This article is based on recent publications of the author mentioned in the text. Parts of it may be found in chapter 9 of a *Handbook on Neutron Spectrometry in Mixed Fields*.

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1. Introduction

The determination of the spectral particle fluence via unfolding of measured detector readings has been investigated by many authors (see, for instance, references \(^2,3,4,5,6,7,8,9,10,11\); this list does not, however, claim to be complete). Many papers are available, which relate to the so-called inverse problem, where solutions for metrological tasks can be obtained by unfolding.

In this paper the overview given in references \(^2\) and \(^3\) will be repeated and extended. The spectrometry performed by means of so-called ‘multichannel’ or ‘few-channel’ measurements will be discussed and attention will be paid to the question of uncertainty analysis and to the propagation of uncertainties in under- and over-determined inverse problems.

The detectors used for spectrometry in mixed neutron-photon fields generally indicate a superposition of readings which is due to the fact that the field has two components of radiation. In the case of isotropic indicating detectors, the reading \(z_i\) of a detector with number \(i\) of a set \(M\) of detectors or the reading \(z_i\) in a channel \(i\) of a multichannel detector can be written as:

\[
z_i = \int dE_\gamma R_i^\gamma(E_\gamma) \Phi_i^\gamma(E_\gamma) + \int dE_n R_i^n(E_n) \Phi_i^n(E_n), \quad (i=1,\ldots,M)
\]

where \(R_i^\gamma(E_\gamma)\) and \(R_i^n(E_n)\) are the response functions for detector \(i\) for photon and neutron irradiation at photon energies \(E_\gamma\) and neutron energies \(E_n\). For non-isotropic indicating detectors the response additionally depends on the direction of the incoming particles.

In spectrometric experiments it is attempted to separate the two contributions by the use of special neutron and photon detectors. In the following, mainly neutron detectors are considered, and the terms “fluence” and “response function” are used without the two components being specifically distinguished:

\[
z_i = \int dE R_i(E) \Phi_i(E).
\]

The response function as appearing in eq. (2) has the properties of a so-called transmission (or transfer) function, where via a linear relationship the “input” quantity “spectral fluence” is connected to the “output” quantity “detector reading”. In physics, within the framework of
the “linear response theory” the left-hand side of eq. (2) is generally called “response” which might lead to some confusion (see also chapter 2 or reference\(^1\) for the definition of the response function). In mathematical terms, the reading \( z_i \) in eq. (2) is a linear functional of the spectral fluence. The kernel of eq. (2) which is here called response function \( R_i(E) \), can be interpreted as the first functional derivative of the reading with respect to the fluence which is sometimes written as \( z_i,\Phi(E) \).

For numerical work, eq. (2) has to be transformed at least approximately into the discretised linear matrix equation

\[
    z = R \Phi
\]

with the group fluence vector \( \Phi^T = (\Phi_1, ..., \Phi_N) \), where the letter \( ^T \) stands for transposition of the matrix. The \( N \) fluence components are here considered as (integral) fluence values in the \( N \) energy intervals, sometimes however, another method of discretisation is used (see, e.g. references\(^4,7\)).

The mathematical approximation leading from eq. (2) to eq. (3) is discussed in chapter 2 of the above-mentioned handbook\(^1\).

2. Uncertainty and Ambiguity in Inverse Problems

The evaluation of the spectral particle fluence vector \( \Phi \) from a relation due to eq. (3) is called “solving the inverse problem of spectrometry”. Eq. (3) represents the idealized model for the evaluation, in principal the actual measured readings \( z_0 \) have a certain amount of uncertainty and may be written as the sum of the ideal quantity and an uncertainty part:

\[
    z_0 = z + \varepsilon,
\]

where the quantity \( \varepsilon \) reflects the fluctuation due to statistical and systematic uncertainty.

For the following evaluation it is assumed that the measured values \( z_0 \) and the uncertainty matrix (covariance matrix) \( S_{0,0} \) of vector \( z_0 \) are known and that the expectation value of the fluctuating quantity \( \varepsilon \) is equal to zero.
From the mathematical point of view, eq. (2) is a degenerate case of the Fredholm-type integral equation of the first kind. It has no unique solution since a finite number of discrete measurements cannot define a continuous function $\Phi_E(E)$. Neither does eq. (3) have a unique solution in case that the number of detector channels $M$ is smaller than the number of the energy groups $N$ considered (under-determined case $M < N$). In the over-determined case of $M > N$ (or for $M = N$), the solution spectrum and its uncertainty matrix are often calculated by the least-squares method (see, for example, references $^2,^3,^4,^7,^9,^{10},^{12},^{13}$), where the quantity

$$\chi^2 = (z_0 - R \cdot \Phi)^T \cdot S_{z0}^{-1} \cdot (z_0 - R \cdot \Phi)$$

is minimized, provided $S_{z0}$ is non-singular. The solution of eq. (5) is obtained from the so-called normal equations

$$R^T \cdot S_{z0}^{-1} \cdot z_0 = R^T \cdot S_{z0}^{-1} \cdot R \cdot \Phi = B \cdot \Phi,$$

which have to be solved for $\Phi$. Eq. (6) has a unique solution if the rank of the matrix

$$B = R^T \cdot S_{z0}^{-1} \cdot R$$

is maximum, i.e. if it equals the number of fluence groups $N$. Matrix $B$ is sometimes called the structure matrix $^{14}$. 

It has been found in many practical cases that the normal equations (6) are very close to singular $^{2,^4,^{10},^{14}}$, even for a maximum rank of $R$. The situation then is similar to that in the underdetermined case ($N > M$), and it must be concluded that, in practice, there exists probably a manifold of possible solutions of eq. (6). This ambiguity may be extremely hard to notice in complicated problems $^{15}$. The concept of ambiguity is considered here similar to the concept of so-called systematic uncertainties. It means that from incomplete knowledge of a measurand (quantity to be measured) there follows a certain amount of uncertainty.

Matrix $B$ generally controls the amount of the ambiguity $^{2,^3}$, and for every inverse problem the condition of this matrix should be investigated before trying to use mathematical programs to find a solution. The number of non-vanishing eigenvalues (see section 9.12) of matrix $B$ is a measure of the condition of the matrix, and it has been found that in most practical problems there are many eigenvalues very close to zero, thus leading to quasi linear dependence of the normal equations.

There are some possibilities of reducing this ambiguity and increasing the values of the very small eigenvalues. First, all information available on the spectrum must be used within the
unfolding algorithm. Sometimes a pre-calculated fluence vector $\Phi_0$ with an uncertainty matrix $S_{\Phi_0}$ is known, and sometimes a smoothing condition for the fluence can be formulated. This \textit{a priori} knowledge can be used with eq. (5) to construct a solvable system of normal equations. If however, $S_{\Phi_0}$ contains large uncertainty components, non-physical results such as negative elements of the fluence vector might be obtained.

It is a \textit{conditio sine qua non} for the resulting fluence vector to be non-negative for all particle energies. The discussion must therefore be extended to algorithms which cover this condition, such as the logarithmic least-squares method\textsuperscript{10,16,17,18} or, more generally, to algorithms based on the principle of maximum entropy with constraints which are due to the information available.

Computer programs based on this principle have been developed and are now available in a great variety of models and examples (see e.g.\textsuperscript{2,3,5,6,16,19}). It is the aim of this paper to review some algorithms used in particle spectra unfolding and to investigate how propagation of uncertainties can be performed.

### 3. Computer Codes

A number of methods have been developed for solving the inverse problem for particle detection and spectrum determination. The inverse problem is a general problem in physics, but here only a brief overview can be given which will be focussed on the algorithms used in the HEPRO program system\textsuperscript{16,20}. During the last few years, however, important progress was achieved in the development of other methods and codes which are not included in the HEPRO package. Some of these methods will also be referred to here.

