariance files of ENDF/B could be used to estimate uncertainties in neutron spectra obtained on the basis of activation data. During the investigation of this topic I realized that this "few-channel unfolding problem" could be solved, taking into account all of the uncertainties in the data, using the least-squares method. I was able to show that the least-squares method provides the best possible estimate of the spectrum, including its uncertainties, and that currently well accepted methods of solving the problem could produce seriously wrong answers. Although this "new method" of unfolding was developed in the context of dosimetry neutron spectrum unfolding, it is very general, can be used in all unfolding problems, and solves exactly the "propagation of uncertainties" in the "response functions," a very important aspect of unfolding which until now had been either ignored or very poorly treated. As a result of this investigation, two papers were written, one for presentation at the Symposium and the other for presentation the following week at an IAEA Technical Committee Meeting on Current Status of Neutron Spectrum Unfolding. Since these two papers are closely related and will appear in two different proceedings which may not be easily available to those who might benefit from using this new approach to their unfolding problem, the papers are reproduced under a single cover for greater ease of access.

UNCERTAINTY ANALYSIS OF DOSIMETRY SPECTRUM UNFOLDING

F. G. Perey

Paper presented at the
Second ASTM-EURATOM Symposium on
Reactor Dosimetry: Dosimetry Methods for
Fuels, Cladding, and Structural Materials

Palo Alto, California
October 3-7, 1977

Abstract

The propagation of uncertainties in the input data is analyzed for the usual dosimetry unfolding solution. A new formulation of the dosimetry unfolding problem is proposed in which the most likely value of the spectrum is obtained. The relationship of this solution to the usual one is discussed.

Introduction

For several years I have been associated within the Cross Section Evaluation Working Group (CSEWG) with the attempt at providing in ENDF/B some information related to how well the data are perceived to be known. This effort has resulted in the creation of new files — the data covariance files. At the last CSEWG meeting as Chairman of the Data Covariance Subcommittee I was asked by the Dosimetry Subcommittee to investigate how these new files, which will be present for the dosimetry cross sections of ENDF/B-V, could be used to estimate the uncertainties in unfolded spectra. It is the purpose of this paper to summarize the results of this investigation.

The Data Covariance Files of ENDF/B

First we should briefly describe the "estimated data covariance files" of ENDF/B. In plain language they are nothing more than a statement of quantities which experimentalists refer to as "errors" in the measurements, except that in ENDF/B they are "errors" in the evaluations. Early in the development of these files we in fact called them "error files." But for various reasons related in large part to misunderstandings arising out of the use of the word error and consequently the lack of precise meaning on how they are to be manipulated, it was decided to borrow a terminology from statistics and they were called "the covariances of the estimated joint probability density functions of the evaluated data" or "covariance files" for short. In order to provide a complete description which would allow firm rules for their manipulation, we also assumed that the distribution law was normal and that the "data files" contained the mean value of the distribution.

It is unnecessary here to go into the details of the formats and procedures available[1] for ENDF/B-V. We place ourselves here strictly as users of the files and need to keep in mind only two important aspects:

1. By their very nature, they contain approximate quantities which we often refer to as uncertainties, synonymously with covariances, whose magnitudes even under the best of circumstances are not known to better than about 30%, at least in the evaluated files.

2. The total uncertainty in a particular cross section, say a dosimetry cross section at a given neutron energy, is usually made up of several contributions which are referred to as components. Each of these components may be common to some other evaluated cross sections which may be for the same reaction at other energies or even other reactions, even for a different nuclide. By and large in the process of performing the evaluation these contributions, which experimentalists refer to as the statistical error, i.e., completely uncorrelated to other cross sections, are much reduced or have even disappeared. In fact, strictly speaking, because cross sections are continuous functions of energy, it is not possible at all to represent such totally uncorrelated errors in ENDF/B. This does not cause any problem, even in principle, because no measurement can be made without a finite energy spread. The end result of adding all these components which have different correlations is to create a covariance matrix which is not diagonal and may have arbitrary overall correlations.

The covariance files of ENDF/B are therefore approximate, but define a covariance matrix of the "distribution" of the cross sections for which they are given whose major characteristic is that in general it is not diagonal.

Finally, because of their formats, these data covariance files can be readily processed to yield the covariance matrix of the processed data. These covariance matrices can also be easily manipulated to perform the "propagation of the uncertainties" to the results of any well defined mathematical operations on the data to yield the covariance matrix of these results.

Possible Approaches to Uncertainty Propagation

The straightforward approach to satisfy the request of the Dosimetry Subcommittee is to perform a standard propagation of the cross section uncertainties including their correlations to the solution produced by the dosimetry unfolding codes.

If a_i is the activation for the reaction i, σ_j^i the dosimetry cross section for reaction i at energy j and ϕ_j the flux in the neutron spectrum at energy j, we have:

$$A = R \cdot \Phi \tag{1}$$

where $A \equiv \{a_i\}$, $R \equiv \{\sigma_j^i\}$ and $\Phi \equiv \{\phi_j\}$ (using capital letters to denote vectors and matrices, and the dot which we place between matrices indicates the ordinary matrix multiplication operation). Given an "observation vector" A° the dosimetry unfolding problem as usually formulated consists in solving for Φ where:

$$A^\circ = R \cdot \Phi \quad . \tag{2}$$

As is well known, this is not a straightforward matter when Φ has more components ϕ_j than there are activation measurements a_i°.

The usual method of finding a solution is to introduce a $\Phi^{(0)}$ known as the "trial spectrum" and to calculate:

$$A^{(0)} = R \cdot \Phi^{(0)} \quad . \tag{3}$$

Based upon the difference between A° and $A^{(0)}$, an algorithm is used to generate a better approximation called $\Phi^{(1)}$ and the procedure is repeated until a $\Phi^{(n)}$ is found such that we have:

$$A^\circ \approx R \cdot \Phi^{(n)} \quad , \tag{4}$$

where the approximate sign indicates that the difference is of the order of the standard deviations of the a_i°'s, and $\Phi^{(n)}$ is called the solution. This method may not be used by all the dosimetry unfolding codes, but is used by the most popular ones based on the algorithms of SPECTRA,[2] SAND-II[3] and CRYSTAL BALL.[4]

To my knowledge, very few codes perform any uncertainty analysis of their solutions beyond stopping the iterative procedure when the approximation (4) is satisfied within the limits of the measurements and this for two reasons: it does not make much sense to match the data better than it is known, and oscillations tend to occur in the solution, which are deemed unphysical when too good a match is attempted.

There is a Monte Carlo code[3] using SAND-II which performs an analysis of the uncertainties in $\Phi^{(n)}$ due to the uncertainties in the matrix elements of R, i.e., the σ_j^i's. This Monte Carlo code in fact at the same time looks at the effects of the uncertainties in the a_i°'s. The standard version has been modified[5] to look at the effect of the uncertainties in $\Phi^{(0)}$, the trial spectrum. Certainly some improvements could be made to this code since basically no correlations of the a°_i's are allowed and only very limited types of correlations are allowed in the σ_j^i's and ϕ_j's. These correlations are in the form of fully correlated errors over very broad energy ranges, called the GAVE structure, and no correlations are allowed in the errors of different reactions. These approximations are not fundamental to the Monte Carlo technique and can in principle be removed to perform the analysis with arbitrary correlations, i.e., non-diagonal covariance matrices. Monte Carlo can indeed only sample quantities which have independent distributions, i.e., a diagonal covariance matrix. However, by means of unitary transformations A°, R and $\Phi^{(0)}$ could be transformed into quantities which have diagonal covariance matrices which would be sampled by Monte Carlo. This method has the disadvantage that we have to diagonalize very large matrices.

Another approach is the standard sensitivity route. We obtain the sensitivity matrix G:

$$\Delta\Phi^{(n)} \equiv G \cdot \Delta P \quad , \tag{5}$$

where P are the "parameters" of the problem, i.e., the a_i°'s, the σ_j^i's and the $\phi_j^{(0)}$'s. The matrix elements of G are the partial derivatives of the $\phi_j^{(n)}$'s with respect to all the parameters, the a_i°'s, the σ_j^i's and the $\phi_j^{(0)}$'s. Since there does not exist a closed form expression which

relates $\Phi^{(n)}$ to any of the elements of P, these numerous partial derivatives would have to be obtained numerically.

However, once G is obtained it is an easy matter to obtain the uncertainties in $\Phi^{(n)}$, i.e., its covariance matrix, which we write as $N_{\Phi(n)}$, since

$$N_{\Phi(n)} = G \cdot N_p \cdot G^{\dagger} \quad , \tag{6}$$

where N_p is the covariance matrix of the parameters and the symbol † stands for the transpose. We may easily express N_p in terms of the covariance matrices of the input data:

$$N_p = \begin{pmatrix} N_{\Phi(0)} & 0 & 0 \\ 0 & N_{\Sigma} & 0 \\ 0 & 0 & N_{A^{\circ}} \end{pmatrix} \quad , \tag{7}$$

where $N_{\Phi(0)}$ is the covariance matrix of $\Phi^{(0)}$, N_{Σ} the covariance matrix of the dosimetry cross sections and $N_{A^{\circ}}$ the covariance matrix of the activations. We have indicated with our notation of the null submatrices 0 that we assume that the different classes of input data, A°, Σ and $\Phi^{(0)}$, are uncorrelated.

The above two methods are entirely equivalent and may be called brute force methods which have the disadvantage of requiring a lot of computation, for the first method the diagonalization of the covariance matrices, and for the second method the calculation of the partial derivatives.

We should be aware when performing such uncertainty analysis that what we obtain — the final covariance matrix — only represents the contribution due to the input data uncertainties. The ultimate user usually does not care much for such an answer unless we can prove that the method of calculation has not introduced uncertainties which are comparable or at worse even greater than those we give him. In many instances such as the solution of neutron transport problems, it is possible to investigate these "methods uncertainties," as they are called, by studying the sensitivity of the results to various

approximations used in the solution. In the case of the dosimetry unfolding problem I am afraid this is where we run into a fundamental problem since it seems that we have no possibility to investigate this question because the method is the algorithm!! We cannot investigate "the approximations in the algorithm" because we do not know what is the "right" algorithm. Whatever we attempt to do in the algorithm only succeeds in generating a different algorithm.

I therefore strongly believe that performing an uncertainty analysis in the solution to the dosimetry problem as it is conventionally obtained is not giving us "the complete solution." However, as is often the case, a partial solution is better than no solution, and such uncertainty analysis may succeed in pushing back the limit of subjective evaluation of how credible the answer is.

A Possible Solution

It is likely that our failure at obtaining a solution to the dosimetry unfolding problem which is free of subjective evaluation is because we are asking too much from too few data and therefore the solution is impossible. I will propose now a formulation of the dosimetry unfolding problem which is slightly different mathematically from the usual one, but admits an exact solution. Although the mathematical question is different, it is difficult to see any difference between the exact solution to it and what we are usually trying to obtain.

Given:
1. some dosimetry cross sections with their uncertainties,
2. an estimated neutron spectrum with its uncertainty,
3. activation measurements performed in the actual neutron spectrum with their uncertainties.

What is the most likely value of the neutron spectrum and its uncertainty?

The "input data" are exactly what are required to solve the usual dosimetry unfolding problem and do the uncertainty analysis of its solution. But we are now requesting the most likely solution and its

uncertainty, which is after all what we are normally trying to obtain. I think that the usual unfolding procedure is an attempt at providing the answer: What is the neutron spectrum? The mathematical difference between the two formulations is so great that there is a unique and well known solution to one and to my knowledge no satisfactory one to the other.

