ACCEPTABLE SOLUTIONS OBTAINED BY UNFOLDING NOISY DATA WITH A CONJUGATE GRADIENT TECHNIQUE

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ABSTRACT

A linear resolution function in a physical measurement leads to data values and standard deviations at, say, N points. We note that the associated resolution functions may require that a number n of particular linear combinations of the data values be each not significantly different from zero. We are left with at most N-n parameters to evaluate. If the resolution functions are reasonably behaved, we can show that one sensible way to describe the underlying spectrum treats it as a linear combination of the given resolution functions and includes all the significant information from the data.

An iterative search for the best component available to minimise the chi-square of the next fit to the data leads to a conjugate gradient technique. Programs based on the technique have been successfully used to obtain neutron spectra as a function of energy; in raw data from a pulse height analysis of proton recoils in a proportional counter, and where the raw data are time of flight spectra from a time dependent pulse of known form. It is planned to incorporate these, together with working programs respectively for photonuclear analysis and to explore the impurity concentration profile in a surface, into a single 'work-bench' type program.

A suitably difficult model unfolding problem has been developed and used to show the strengths and weaknesses of a number of other methods that have been used for unfolding.

The work to be discussed is part of a larger study.

Activation foil techniques for obtaining neutron fluxes are still work in progress, and progress is reported separately by Cook and Ferguson in this workshop.

It is planned to attempt the dangerous process of amalgamating

several working programs into one 'work-bench' program with multiple options. Such projects should be reported on at completion, or after two new types of unfolding problems have been processed without major modification. The aspects that are complete are written up; they are in fact, typed up and accompanied by figures and references. Printing takes a little longer, but an AAEC report is expected this year.

From the material included there and referred to in my abstract, I am passing over three profitable topics.

1. The working programs for analysis of data.
2. The analysis that leads to conjugate gradient techniques for unfolding over the experiment of a technique for specific problems.
3. The error analysis associated with the second type.

There is room, at best, to present a model designed with malice aforethought to test the usefulness of a variety of unfolding techniques.

We want our model to be simple to program and to understand, but beyond the capabilities of at least half of unfolding techniques. Accordingly, we use a resolution function R that averages the 'natural spectrum' over a considerable number (93) of channels. The chosen natural spectrum $\vec{X}$ has a flat background of 10^5 counts per channel plus a spike of 4.65×10^5 counts in channel 47. To avoid end effects we wrap around. The full circle is divided alternately into 186 channels or 187 channels. The predicted yield $\vec{Y}$ is then 1.05×10^5 counts per channel in channels 1 to 93 and 1.00×10^5 for the rest. Each method of unfolding was tested for the four cases given by 186 and 187 channels and 'measured data' $\vec{M}$ equal to predicted yield $\vec{Y}$, or with Poisson statistics on the count rates, $\vec{M} = \vec{Y} + \vec{\epsilon}$. The 'data' are shown in Fig. 1 and the results are summarised in Tables 1 and 2.

A formal exact solution exists in the case of 187 channels. Even without statistical errors the round-off error in single precision floating point arithmetic on an IBM 360 prevents exact implementation, but those errors are negligible compared with statistics. We recover the given natural spectrum as the mean value of our calculated spectrum with