In reactor dosimetry for ‘few-channel’ unfolding the codes based on linear least-squares methods were successfully applied in the REAL-84 exercise\textsuperscript{21}. STAY’SL\textsuperscript{9}, LEPRICON\textsuperscript{22}, LSL\textsuperscript{17}, DIFBAS\textsuperscript{23}, DIFMAZ of the HEPRO package\textsuperscript{16} and MSITER and MINCHI (“PTB STAY’SL versions”)\textsuperscript{16,24} are representative of a large number of available least-squares adjustment codes using \textit{a priori} information on the fluence. These codes are also successfully applied to the unfolding of measured data obtained by Bonner spheres. As a second group,
the codes excluding negative fluence values, e. g. SAND-II \cite{18}, GRAVEL (based on an improved SAND-II algorithm)\cite{16}, LSL-M2 \cite{17}, LOUHI \cite{25}, BUNKI \cite{26}, RADAK \cite{27} have to be mentioned. These codes in principle perform a non-linear least-squares adjustment, with the constraint of non-negative particle fluence. In this context, the approach by F. Schmittroth \cite{10} has to be mentioned, who uses a log-normal distribution of the variables to avoid negative fluence values. Secondly, Schmittroth uses correlations in the \textit{a priori} spectrum as a means of ensuring smoothness. Some of the least-squares codes employ other smoothing or regularizing procedures to construct a non-singular matrix $B$ in eq. (7), e. g. a Tikhonov regularization \cite{28} or a condition of small curvature or small fluctuation, e. g. the FERDOR or the FORIST code \cite{29,30}. In this context, the singular value decomposition \cite{5,7,15,31} should be mentioned here, where only the positive eigenvalues of $B$ are taken in a special approximation and the other eigenvalues are neglected.

Recently, genetic algorithms (e. g. those of Freeman et al. \cite{32} and Mukherje \cite{33} where applied in particle spectrometry using an evolution model together with a “survival” strategy to solve complex mathematical equations. Here, the optimisation criterion (definition of the fittest) is an important model parameter. Up to now, in particle spectra unfolding, these codes give very poor results. Some of the codes mentioned here allow an uncertainty analysis to be performed, namely those codes based on the least-squares method. Up to now it has not been quite clear how to propagate the uncertainties for the evolution models or the models relating to neural networks. Some progress has been made in this field by applying Bayesian methods in neural network theories \cite{34,35,36}.

Bayesian methods or methods based on the maximum entropy method have been realised in the MIEKE and UNFANA programs of the HEPRO package \cite{16} and in the MAXED code, recently developed \cite{19,37}. These codes make consistent uncertainty propagation possible, however, it is not yet completely understood how the uncertainty resulting from the “ambiguity” of the solution (singularity of matrix $B$) can be taken into account; a first trial is contained in the MIEKE code (see below).
4. Least-Squares Methods

It is assumed that a pulse height spectrum or a number of detector readings \( z_0 \) with the uncertainty matrix \( S_{z0} \) have been determined (see eq. (5)). For \( S_{z0} \), only a diagonal form is sometimes used with the variances of \( z_0 \) (often determined by Poisson statistics). It is further assumed that pre-information \( R_0 \) on the response matrix is available (or that some parameters \( p_0 \) of the response matrix are known before) with the uncertainty matrix \( S_{p0} \) or \( S_{\phi 0} \). If, in addition, the particle fluence \( \Phi_0 \) was previously calculated or measured by another independent “measurement” (e.g. by a transport code calculation) with the uncertainty matrix \( S_{\phi 0} \), the general \( \chi^2 \) expression:

\[
\chi^2 = (z_0 - z)^T \cdot S_{z0}^{-1} \cdot (z_0 - z) + (R_0 - R)^T \cdot S_{R0}^{-1} \cdot (R_0 - R) + (\Phi_0 - \Phi)^T \cdot S_{\phi 0}^{-1} \cdot (\Phi_0 - \Phi)
\]  

(8)

has to be minimised under the constraint \( z = R(p) \cdot \Phi \) with respect to \( z, R \) (or \( p \)) and \( \Phi \). Eq. (8) is the general \( \chi^2 \) expression for an adjustment procedure, when the parameters or the fluence are already known to a certain extent and the new measurement \( z_0 \) is used only for adjustment. Eq. (8) can be considered as a typical least-squares task, where the fluence components have to be determined from an over-determined problem. The various algorithms used to find the minimum of eq. (8) make a distinction as regards the modelling of the last two terms. There are only some codes, mainly used in reactor dosimetry, where the \textit{a priori} information on the response matrix can be taken into account (e.g. STAY'SL \(^9\), LSL \(^17\), LEPRICON \(^{22}\), MSITER and MINCHI of PTB \(^{24}\); in all other cases, the second term in eq. (8) is missing. If nothing is known \textit{a priori} on the fluence, the last term in eq. (8) may be replaced by a smoothing or shape condition (see e.g. \(^{25,29,30,38}\)) in order to obtain a non-singular system of normal equations for the solution as mentioned in the previous sections. This is the essential content of the Tikhonov regularization \(^{28}\).

With the constraint \( z = R \cdot \Phi \), the minimisation of eq. (8) leads to non-linear normal equations. Since it can be assumed that the adjusted values will not be too far from the \textit{a priori} information values, this constraint equation is replaced by a Taylor approximation in the vicinity of \( R_0 \) and \( \Phi_0 \) \(^{16}\), leading to the linear expression

\[
z - R \cdot \Phi \Rightarrow z - z_i - z_R \cdot (R - R_i) - z_\Phi \cdot (\Phi - \Phi_i),
\]  

(9)

where \( z_i = R_0 \cdot \Phi_0 \), and \( z_R \) and \( z_\Phi \) are matrix derivatives of \( z \) at \( R_0 \) and \( \Phi_0 \), with \( z_\Phi = R_0 \) and \( z_R = \Phi_0 \).
With eq. (9), the linear least-squares adjustment is performed. The solution for the fluence vector and its uncertainty matrix is:

\[
\Phi = \Phi_0 + S_{\phi 0} \cdot z_{\phi} \cdot W^{-1} \cdot (z_0 - R_0 \cdot \Phi_0), \quad S_{\phi} = S_{\phi 0} - S_{\phi 0} \cdot z_{\phi} \cdot W^{-1} \cdot z_{\phi} \cdot S_{\phi 0}.
\]  

(10)

with the weighting matrix

\[
W = S_{z_0} + z_R \cdot S_{R_0} \cdot z_R + z_{\phi} \cdot S_{\phi 0} \cdot z_{\phi}
\]  

(11)

(transposition not indicated here and in the following).

From eqs. (10) and (11) it is apparent that the introduction of a priori information into the least-squares formalism leads to normal equations, where only an inversion of the \( M \times M \) matrix \( W \) instead of the \( N \times N \) matrix \( B \) of eq. (7) is required. Due to the minus sign in the uncertainty equation, the uncertainty is reduced after adjustment. From eqs. (10) it is also apparent that the solutions and their uncertainty matrices strongly depend on the a priori information values \( \Phi_0 \) and the a priori uncertainty matrix \( S_{\phi 0} \). It is also seen that negative fluence values may appear here.

In practice, the a priori spectrum often is not known in an absolute scale. In this case, the scaling factor for the fluence has also to be determined by the unfolding code. A non-linear evaluation of this factor has been included in the MSITER(MINCHI)\(^{24}\) program. It is not included in the least-squares codes STAY’S\(^{9}\), DIFBAS\(^{23}\) and DIFMAZ\(^{16}\).

From eq. (8) it can be concluded that the a priori information on both, the response matrix \( R_0 \) and the fluence \( \Phi_0 \) is considered in the same way, i.e. as if both quantities are to be adjusted. This is the philosophy of the ISO Guide\(^{39}\), the German DIN Standard DIN 1319\(^{40}\) and the LEPRICON\(^{22}\) methodology: all measured quantities, those currently measured and data quantified before, have to be included in the adjustment procedure, i.e. the “properties of the entire world” are influenced by the current measurement.

There is another way of adjustment not yet established in particle fluence unfolding, namely to consider the response function as a so-called “parameter” and employing the adjustment procedure with this “parameter” being constant during the unfolding procedure, and performing the uncertainty propagation afterwards. In this case, the second term of the right-hand side of eq. (8) is missing. The solution of this model is similar to eq. (10), but the term
with $S_{R0}$ is missing in the expression for matrix $W$. From the uncertainty propagation one finds (with new matrix $W_1$ instead of $W$):

$$S_\Phi = S_{\phi_0} - S_{\phi_0} \cdot z_\Phi \cdot W_1^{-1} \cdot z_\Phi \cdot S_{\phi_0} + S_{\phi_0} \cdot z_\Phi \cdot W_1^{-1} \cdot z_R \cdot S_{R0} \cdot z_R \cdot W_1^{-1} \cdot z_\Phi \cdot S_{\phi_0}$$  \hspace{1cm} (12)

This model is different from that usually used for least-squares adjustment, and it has obviously not been employed to date in standard software like STAY’SL. It offers advantages in cases the response functions are known with small uncertainties.