The Mathematical Solution

Not only is there a unique solution to the problem as formulated, there are several well known ways[6] to obtain it. We will here only explore one of these, the least-squares method. As the problem was formulated, we have to minimize the χ^2-function:

$$\chi^2 = \begin{pmatrix} P - \bar{P} \\ A^\circ - \bar{A} \end{pmatrix}^\dagger \cdot \begin{pmatrix} N_p & 0 \\ 0 & N_{A^\circ} \end{pmatrix}^{-1} \cdot \begin{pmatrix} P - \bar{P} \\ A^\circ - \bar{A} \end{pmatrix} \quad , \tag{8}$$

where P stands for the "parameters" Φ and Σ, i.e.,

$$P \equiv \begin{pmatrix} \Phi \\ \Sigma \end{pmatrix} \quad , \tag{9}$$

and N_p the covariance matrix of P, i.e.,

$$N_p = \begin{pmatrix} N_\Phi & 0 \\ 0 & N_\Sigma \end{pmatrix} \quad . \tag{10}$$

In the χ^2-function we introduce P and N_p since we want the solution, the value of $\bar{P}$, which minimizes χ^2, to be the most likely value based upon our *a priori* knowledge of $\bar{P}$ given by P and N_p. Details of the solution will be given in a subsequent paper.[7] If we label by P' the value of $\bar{P}$ which minimizes the χ^2-function and by $N_{p'}$ its covariance matrix, we have:

$$P' - P = N_p \cdot G^\dagger \cdot (N_A + N_{A^\circ})^{-1} \cdot (A^\circ - A) \quad , \tag{11}$$

and

$$N_{p'} - N_p = -N_p \cdot G^{\dagger} \cdot (N_A + N_{A^\circ})^{-1} \cdot G \cdot N_p^{\dagger} \quad , \tag{12}$$

where A is computed from Φ and Σ, G is the sensitivity matrix defined by:

$$\Delta A \equiv G \cdot \Delta P \quad , \tag{13}$$

this G matrix is different from (5). The matrix N_A is the covariance matrix of A calculated using N_p and is given by:

$$N_A = G \cdot N_p \cdot G^{\dagger} \quad . \tag{14}$$

The solution (11) is most likely by virtue of the fact that it minimizes the χ^2-function (8), but also the best in the sense that it is unbiased and satisfies a minimum variance theorem.[6]

The solution, (11) and (12), can be very easily obtained since it only involves simple matrix multiplications and the matrix to be inverted $N_A + N_{A^\circ}$ has only the dimensions of the number of activations, which is small, and the matrix $N_A + N_{A^\circ}$ is almost never singular.[7] Contrary to the G matrix given by (5), which required computations of very many derivatives by numerical methods, the G matrix now needed as defined by (13) has for elements the parameters P themselves. If we define by Σ^i the activation cross sections for the reaction i, i.e., $\Sigma^i \equiv \{\sigma_j^i\}$, then the G matrix now needed is explicitly:

$$G = \begin{pmatrix} \Sigma^{1\dagger} & \Phi^{\dagger} & 0 & 0 & \cdots \\ \Sigma^{2\dagger} & 0 & \Phi^{\dagger} & 0 & \cdots \\ \Sigma^{3\dagger} & 0 & 0 & \Phi^{\dagger} & \cdots \\ \vdots & & & & \end{pmatrix} \quad . \tag{15}$$

A computer code named STAY'SL has been written[8] and is now available from RSIC to provide the solution, (11) and (12). The code STAY'SL only solves for the values of Φ' and $N_{\Phi'}$ instead of for the whole vector P' and $N_{p'}$. A code TRY'SL, soon to be released, will provide the complete solution P' and $N_{p'}$ and its purpose will be explained later.

Discussion

With our assumption that the covariance matrix of the parameters is diagonal in Φ and Σ the expression (8) for the χ^2-function can be written:

$$\chi^2 = (\Phi-\overline{\Phi})^{\dagger} \cdot N_{\Phi}^{-1} \cdot (\Phi-\overline{\Phi}) + (\Sigma-\overline{\Sigma})^{\dagger} \cdot N_{\Sigma}^{-1} \cdot (\Sigma-\overline{\Sigma}) + (A^{\circ}-\overline{A})^{\dagger} \cdot N_{A^{\circ}}^{-1} \cdot (A^{\circ}-\overline{A}) \ , \tag{16}$$

which indicates clearly that the solution Φ' and $N_{\Phi'}$ takes into account the uncertainties in all of the input data. How realistic and credible is our solution will therefore depend directly upon how realistic and credible are our estimates of the covariance matrices $N_{A^{\circ}}$, N_{Σ} and N_{Φ}. This is not really new, since it is perceived[9] with our usual methods, using the trial solution, that the solution $\Phi^{(n)}$ should be viewed with great caution and cross sections Σ should have in some sense been "validated," i.e., a "good" N_{Σ}, and the trial spectrum should be a "physical" one. Furthermore, it is recommended[9] that several different trial spectra $\Phi^{(0)}$ be used to ascertain the reliability of the solution, i.e., $N_{\Phi'}$. The usual methods should not be used as black boxes which produce "the solution."[9] In other words the usual methods seem to substitute a large amount of subjectivity to assess all of the covariance matrices N_{Φ}, N_{Σ} and finally $N_{\Phi'}$. The least-squares method removes any concern we have about biases in the algorithm since it is an unbiased algorithm.[6] A usual problem concerning the use of the least-squares method does not strictly speaking occur for the dosimetry problem, namely how good is the model? i.e., the formula which connects the observables A, a_i, and the parameters, Σ^i and Φ. In our case by definition the formula is exact:

$$a_i = \Sigma^{i\dagger} \cdot \Phi \quad . \tag{17}$$

However, in practice we have to worry about two problems. First, the group structure has to be fine enough not to make serious approximations in the use of relation (17). Second, through the relation $\Delta A \equiv G \cdot \Delta P$ we have linearized the problem and although strictly speaking we could use a nonlinear least-squares method, i.e., iterate to find G,

in practice there are serious problems because we are inserting *a priori* information about the solution Φ' through Φ, and Φ is used in G. It is not clear at this stage what can be done concerning this problem. Does it make much sense to request that the solution Φ' be consistent with the *a priori* knowledge of it, i.e., Φ and N_Φ, while we find that it is a poor estimate to obtain G? We have not investigated the implications of this apparent dilemma, but believe there is a logical inconsistency of sort even if in principle it could be justified. Consequently, we believe that the least-squares method is only in a very secure position and straightforward when the set of input data is not too unlikely. We do not believe that the solution should be iterated without some clear understanding of what this means. It is quite likely that such a conservative position is justified presently. Although iterations could easily be done, the meaning of the solution may be somewhat different. We believe that it may be safe to iterate to find G only when the values of Φ', although substantially different from Φ, are well within the uncertainties of Φ. In such cases, however, it could very well be that the joint probability density function given by Φ' and N_Φ, at the first step is not very different from the one obtained after one or two iterations. In common language, within the errors the two solutions agree.

Prospects for Application of the Least-Squares Method

The method of least-squares, with its better theoretical foundation and by making explicit the assumptions upon which the solution is based, has the potential for generating much more credible answers than we currently obtain. It is evident that considerable effort will have to be invested in order to obtain the most likely covariance matrices N_{A°, N_Σ, and N_Φ needed to solve for the most likely solution. During the course of testing the dosimetry least-squares code STAY'SL, and in particular when trying to compare its solution in a particular case[9] to those of other codes, we developed the concept of better and better solutions generated using very crude covariance matrices. Since this concept allows us to guarantee more likely answers than we currently get, even when we have a poor idea of what the best covariance matrices are, immediate benefits can be obtained using the method of least-squares.

solutions which is guaranteed to converge to the true or most likely solution and we can say that these solutions are better and better. This is so because there is a unique solution to the least-squares method for a given set of input quantities.

Now to complete our proof, we need to note that the least-squares method is known to give us the best unbiased estimate of the solution.[6] Therefore, it is guaranteed to give us a solution which is no worse than our current methods if we use it with either the implicit or effective covariance matrices which they use. If these covariance matrices are close to what we have called the "absolutely best" or "absolutely worst" ones, we can easily obtain a better solution by approaching in a well defined manner the most likely covariance matrices. How close we can come to the most likely answer depends of course upon how well we perceive to know the most likely covariance matrices. How much we "improve our solutions" depends also upon how far we go away from the "absolutely best" and "absolutely worst" covariance matrices. We shall now indicate the implicit or effective covariance matrices we use in our current methods.

For N_{A° we use only the diagonal elements at best, i.e., the variances of the a_i°'s. There is in fact no need to create any sequences of matrices. We should always use the most likely covariance matrices N_{A° as obtained from an analysis of the experiments. The experimentalists should give us with A° the full covariance matrix N_{A° or communicate the results of their "error analysis" in such a manner that the full covariance matrix can easily be generated. For N_Σ all of the current methods obtain the equivalent of Φ' assuming that the cross sections are perfectly well known. They are therefore implicitly using the "absolutely best" covariance matrix N_Σ, and we could readily improve upon them. When the Monte Carlo method is used with SAND-II,[3] this is no longer true since a definite N_Σ is used. However, we believe that some improvements could easily be made because we think that some of the correlations currently ignored could be used as well. For N_Φ we cannot so readily define the implicit covariance matrices used. However, all codes have been designed so that the solution $\Phi^{(n)}$ is influenced as

little as possible by the value of $\Phi^{(0)}$ through the various algorithms used. To the extent that they largely succeed, and it is impossible to succeed completely since the response matrix is singular, the effective covariance matrix N_Φ which they use can be said to be an "absolutely worst" one. Although such "absolutely worst" covariance matrices may be the only ones to use in some circumstances, in many others where we have some *a priori* knowledge of the spectrum it is very easy to improve upon them to get better solutions.

We conclude this discussion by noting that although a lot of work may be required to provide credible most likely covariance matrices, if we are only claiming to obtain a more likely answer than we do now, all we need to do is use credibly "absolutely better" or "absolutely worse" covariance matrices than we do now and we need not be very close to the most likely covariance matrices. Together with the code STAY'SL, we release the utility programs FCOV and XCOV which allow one to prepare such crude covariance matrices.