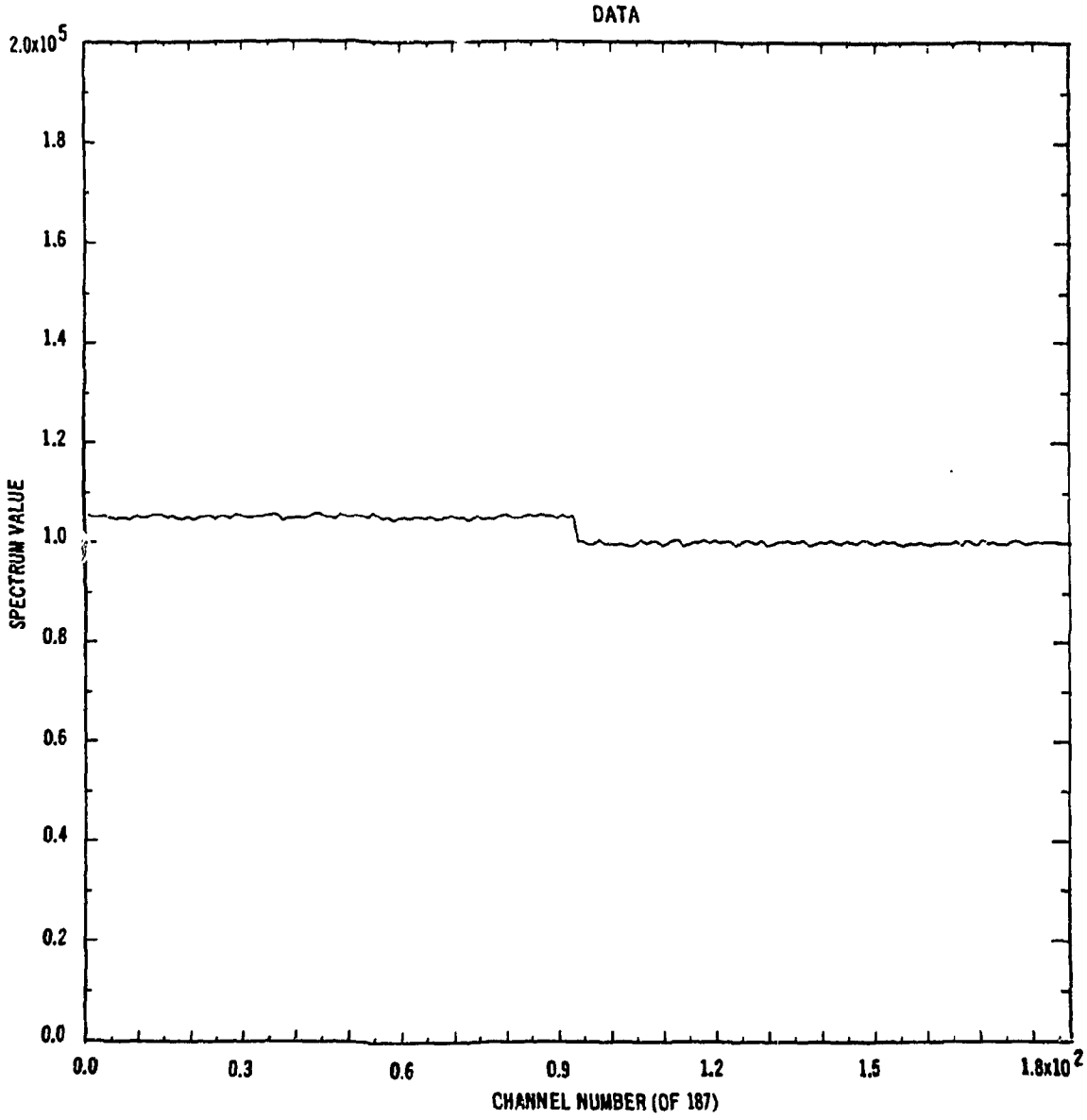

Fig. 1. Noisy data used to test unfolding methods. The 'step' down after channel 93 requires a spike up in the spectrum at channel 47 or downward in channels 140 and 141, but the data distinguish the two cases only on the basis of the content of channel 187.

Table 1. Results Obtained after Ten Iterations by Various Unfolding Methods

Number of channels in circumference		186	186	187	187
Method of iteration	Data with (+), without (-) statistical error	+	-	+	-
Conjugate gradient	S^2	3.25	1.98	3.88	2.14
	C	3.61	3.33	3.10	2.88
Conjugate gradient (positive eigenvalues)	S^2	2.97	1.48	3.34	1.68
	C	3.63	3.71	3.73	3.18
Series	S^2	390	351	387	358
	C	-	-	-	-
Series (positive eigenvalues)	S^2	17.1	14.6	17.6	-
	C	0.54	0.53	0.47	-
'Appropriate'	S^2	397	355	392	364
	C	-	-	-	-
'Appropriate' (alternating ratios)	S^2	17.1	16.4	17.6	16.4
	C	0.55	0.54	0.47	0.48

The quantity $S^2 \times 10^7$ is the sum of the squares of the remaining discrepancies and has a target value of about 2.0 if all remaining discrepancies are statistical. The quantity $C \times 10^5$ is the concentration of variation from the mean in the recovered spectrum into channels around 47 and 140. The target value is 4.65.