Some remarks have to be made on the construction of the matrices $S_{\phi_0}$ and $S_{R0}$, which up to now have not been made available from the transport code calculation used to derive $\Phi_0$ and $R_0$. In many cases, one has a rough idea of the slope of the particle spectrum. In a reactor moderator, for instance, a moderated fission spectrum is expected, expressed as a sum of parameterised subspectra with a number $k$ of parameters (e. g. the temperature parameter of a Maxwell spectrum or the slope of a $1/E$ spectrum). If the subspectra and the uncertainties of their parameters are used to construct the matrix $S_{\phi_0}$, it turns out that $S_{\phi_0}$ has deficient rank $r=k$. Generally, $S_{\phi_0}^{-1}$ then is non-existent, however, a solution vector $\Phi$ may be compiled from eq. (10). It can be shown that the possible solution spectra are restricted to a very small subspace spanned by the $r=k$ eigenvectors of $S_{\phi_0}$, which in principle means that the solution spectrum is a superposition of the $k$ subspectra defined $a$ priori, thus putting severe constraints on the solution spectrum by the specific choice of the $a$ priori covariance matrix $\Phi_0$. It is, therefore, preferable to use a diagonal $S_{\phi_0}$ instead, so that the entire solution space is available. This in compliance with the German standard DIN 1319: “If nothing is known on the correlations, a diagonal uncertainty matrix must be used”.

In practical examples the uncertainty matrix $S_{R0}$ should be constructed in a way already outlined in the ENDF uncertainty file, and it is recommended that the format used there should also be used, for instance, for establishing the uncertainty matrix of the Bonner spheres response function. Apart from reactor dosimetry where the use of a full uncertainty matrix $S_{R0}$ compiled from ENDF data is considered to be state-of-the-art, only a few attempts were made in the past to include response matrix uncertainties in the unfolding process for other problems. The HEPRO package provides the possibility of including uncertainties of energy calibration and resolution parameters of the response functions in multichannel unfolding problems. There is a fairly recent paper by Dose, Fischer and von der Linden that
does discuss a rigorous approach for introducing the uncertainty of the response functions into the unfolding process (although not in the context of neutron spectrometry)\(^{44}\).

### 5. Non-linear Least-Squares Methods

The linear least-squares method, well established in the STAY’SL\(^9\) code, the DIFBAS\(^{23}\) and the DIFMAZ\(^{16}\) code and in the LEPRICON methodology\(^{22}\), is the unfolding algorithm recommended for use when good \textit{a priori} information and consistent measurement results are available (see e.g. ISO Guide\(^{39}\)). The disadvantage is that negative fluence values cannot be excluded (see examples below). To take the condition of non-negative fluence into account, a method first realised in the SAND-II code\(^{18}\) and used later in the LSL-M2\(^{17}\) and GRAVEL\(^{16}\) codes, can be applied. In this case, not the group fluence elements \(\Phi_v\) but their logarithms \(\ln(\Phi_v)\) are determined by a special iteration procedure minimising an expression similar to eq. (5) with the logarithms of the \(z_{oi}\) instead of \(z_{oi}\). A similar method is used in the LOUHI code\(^{25}\), where the unknown quantities \(\Phi_v\) are expressed as squares of real numbers.

More recent developments in data analysis have resulted in better ways of unfolding “when good a priori information and consistent measurements are available”- a wide range of Bayesian methods, as well as the theory on which MAXED\(^{19}\) is based. A good summary of this theory can be found in the paper by W. von der Linden\(^{45}\).

The SAND-II (GRAVEL) solution is determined by a special gradient method\(^{16}\): iteration is started with a spectrum \(\Phi_v^{(1)}\). Weights \(w^{(i)}_\mu = R_v \cdot \Phi_v^{(1)}(i)\) with \(z^{(1)}_i = \sum_v R_v \cdot \exp(\ln \Phi_v^{(1)})\) are calculated. In each iteration step the current solution (k+1) is obtained from the previous solution (k) by

\[
\ln \Phi^{(k+1)}_\mu - \ln \Phi^{(k)}_\mu = \lambda^{(k)}_\mu \cdot \sum_i (\ln z_{0i} - \ln z^{(k)}_i) \cdot \frac{w^{(k)}_\mu}{\rho_i^2}, \quad \text{where} \quad \lambda^{(k)}_\mu = \left( \sum_i \frac{w^{(k)}_\mu}{\rho_i^2} \right)^{-1} \tag{13}
\]

The \(\rho_i\) are the relative standard deviations of the \(z_{0i}\), namely \(\rho_i = \sigma_{0i}/z_{0i}\) which were not included in the original SAND-II codes.
It should be mentioned that the BUNKI (SPUNIT) algorithm \(^{26}\) is similar to the SAND-II (GRAVEL) algorithm. Starting from the SAND-II iteration formula, eq. (13), and developing the right-hand side around \( z_i^k = z_{i0} + \delta_i^k \), one obtains in first order:

\[
\Phi^{(k+1)}_\mu = \Phi^{(k)}_\mu \frac{\sum_i R_{i\mu} z_i^k \frac{\delta_i^k}{z_{i0}}}{\sum_i \frac{R_{i\mu}}{z_{i0}} \frac{1}{\rho_i^2}}
\]

which is equal to the corresponding equation used in the SPUNIT code \(^{46}\). It has been found that the results obtained by the two codes are nearly identical.

For the iteration procedure in the SAND-II (GRAVEL) codes, an initial input spectrum is needed when iteration is started. A solution always exists, but the solution spectrum depends on this input spectrum in a way which is not quite transparent so that an uncertainty propagation cannot be easily performed. It has been found \(^{16}\) that matrix \( B \) of eq. (7) controls the various solutions; for non-singular \( B \) a unique solution exists, whereas for ill-conditioned \( B \) a manifold of solutions may exist, depending on the rank of \( B \).

For the uncertainty analysis, the method of randomly chosen start spectra has been tried \(^{47,48,49}\), with final averaging over all solutions. This provides a (model-dependent) plausible uncertainty for the solution spectrum, including correlations. This uncertainty represents the variety (ambiguity) of solutions and cannot take the normal uncertainty propagation of the uncertainty matrices \( S_{z0} \) and \( S_{R0} \) into account.

The other available non-linear least-squares methods may be considered as special unfolding models used to regularize matrix \( B \) (e. g. \(^{25,28,29,30,31}\)). Additional parameters (e. g. for smoothing) are introduced to get a unique solution. Uncertainty propagation can be performed by these algorithms but has obviously not yet been established in the codes available.
6. Maximum Entropy

The existing models for solving the inverse problem can be treated from two points of view. In the first method the minimum least-squares solution according to eq. (5) is determined. A solution of eq. (6) should in principle always exist for realistic physical problems but in many cases, the solution may not be unique. In the second method, the ambiguity is taken into account and a probability distribution of the possible fluence components is determined. Both ways can be traced back to Bayesian theory; together with the principle of Maximum Entropy\(^{50}\), they describe two ways of inference.

The Bayesian method is used to provide a formal foundation for the use of \textit{a priori} information. The \textit{a priori} information is not limited to data values and uncertainties but can include correlations and various physical constraints\(^ {10}\). Sometimes the only \textit{a priori} information might be that all the fluence values should be non-negative. Starting from an \textit{a priori} probability distribution (called Prior), the a posteriori probability (called posterior) of Bayes’ theorem can be obtained from the well-known relation \(^ {51}\) “posterior proportional to likelihood times prior”.

Generally, to establish the joint posterior probability distribution \(P(\mathbf{x})\) of a set of variables \(\mathbf{x}\), the distribution \(P(\mathbf{x})\) is factorised by

\[
P(\mathbf{x}) = P_L(\mathbf{x}) \cdot w(\mathbf{x})
\]

into the unknown likelihood \(P_L(\mathbf{x})\) and the prior \(w(\mathbf{x})\). The distribution \(P(\mathbf{x})\) is then obtained by the Lagrange method using the principle of maximum entropy

\[
S = -\int P(\mathbf{x}) \log \left( \frac{P(\mathbf{x})}{w(\mathbf{x})} \right) \, d\mathbf{x} \Rightarrow \max
\]

and observing the normalisation condition and certain constraints on \(\mathbf{x}\)\(^ {50}\). The likelihood, too, may be the result of maximising the entropy where as a prior the so-called data prior is used. Most of the unfolding models applied use as the likelihood function the probability distribution of the fluence vector:

\[
P_L(\Phi) = C_1 \cdot \exp\left( -\frac{\beta}{2} \cdot \chi^2(\Phi) \right)
\]

with a normalisation constant \(C_1\), with \(\chi^2(\Phi)\) defined by eq. (5), and where the parameter \(\beta\) is determined (see below) from the condition that the expectation value of \(\chi^2(\Phi)\) in the
posterior probability distribution (with the notation $< \chi^2(\Phi) >$) be equal to the number of degrees of freedom $M$. Obviously, the minimum least-squares method is equivalent to maximising the likelihood but obviously the two ways mentioned are based on different models as regards the value of $\chi^2(\Phi)$ ($\chi^2 \to \min$ or $< \chi^2 > = M$). It can, however, be shown that both ways lead more or less to the same result in case the minimum least-squares solution exists and the uncertainties of the readings are small.