Finally, we would like to discuss one aspect of obtaining the most likely Σ and N_Σ to use in dosimetry unfolding problems. It is evident that since we have very carefully performed activation measurements in standard fields we would like to use these integral measurements to "improve" upon our knowledge of the dosimetry cross sections obtained from differential measurements. We are extending STAY'SL to solve explicitly for Σ' and N_Σ' so that this code called TRY'SL may be used to analyze these experiments. Although this can be viewed strictly as an adjustment procedure if we use the most credible values for Φ and N_Φ as well as A° and N_{A° and the least-squares method, this adjustment is perfectly justified and may in fact be properly called evaluating the cross sections on the basis of both integral and differential data. Now let us consider that we use the output values Σ' and $N_{\Sigma'}$ as our most likely cross sections to perform another analysis using activation data A^1 and N_{A^1} obtained in a spectrum which is characterized by an estimated Ψ and N_Ψ. We, of course, are only interested in obtaining Ψ' and $N_{\Psi'}$, but getting these is equivalent to performing a new adjustment of Σ' and $N_{\Sigma'}$ to obtain say Σ'' and $N_{\Sigma''}$. It is here that we run into a problem

which is, we believe, unique to the dosimetry field. Even though we are only interested in Ψ' and $N_{\Psi'}$, we effectively readjust the Σ' and $N_{\Sigma'}$ on the basis of A^1 and N_{A^1} as well. If there are any correlations between A° and A^1, as there will very likely be, we cannot use the simple method we have discussed so far because in effect we have some correlations between Σ' and A^1. We emphasize that this is not a fundamental limitation of the least-squares method and that in principle we could solve the problem if we knew what the correlations between Σ' and A^1 are. The practical problems would be very large and involve diagonalizing essentially $N_{\Sigma'}$. In addition to this problem, we have the even more formidable task of generating these correlations. The usual method of handling such problems is not to perform two consecutive adjustments but rather a single one where we only need to know the covariance matrix of A° and A^1 which we refer to as Y. What we propose to do, therefore, is to solve the following least-squares problem:

$$\chi^2 = \begin{pmatrix} P - \overline{P} \\ A^t - \overline{A} \end{pmatrix}^\dagger \cdot \begin{pmatrix} N_P & 0 \\ 0 & N_{A^t} \end{pmatrix}^{-1} \cdot \begin{pmatrix} P - \overline{P} \\ A^t - \overline{A} \end{pmatrix}$$

which is our original problem but where now in an obvious notation we have

$$P = \begin{pmatrix} \Psi \\ \Phi \\ \Sigma \end{pmatrix} \quad , \qquad N_P = \begin{pmatrix} N_\Psi & 0 & 0 \\ 0 & N_\Phi & 0 \\ 0 & 0 & N_\Sigma \end{pmatrix} \quad ,$$

and

$$A^t = \begin{pmatrix} A^\circ \\ A^1 \end{pmatrix} \quad , \qquad N_{A^t} = \begin{pmatrix} N_{A^\circ} & Y \\ Y & N_{A^1} \end{pmatrix} \quad .$$

We would solve explicitly only for Ψ' and $N_{\Psi'}$ and never calculate the adjusted cross sections nor Φ' and $N_{\Phi'}$ in this problem. What this least-squares solution would be is the most likely flux Ψ on the basis of our *a priori* knowledge of 1) the flux itself, Ψ and N_Ψ; 2) measurements made in this spectrum A^1 and N_{A^1}; 3) differential cross section data, Σ and N_Σ; and 4) activation measurements, A° and N_{A°, made in a standard field characterized by Φ and N_Φ.

We believe that through proper reporting of the error analysis of A° and A^{1} one could easily obtain Y. The solution to this problem should be easily obtained since it has only twice the dimensions of the original problem. In fact, when $Y \approx 0$, we believe that the inconvenience of solving this problem is compensated by the fact that we do not need to handle Σ' and the large covariance matrix N_{Σ}, which could not be approximated without loss of information.[7] In addition, we could readily improve our solutions Ψ' and N_{Ψ}, on the basis of improvements made to Σ, N_{Σ} and Φ, N_{Φ}. We plan to extend the code STAY'SL to provide the solution to the above problem.

Conclusions

In this paper we have discussed the question of propagations of uncertainties in the input data, particularly in the dosimetry cross sections, to the solution of the dosimetry neutron unfolding problem. We have reformulated the problem as a general least-squares one using non-diagonal covariance matrices where all of the uncertainties in the input data are explicitly used to arrive at the solution which we have compared with those of other often used unfolding codes. The method we propose is closely related to the well known data adjustment methods[10] and in fact identical to the one used in DANTE[11] in its handling of the spectrum and activation data. Although DANTE was proposed some time ago, we do not believe that the advantages of a general least-squares method are fully appreciated, probably because DANTE did not consider the dosimetry cross sections as parameters in the problem and therefore its solution was a particular case of the method we have outlined. We strongly believe that the general least-squares method we propose, because of its greater theoretical foundation, the fact that the credibility of the solutions can be inferred from the credibility of the input data and its great convenience in obtaining numerically the solution, has not only great potential in obtaining the most likely solutions, but also can be used in the near future to improve upon the current solutions. Much can be inferred about the solution from the input data due to the closed form expression of the solution without performing extensive numerical experiments as we will demonstrate in another paper.[2]

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SPECTRUM UNFOLDING BY THE LEAST-SQUARES METHOD

F. G. Perey

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ABSTRACT

The method of least squares is briefly reviewed, and the conditions under which it may be used are stated. From this analysis, a least-squares approach to the solution of the dosimetry neutron spectrum unfolding problem is introduced. The mathematical solution to this least-squares problem is derived from the general solution. The existence of this solution is analyzed in some detail. A χ^2-test is derived for the consistency of the input data, which does not require the solution to be first obtained. The fact that the problem is technically nonlinear, but should be treated in general as a linear one, is argued. Therefore, the solution should not be obtained by iteration. Two interpretations are made for the solution of the code STAY'SL, which solves this least-squares problem. The relationship of the solution to this least-squares problem to those obtained currently by other methods of solving the dosimetry neutron spectrum unfolding problem is extensively discussed. It is shown that the least-squares method does not require more input information than would be needed by our current methods in order to estimate the uncertainties in their solutions. From this discussion it is concluded that the proposed least-squares method does provide the best complete solution, with uncertainties, to the problem as it is understood now. Finally, some implications of this method are mentioned regarding future work required in order to exploit fully its potential.

Introduction

The usual solution to the dosimetry neutron spectrum unfolding problem is an attempt at providing a detailed spectrum based upon activation measurements obtained in this spectrum given *a priori* knowledge of the corresponding dosimetry cross sections. As is well known, a very detailed, exact (i.e., unique) spectrum cannot be obtained for this problem. Most popular dosimetry unfolding codes such as SAND-II,[1] SPECTRA,[2] and CRYSTAL BALL,[3] or those based on their algorithms, obtain their solution by introducing some additional information in the form of a "trial spectrum." This trial spectrum is clearly some form of *a priori* information about the solution. In a recent paper[4] we analyzed the propagation of the uncertainties in the input data to the solution of these codes. While it is clear what the meaning of the uncertainties is for the activation data and the cross sections, some discussion of the "uncertainties in the input trial spectrum" and their effects upon the solution is desirable. In many favorable cases of activation data analysis, if the trial spectrum is selected "close to a physical one," the solution of these codes exhibits a weak dependence upon the trial spectrum.[5] This aspect of the uncertainties in the solution is usually handled by means of several calculations performed using "several different physical trial spectra," and a subjective evaluation of the reliability of the solution due to "trial spectrum sensitivity" is made.[5] If we wanted to be quantitative about these uncertainties, we could explore in some fashion the whole space of "physically valid trial spectra" by say numerical methods and extract some measure for these uncertainties.

Certainly, if we did this, we would somewhat improve the credibility of the solution since in essence we would convert the somewhat arbitrary trial spectrum used to obtain the solution to a rather complete statement of the *a priori* knowledge about the solution, including its uncertainties. We believe, therefore, that part of the difficulties associated with the credibility of our usual solutions are related to the lack of precision in the statements which we either directly or indirectly make about the *a priori* information used and in some sense lower that information to the rank of "intuitive information,"[6] which calls for subjective evaluation. The second problem with our current methods is the fact that we in general cannot prove *a priori* what desirable or undesirable features our algorithms have in addition to those purposely put in. Such knowledge must be obtained through numerical experiments, inter-comparison of codes in special cases, etc.;[7] and such knowledge obtained *a posteriori* in specific examples may not necessarily be valid for somewhat new situations. It is for this reason that we proposed a new approach to the problem[4] which we think goes a long way toward eliminating these difficulties. In this paper we discuss at greater length this least-squares approach and some of the features and advantages of the solution.

The Least-Squares Approach

We review first briefly the general method of linear least-squares in order to establish a notation and state clearly the assumptions upon which the solution is obtained. We shall use as much as possible a description based on the physics of the situation rather than the more precise statistical language.[8]

Given some "observations" y_i° of n "quantities," $\overline{y}_i$, forming the abstract vector Y°, $Y^\circ \equiv \{y_i^\circ\}$. Let these observations, y_i°, have "errors," e_i, associated with them. We consider the quantities $\overline{y}_i$ to be random variables and the abstract vector $\overline{Y} \equiv \{\overline{y}_i\}$ to be therefore a multivariate. If the experimental results are unbiased, we can say that they provide us with an estimate of the joint density function of $\overline{Y}$ if we identify Y° with its expectation value, $Y^\circ = E[\overline{Y}]$, and from the e_i's we obtain its covariance matrix $M \equiv \{m_{ij}\}$, with $m_{ij} = E[e_i, e_j]$. No assumptions need be made about the form of the joint density function of $\overline{Y}$, and we emphasize that only its second moments, the m_{ij}'s, are specified. We introduce a "model" whereby $\overline{Y}$ is defined in terms of m "parameters," $\overline{p}_i$, which form the abstract parameter vector $\overline{P}$. Therefore, $\overline{P}$ is also considered to be a multivariate. Let us first take a model for $\overline{Y}$ which is linear in $\overline{P}$; we may write:

$$\overline{Y} = D \cdot \overline{P} \quad , \tag{1a}$$

where the dot we place between vectors and matrices denotes ordinary matrix multipliation and the n x m "design matrix" D is not a function of $\overline{P}$. When n = m, the equation (1a) can be solved exactly, to obtain the estimated joint density function of $\overline{P}$ from the estimated joint density function of $\overline{Y}$, if the design matrix D is not singular. For the case of n > m, our system of equations (1a) is overdetermined and what we seek is a "best average solution" in some sense. The method of least-squares obtains this solution by minimizing the "χ^2-function":

$$\chi^2 = (Y^\circ - \hat{Y})^\dagger \cdot M^{-1} \cdot (Y^\circ - \hat{Y}) \quad , \tag{2a}$$

where the symbol † denotes the transpose of vectors and matrices and $\hat{Y}$ denotes some estimate of the expectation value of $\overline{Y}$ based upon some estimate $\hat{P}$ of the expectation value of $\overline{P}$, $\hat{Y} = D \cdot \hat{P}$. The vector $Y^\circ - \hat{Y}$ is the "residual vector" and in this case is just $Y^\circ - D \cdot \hat{P}$. The minimum value of the χ^2-function is obtained by adjusting $\hat{P}$ and provides us with an "unbiased" estimate[8] for the joint density function of $\overline{P}$ characterized also only by its expectation value P' and its covariance matrix N'_p. This least-squares solution for the joint density function of $\overline{P}$ is often said to be "best" or "most likely" by virtue of the "minimum variance theorem"[8] which guarantees that it minimizes the variance of any linear combination of the parameters $\overline{p}_i$. We shall not prove here these very important properties of the least-squares solution, nor derive the solution, which is:[8]

$$P' = (D^\dagger \cdot M^{-1} \cdot D)^{-1} \cdot D^\dagger \cdot M^{-1} \cdot Y^\circ \quad , \tag{3a}$$

$$N'_p = (D^\dagger \cdot M^{-1} \cdot D)^{-1} \quad . \tag{4a}$$

When we refer to the solution of the problem, we mean both P' and N'_p since they are required for a somewhat meaningful specification of the joint density function of $\overline{P}$. We are indeed extremely limited in the kinds of useful statements we can make if we only obtain P'. The solution, (3a) and (4a), will always exist since the covariance matrices M and $D^\dagger \cdot M^{-1} \cdot D$ are in principle nonsingular. This is the case because the covariance matrix M is symmetric, as well as positive definite, and at least one "independent piece of information" is required to be associated with each observation y_i°. The "error" associated with this "independent piece of information" will contribute only to the diagonal of M and this

is sufficient to make the matrix M nonsingular. Therefore, if in practice a singular covariance matrix M is found, it is due to an oversight or mistake. The same arguments can be made about the covariance matrix $D^{\dagger} \cdot M^{-1} \cdot D$, although here it is relatively easier to overlook the fact that although two different "labels" were used for two parameters they are the same quantity, since they enter in the model in exactly the same way. Such singularities can therefore be removed easily.