Table 2. Results Obtained by the Least Structure Method of Unfolding for Various Values of Gamma

Number of Channels in Circumference		186	186	187	187
Gamma	Data Statistical (+) Bare (-)	+	-	+	-
32.0	S^2	4.19	2.41	4.05	2.45
	C	2.59	2.51	2.34	2.37
8.0	S^2	3.77	2.06	3.67	2.10
	C	2.93	2.86	2.68	2.71
2.0	S^2	3.43	1.76	3.30	1.80
	C	3.32	3.24	3.07	3.10
0.5	S^2	3.15	1.47	2.94	1 52
	C	3,70	3.66	3.51	3.52

The quantities S^2 and C are as in Table 1.

an RMS noise component of 0.4×10^5 counts per channel. The chi-square value of the fit to data is zero, associated with the 'hairy' nature of the recovered spectrum.

The zero eigenvalue of the resolution matrix R prevents an exact solution for 186 channels. We can, however, throw away all components that would be suppressed by a resolution function, leaving information about the mean value of the spectrum on all channels and the difference of the spectrum in opposite channels. From these we recover a formal spectrum which fits the data as far as they are self consistent. The chi-squared value is predicted to be close to half the number of channels. The recovered spectrum has mean value 1.025×10^5 counts per channel as background, with an upward spike of 2.325×10^5 counts in channel 47 and a matching downward spike on channel 140. The RMS noise component, still containing large long range correlations, is 0.14×10^5 counts per channel.

Experimentally, we would not expect to distinguish the change in total channel numbers. We might have a preference for positive spikes over negative ones, particularly ones leading to emission of particles from our counters. An unfolding method that shows the positve bump centred at channel 47 and a negative bump (compared to background) at channel 140, would be adequate with less demanding data. We seek methods that are better. They should not introduce spurious structure into the spectrum. They should fit the data adequately, i.e. so that the chi-squared value is approximately equal to the number of channels, and they should be simple to program. High precision arithmetic to deal with low precision data is suspect. Iterative methods can easily incorporate negative feedback of residual discrepancies and were used first. We also use the wrap-around nature of the problem to produce a Fourier component arrangement in which least structure solutions can be produced by inversion of a diagonal matrix instead of its ill-conditioned equivalent.

Two methods failed completely. With a superscript (n) to indicate the number of the iteration, a series solution given by

$$\vec{X}^{(n+1)} - \vec{X}^{(n)} = \vec{M} - \vec{Y}^{(n)} \qquad (1)$$

diverges without limit.

The 'appropriate solution',

$$X_j^{(n+1)} = X_j^{(n)} \times M_j / Y_j^{(n)} \quad , \tag{2}$$

converges eventually to a solution that does not fit the data. The reason is well understood and in both cases depends on the existence of negative eigenvalues of the matrix R giving positive feedback in the iteration process.

Slow convergence can be obtained in both cases using essentially the square of the matrix. We use

$$\vec{X}^{(n+1)} - \vec{X}^{(n)} = R^T (\vec{M} - \vec{Y}^{(n)}) \quad . \tag{3}$$

For the general case we would use the transpose R^T of the matrix as written, but with R a real symmetrical matrix, it makes no difference. The 'appropriate alternating solution' uses

$$X_j^{(2n+1)} = X_j^{(2n)} \times M_j / Y_j^{(2n)} \tag{4}$$

and

$$X_j^{(2n+2)} = X_j^{(2n+1)} \times Y_j^{(2n+1)} / M_j \quad . \tag{5}$$

For the particular case of our problem, the results are barely distinguishable (Fig. 2).

To improve the series method we can optimise the size of each term to be added to $\vec{X}^{(n)}$. Doing this by least squares leads to making sure that previous steps are not undone and the conjugate gradient technique. A further refinement depends on the eigenvalues of $R^T R$ being non-negative (bunched). Ten iterations then give Fig. 3.