The minimum least-squares method is often used to fit data, assuming at the same time that the model applied is true. This is the first level of inference. At the second level of inference it is intended to infer which model is most plausible given the data, which means discussing probability distributions and expectation values.

The properties of the minimum least-squares codes are less satisfactory, when there is a lack of pre-information on the particle spectrum. In this case, the singularity or quasi singularity of matrix $B$ of eq. (7) may lead to ambiguity of the solutions even if the constraint of non-negative fluence is included in the least-squares algorithm. For the equivalent maximum likelihood method it follows that a unique, most probable particle spectrum might not exist. However, similar to the maximum likelihood method, it is possible to construct an a posteriori probability density of the fluence using Bayes’ theorem with eq. (14). The solution spectrum can then be defined as the expectation value of $\Phi$, denoted by $< \Phi >$, which can be calculated from the probability density. This method was used in reference; later, a more modern interpretation was given in references using the principle of maximum entropy.

In fluence spectrum unfolding, together with eq. (15), certain constraints are usually formulated and used with the maximum entropy method. When the constraints to be imposed are included in eq. (15), it is possible to formulate the extremum principle for the determination of the fluence probability density $P(\Phi)$ using the constant probability distribution as the prior (“equal distribution of ignorance”). In the case realised in the MIEKE code, two constraints are assumed to exist: (a) all group fluence values should be non-negative, and (b) the expectation value $< \chi^2 >$ of $\chi^2$ (see eq. (5)), should be equal to the number of degrees of freedom involved, which is equal to the number $M$ of elements in $z_0$. By means of the extremalisation procedure, the probability density
\[ P(\Phi) = C_1 \cdot \exp\left(-\frac{\beta}{2} \cdot \chi^2(\Phi)\right) \quad \text{for all } \Phi \geq 0 \] (17)

is obtained, and the prior of eq. (14) is taken as a constant value, defined for all \( \Phi \geq 0 \) and vanishing for negative values due to condition (a). \( C_1 \) is the normalisation constant. \( \beta \) is a "temperature" parameter to be determined from condition (b). The probability density \( P(\Phi) \) represents a multivariate normal distribution with a \( \chi^2 \)-exponent, truncated because of condition (a). Although the exponent is degenerate in case \( N > M \) (or for an ill-conditioned matrix \( B \)), the distribution can be normalised and the expectation value \( < \Phi > \) with its uncertainty matrix

\[ S_\Phi = <\Phi\Phi> - <\Phi><\Phi> \] (18)

can be calculated. For \( \beta = 0.5 \) and excluding the constraint of non-negative fluence values, \( P(\Phi) \) is equivalent to the likelihood expression used in Bayes’ theorem if a normal distribution is assumed for the measured data.

The probability density of eq. (17) is introduced into the MIEKE code of the HEPRO package \(^{16}\). A Monte Carlo code with importance sampling is used to calculate expectation values. For the MIEKE code, the computing time turned out to be very long, in particular for \( M \ll N \). K. Weise \(^6\) therefore proposed an analytical approach to the Monte Carlo results to reduce the computing time. Weise replaced the distribution of eq. (17) by the simpler exponential ansatz \(^4,6\):

\[ P(\Phi) = C_1 \cdot \exp(-\mathbf{b}^T \cdot \mathbf{R} \cdot \Phi) \] (19)

and used the same constraints for the extremum principle of maximum entropy. The parameters \( \mathbf{b} \) for maximum entropy can be obtained by a simple solution of a non-linear matrix equation. Here, the expectation values can easily be calculated. The covariance matrix \( S_\Phi \) of the distribution turns out to be diagonal and must be properly interpreted. To obtain the uncertainty associated with the expectation value \( <\Phi> \) due to the uncertainty matrix \( S_{\Phi\Phi} \) the Gaussian law of uncertainty propagation is used. The subroutine UNFANA \(^6\) of the SPECAN code uses eq. (19) and performs this analysis.

Weise \(^6\) has shown that for \( N \to \infty \) the expectation values \( <\Phi> \) obtained are identical for both distributions of eqs. (17) and (19). It has been found from a variety of examples that there is also good agreement for \( M \approx N \).
It should be noted that, in principle, \textit{a priori} information could be included in both distributions (eq. (17) and eq. (19)) by using for $\chi^2$ an expression similar to eq. (8) instead of eq. (5) or by using the corresponding term in the prior, i.e. the \textit{a priori} probability distribution in a Bayesian formulation. For the algorithm used in the MAXED code \textsuperscript{19,37}, this \textit{a priori} information is included as a prior in the maximum entropy formulas. In MAXED, the (normalised) spectral fluence is taken as a probability density.

Although MIEKE, UNFANA and MAXED are all based on the maximum entropy principle, they apply this principle in very different ways. MIEKE and UNFANA refer to the original definition of maximum entropy due to Shannon (see e.g. Weise et al.\textsuperscript{50}, Jeffreys\textsuperscript{51}, Jaynes\textsuperscript{53}), where the entropy is a measure of the amount of uncertainty expressed in a multivariate distribution of the individual fluence components and where the prior $w(x)$ in equation (15) is set to constant (see also appendix A in reference \textsuperscript{19}). In MAXED, the probability density of the spectral fluence is derived from the principle of cross-entropy\textsuperscript{19} (see also Skilling\textsuperscript{54}), where in equation (15) the one-dimensional distribution $P(x)$ corresponds to the (normalized) spectral fluence $\Phi_{E}(E)$ and $w(x)$, the prior probability distribution, incorporates the \textit{a priori} information on the spectral fluence. MAXED is one of the modern unfolding codes that brings new ideas (from information theory and Bayesian theory). It has been successfully used at a number of different places. The uncertainty propagation\textsuperscript{37} has been implemented recently; the code runs with the same format of input data as the other functions within the HEPRO package.

7. \textbf{Approach to Uncertainties}

For the uncertainty analysis it must be taken into account that, in principle, two fluctuation components exist, one resulting from the uncertainties of the input quantities $x_0$ (readings, response functions, \textit{a priori} information on the fluence) and the other from the ambiguity of the solution (compare, for example with the microscopic and macroscopic fluctuations in particle statistics). The fluctuation of the resulting fluence can be considered composed of the two contributions:
\[ \delta \Phi = < \frac{\partial \Phi}{\partial x_0} > \delta x_0 + \delta \Phi_i \]  

(20)

which are perpendicular to each other, i. e. \( < \delta x_0 \delta \Phi_i > = 0 \). The resulting covariance matrix thus is the sum of two components: \( \frac{\partial < \Phi >}{\partial x_0} S_{x0} \frac{\partial < \Phi >}{\partial x_0} + S_{\phi_i} \). For the MIEKE algorithm, the corresponding formulas are quite easy to obtain from the probability distribution.

Considering only the uncertainties \( S_{z0} \) of \( z_0 \), it can be shown that \( \frac{\partial < \Phi >}{\partial z_0} = -\beta S_{\phi} \cdot R \cdot S_{z0}^{-1} \), and with the definition of \( B \) (eq. (7)) one finds \( S_{\phi i} = S_{\phi} - \beta^2 S_{\phi} \cdot B \cdot S_{\phi} \). In linear least-squares methods, \( \beta^2 S_{\phi} = B^{-1} \), which holds for non-singular \( B \) and for a Gaussian distribution. In this case, the solution is unique and \( S_{\phi i} \) vanishes. The ambiguity part \( S_{\phi i} \) cannot be obtained so easily for the other maximum entropy models. For UNFANA and MAXED, only the conventional uncertainty propagation corresponding to \( z_0 \) and (in principle to \( R_0 \)) is included. It has been found that the part from the uncertainty propagation of \( z_0 \) for the MIEKE code (\( \beta^2 S_{\phi} \cdot B \cdot S_{\phi} \)) agrees well with the corresponding result of UNFANA.