The above statement of the problem is known as a linear least-squares one, for obvious reasons. In many situations the model for $\overline{Y}$ is nonlinear in the parameter $\overline{P}$, $\overline{Y} = F(\overline{P})$, and the solution cannot be obtained as indicated above. In such cases an approximate solution can still be found using the least-squares method by linearizing the model. To do so we expand the model in a Taylor series in the parameters, which is truncated after the second term:

$$\overline{Y} \approx Y + D \cdot (\overline{P} - P) \quad , \tag{1b}$$

where the design matrix D is made up of the partial derivatives of the model, $F(\overline{P})$, with respect to the parameter $\overline{P}$ and evaluated at $\overline{P} = P$. The linearization of the model by (1b) is good only for $\overline{P}$ close to P. Since $\overline{P}$ is a multivariate which can assume a large range of values, the approximation (1b) can be said to be always bad in some domain of $\overline{P}$. However, if we choose P in the neighborhood of the solution, P', assuming that it exists, and if the standard deviations of the joint density function of $\overline{P}$ are small compared to the expectation values and/or if the model is not very nonlinear in the sense that the elements of D are not very sensitive to P, the approximation (1b) may be a relatively good one.

A general discussion of the consequences of the linearization of the model is not our purpose since we will return to it later in commection with the dosimetry problem. Therefore, assuming the linear approximation (1b) can be made, we can proceed as for the linear case and write down explicitly the χ^2-function:

$$\chi^2 = (Y^\circ - Y - D \cdot (\hat{P}-P))^\dagger \cdot M^{-1} \cdot (Y^\circ - Y - D \cdot (\hat{P}-P)) \quad . \qquad (2b)$$

The comparison of (2b) with (2a) allows us to write immediately the solution for the minimum value of χ^2 which is obtained from (3a) and (4a) by substituting Y°-Y for Y° and P'-P for P' to get:

$$P' - P = (D^\dagger \cdot M^{-1} \cdot D)^{-1} \cdot D^\dagger \cdot M^{-1} \cdot (Y^\circ - Y) \quad , \qquad (3b)$$

$$N'_p = (D^\dagger \cdot M^{-1} \cdot D)^{-1} \quad . \qquad (4b)$$

Since frequently the initial choice of P is a poor one for the expansion (1b), the solution is then obtained by iteration in the hope that the solution will converge. It is important to note that the need to iterate is not an essential aspect of the method if the initial expansion "point" P yields a solution P' which is close to it. Iterating is, however, necessary if the model is highly nonlinear and P' is far from P. In this case the convergence of the process may or may not occur and when it does occur it may be at a "local minimum" which is a function of the starting value P.

If we can formulate our dosimetry data analysis problem as a least-squares one, the solution will be the most likely one and therefore better, or at least no worse, than any other one not based upon minimizing the χ^2-function. In addition, the properties of this solution will be well known and fully understood.

It is evident that our activation measurements in the spectrum, the a_i°'s and their uncertainties, meet the requirements to be some observations of the type y_i° needed for a least-squares problem. The activations $\bar{a}_i$ can be defined in terms of the fluxes $\bar{\phi}_j$ and cross sections $\bar{\sigma}_j^i$; our model for these quantities is clearly:

$$\bar{a}_i = \sum_j \bar{\sigma}_j^i \bar{\phi}_j \quad . \tag{5}$$

Since we can approximate our integral statement by expression (5) to any degree of accuracy, the "model" is exact by virtue of the definition of the quantities called the $\bar{\sigma}_j^i$'s. We may rewrite (5) in a more compact notation if we introduce the vector $\bar{\Phi}$ for the $\bar{\phi}_j$'s, $\bar{\Phi} \equiv \{\bar{\phi}_j\}$, and the vectors $\bar{\Sigma}^i$ for the $\bar{\sigma}_j^i$'s, $\bar{\Sigma}^i \equiv \{\bar{\sigma}_j^i\}$. Equation (5) then becomes:

$$\bar{a}_i = \bar{\Sigma}^{i\dagger} \cdot \bar{\Phi} \quad . \tag{6}$$

It is clearly implicit in our use of the name "dosimetry neutron spectrum unfolding" for dosimetry data analysis, that the "flux quantities" are usually considered as "parameters" in the problem and we have indicated this in Eq. (5) by treating them as variates by our notation $\bar{\Phi}_j$. The code DANTE,[9] which to our knowledge is the only current code which approaches dosimetry data analysis as a general least-squares problem as we do, treats the $\bar{\phi}_j$'s as the only parameters entering the model for the $\bar{a}_i$'s. DANTE does so by treating the cross sections as constants and solves the corresponding linear least-squares problem. Since at this stage of our knowledge of the dosimetry cross sections their estimated accuracies are often poorer than the estimated accuracies of the measured activations, ignoring the cross section uncertainties by treating the cross sections as constants

will significantly affect the estimated uncertainties in the spectrum. This point does not appear to have been generally appreciated for the "dosimetry unfolding problem" or even for the "many channel unfolding problem" where the "response matrix," which plays the role of the dosimetry cross sections in the dosimetry problem, is not considered as a variate on the same footing as the spectrum and consequently the uncertainties in the response matrix are not handled adequately.

In a dosimetry analysis problem we always have fewer activation measurements a_i° than we have quantities $\bar{\sigma}_j^i$ and $\bar{\phi}_j$, or even $\bar{\phi}_j$'s. There is, therefore, no unique solution for the $\bar{\phi}_j$'s, even if the a_i°'s were known perfectly, unless we are willing to add more information than just the activation measurements. Of course we could solve the problem of activation data analysis by representing the $\bar{\phi}_j$'s by a few parameters and this has been done in the past, but such ways of handling the difficulties are generally considered inadequate. In the least-squares method information is in the form of "observations" and therefore what we seek in solving the problem by this method is to supplement the a_i°'s with "other observations" which will produce an overdetermined set of equations for the $\bar{\sigma}_j^i$'s and $\bar{\phi}_j$'s. Two requirements must be met by the "quantities" used as "other observations": they must have "errors" associated with them and must be related to the parameters $\bar{\sigma}_j^i$ and $\bar{\phi}_j$ by means of a "model." Preferably this model must be exact, or considered so, since otherwise we need to introduce still more "observations" to overdetermine the approximate quantities in the model. It is evident that from a formal point of view the choice of "other quantities" to obtain an overdetermined set of equations is arbitrary and a solution can be found for each set of "other "quantities" which meet the two basic requirements stated above. This

arbitrariness in the choice of "other observations" can be largely removed if we consider the intended use of the solution sought. From the concept that we want the "best solution" for a specific use, it often becomes very clear what "best set of other observations" is needed, in addition to the measured a_i^o's of the problem. In the remainder of this paper we shall assume that what we are after is in some sense the "very best solution" consistent with our current knowledge. It is not evident that this particular solution is always the one desired, but we believe that it is the one which will be most useful for many uses and will serve to indicate the methodology. The idea of "very best solution" has implicit in it the fact that we have used to obtain it all observations which were ever made, for whatever purpose, related to the $\bar{\sigma}_j^i$'s and $\bar{\phi}_j$'s of this problem and that these observations are exploited to the fullest extent of our current knowledge.

We will first consider the $\bar{\sigma}_j^i$'s and show how this can be accomplished. The direct use of every experimental result related to the $\bar{\sigma}_j^i$'s is not practical even if in principle feasible. However, we can come close to achieving our goal if we consider that our "evaluations" of the $\bar{\Sigma}^i$'s attempt to represent all previous measurements and can be used directly as observations if they have "errors," or covariance matrices, associated with them. If we treat such evaluations of the $\bar{\Sigma}^i$'s as observations, their "model" becomes exact since it is the identity matrix. It is unfortunate that most of our evaluations of the $\bar{\Sigma}^i$'s do not have data covariance information associated with them since they cannot be used for our purpose until such information has been added to them. A formalism has been developed within the context of ENDF/B to represent such data

covariance information,[10] and hopefully all the dosimetry cross sections of ENDF/B-V will have "data covariance files" and could be used directly. We shall therefore assume that it is practical to use evaluated $\bar{\Sigma}^i$'s to generate our "best solution" even if now the needed covariance matrices, $N_{\Sigma^{ij}}$, must be added to them. By doing so we have added to the a_i°'s one "observation" per $\bar{\sigma}_j^i$ and the required overdetermination of the $\bar{\sigma}_j^i$'s is achieved.

Let us now turn our attention to the $\bar{\phi}_j$'s. It is evident that we have a very efficient method in overdetermining the $\bar{\sigma}_j^i$'s since only one "observation" is used for each $\bar{\sigma}_j^i$ and the same technique can be utilized for the $\bar{\phi}_j$'s. A method which can always be used is to estimate the $\bar{\phi}_j$'s by means of calculations based upon a "model" of the system which produced the spectrum in which the foils were irradiated. Because our model for these calculations is bound to be approximate and we must use imperfectly known nuclear data as input, these estimates for the $\bar{\phi}_j$'s will only be approximate and have "errors" associated with them. If we do estimate the uncertainties in these calculations, then the result is that we may use the calculated fluxes directly as observations. Of course, we should supplement these calculations of the $\bar{\phi}_j$'s with direct measurements of the $\bar{\phi}_j$'s if these are available and obtain effectively an evaluation for $\bar{\Phi}$, complete with covariance matrix N_Φ. The approach we advocate in the treatment of the spectrum is related to what is done in the code RADAK.[11] RADAK is a general purpose "spectrum analysis code" which does a "simultaneous unfolding" from several detectors. It is primarily intended to be used with "many channel" detectors, but some activation foils may be included. As such, it is not a dosimetry unfolding code, but since no

correlations are allowed between the "many channel" detectors output and the activation data, it is effectively equivalent to one where the $\bar{\phi}_j$'s are first obtained from the many channel detectors and then used to analyze the dosimetry data. In the cases where RADAK can be used, i.e., there are many channel detector data available for the complete spectrum, the solution we seek, the "best possible one," can be obtained by combining the output of RADAK with the results of model calculations. It is, therefore, merely a question of strategy about how to proceed in this case, and the result should be independent of the approach. However, when the dosimetry cross sections extend below the energy range of the many channel detectors, we must make use of model calculations to provide the necessary overdetermination of the spectrum, in that energy range at least, before we can exploit the activation data.

If we proceed as outlined above, by supplementing our measured activations a_i°, and their covariance matrix N_{A°, with a synthesis of all our previous observations concerning the $\bar{\sigma}_j^i$'s in the form of fully "evaluated cross sections," with expectation values Σ^i and covariance matrices $N_{\Sigma^{ij}}$, and a synthesis of all our previous knowledge of the $\bar{\phi}_j$'s in the form of a fully "evaluated spectrum," with expectation value Φ and covariance matrix N_Φ, we will have in a direct sense the "best input data" and our solution can be called the "best possible solution." It should be clear that whatever is our intended use of the solution spectrum it can never be called "best" if we do not use fully all the information concerning the dosimetry cross sections in the form of "best evaluations" for the $\bar{\Sigma}^i$'s. Therefore, our different "best solutions" can only come from what we use as "best evaluations of $\bar{\Phi}$." It is conceivable that

different intended use of the solution will dictate different "best assumptions" to be made in the evaluation of $\overline{\Phi}$ and therefore we will have different "best evaluations" of $\overline{\Phi}$. It should be clear, however, that in order to be used in our problem the evaluations of $\overline{\Phi}$ must be complete in the sense of having a covariance matrix N_{Φ} which corresponds to the assumptions made in the evaluation.

In this lengthy introduction we have attempted to justify in detail and in a logical manner the use of what is often called "*a priori* information about the solution." It is often perceived that only some class of *a priori* information such as non-negativity of the spectrum is "non-controversial."[6] We hope to have shown that this need not be the case and that the often perceived failure[6] of having found a satisfactory solution to the "few-channel unfolding problem" does not lie in the need for "detailed" *a priori* information, but rather in the fact that the detailed *a priori* information used in the past was poorly quantified. We contend that any amount of detailed *a priori* information about the solution, if it succeeds in overdetermining the parameters of the problem, can provide a satisfactory solution if it is complete, i.e., has "uncertainties" associated with it, and the assumptions under which the complete *a priori* information is generated are justified and understood. From a purely mathematical point of view, the statement of the "input values of Σ^i, $N_{\Sigma ij}$, Φ and N_{Φ}" constitute the assumptions under which the solution is obtained and there is therefore nothing "controversial" about the solution since the assumptions are clearly stated.