Photonuclear cross sections have been associated with least structure techniques. Minimising (say) second differences leads to the equation,

$$(R^T \omega^2 R + \gamma H^T H) \vec{X} = R^T \omega^2 M \quad , \tag{6}$$

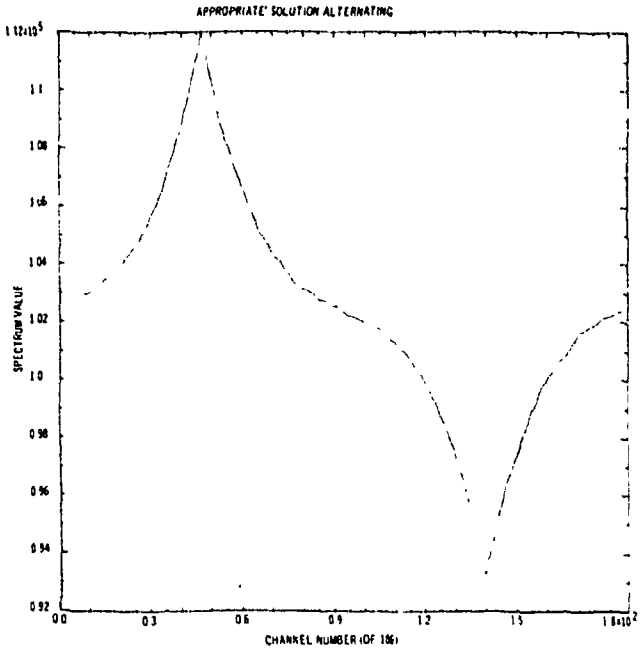

Fig. 2. Example of a method of unfolding that finds major trends of the spectrum.

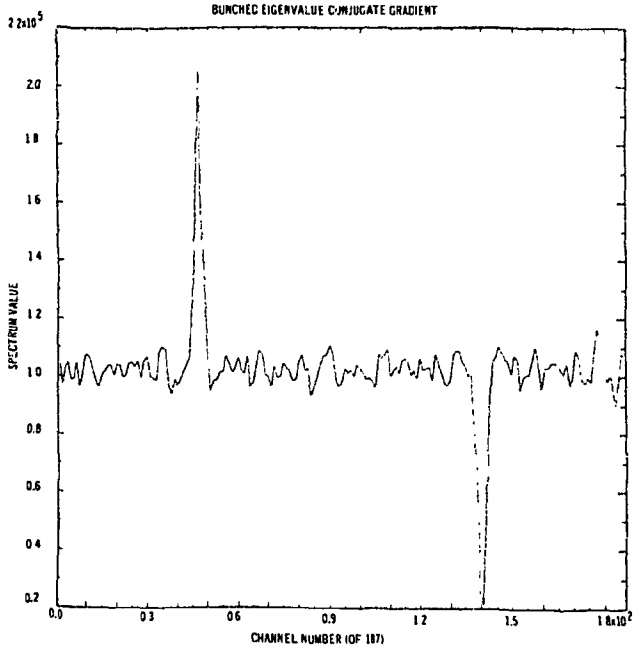

Fig. 3. Example of a method of unfolding that uses most of the information from the data.

where ω_j^{-1} is the standard deviation of the j^{th} data value, H is an operator evaluating second difference and γ is initially an arbitrary parameter. The method is successful, if undesirable small eigenvalues of the product matrix $R^T \omega^2 R$ are associated with large diagonal matrix elements of the product matrix $H^T H$. It works well with the Fourier transformed matrix and 186 channels since only non-zero eigenvalues of $R^T \omega^2 R$ are included. For 187 channels there are small eigenvalues. The corresponding eigenvectors are randomly present in $\omega\vec{M}$ and hence in $(R\omega)$ $(\omega\vec{M})$. Not all such are associated with large eigenvalues of $(H^T H)$ and hence structure appears in the recovered spectrum without significant support from the data (Fig. 4).