It has to be mentioned that sometimes, when a rather large temperature parameter has to be used, the fluence uncertainty due to uncertainty propagation \( \beta^2 S_{\phi} \cdot B \cdot S_{\phi} \) turns out to be greater than the part \( S_{\phi} \) which combines the two contributions (including ambiguity). This makes no sense and possibly shows the limits of practical unfolding work: a high temperature parameter limits the ambiguity.

For the MIEKE algorithm one obtains in obvious matrix notation (indices have to be chosen carefully):

\[ \frac{\partial < \Phi >}{\partial R} = \beta \{ S_{\phi} \cdot S_{z0}^{-1} \cdot z_0 - ( < \Phi \Phi \Phi > - < \Phi > < \Phi > < \Phi > ) \cdot R \cdot S_{z0}^{-1} \} . \]

As is usual in uncertainty propagation, the triple correlation function can be written in Gaussian approximation: \( < (\Phi_i - < \Phi_i >)(\Phi_j - < \Phi_j >)(\Phi_k - < \Phi_k >) > = 0 \).
This means that the usual propagation of uncertainties even for the response matrix, can be compiled after an unfolding run provided the resulting covariance matrix $S_\Phi$ given by eq. (18) is calculated by the code.

It should be noted that the maximum entropy algorithms allow other probability distributions to be constructed $^{3,55}$. In the MIEKE code the evaluation of $P(H^*)$ for the dose equivalent 

$$H^* = \sum \nu h_{\nu} \Phi_{\nu} = h_{\Phi} \cdot \Phi$$

is performed ($h_{\Phi}$: fluence-to dose conversion factor):

$$P(H^*) = \langle \delta (H^* - h_{\Phi} \cdot \Phi) \rangle$$

(21)

The variance $\langle H^* H^* \rangle - \langle H^* \rangle \langle H^* \rangle = h_{\Phi} S_\Phi h_{\Phi}$ of the distribution again includes contributions from the uncertainty propagation and the ambiguity.

Instead of the dose equivalent probability distribution the corresponding probability distribution of a certain detector reading $z$ can be calculated. From $z = \sum \nu R_{\nu} \Phi_{\nu} = R \cdot \Phi$ the probability distribution

$$P(z) = \langle \delta (z - R \cdot \Phi) \rangle$$

(22)

is obtained.

8. Results Obtained by Practical Examples.

The unfolding tasks to be solved in particle spectrometry may be considered from two points of view as “few-channel” or “multichannel” problems. As examples of “few-channel” spectrometry, the measurements in reactor dosimetry have to be mentioned (e. g. $^{21,24}$), where activities or reaction rates of different irradiation probes are determined. It was shown in the past that exact uncertainty propagation is possible in this field of metrological problems $^{2,3,21,22,24}$, provided real (or specific) pre-information on the spectrum is available, no guess! During the REAL-84$^{21}$ to the REAL-88$^{24}$ exercises, integral damage parameters for reactor pressure vessels had to be determined. It turned out that consistent determination of the parameters with a sufficiently small uncertainty was not possible without using pre-information. It was also found that with guess spectra used as pre-information the resulting uncertainties of the damage parameters might be wrong. It was recommended only to use
consistent pre-information in the unfolding codes, e.g. results of a Monte Carlo calculation with appropriately estimated uncertainties. It was also found that the rank of the correlation matrix of the pre-information spectrum is conserved during the unfolding process, which is a mathematical consequence of the linear least-squares adjustment\(^\text{41}\). Therefore, if nothing is known on the correlations, it might be better to use a diagonal correlation matrix than artificial correlations.

Other important examples of “few-channel” unfolding stem from neutron dosimetry, namely the Bonner sphere detectors (e.g. \(^\text{49,56}\)) and the superheated drop (bubble) detectors (e.g. \(^\text{57}\)). Here, the same statements as for reactor dosimetry have to be made. However, in reactor dosimetry, the propagation of response function uncertainties (uncertainties of the cross sections) is consistently possible. An uncertainty description is still missing for the response functions of the Bonner sphere detectors and the bubble detectors.

In practice, it is not so easy to obtain consistent pre-information on the spectrum for measurements at arbitrary places. In most cases guess spectra are used, sometimes without a good physical foundation. The use of estimated guess spectra as pre-information without quantifying the pre-information uncertainty may lead to an inconsistent uncertainty determination of the results. Further work is required to find an algorithm for better quantifying pre-information and its uncertainties.

The pre-information is not such a great problem in “multichannel” unfolding, since much more information is available there from the measurements. Here, the problem of quantifying uncertainties of the response matrices is not solved. This basically is only a data handling problem, e.g. a multichannel response matrix for 1000 particle energies and 1000 channels i. e. \(10^6\) elements has to be described by a \(10^6 \times 10^6 = 10^{12}\)-element uncertainty matrix.

It should be noted that unfolding with a neglected response uncertainty matrix might lead to wrong unfolded spectra in case the uncertainty of the measured multichannel spectrum is smaller than the (not directly quantified) response uncertainty. This means that very good measurements (good “statistics”) cannot be used unless the response function is known with a smaller uncertainty. It should also be pointed out that the “problem of good statistics” (relative to the response functions) can be dealt with by assigning more realistic uncertainties to the measurements. This can be done by adding by quadrature an estimated additional
uncertainty to each measurement to account for response functions that are not exact, or by unfolding to a higher-than-one value of the chi-square per degree of freedom. There is the possibility within the HEPRO codes and within MAXED for choosing by input the wanted final value of $< \frac{\chi^2}{M} >$. These methods are not perfect, but they help.\(^{58}\)

9. “Few-channel” Analysis

9.1 Bonner Spheres System

The determination of neutron spectra from the readings $z_0$ of a Bonner sphere system is a representative example of "few-channel" unfolding. Count rates for $M$ detectors are measured ($M$ being of the order of 10), and it is intended to evaluate the spectral neutron fluence or the dose equivalent in 50 to 100 energy groups. Obviously, the $a$ priori information on the fluence is more important here than in the multichannel case. Adding of $a$ priori information during unfolding is equivalent to increasing the number of measurements from $M$ to $M + N$. This means that $a$ priori information controls the results as well as the measured values. The results obtained in various examples confirm this conjecture.

In the present version of the MIEKE and UNFANA codes, $a$ priori information cannot be taken into account. If real $a$ priori information is available (no guess!), the only codes which should be used are those based on eq. (8), e.g. STAY’ SL, LEPRICON, DIFBAS, DIFMAZ, MSITER(MINCHI) and LSL, also MAXED is highly recommended to be used in such cases. However, there is a multitude of examples (e. g. references\(^ {14,59}\)), that neutron spectra have also been successfully unfolded using only guess functions together with the SAND-II (GRAVEL) program. Careful investigation of these methods allows the conclusion to be drawn that $a$ priori information is introduced as well, although in an interactive procedure, which is not easy to quantify mathematically.

A lot of experience is needed for successful unfolding of neutron spectra employing the SAND-II or the GRAVEL code. For instance, in the energy region of thermal neutrons, there is poor spectral resolution, since only the blank sphere and the cadmium covered sphere provide sufficient response. In most cases a Maxwellian spectrum is assumed within this
range. The use of such a thermal spectrum or in the fast region, the use of a fission spectrum as the starting guess spectrum in SAND-II or GRAVEL means quantifying \textit{a priori} information. On the other hand, when codes are used which need no pre-information at all, like MIEKE and UNFANA, it is difficult to unfold a reasonable neutron spectrum. However, due to negative correlations between adjacent neutron groups of the solution spectrum, resulting from the matrix $S_{\phi_1}$, it has been shown that integrals over the fluence, such as the total dose equivalent, can be calculated with much smaller uncertainties $^{2,3,16}$.

The following example represents the results of measurements with Bonner spheres performed in a moderated $^{252}$Cf reference field $^{60}$. 12 Bonner spheres were irradiated; the relative uncertainties of the readings (uncertainty of a common scaling factor of the response functions included) were between 1.2% and 4%. \textit{A priori} information was available from MCNP calculations $^{61}$, and the relative uncertainties of the MCNP calculations were estimated to be 15% below 100 keV and 10% above this value.

Fig. 1: Spectral fluence of a moderated $^{252}$Cf neutron field unfolded from the readings of 12 Bonner spheres.