The Mathematical Formulation

In this section we merely transcribe in mathematical language the ideas discussed in the previous section. To simplify the notation we introduce the abstract cross section vector $\overline{\Sigma}$,

$$\overline{\Sigma} \equiv \begin{pmatrix} \overline{\Sigma}^1 \\ \overline{\Sigma}^2 \\ \overline{\Sigma}^3 \\ \vdots \end{pmatrix} , \tag{7}$$

and the abstract parameter vector $\overline{P}$,

$$\overline{P} \equiv \begin{pmatrix} \overline{\Phi} \\ \overline{\Sigma} \end{pmatrix} . \tag{8}$$

We shall refer to the evaluations of $\overline{\Phi}$ and $\overline{\Sigma}$, treated as "observations," by the abstract vector P and its covariance matrix N_p:

$$P \equiv \begin{pmatrix} \Phi \\ \Sigma \end{pmatrix} , \qquad N_p \equiv \begin{pmatrix} N_\Phi & 0 \\ 0 & N_\Sigma \end{pmatrix} . \tag{9}$$

We have shown in Eq. (9) by the symbol 0 for the off-diagonal matrices of N_p that we assume, as will be generally the case, that the evaluations of $\overline{\Phi}$ and $\overline{\Sigma}$ are uncorrelated. This is not necessarily always the case, since it is possible that some of the dosimetry cross sections of the problem, some $\overline{\Sigma}^i$, enters also in the evaluation of $\overline{\Phi}$ as could be for instance the case of the ^{235}U fission cross section. In such cases the off-diagonal matrices of N_p will not be zero. It is not essential for the problem that N_p be diagonal in the space of Φ and Σ which should therefore represent the true situation. However, it is convenient later to consider N_p to be diagonal in the space of Φ and Σ purely from a

presentation point of view. We shall therefore state that without loss of generality we consider N_P to be diagonal in the space of Φ and Σ, which does not mean that we consider N_Φ and N_Σ to be diagonal.

As previously discussed, we consider our evaluations of $\bar{\Phi}$ and $\bar{\Sigma}$ as "observations" as well as the abstract vector A° made up of the measured activations a_i°, $A^\circ \equiv \{a_i^\circ\}$. In the notation of the previous section we have therefore:

$$Y^\circ \equiv \begin{pmatrix} P \\ A^\circ \end{pmatrix} , \qquad M \equiv \begin{pmatrix} N_P & 0 \\ 0 & N_{A^\circ} \end{pmatrix} . \tag{10}$$

In Eq. (10) we indicate, by our notation 0 for the off-diagonal matrices of M, that the "observations" A° and P are uncorrelated. It is strictly not necessary to make this assumption, in order to use the least-squares method, if we are willing to invert the full matrix M, as shown by (3) and (4). However, as we will show in the next section, if M is diagonal in the space of P and A°, it is only necessary for us to "formally" invert the matrix N_P without actually doing so explicitly. When M is not diagonal in the space of P and A°, we have to invert it explicitly to get the solution and this may not be practical since the rank of M may well be of the order of a few hundred or even a few thousand. We shall therefore assume that in order to be practical our method requires that P and A° be uncorrelated. The meaning of this requirement is that in our evaluations of $\bar{\Phi}$ and $\bar{\Sigma}$ we must not use any data which are correlated to A°. This restriction appears at first sight to be a strong limitation of the method since it might force us to exclude from the evaluations some types of data obtained in standard and benchmark fields. We have already discussed a procedure for by-passing such

difficulties[4] and we shall not return to it in this paper. (Mathematically speaking, it is the fact that M is diagonal in the space of P and A° which justifies our use of the term prior information to describe the evaluations of $\overline{\Phi}$ and $\overline{\Sigma}$, i.e., they can be made without using our knowledge of A°.)

Having identified the "observations," Y° and M, for our least-squares problem we must now establish a "model" for the quantities $\overline{Y}$, i.e., obtain the complete design matrix. It is clear that P stands for the quantity $\overline{P}$ and therefore our model for these observations is the identity matrix!! It is therefore linear and exact. Our "observations" A° stand for the quantity $\overline{A}$, with $\overline{A} \equiv \{\overline{a}_i\}$ and $\overline{a}_i$ is defined by Eq. (6). Since $\overline{a}_i$ is a bilinear product of some of the elements of $\overline{P}$, our model for $\overline{A}$ is non-linear. In order to obtain our design matrix we must linearize the model. We shall do so by performing an expansion about the estimated expectation values of $\overline{\Phi}$ and $\overline{\Sigma}$, i.e., Φ and Σ, we get:

$$\overline{a}_i = \Sigma^{i\dagger} \cdot \Phi + \Phi^{\dagger} \cdot (\overline{\Sigma}^i - \Sigma^i) + \Sigma^{i\dagger} \cdot (\overline{\Phi} - \Phi) + (\overline{\Sigma}^i - \Sigma^i)^{\dagger} \cdot (\overline{\Phi} - \Phi) \quad , \quad (11)$$

since the expansion terminates the expression (11) is therefore exact regardless of the values of Φ and Σ^i, as can be verified by performing the operations indicated. The linearization of (11) is accomplished by dropping the last term only. It is clear that "very little approximation" is made by dropping the last term since if our evaluations are "reasonably close" to the solution the contributions of this term will be small. This is so because to contribute significantly both Σ^i and Φ must be significantly wrong in the same energy region; the signs of the differences must be such that no appreciable cancellations occur in the summations over energy and this sum is to be compared with the total activation. These three requirements to make the approximation poor must be met simultaneously

and therefore we can already conjecture that the model being "quasi-linear" most of the time we expect the linearization to be a good approximation and consequently our need to iterate to find the solution will be infrequent. We shall return later to a discussion of this point. In order to find the design matrix, we must rewrite (11) in a form similar to (1b):

$$\overline{A} \approx A + G \cdot (\overline{P} - P) \quad , \tag{12}$$

where $A \equiv \{a_i\}$ and $a_i = \Sigma^{i\dagger} \cdot \Phi$. The "sensitivity" matrix G is therefore given by:

$$G = \begin{pmatrix} \Sigma^{1\dagger} & \Phi^{\dagger} & 0 & 0 & \cdots \\ \Sigma^{2\dagger} & 0 & \Phi^{\dagger} & 0 & \cdots \\ \Sigma^{3\dagger} & 0 & 0 & \Phi^{\dagger} & \cdots \\ \vdots & \vdots & \vdots & \vdots & \end{pmatrix} \quad . \tag{13}$$

Because the quantities $\overline{A}$, for which we have observations A°, have a non-linear model, it is convenient to write $\overline{P}$, for which we have observations P, as if it also had a non-linear model. This can be accomplished exactly as follows:

$$\overline{P} = P + I \cdot (\overline{P} - P) \quad , \tag{14}$$

where I is the identity matrix. Using (12) and (14) and (1b) we find by inspection that for our non-linear least-squares problem we have:

$$Y = \begin{pmatrix} P \\ A \end{pmatrix} \quad , \qquad D = \begin{pmatrix} I \\ G \end{pmatrix} \quad . \tag{15}$$

This completes the mathematical formulation of our non-linear dosimetry least-squares problem since we have defined or derived appropriately the quantities: Y°, M, Y, D and $\overline{P}$, which were introduced in the previous section as needed to state such a problem.

It is clear from the above mathematical formulation of the problem that what we are solving for in our least-squares approach is:

Given,

1. activation measurements in a spectrum, A° and N_{A°,
2. *a priori* information about the dosimetry cross sections, Σ and N_Σ,
3. *a priori* information about this spectrum, Φ and N_Φ.

what is the most likely value of the spectrum and its uncertainty, Φ' and N'_Φ?

Because we have also used the dosimetry cross sections as parameters, we could also answer the question, "What is the most likely value of the dosimetry cross sections and their uncertainties, Σ' and N'_Σ?" if we so desired.

The Mathematical Solution

In the preceeding sections we have stated the general least-squares method, given its solution, and formulated a least-squares problem for dosimetry data analysis. In this section we obtain the solution explicitly in terms of the input data and emphasize that it is extremely easy to compute and always exists. We could rewrite (2b) using the previous section as:

$$\chi^2 = \begin{pmatrix} P - \hat{P} \\ A^\circ - A - G\cdot(\hat{P}-P) \end{pmatrix}^\dagger \cdot \begin{pmatrix} N_p & 0 \\ 0 & N_{A^\circ} \end{pmatrix}^{-1} \cdot \begin{pmatrix} P - \hat{P} \\ A^\circ - A - G\cdot(\hat{P}-P) \end{pmatrix}, \quad (16)$$

and proceed, using standard techniques,[8] with the direct minimization of χ^2 by varying $\hat{P}$. In doing so we would not make use of the previously

stated results (3b) and (4b). After some suitable manipulation we would obtain the solution:

$$P' - P = N_p \cdot G^{\dagger} \cdot (N_A + N_{A^\circ})^{-1} \cdot (A^\circ - A) \quad , \tag{17}$$

$$N_p - N_p' = N_p \cdot G^{\dagger} \cdot (N_A + N_{A^\circ})^{-1} \cdot G \cdot N_p \quad , \tag{18}$$

where the symbol not previously defined is N_A which is defined as:

$$N_A \equiv G^{\dagger} \cdot N_p \cdot G \quad . \tag{19}$$

N_A is the covariance matrix of the vector A. We recall that the vector A is calculated from the input vector P, more specifically if $A \equiv \{a_i\}$, a_i is given by:

$$a_i = \Sigma^{i\dagger} \cdot \Phi \quad . \tag{20}$$

Therefore, A and N_A are the predictions, based upon our *a priori* evaluations of $\overline{\Phi}$ and $\overline{\Sigma}$, for the observed activities A° and N_{A°. A and N_A play a crucial role in obtaining the solution P' and N_p', as is evident from (17) and (18), since it is through them that we can make use of the dosimetry data of the problem: A° and N_{A°.

We shall now indicate how we can obtain the results (17) and (18) from (3b) and (4b) using the definitions for the quantities Y°, M, Y, D and $\overline{P}$ presented in the previous section. We shall consider this a proof of the results (17) and (18) since the derivation of (3b) and (4b) is well known.

Since N_p and N_{A° are square matrices, the inverse of M is:

$$M^{-1} = \begin{pmatrix} N_p^{-1} & 0 \\ 0 & N_{A^\circ}^{-1} \end{pmatrix} \quad . \tag{21}$$

Similarly, the inverse of N_p in (21) is obtained from the inverse of N_Φ and N_Σ under the assumption that N_p is diagonal in the space of Φ and Σ, as we shall take it to be for purposes of the following discussion. We have already discussed the reasons why if M is a "correct" covariance matrix of some observations it must be non-singular and therefore its inverse exists. The arguments apply directly to N_{A° since in our problem A° corresponds to actual measurements. They should also apply to N_Φ and N_Σ since these are taken as observations and if our evaluations are done correctly they can be traced to direct observations. In practice, however, N_Φ and N_Σ are likely to be singular for several reasons. We shall return later to a discussion of the covariance matrices N_Φ and N_Σ since they play an important role in our problem. We will therefore now proceed with the proof, as if N_Φ and N_Σ were non-singular, postponing until later our justification for doing so.