Our current conclusion is that the best method to use if starting a new unfolding program is one using conjugate gradients.

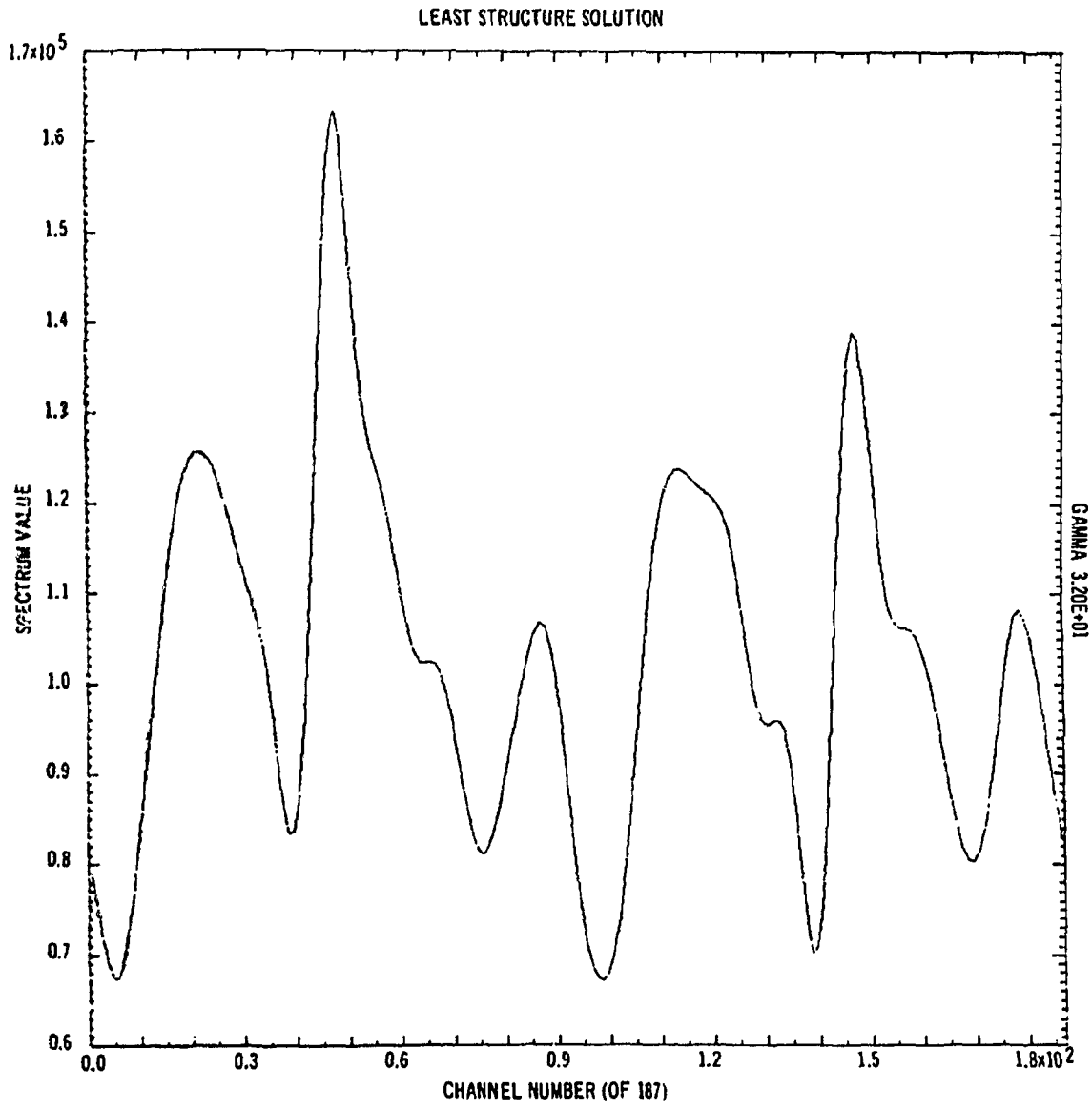

Fig. 4. Example of a method of unfolding that gives features in the recovered spectrum not required by the data.