From fig. 1 it is apparent that the MINCHI result is nearly the \textit{a priori} spectrum with the exception of the thermal part, for which the MCNP results are uncertain because the components of reflecting concrete are not well-known. The SAND-II result $^{60}$ was obtained by an educated guess using various combinations of thermal, intermediate and fission spectra. From the UNFANA result the spectrum can hardly be recognized, since available \textit{a priori}
information was not included. Nevertheless, it was found that integral values such as the total fluence or the total dose equivalent agree within the uncertainties.

This also holds for the integral values obtained with the MIEKE code. The uncertainty of the dose equivalent is the sum of two almost equal parts (from ambiguity matrix $S_0$ and from uncertainty propagation) which can be seen in fig. 2, in which the probability distribution of $H^*$ (as obtained by MIEKE) is given.

![Probability density of $H^*$ in a moderated $^{252}$Cf neutron field due to eq. (21). There are two contributions to the uncertainty coming from ambiguity and from the usual propagation of uncertainties. The peak is asymmetric.](image)

Considering the other examples of Bonner sphere unfolding given in the literature, it must be concluded that in moderated fission spectra like reactor surroundings the fluence can generally be determined with a relative uncertainty of about 5% and the total dose equivalent with an uncertainty of less than 15%.

### 9.2 Superheated Drop (Bubble) Detectors

Bubble detectors consist of numerous superheated droplets dispersed in a gel. They can be used as active neutron detectors: charged particles (neutron recoils) nucleate a sudden phase transition generating macroscopic bubbles combined with a sharp sound. The sound is recorded by an electronic device containing a piezo crystal.$^{57,62}$
The detector response depends on the chemical properties of the suspension and on the temperature (degree of superheating). It has the characteristic structure of a threshold detector, i.e. below a certain threshold energy the response is nearly zero increasing from that threshold energy to a flat plateau. With two types of bubble detectors and appropriate variation of the temperature (25 °C to 40 °C), threshold energies between 0.01 MeV and 10 MeV can be achieved.

The response as a function of neutron energy was investigated in the PTB’s monoenergetic reference neutron fields for eight detectors. Test measurements for neutron spectrometry were performed in the broad spectra of \(^{252}\text{Cf}\) and Am-Be neutron sources\(^{63}\).

![Spectral fluence in a \(^{252}\text{Cf}\) californium field obtained by unfolding the readings of a set of eight bubble detectors\(^{63}\).](image)

The adjustment run with the MSITER code for the \(^{252}\text{CF}\) field was performed using numerical data for a \(^{252}\text{CF}\) fission spectrum in a broad group structure as \textit{a priori} information. Uncorrelated relative uncertainties of 2% were associated with the values in the individual energy groups. With these assumptions, virtually no differences resulted between input and output spectra. A reduced \(\chi^2\) value of 0.6 after adjustment proved consistency of all the data.
For successful unfolding of a measured pulse height spectrum the particle response function for each particle energy and each channel must be known. The progress made over the last few years in Monte Carlo calculations of response functions induced progress in unfolding techniques, too. Concerning gas-filled neutron detectors, the GNSR code\textsuperscript{64} has to be mentioned which calculates the neutron response function in various neutron beam configurations for cylindrical detectors using Monte Carlo techniques. Included are recoil detectors filled with H\textsubscript{2}, \textsuperscript{3}He, \textsuperscript{4}He, and mixtures with commonly used quenching gases. For organic scintillators, the codes NRESP\textsuperscript{65}, EGS\textsuperscript{466}, and MCNP4A \textsuperscript{61} have been used to calculate neutron and photon response functions for NE-213 \textsuperscript{67,68,69}. In practice, only the so-called ideal response function for an energy $E_n$ of an incoming particle is calculated by determining the distribution of energy $E_{\nu}$ deposited within the detector. The other parameters, relating to energy calibration and resolution, have to be determined separately by the experimenter. The ideal response function $W(E_n \rightarrow E_{\nu})$ has to be folded with the so-called resolution function $G(E_{\nu} \rightarrow E_i)$\textsuperscript{16,70,71} to obtain the response matrix for channel $i$:

$$R_i(E_n) = \sum_{\nu} G(E_{\nu} \rightarrow E_i) \cdot W(E_n \rightarrow E_{\nu}).$$

(23)

$G(E_{\nu} \rightarrow E_i)$ is the probability that an event releasing energy in the interval at $E_{\nu}$ will be registered in the counter in channel $i$ at energy $E_i$. The functional relationship between $E_i$ and the channel number $i$ generally is non-linear; sometimes it can be approximated by a linear energy calibration law $E_i = A + B \cdot i$, where $A$ and $B$ are energy calibration parameters. The resolution function can be approximately represented as a Gaussian distribution around $E_{\nu}$, whose width (full width at half maximum, FWHM) can be parameterised by\textsuperscript{72}:

$$\Gamma^2(E_{\nu}) = a + b \cdot E_{\nu} + c \cdot E_{\nu}^2$$

(24)

Parameters $a$, $b$, $c$ have to be determined by the experimenter.

For practical unfolding work the question arises of how many multichannel and fluence groups are reasonable. It has been found in reference \textsuperscript{16} that the bin width of the pulse height channels should be in the order of 1/5 of the FWHM, and the same holds for the corresponding fluence groups.
In the following, two examples are discussed which were in part described in the manual for the HEPRO package\textsuperscript{16}: the unfolding of a neutron spectrum from $^3$He proportional counter measurements, and of a photon spectrum from NE-213 pulse height distributions.

11. Multichannel Analysis

11.1 Proportional Counter with $^3$He

In neutron metrology, $^3$He proportional counters can be profitably used as neutron spectrometers for neutron energies between 20 keV and 2 MeV\textsuperscript{70,71}. Neutron-induced $^3$He break-up into proton and triton ($Q = 764$ keV) enables peaks in the neutron spectrum at energies $E_n$ to be detected directly in the multichannel pulse height spectrum at energies $E_C = E_n + Q$.

Measurements were performed in an iron-filtered reactor beam with a 5,08 cm diameter cylindrical $^3$He counter filled with 26.7 kPa of $^3$He\textsuperscript{25}. The ideal response function was calculated by the GNSR\textsuperscript{36} code. The energy calibration was assumed to be linear, the calibration parameters $A$ and $B$ were determined from pulser measurements and using the "thermal" peak at $E_C = Q$, which always occurs in the pulse height spectrum of $^3$He. The resolution parameters (full width at half maximum) were obtained from the measurements in a quasi monoenergetic Si-filtered reactor beam (144 keV) to be 16.8 keV at the thermal peak and 18.6 keV at $Q + E_n$, with $E_n = 144$ keV. The resolution for neutrons of $E_n = 1,1$ MeV was estimated from first unfolding runs at 31.6 keV. A calculated \textit{a priori} fluence spectrum was available assuming a "white" neutron spectrum at the reactor side of the filter and calculating the transmission through the iron filter\textsuperscript{71}. Since the incoming reactor spectrum was not taken into account, only the peak structure of the spectrum was known \textit{a priori}, not the absolute values.

The results for the MIEKE unfolding run are shown in fig. 4 together with the measured pulse height spectrum (scaled in the abscissa to neutron energies) and the \textit{a priori} spectrum. It is seen that the peaks expected from filter calculation are entirely reproduced.
Using the calculated spectrum as *a priori* spectrum in the DIFMAZ code \(^{16}\), the spectrum was nearly reproduced in the solution\(^{71}\). However, negative fluence values were found in the neighbourhood of some peaks\(^{71}\). This effect is more pronounced if a constant *a priori* spectrum with a diagonal uncertainty matrix of 100% relative standard deviation is used as input in the DIFMAZ code \(^{16}\). The result is shown in fig. 5 for the neutron energy range between 50 keV and 400 keV.

Compared with the GRAVEL and MIEKE results, the DIFMAZ spectrum is poorly resolved and shows strong oscillations between positive and negative values. In fig. 5, only small differences between the MIEKE and GRAVEL results can be observed. The results of the next section show more clearly that spurious peaks sometimes occur after a high degree of GRAVEL iterations.