If we rewrite (3b) as:

$$(D^\dagger \cdot M^{-1} \cdot D) \cdot (P' - P) = D^\dagger \cdot M^{-1} \cdot (Y^\circ - Y) \quad , \qquad (22)$$

and substitute the appropriate expressions for D, M^{-1}, Y° and Y, we get:

$$(N_p^{-1} + G^\dagger \cdot N_{A^\circ}^{-1} \cdot G) \cdot (P' - P) = G^\dagger \cdot N_{A^\circ}^{-1} \cdot (A^\circ - A) \quad . \qquad (23)$$

From (4b) we also get:

$$N_p' = (N_p^{-1} + G^\dagger \cdot N_{A^\circ}^{-1} \cdot G)^{-1} \quad . \qquad (24)$$

We can readily rearrange the terms in (23) to obtain:

$$N_p^{-1} \cdot (P' - P) = G^\dagger \cdot N_{A^\circ}^{-1} \cdot (A^\circ - A - G \cdot (P'-P)) \quad . \qquad (25)$$

A very elegant way to proceed from (25) is to introduce after Dragt *et al.*[12] the auxiliary quantity:

$$X \equiv N_{A^\circ}^{-1} \cdot (A^\circ - A - G \cdot (P'-P)) \quad , \tag{26}$$

and write (25) as:

$$P' - P = N_p \cdot G^\dagger \cdot X \quad . \tag{27}$$

If we then multiply (27) from the left by G, use the definition (19), after substitution of G•(P'-P) in (26), we get:

$$X = (N_A + N_{A^\circ})^{-1} \cdot (A^\circ - A) \quad . \tag{28}$$

We need not worry about the existence of the inverse of $N_A + N_{A^\circ}$ since it will always exist because the covariance matrix N_{A° is non-singular and N_A is symmetric. Substitution of (28) back into (27) yields our solution. In a similar fashion we can derive (18) from (24).

This basically concludes our proof and we can see that the expressions to obtain the solution P' and N_p' are very simple to calculate. This is clearly so when we show the simple form that N_A takes. From the definition (19) and using for N_p we have:

$$N_A = G \cdot \begin{pmatrix} N_\Phi & 0 \\ 0 & N_\Sigma \end{pmatrix} \cdot G^\dagger \quad , \tag{29}$$

N_A can therefore be written as the sum of two contributions:

$$N_A = N_A^\Phi + N_A^\Sigma \quad , \tag{30}$$

where:

$$N_A^\Phi \equiv \{n_{ij}{}^\Phi\} = \{\Sigma^{i\dagger} \cdot N_\Phi \cdot \Sigma^j\} \quad , \tag{31}$$

and:

$$N_A^{\Sigma} \equiv \{n_{ij}^{\Sigma}\} = \{\Phi^{\dagger} \cdot N_{\Sigma ij} \cdot \Phi\} \quad . \tag{32}$$

When N_p is not diagonal in the space of Φ and Σ, an additional "cross term" is required in N_A.

Covariance Matrices of Evaluations

The primary purpose of this section is to justify some statements made in the previous section and clearly indicate some of the consequences for our solutions of certain approximations we are likely to make in the handling of covariances of evaluations. We claimed that the solution to the least-squares problem always existed because the covariance matrix M was always non-singular. However, during the course of our proof when we came to invert the covariance matrices N_{Φ} and N_{Σ} we pointed out that in practice they were likely to be singular, but that we should proceed as if they were not. It is clear that since the matrix M cannot be in principle singular, we can say that its singularity resulted from a "mistake." We argue that this is possibly true, but wish to consider that the "mistake" was intentional in the sense that it corresponds to some approximation we intend to make and we are interested in obtaining a solution under such conditions. We shall show that we need not explicitly change our formulation to recognize this fact and can proceed as if these approximations had not resulted in a singular matrix for N_{Φ} or N_{Σ}. This property of our least-squares problem has very important practical consequences. On the one hand, if we have written a computer code to solve it, we can use it for obtaining solutions under various approximations which result in singular covariance

matrices without having to change the code or otherwise communicate this fact to the code. On the other hand, it may be a disadvantage since we may not recognize that we have made some approximations we did not intend to make. Since this discussion will shed light upon the role which the covariance matrices of our evaluations play in general, and in the least-squares problem in particular, we shall carry it in some details. However, because a complete discussion of this interesting and possibly not well appreciated aspect of "uncertainties" in evaluations would carry us too far from our subject, we will not approach it in its greatest generality, but rather from a practical point of view.

We first emphasize that the covariance matrices N_Φ and N_Σ need not be singular. However, we conjecture that they may be singular under the assumptions we are likely to make at this stage in the handling of uncertainty information in evaluations and if we follow in the use of the least-squares method the same practices used with our current codes. We shall not argue against these assumptions and practices since they may be justified if only on grounds of convenience. Since at this stage rather little experience exists in the treatment of uncertainties in evaluations we are likely to concentrate on the description of the major or gross features of the problem and therefore the statement of the uncertainties is bound to be crude in the sense of having not too much detail. We may also, as is done in ENDF/B,[10] make some rather crude approximations which have great convenience as far as representing and processing the information to generate covariance matrices of processed data. These approximations being fully consistent with the perceived accuracies of the estimated uncertainties. Also, as a matter of convenience we may select a standard group structure to do our analyses with the result that it is not

tailored to each problem, and in any problem this group structure is likely more detailed than is really needed or justified on the basis of information available, at least in some energy regions. The combination of the above two practices, which are likely to occur, will almost surely result in covariance matrices N_Φ and N_Σ which are singular. This is so because the dimension of our covariance matrices, the number of groups we use, will almost surely exceed their rank, which in a very direct sense corresponds to the "amount of information" we have included in our evaluations regarding their "uncertainties."

In order to facilitate the discussion let us consider some specific examples which we think embody the essence of the problem and may easily be generalized. For example, we take the spectrum in an energy region where there are several group fluxes ϕ_j. We suppose that in our evaluation of the spectrum the statements concerning the uncertainties are such that the several group fluxes ϕ_j should be considered as fully correlated. The covariance matrix of these group fluxes will have a dimension equal to the number of groups, but its rank will be one; it will therefore be singular and consequently the full covariance matrix N_Φ will also be singular and cannot be inverted. It is important to note that since our covariance matrices are symmetric and positive definite the above mechanism is the only one which can be responsible for their singularity, a statement we shall not prove here. It is clear that since the several ϕ_j's are fully correlated they can be replaced by a single auxiliary variable and an exact linear transformation which relates it to the ϕ_j's. If these ϕ_j's were from "real independent measurements," this would be an inconsistency of sorts, but since we are dealing with "evaluations taken as measurements" this may not be a

mistake and we can easily handle the problem. We could do so by formally replacing these ϕ_j's by the single auxiliary variable and the exact linear transformation, which could be obtained by inspection. The singularity of our covariance matrix of the parameters would then be removed and we could solve for the auxiliary parameter directly instead of these ϕ_j's. However, having obtained the solution for this auxiliary parameter, we could use our exact transformation to obtain the solution for the ϕ_j's and the resulting spectrum would be identical to the one obtained by the direct application of (17) and (18). We shall not formally introduce the transformation and prove this point by mathematical manipulations because it should be clear that what we have done is merely change the definition of the "parameter vector" and the transformation is already embedded in our sensitivity matrix G. In conclusion we see that we can always ignore the fact that the covariance matrices of our evaluations are singular and proceed formally as if they were not!

This discussion should make it clear that in a dosimetry problem the number of groups we use to analyze the problem does not at all correspond to the number of parameters we have. The number of parameters is determined by the rank of the covariance matrices from our evaluations. In practice we do not need to know how many parameters we really have to solve the problem, but it can easily be determined by inspection of the correlation matrix of Φ and Σ. It should also be clear now that any structure we have in our input spectrum in energy regions where the evaluations state that the spectrum is fully correlated is reproduced in our solution exactly. An extreme example of this is when our covariance matrix is fully correlated over the whole energy range.

The auxiliary parameter is the normalization of the spectrum and the transformation is the shape of the spectrum. In this case, no matter how many activation measurements we have, the shape of the spectrum will remain unchanged and only its normalization will be determined. On the other hand, even with a single activation measurement, if the input covariance matrix N_Φ does not correspond to a fully correlated spectrum, both the shape and normalization of the spectrum are adjusted. It is important to keep in mind that what is being adjusted in the spectrum is entirely determined from the structure of the input covariance matrix based upon the uncertainties in the evaluation and is unrelated to the number of groups used or the number of activations available.

A Test for Consistency of the Data

We have already stressed the fact that the least-squares solution does not require that the joint density functions of the input data be normal. The only requirement is that the covariance matrices represent the second moment of the density functions. If the form of the density functions were known, or assumed to be known, we could go further than just obtain the solution (17) and (18); we could extract some additional information from the numerical value of the minimum of the χ^2-function in the sense of being able to test the "likelihood" of the input data. Since such tests are often very useful in detecting mistakes, we believe that at least for purposes of such investigations we should assume that the density functions are known and argue on the basis of the "central limit theorem"[8] that we should take them to be normal. It is then possible to perform two tests on the distribution of the input data.

The well-known χ^2-test may be used to estimate the likelihood of the input data set on the basis of the minimum value of χ^2. In order to do so one needs to establish the number of degrees of freedom in the problem. If we have m cross sections and fluxes and n activation measurements, the total number of input quantities is m + n, but since we solve for m parameters we have only n degrees of freedom. Therefore, the χ^2 minimum corresponds to n degrees of freedom. We shall now show that the minimum value of χ^2 is entirely determined from the values of the input data. The minimum value of χ^2, χ^2_m, is obtained by substituting the value of P' given by (17) for $\hat{P}$ in (16). We therefore have,

$$\chi^2_m = (P-P')^\dagger \cdot N_p^{-1} \cdot (P-P') + (A^\circ-A')^\dagger \cdot N_{A^\circ}^{-1} \cdot (A^\circ-A') \quad . \tag{33}$$

We may rewrite (33) as:

$$\chi^2_m = \chi^2_p + \chi^2_A \quad . \tag{34}$$

Using (27) we may evaluate χ^2_p as:

$$\chi^2_p = (A' - A)^\dagger \cdot X \quad , \tag{35}$$

and also from (27), operating upon it with G, we get:

$$A' - A = N_A \cdot X \quad . \tag{36}$$

Substituting (36) into (35), we have:

$$\chi^2_p = X^\dagger \cdot N_A \cdot X \quad . \tag{37}$$

To evaluate χ^2_A we rewrite (26) as:

$$A^\circ - A' = N_{A^\circ} \cdot X \quad , \tag{38}$$

substituting (38) into the expression for χ^2 in (33), we have:

$$\chi_A^2 = X^\dagger \cdot N_{A^\circ} \cdot X \quad . \tag{39}$$

Using now (37) and (39), we obtain the desired result, if we use the expression (28) for X:

$$\chi_m^2 = (A^\circ - A)^\dagger \cdot (N_A + N_{A^\circ})^{-1} \cdot (A^\circ - A) \quad . \tag{40}$$

It is therefore clear from (40) that the minimum value of χ^2 can be evaluated easily from the input data. We can then test the likelihood of the input data, prior to obtaining the solution, by means of a χ^2-test on χ_m^2 using as the number of degrees of freedom the number of activation measurements.

The second test on the input data can also be made from (40) by looking at the "randomness" of the terms which make up χ_m^2. There are n terms which we must sum in the final stage of the computation of χ_m^2 in (40), and to each term we can associate a particular activation. The "fit" may not be good if one or a few activations contribute mostly to χ_m^2 and should be taken as a possible indication of a mistake to be investigated.