![Graph](image.png)

**Fig. 4:** Calculated and unfolded spectrum using the MIEKE code. The calculated spectrum was negatively scaled. For comparison, the measured pulse height spectrum is shown, too. All spectra are properly scaled.
The good results obtained here for $^3$He proportional counter are not very surprising, since the response functions used show a peak structure for these counters, so that, in principle, only an unfolding of the Gaussian broadened pulse height spectrum has to be performed. For the example considered here, the energy calibration parameters could easily be determined from known neutron peaks. In the energy range considered, there was no indication that counters of the type used in the experiments deviate more than about 1.5% from the linear energy calibration law. The situation is not so simple for high-pressure $^4$He counters and for the NE-213 scintillation counters considered in the next subsection.

### 11.2 NE-213 Scintillation Counter

The organic liquid scintillator NE-213 is very well suited for measurements in mixed neutron-photon fields owing to its excellent neutron-photon discrimination capabilities. Photons produce scintillations by the Compton and pair-production interactions, which, together with wall effects, lead to a broad response function for incoming monoenergetic photons. In the following, the photon unfolding example of a cylindrical NE-213 detector
(5 cm in radius, 5 cm in height) irradiated in the high-energy reference photon field of the PTB \(^{67}\) is considered. Details of the experiment can be found in reference \(^{74}\). Another interesting example recently published can be found in reference \(^{75}\).

The response functions for monoenergetic photons were calculated by T. Novotny\(^{74}\) using the EGS4 code\(^{66}\). There is a non-linear relationship between the measured pulse height and the corresponding calculated light output. This relationship was experimentally determined together with the resolution parameters from irradiations in reference photon fields.

The unfolding of the measurements performed in the high-energy photon field of the PTB (main peaks around \(E_\gamma=7\) MeV) is described below. In the photon spectrum, apart from a peak at 0.5 MeV, three lines were expected between 1.2 MeV and 1.5 MeV and, in addition, lines at 6.1 MeV, 6.9 MeV and 7.1 MeV. In fig.6, the measured pulse height distribution (abscissa in electron-equivalent energy units as calculated by EGS4) is shown. The smooth curve is the refolded pulse height distribution using the UNFANA results of fig. 7, which is an indication of the consistency of the unfolding process.

For comparison, the Gaussian broadened response function for 7 MeV photons is also shown (dashed curve). The resolution for a pulse height of 6 MeV amounts to about 380 keV\(^{74}\) (full width at half maximum).

![Fig. 6: Experimental and from the UNFANA result of fig. 7 refolded (smooth full curve) pulse height spectrum. The pulse height is given in electron-equivalent energies.](image-url)
Fig. 7: Results of unfolding the photon fluence spectrum.

The unfolded results are shown in fig 7. The results of the DIFMAZ program\(^{16}\), calculated assuming a constant a priori fluence with 100% relative standard uncertainty and neglected correlations, again show poor resolution and strong oscillations. When the FORIST code\(^{30}\) with appropriate group structure and energy-dependent smoothing option is used, these oscillations can be reduced.

With the GRAVEL code, some narrow peaks can be produced, the width of which depends on the number of iterations. Spurious peaks sometimes occur (indicated by an arrow), resulting either from the statistical fluctuations of the pulse height distribution or errors in the response matrix. It has been found that for this multichannel unfolding the solution spectrum is nearly independent of the GRAVEL starting spectrum.

Consistent results were obtained with the MIEKE and SPECAN(UNFANA) codes. There was good agreement between the unfolded photon spectra determined previously with a germanium detector\(^{67}\). Integrals over peak areas were reproduced within the range of uncertainties\(^{74}\).
In the previous examples of multichannel unfolding, the number of particle fluence groups \( N \) was of the same order of magnitude as the number \( M \) of channels measured. Unfolding means only a redistribution or a transformation of information from \( M \) measured to \( N \) unfolded channels. As was explained above, the matrix \( B \) of eq. (7) plays an important role for the structure of the solution spectrum. An ill-conditioned matrix \( B \) results in large uncertainties for the individual fluence values. The uncertainties obtained by MIEKE and UNFANA unfolding consist of two parts: one resulting from an uncertainty propagation of the uncertainties of the measurements and another stemming from the ambiguity of the solution. The second part always remains, even for highly precise measurements. In the "few-channel" unfolding case \( M \ll N \), the second part will dominate if no a priori information is available.

The resolution of the unfolded peaks of fig. 7 (e.g. by the MIEKE code) depends strongly on the uncertainties of the measured pulse height spectrum and on the resolution of the detector used.

The spectra (a) and (b) of fig. 8 were obtained from the same pulse height spectrum of fig. 6 but with an uncertainty of the multichannel counts assumed to be twice or four times higher. In the lower curve (c) the results of a simulation are shown, the resolution of the detector being assumed to be twice the resolution of the detector from fig. 6.

There was good agreement between the unfolded photon spectra and the spectra previously determined with a germanium detector \(^{67}\). Integrals over peak areas were reproduced within the range of uncertainties \(^{69}\).
12. Eigenvalues and Limits of Unfolding

It has been shown in references\(^2,3,14\) that there is a criterion to quantify the amount of information available in an unfolding process. The number of non-vanishing eigenvalues of matrix \(B\) (eq. (7)) determines the amount of ambiguity, or, which is equivalent, the number of independent parameters available in the solution spectrum. Values near zero of the ratio \(r\) (ratio of an individual eigenvalue to the largest one) cause high uncertainties in the solution spectrum and are related to the ambiguity involved. Non-negative eigenvalues with low ratio \(r\) close to the floating point precision of the computer may in addition lead to numerical
errors in unfolding. This eigenvalue decomposition of matrix $B$ corresponds to the singular value decomposition \cite{31}, for which similar problems are discussed.

To quantify the resulting precision of an unfolding process, the number $n_\lambda$ of eigenvalues, with a ratio $r$ above a certain limit (e. g. $r > 10^{-4}$), should be compiled. $n_\lambda$ might be compared with the maximum possible rank $n_r$ (number of neutron groups) of matrix $B$.

For the Bonner sphere example of fig. 1, $n_\lambda = 5$ ($n_r = 52$) has been obtained, which means that in principle only five “parameters” of the solution spectrum can be determined and that \textit{a priori} information is needed for successful unfolding (see results shown in fig. 7). From fig. 7 it can be seen that considering only the energy range above 0.1 MeV, the bubble detector system has slightly better spectrometric properties than the Bonner sphere system.

For the NE-213 example, a strong dependence of $n_\lambda$ on the resolution function was found. The data used for fig. 6 and fig. 7 lead to $n_\lambda = 70$ ($n_r = 278$) for unfolding with the “ideal” response function (ideal resolution), to $n_\lambda = 45$ ($n_r = 278$) for the experimental resolution available (used in fig. 6) and to $n_\lambda = 26$ ($n_r = 278$) for the resolution used in fig. 8c. $n_\lambda$ does not depend on the uncertainties of the measured values $z_0$. The loss of resolution in an unfolding process due to “poor statistics” is a consequence of the principle of maximum entropy (from all possible solutions those of minimum curvature are taken).

For the $^3\text{He}$ example 440 measured channels were used to unfold for 248 neutron channels. It is apparent from fig. 8 that, due to the Gaussian broadening, a lot of eigenvalues are decreased.

For an increasing number $N$ of fluence groups (decreasing bin width), the curves in figs. 7 and 8 are only changed on the right, i. e. some very small eigenvalues are added, which have no influence on the fluence results. As mentioned in \cite{16}, the optimum choice of the bin width is of the order of 1/5 of the FWHM; a smaller bin width cannot improve the unfolding results.

There are two recent references that discuss the issue of eigenvalues (although from a somewhat different point of view). They are from D. S. Sivia\textsuperscript{76} and from W. von der Linden\textsuperscript{45}. 

Fig. 7: Eigenvalues for the Bonner spheres and the bubble detector examples.

Fig. 8: Eigenvalues for the examples $^3$He and NE-213. The decrease of information due to Gaussian broadening can be clearly seen.
The ambiguity part $S_{\Phi}$ always leads to large uncertainties but strong anticorrelations of the fluence values in adjacent energy groups so that integral values can be obtained with much lower uncertainty. Recently attempts have been made to unfold the full energy- and angle-dependent differential neutron fluence from the measurements of six electronic dosimeters mounted on a sphere \(^{77}\) (see next section). High uncertainties were obtained for the unfolded fluence, since $n_\lambda = 13$ ($n_e = 450$) was found \(^{77}\). However, integral values like the personal dose equivalent could be obtained after unfolding with a reasonably small uncertainty \(^{77}\).