Finally, we should indicate that the predictions for the activations one will obtain from the solution P' can be obtained without solving for P'. If we operate on (17) with G from the left, we immediately get:

$$A' = A + N_A \cdot (N_A + N_{A^\circ})^{-1} \cdot (A^\circ - A) \quad . \tag{41}$$

If we now multiply (18) on the left by G and on the right by $G^{\dagger}$, we obtain:

$$N'_A = N_A - N_A \cdot (N_A + N_{A\circ})^{-1} \cdot N_A \quad , \tag{42}$$

which gives us the covariance matrix of the activations calculated from the solution without having to explicitly calculate N'_p either.

The Non-Linearity of the Problem

Our problem is a non-linear least-squares one. Since such problems are usually solved by iteration, as well as all of our current methods, we must now discuss when we may gain from an iterative scheme to get our solution. We shall show that, although an iterative procedure will always somewhat improve the solution, in many practical situations such improvements may not be very significant and therefore some doubt always exists about its usefulness.

When solving a non-linear least-squares problem we must always linearize the model and in so doing make an approximation; in our case this was done in (12). Such linearization procedure involves an expansion, and the best expansion to make is about the solution. Since we usually do not know the solution, such expansion must be made about some "trial value" from which a trial solution is obtained. This "trial solution" is then used as a new "point" about which the model is expanded again. Therefore an iterative procedure is developed and progress toward a "converged solution" is usually monitored by observing the successive improvements in the χ^2 minimum at each step. In our case we chose as an expansion point the *a priori* evaluations P in order to generate P' and N'_p. It would appear that if we now go back and expand again our model

using P' in (12) instead of P, we would get a better solution. We will now develop such an iterated solution. In order to develop a notation which incorporates iteration numbers in it, let us expand the model about P_n, instead of P in (12), and call the solution P_{n+1} instead of P'. If we proceed exactly as we did to obtain (17) and (18), we get:

$$P_{n+1} - P = N_p \cdot G_n \cdot (N_{A_n} + N_{A^\circ})^{-1} \cdot (A^\circ - A_n - G_n \cdot (P - P_n)) \quad , \quad (17a)$$

$$N_p - N_p^{n+1} = N_p \cdot G_n^\dagger \cdot (N_{A_n} + N_{A^\circ})^{-1} \cdot G_n \cdot N_p \quad , \quad (18a)$$

where A_n is the activation vector calculated using P_n, G_n is the sensitivity matrix (13) calculated using P_n and the quantity N_{A_n} is defined analogously to N_A in (19) and is:

$$N_{A_n} = G_n^\dagger \cdot N_p \cdot G_n \quad . \quad (19a)$$

If we now calculate the χ^2-minimum for our iterated solution (17a), $\chi^2_{m,n+1}$, by proceeding exactly as we did to derive (40) from (17), we get:

$$\chi^2_{m,n+1} = (A^\circ - A_n - G_n \cdot (P - P_n))^\dagger \cdot (N_{A_n} + N_{A^\circ})^{-1} \cdot (A^\circ - A_n - G_n \cdot (P - P_n)) \quad . \quad (40a)$$

If we compare the above results to those obtained from the expansion about the *a priori* evaluations, we see two differences. The first one is the replacement of G and N_A by G_n and N_{A_n}, and the second one the replacement of A by $A_n + G_n \cdot (P - P_n)$. It is clear that if our input data A°, N_{A° and P, N_p are "fairly consistent" to the extent that our *a priori* evaluations predict "well" the measurements A°, that is we may compute A such that it agrees with A° within the combined uncertainties N_A and N_{A°, then the χ^2_m calculated using (40) will correspond to approximately one per degrees of freedom. In such cases within the uncertainties we will have $A \approx A_n$.

Even if our data are somewhat "inconsistent" but not very improbable, say with a χ^2_m less than 2 per degrees of freedom, then the approximation $A \approx A_n$ may not be very good, but it is likely that within the uncertainties we will have $A \approx A_n + G_n \cdot (P-P_n)$. What we are arguing is that as long as our data are not too inconsistent then a linear model is very good; the non-linearity of the model is not important. As is well known,[8] if the model is exactly linear, it is not necessary to iterate to find the solution. In our case this should be reflected in our results (17a), (18a) and (40a) which will be close to (17), (18) and (40) if the data are not too inconsistent. We can see that directly if we substitute in (17a), (18a) and (40a) $A = A_n + G_n \cdot (P-P_n)$ to get:

$$P_{n+1} - P = N_p \cdot G_n \cdot (N_{A_n} + N_{A^\circ})^{-1} \cdot (A^\circ - A) \quad , \tag{17b}$$

$$N_p - N_p^{n+1} = N_p \cdot G_n^\dagger \cdot (N_{A_n} + N_{A^\circ})^{-1} \cdot G_n \cdot N_p \quad , \tag{18b}$$

$$\chi^2_{m,n+1} = (A^\circ - A) \cdot (N_{A_n} + N_{A^\circ})^{-1} \cdot (A^\circ - A) \quad . \tag{40b}$$

Our solution (17b) and (18b) still does not quite look like the original one (17) and (18) since we have G_n and N_{A_n} instead of G and N_A. However, since $N_{A_n} \approx N_A$ within the uncertainties of these quantities which are controlled by N_p, the χ^2-minimum (40b) is not very different from the χ^2_m given by (40) and therefore the results (17b) and (18b) are equivalent to (17) and (18) or more exactly the differences are not measurable from the χ^2-minimum. We conclude then that if our data are not too unlikely, in the sense that χ^2_m given by (40) is less than about 2 per degrees of freedom, we have little to gain by iterating in order to find the solution, the improved precision in the solution being not justified by its accuracy.

We see from the above analysis that the value of χ^2_m, the "consistency" of our input data, indicates to us when we may gain significantly by an iteration scheme to get the solution. Such potential gains exist only when χ^2_m per degrees of freedom is large. Unfortunately, in such cases we may not exploit fully the benefit of iterating to improve our results since the data are then so unlikely that the credibility of the solution is low. We must assume that very likely a mistake has been made somewhere and should be corrected to restore some credibility in the answer. We will not discuss the various methods which may be used in such situations; these different strategies, however, have all the same result, which is to reduce effectively χ^2_m to be about one per degrees of freedom. There is then very little need to iterate in order to find the solution which would not become much more credible.

The above result which may appear surprising — very little use of the non-linearity of the model can be taken advantage of by iterations which would improve the solution — is not unique to our dosimetry problem. This feature is common to all non-linear least-squares problems where a "few integral results" are available and *a priori* knowledge about the solution is introduced in the form of "fully evaluated differential data" to exploit these "integral results." In this strategy we merely want our "*a posteriori* evaluations" to reflect the "new information" present in the integral data. It is clear that through the "integral data" we cannot learn much about the "differential quantities" unless we have "strong inconsistencies." When the integral data are relatively consistent with our differential data, the integral results will not cause our knowledge of the individual differential quantities to be modified. Their values and their variances will not be changed significantly, i.e. $P' \approx P$ and the diagonal elements of the

covariance matrices N_p' and N_p will also be about the same. What the least-squares method does is change as little as possible each parameter, but modifies as many as possible in such a highly correlated fashion to reproduce as best it can the integral results. In such conditions the only significant information we get deals with the correlations of the differential quantities and these are expressed by the off-diagonal elements of N_p' the output or *a posteriori* covariance matrix. The potential for improvements in our knowledge of the individual differential quantities exists, and therefore the need for an iterated solution, only when there are very significant differences between, or inconsistencies in, our two types of input data. Their usefulness in improving our knowledge of the individual differential quantities is, however, limited by our inability to claim with confidence that the "inconsistencies" are "real" and not the results of "mistakes."

The above discussion is very general and does not make use of the explicit form of the "model" of the integral quantities in our dosimetry problem. There are two situations where the dosimetry method is often used, and the model becomes "effectively linear" even though χ^2_m may be large. These situations occur when either $\overline{\Phi}$ or $\overline{\Sigma}$ is known *a priori* to a much higher relative accuracy than the other. In such cases the model is "quasi-linear" because the non-linear terms $(\overline{\Sigma}^i-\Sigma^i)^\dagger\cdot(\overline{\Phi}-\Phi)$ become effectively small in an absolute sense whether we choose our *a priori* or *a posteriori* estimates to expand the model. In these cases again iterations are not needed, even though χ^2_m may be large, because the model is "effectively linear" and the "differential quantities" which are not as well known relatively will be the only ones changed significantly. These situations may occur in "standard fields applications" when N_Φ is relatively much better known and in "practical applications" where it is N_Σ which is relatively much better known.

The Least-Squares Analysis Code STAY'SL

The above method of analysis of dosimetry data has been incorporated into a computer code STAY'SL which has been documented[13] and is available from the Radiation Shielding Information Center (RSIC) at Oak Ridge National Laboratory.

In STAY'SL we calculate explicitly only the values of Φ' and N'_{Φ}; therefore, two possible interpretations of the code output can be made. The first one is that the full solution for P' is not obtained, although both Φ and Σ are "adjusted." A code for generating the full solution (i.e., including Σ' and N'_{Σ}) will soon be released. The other interpretation is that in STAY'SL the cross sections (i.e., Σ) are assumed to be only "formally adjustable" during the analysis in order to propagate their uncertainties to the solution. The covariance matrix $N_{A\circ}$ of the measured activations was modified by adding to it the matrix N_A^{Σ}, given by (31), and obtained from an estimate of N_{Σ}, in order to take into account the fact that our "model" [i.e., expression (5)] is inexact. In doing so we claim to have properly taken into account the "approximations" in our model (i.e., the cross sections). This second interpretation of the solution of STAY'SL has, we believe, some interesting implications concerning the general use of the method of least-squares when the "model" is known to be deficient and suitable "methods" or "approximation" parameters may be introduced, with assigned uncertainties, such that within these uncertainties the "model" can be claimed to be exact.

Comparison with Other Methods

It is evident from the above discussion that the least-squares method has the potential for providing a solution which incorporates in principle

all of the available information concerning the problem in a straightforward manner and at the same time giving us the "best" such solution in the sense of the minimum variance theorem. In practice this potential can only be realized at some costs. We will first discuss briefly each type of information used as input and analyze how close in practice, and at what costs, we can come to utilize "all of the information" available.

Concerning the activation measurements, it should be relatively easy to use all of the information available. In particular, the correlations of the different activations, which are not used at all presently or are used in an unknown manner through the use of so-called "calibrated methods," should be easily handled. In order to do so, however, the experimentalist must provide the covariance matrix of the measurements or preferably report the analysis of the uncertainties in the data in such a way that these estimates may be evaluated and the covariance matrix easily generated from the information. In the past such types of information were not used very explicitly; therefore, there was little incentive to provide it in a clear fashion and only the standard deviations of the activations were usually reported.

Concerning the dosimetry cross sections, it should also be possible to come close to utilizing most of the information available. The starting point is always a detailed evaluation of the differential data. In the past very few evaluations were made with enough details available concerning the uncertainties in the evaluated data to allow the covariance matrices to be generated. In the ENDF/B files it is now possible to communicate this information[10] and hopefully in ENDF/B-V all dosimetry cross sections will have data such that the covariance matrices can be generated for any group structure. Our knowledge of the dosimetry cross

sections does not come only from differential measurements. However, if we have evaluated differential data files with correlations indicated, they can be exploited, using the same least-squares method discussed here, to generate new evaluations which incorporate the results of integral measurements obtained in benchmark and standard fields. We have already discussed[4] that some care must be exercised regarding how we accomplish this last step if we are not to run into large computational problems. We therefore believe that the methodology exists for generating dosimetry cross sections which will come close to reflecting adequately almost all of our information regarding how well we know them.

We believe then that the major obstacle which must be overcome to use "all of the information" available in our solution to the dosimetry analysis problem is the determination of appropriate Φ and N_Φ. Because this problem is specific to every spectrum being analyzed, we can only discuss it in general terms. The approach to this problem is, however, straightforward even if we will usually run into practical difficulties in finding its solution. The *a priori* spectrum Φ can always be obtained as a combination of whatever data are available and the results of appropriate transport calculations. Since this is what is often done now in order to generate the "input spectrum" to our current methods, we shall not discuss this aspect further. Therefore, it may be perceived at this stage that the major obstacle will be the generation of an appropriate covariance matrix N_Φ. The procedure for obtaining N_Φ is in principle easy since it is merely a statement of how well we believe we know Φ. Although some subjective elements will always exist in our estimation of N_Φ, some degree of credibility can be achieved if we

analyze with care the source of our uncertainties in Φ. It is often perceived that the "uncertainties" in Φ come from two major sources: uncertainties in the basic nuclear data used in the computations and approximations made in the computations. Using sensitivity methods, it is in principle straightforward to propagate the uncertainties of the input data to the resulting spectrum. The question of the approximations made in the computations is more difficult, but the covariance matrix N_Φ must certainly reflect the uncertainties in Φ due to them.

In the near future, since much of our information is not codified in the appropriate form, some of the benefits of the method may not be realized. We have already discussed[4] the fact that in such cases all we can expect is more credible answers than we currently obtain merely by using more credible input data. In the past, various methods[7] have been devised to compare the various unfolding codes. A particularly useful one is to obtain the solution to a given problem using the same input data by different codes and compare the ratios of the output and input spectra. The comparison of these ratios for different codes such as SAND-II, SPECTRA and CRYSTAL BALL is very instructive since it shows rather large differences which are indicative of the various algorithms used. For these codes this ratio is not unique for a given problem, but also depends upon a number of input quantities having to do with the algorithms and not related to the problem being solved. In the case of the least-squares method, this ratio can easily be obtained from (17) and is simply:

$$\frac{\phi'_j}{\phi_j} = 1 + \sum_{i,k,\ell,r} m_{\phi_{j\ell}} \sigma^i_\ell \phi_\ell w_{ik} (a^\circ_k - \sigma^k_r \phi_r) \quad , \tag{43}$$

where $m_{\phi_{j\ell}}$ is the relative covariance of the flux ϕ_j and ϕ_ℓ and the w_{ik}'s are the matrix elements of the matrix $(N_A + N_{A\circ})^{-1}$, the weight matrix W, all other symbols in (43) having been defined previously.

It is evident that the purpose of any dosimetry spectrum unfolding code is to modify the "input spectrum" in order to obtain an output spectrum which is consistent with the measured activations. It is also clear that we want these modifications of the input spectrum to occur in such a way that they are consistent with how well we know various features of the input spectrum. How well we know the various features of the input spectrum is, of course, problem-dependent and is communicated by means of the covariance matrix N_Φ. Even though the unfolding codes SAND-II, SPECTRA, and CRYSTAL BALL do not require that we directly input N_Φ, we may view them as strategies to obtain the solution (43) and therefore look upon the algorithms as having built into them an effective covariance matrix N_Φ. A difficulty with these codes is that this effective covariance matrix is unknown, fixed once and for all, and to be used in all unfolding situations regardless of how well we know the input spectrum Φ. It is also evident that this effective covariance matrix is different for each one of these codes. Consequently, it is difficult to compare the solutions of these codes with the output of STAY'SL since we cannot use exactly the same input data. In fact, it is difficult to compare the output of these codes among themselves because they all in a direct sense do not solve exactly the same problem due to their different effective N_Φ.

It is clear from the algorithms of SAND-II, SPECTRA, and CRYSTAL BALL that these codes can produce a solution which will reproduce as well as we care to state the measured activities. However, we know that

often this is done by introducing in the solution what is referred to as "unphysical oscillations." In fact, we use that name to indicate that these features of the solution are thought inconsistent with our *a priori* knowledge of the spectrum. Therefore, we must conclude that it is possible to operate these codes in such a manner that their effective covariance matrices are unreasonable. This fact is well known and is often expressed by saying that these codes cannot be used as "black boxes" and require considerable expertise to be used to generate acceptable solutions.[5] It is therefore not possible to use as a figure of merit for the solutions how well the input activities are numerically reproduced.

There exists a very straightforward way to compare the various methods. It is to ask, "How well do the different solutions predict the results of computations based upon them?" By "how well," we mean how small are the uncertainties in the results of computations using the solution. A measure of these uncertainties is the variance of the results in question. In order to be able to answer this very important question we need to know what are the uncertainties in the solution (i.e., its covariance matrix N'_Φ). In the case of the least-squares method, N'_Φ is given simply using relation (18). In the case of the other methods, we do not know what the uncertainty in their solution is since it is usually not calculated in any well defined manner. We have discussed previously[4] how to generate the uncertainties in the solution of the usual unfolding codes on the basis of the input data uncertainties, but will repeat here some of the method since it will allow us to make a very strong argument as to why not only in theory but also in practice we should use the least-squares method.

The solution to the problem, Φ', by whatever method it is calculated, is a function of the input quantities A°, Φ and Σ. A straightforward method to propagate to the solution the uncertainties in the input data is to calculate the sensitivity of the solution to the input parameters. Let us construct such a sensitivity matrix S given by:

$$d\Phi' = S \cdot \begin{pmatrix} dA^\circ \\ d\Phi \\ d\Sigma \end{pmatrix} \quad . \tag{44}$$

The elements of the matrix S are the partial derivatives of the output fluxes with respect to all the input data. Since in our usual methods we do not have a simple expression which relates the solution to the input data, the matrix S must be obtained by numerical methods and this may be a very large computational task which can be carried out at least in principle. (Some of the diagonal elements of the matrix S are related to the often used "improvement ratios."[7]) Once one has the matrix S, we can obtain the covariance matrix N'_Φ by the relation:

$$N_{\Phi'} = S \cdot \begin{pmatrix} N_{A^\circ} & 0 & 0 \\ 0 & N_\Phi & 0 \\ 0 & 0 & N_\Sigma \end{pmatrix} \cdot S^\dagger \quad , \tag{45}$$

where the matrices N_{A°, N_Φ and N_Σ are the very same quantities which were discussed in connection with the least-squares method. Expression (45) indicates that if we are interested in obtaining the uncertainties in the solution of our usual methods we must generate and use the same covariance matrices required by the least-squares method. The problems which may be perceived in using the least-squares method due to the requirement of having such covariance matrices are therefore not unique to it but also present when we want to answer the question, "What are

the uncertainties in the solution?", regardless of how we obtain the solution. If we obtained N'_{ϕ}, using (45) for our current methods, we then could answer the question: How good are the predictions which we can make using the solutions?. In order to pick a large class of possible applications in which we might use Φ', let us consider a "result" r which is obtained as a linear combination of the ϕ'_j's. We define r in terms of the vector R whose elements are the coefficients of the linear combination of the ϕ'_j; we therefore write

$$r = R^{\dagger} \cdot \Phi' \quad . \tag{46}$$

Then the variance of r, which we write as V_r, is just:

$$V_r = R^{\dagger} \cdot N_{\Phi'} \cdot R \quad . \tag{47}$$

The vector R is completely arbitrary and we might suggest that several such vectors R may be of particular importance in our dosimetry problem. For instance, we might think of r as being one of the activations which were measured, in which case R is just Σ^i. Another pertinent example is one where r is some damage parameter, in which case R is the corresponding "damage function."

In some very real sense, if we carried out the above calculations, we could say that the better method is the one which produces the smaller value of V_r. The minimum variance theorem guarantees that whatever is the set of input data and the vector R the solution from the least-squares method is guaranteed to give the smallest variance V_r. We can now continue our discussion of the comparison of the different codes on the basis of how well their solutions reproduce the measured activations. As we discussed before, the codes SAND-II, SPECTRA, and CRYSTAL BALL could be run

such that the numerical values of the "output activations" agree with the measured values better than the output of STAY'SL, but we would be wrong to conclude that their solution is therefore better. We have just proven that this "numerically better agreement" is purely fortuitous since the uncertainties in these numbers, whether we actually compute them or not, are likely to be bigger and can be no smaller than those obtained by the least-squares method. In addition, the running time by the least-squares method is not larger for the same size problem.

Summary and Conclusions

The problem of dosimetry neutron spectrum unfolding has received considerable attention and much progress has been made in developing algorithms (SAND-II, SPECTRA and CRYSTAL BALL) which are perceived to give much promise even though their solutions to the same problem are sometimes quite different. Through extensive comparisons of the output of these codes for the same problem and the development of various quantities to allow some aspects of the solutions to be investigated, much insight has been gained into these algorithms and the nature of the few-channel unfolding problem. Dosimetry spectrum unfolding, as practiced now with these codes, still remains difficult and requires much expertise to produce generally acceptable solutions. Until now very little attention has been given to the problem of analyzing in a credible manner the uncertainties in the solutions, with the exception of the SAND-II code where Monte Carlo is used to provide an estimate of some of the uncertainties. We have shown that the propagation to the solutions of these codes of the uncertainties in the input data was in principle straightforward.

The uncertainty in the solution due to all of the input data uncertainties, as given by their covariance matrices, can be obtained by generating the sensitivity matrix of the solution with respect to the input data. This method of obtaining the uncertainties in the solution of these codes requires, however, a large computational effort which probably would be prohibitive for routine use. The approach to uncertainty estimate of SAND-II could also be improved to take into account important correlations which are currently neglected, but this method[4] also runs rapidly toward large computational problems. We believe that, if these calculations were made, a large part of the subjectivity currently needed to assess the "goodness" of these solutions would be eliminated. There would, however, still remain a problem related to the heuristic nature of these algorithms for the solution.

We have shown in this paper, and a previous one,[4] that given the input data required to obtain our current solutions and estimate the uncertainties due to the input data, a solution can be obtained using the least-squares method. We have reviewed in some detail the assumptions of the least-squares method and some of the properties of its solution in an effort to establish that this least-squares method did not require any more assumptions than we currently make. The solution by the least-squares method is extremely easy to obtain given the required input data, is unique and in a very real physical sense provides the best possible solution under the circumstances (i.e., the assumptions made and the intended use of the solution), and also easily provides the uncertainties in the spectrum. We, therefore, believe that this least-squares method provides the solution which we have sought for the dosimetry spectrum unfolding. A computer code STAY'SL, which calculates this solution, is now available.

Although the method now exists for computing a satisfactory solution to the dosimetry unfolding problem, much work remains to be done in most cases in order to obtain the best answers. We believe that most of our efforts should be devoted to the codification of our uncertainties in the evaluations used as input data to be able to generate covariance matrices. Although this is likely to be a substantial amount of work, we also think that much of the methodology exists to carry out this task. In particular, with respect to dosimetry cross sections, where much thought has already gone into this problem and a formalism created in ENDF/B to handle the covariance matrix information, hopefully most of these data will soon become available with ENDF/B-V. Regarding the uncertainties in the input spectrum, much progress has already been made in the area of computing the sensitivity coefficients in transport applications in order to propagate nuclear data uncertainties. However, much work remains to be done regarding the estimation of uncertainties in transport problem solutions due to the various approximations made.

Finally, although the method of least-squares we propose is very likely satisfactory for most problems, in some situations it may not be entirely adequate to obtain only the second moment of the joint density function of the spectrum as the least-squares method does. We believe that as we gain experience with the least-squares method and improve considerably our perception of the uncertainties in nuclear data the need may arise to go beyond their representation in terms of only the second moment of the density functions. Then more powerful methods capable of dealing with higher moments of the density functions will be needed. How urgently we need to explicitly develop such methods for the dosimetry problem is a matter of conjecture now and will depend, we

believe, very much upon the progress we make in understanding the nature of the uncertainties in nuclear data and the problems we face when trying to handle only the second moments of their estimated joint density functions. To a large degree the nature of those more powerful methods will be dictated by the kinds of problems we encounter.

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