### 13. Unfolding of Energy and Direction Distributions

The estimation of non-isotropic dose quantities in multidirectional neutron fields requires knowledge of the spectral neutron radiance (i.e. the differential distribution of the neutron fluence rate in energy and angle, sometimes called directional distribution of spectral fluence rate). No ideal measuring instrument is available which would allow both the energy and the angle to be analysed. The detectors customarily used in neutron dosimetry for the determination of the ambient dose equivalent or for spectrometry have a more or less isotropic response. Personal dosemeters mounted on a phantom are better suited, since their response shows directional dependence, due to the shielding of the neutrons by the phantom. Several approaches were made in the past to enable directional spectrometry with such instruments (see e.g. references \(^{78, 79, 80, 81, 82, 83, 84, 85, 86, 87, 88}\)), most of them relating to spherical phantoms, where neutron detectors are mounted and irradiated at selected points on the surface of a moderating sphere \(^{80, 81, 82, 85, 87}\).

After irradiation of such detectors, the evaluation of orientation-dependent integral quantities (such as the prediction of the directional dose equivalent or of the personal dose equivalent) is performed in two steps. In a first step the directional spectral fluence is determined by unfolding, resulting in rather high uncertainties in the single directional and spectral groups. In a second step the relevant dose quantities are calculated as weighted integrals, and it is obvious that such integral quantities can be calculated with much smaller uncertainty.
The quantity determined by unfolding is the directional distribution of the spectral fluence defined by \( \Phi_{\Omega,E}(\Omega,E) \), where the unit vector \( \Omega \) defines the direction of the radiation (or the solid-angle element at the surface of the unit-sphere, see chapter 2 of \( \Gamma \)). If the coordinate system is chosen so that the origin is positioned in the centre of the sphere and the \( z \)-axis is crosses the poles, \( \Omega \) may be represented by
\[
\Omega = (\cos \varphi \sin \vartheta, \sin \varphi \sin \vartheta, \cos \vartheta),
\]
where \( \vartheta \) and \( \varphi \) are polar angles.

A number \( S \) of neutron detectors are thought to be mounted at certain points of the surface of the moderating sphere. The orientation of each detector \( i \) \( (i = 1,...,S) \) is characterised by its normal vector \( \mathbf{u}_i = (x_i, y_i, z_i) \), pointing to the centre of the sphere.

For the detectors considered here, cylindrical symmetry is assumed, i.e. the response to incident neutrons of the direction \( \Omega = (\cos \varphi \sin \vartheta, \sin \varphi \sin \vartheta, \cos \vartheta) \) depends for each energy only on
\[
\cos \Theta_i = \mathbf{u}_i \cdot \Omega = x_i \cos \varphi \sin \vartheta + y_i \sin \varphi \sin \vartheta + z_i \cos \vartheta.
\]

If every detector \( i (i = 1,...,S) \) provides information in \( K \) channels, a total sum of \( M = S \cdot K \) channels is registered and the reading of the detector \( i \) in channel \( K \) is given by the model equations:
\[
Z_i^k = \int \int dE \ d\Omega \ R_k(\mathbf{u}_i \cdot \Omega,E) \ \Phi_{\Omega,E}(\Omega,E), \quad (i = 1,...,S) \quad (k = 1,...,K)
\]
where \( \Phi_{\Omega,E}(\Omega,E) \) is the directional distribution of the spectral neutron fluence assumed to be space-independent over the sphere volume, and \( R_k(\mathbf{u}_i \cdot \Omega,E) \) is the corresponding response function for neutrons of energy \( E \) incident under the solid angle \( \Omega \). Up to six detectors \( (S = 6) \) are considered; each with a number of \( K \) channels. For the active electronic personal dose meter system \( K \) is of the order of a few hundred.

Using a suitable group representation for \( \Phi_{\Omega,E}(\Omega,E) \) with solid-angle elements \( \Delta \Omega_i \) \( (l = 1,...,L) \) and energy elements \( \Delta E_j \) \( j = (1,...,J) \), the integrals in Eq. (27) may be replaced by a double sum:
\[ Z_i = \sum_{j=1}^{J} \Delta \Omega_i \sum_{j=1}^{J} \Delta E_j \, R_i (\mathbf{u}_i \cdot \Omega_j, E_j) \Phi_{\Omega,E} (\Omega_j, E_j) \]  

with \( \Delta \Omega_i = \sin \vartheta_i \Delta \vartheta_i \Delta \phi_i \).

In eq. (28) measured readings in a number of \( M = S \cdot K \) channels are related to \( N = L \cdot J \) unknown components of the fluence, i.e. eq. (28) represents a system of \( M \) equations with \( N \) unknown variables. In the case considered here, \( M \ll N \), i.e. the number of unknown parameters exceeds the number of measured parameters, and the system of equations is considerably underdetermined. Eq. (28) may be abbreviated to the vector-matrix model equation \( \mathbf{z} = \mathbf{R} \cdot \mathbf{\Phi} \) with the \( M \)-dimensional multichannel vector \( \mathbf{z} \), the \( N \)-dimensional group fluence vector \( \mathbf{\Phi} \) and the \( N \times M \) response matrix \( \mathbf{R} \). For the unfolding solution the methods mentioned above may be used. It has been found that a number of 20 angle groups represented by an icosahedral structure of the sphere surface is suitable together with about 50 energy groups \(^{85}\).

Using the codes described above, not only the expectation values \( \langle \Phi_{\Omega,E} (\Omega_j, E_j) \rangle \) and their covariance matrices may be calculated but also further interesting integrals such as the ambient dose equivalent \( H^*(10) \) or the current through a fixed plane. Also, values relevant to personal dosimetry such as the directional dose equivalent, the personal dose equivalent or the effective dose, or other dose quantities, which might be created in future, can be determined from the integrals: \( \int dE \, d\Omega \, W(\Omega, E) \, \Phi_{\Omega,E} (\Omega, E) \) where \( W(\Omega, E) \) is the corresponding weighting function. Examples of the weighting function are the ambient dose equivalent conversion function \( h^*_\phi(E) \) which is independent of the angle of incidence, and the directional dose equivalent conversion function \( h^*_{\phi} (\mathbf{u}_p \cdot \Omega, E) \) where \( \mathbf{u}_p \) characterises the direction of interest  (\( \cos \alpha = \mathbf{u}_p \cdot \Omega \)).

14. Experiences from Practice and Summary of Unfolding Methods

In the previous sections it has been tried to review some of the unfolding algorithms used in neutron physics and to quantify the amount of information involved in an unfolding process.
As a first attempt the ambiguity part due to the underdetermination was analysed by means of the MIEKE code. On the basis of the results of the discussion of the algorithms and the examples presented here, the following statements can be made:

Unfolding of measured detector readings in particle spectrometry often constitutes a system of ill-conditioned normal equations, even in case $M > N$. The matrix $B$ to be inverted might be numerically unstable, in particular for Gaussian broadened response functions.

As a consequence, to increase the condition of matrix $B$, all information known before has to be included in the unfolding algorithm. Modern methods based on maximum entropy are available, however, the most important problem in this context seems to be the quantifying of pre-information. Quantifying pre-information in a mathematically consistent way means to estimate the pre-information fluence values as well as their covariance matrix. General numerical methods for this purpose are not yet available. Quantifying pre-information and including in the unfolding work leads to a decrease in ambiguity. In principle, if pre-information can be quantified in a consistent way, the unfolding codes perform only an adjustment of the spectrum within the “area” covered by the pre-information.

It is another problem that up to now the uncertainties of the response matrices have been neglected in most codes. It has to be emphasised that in unfolding work unfolding results, which obviously are not „convenient“, can often be traced back to inconsistent data rather than something being lacking in the unfolding codes. Consistency means that all uncertainties are included in a realistic way. As a consequence: neglecting the uncertainties of the response functions (as is to date done by most unfolding codes) means that the uncertainties of the measured channel contents should not be too small. In practice, the time for a multichannel measurement should be chosen in such a way that the resulting statistical uncertainties of the channel contents are greater than the existing uncertainties of the response function.

The MIEKE code seems to be the only code, which at present would allow consistent uncertainty propagation. The advantage for the inverse problem here lies in the fact that in the MIEKE unfolding a distinction can be made between the usual propagation of uncertainties and the ambiguity which obviously always exists. The ambiguity part can be quantified.
Unfolding codes generally should not be used as "black boxes". Some experience is required, and it is recommended using more than one of the codes mentioned here. In the HEPRO package, the GRAVEL, MIEKE and UNFANA codes may be used in succession.

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**References**


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