DECONVOLUTION OF SPECTRA

The SATAN command ADECON provides the interactive deconvolution of spectra [1,2,3]. A measured spectrum “anlin” is expected to be a convolution of an ideal spectrum “anlout” with a calculated detector response function “anlres”.

$$anlin = anlres \times anlout$$

The spectrum “anlout” is calculated by an iterative procedure.

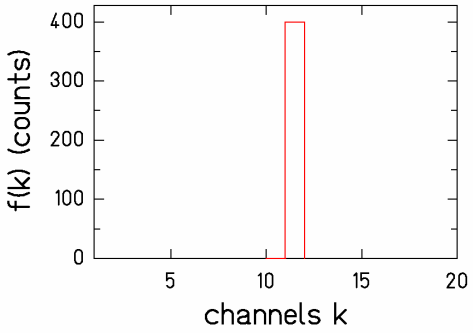
The region of the analyzer “anlin” that is to be deconvoluted must be displayed; the names of “anres” and “anlout” are given within the command. A “check-analyzer” may be specified to contain the reconvoluted resulting spectrum for comparison with the input spectrum.

The Response Matrix

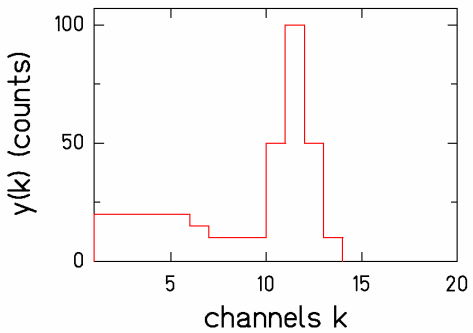
Theoretically the energy distribution of the radiation of a monenergetic source is a δ function. Subdividing the range of energy in small intervals

$$\Delta E = E(k+1) - E(k)$$

one expects an ideal spectrum f(k) with the observed counts in one channel:



In practice the spectrum y(k) (e.g. γ-rays) is measured:



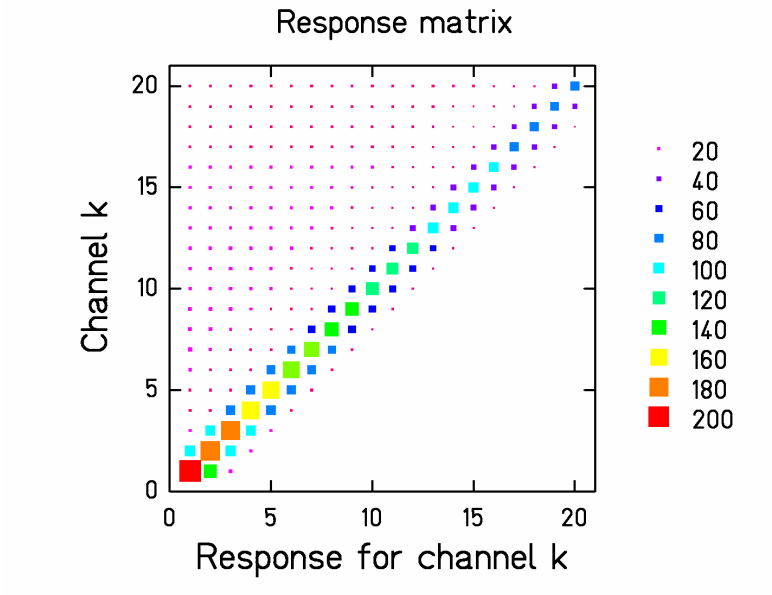
Mathematically this can be expressed as:

$$y(k) = \Sigma_l \, (r(k,l) \times f(l))$$

where the summation is performed over index l. r(k,l) is the response matrix. In case the ideal spectrum f contains one discrete energy E_0 in channel l_0 (δ-function), one column of the response matrix is projected onto vector y:

$$y(k) = r(k,l_0)$$

Hence to construct the matrix the detection system has to be calibrated with monoenergetic sources; a calibration spectrum y(k) measured at the energy E(l) is stored in column l of the response matrix r(k,l) as illustrated in the two-dimensional representation below.



Generally a sufficient number of sources of different energies to fill the whole matrix is not available. This means that the measured response spectra have to be interpolated. Finally the columns of the response matrix must be normalized to unity, because only on this condition the detector efficiency can be mathematically separated from the total response function.
Generating the response function it should be considered that a matrix needs a lot of storage (4 bytes per element).

The Deconvolution Procedure

The following section describes the principle of operation of the deconvolution procedure. For detailed information refer to the original publications.

The deconvolution works iteratively according to the following equation:

$$f_i(k) = c(k) \times f_{i-1}(k)$$

where k labels the elements of spectrum y and i is the number of the current approximation to the exact solution. Each element is corrected individually by a correction factor c(k) . As zeroeth approximation the input spectrum is taken:

$$f_0(k) = y(k)$$

In every iteration step i a check spectrum

$$d_j(k) = \Sigma_l \, (r(k,l) \times f_i(l))$$

is computed to test the quality of the solution $f_i(l)$ by folding it with the matrix. The result should be a good approximation to the input spectrum. An expression for chi-square is evaluated:

$$X^2 = \Sigma_k \, ((d_i(k) - y(k)) / \Delta y(k))^2 / N$$

(Δy = errors of input spectrum, N = number of spectrum elements) which should be of the order of 1 or less. If the relative change of chi-square becomes less than the value in the accuracy parameter the iteration process is stopped even if the maximum number of iteration steps defined by the ITER-parameter is not executed.

The algorithm to evaluate the correction factor is based on the formula

$$c(k) = \Sigma_l \, (r(l,k) \times y(l) / d_i(l)) / \Sigma_l \, r(l,k)$$

where the summation is performed over the index l extending from l_{min} to l_{max} which are implicitly determined by the range parameter n to

$$l_{min} = k - n \;, \quad l_{max} = k + n$$

(l_{min} and l_{max} are truncated when k reaches the spectrum bounds).

For $n > 0$ this procedure has a smoothing effect, since the neighbouring points are taken into account and a weighting with the matrix elements is done ("response weighted method"). This option works best with continuous spectra where no sharp peaks are expected. The default value of $n = 2$ is an optimum based on experience in deconvoluting $ß^{+-}$ and continuous γ-spectra.

For $n = 0$ the correction factor is equal to

$$c(k) = y(k) / d_i(k) \; .$$

This is known as the "quotient method". It is useful for spectra with a lot of peaks where the intensity from the tail contributions shall be stored into separate peaks. It is possible that even small "hidden" peaks hooked on the shoulder of dominating peaks (e.g. conversion electron spectra where an L-line may be located very close to the K-line) appear after applying this deconvoluting technique. On the other hand the quotient method may interpret statistical fluctuations in the spectrum as nearly hidden peaks and emphasize them during deconvolution.

If the conformity between refolded and measured spectrum is found to be too poor ($X^2 > 1$) an iteration step is calculated from the derivatives of X^2 with respect to the f(k) ("gradient search algorithm"). Since the evaluation of the gradient is time-consuming for large spectra (more than 100 bins) the number of steps is limited automatically depending on the spectrum size.

Negative elements of the input spectrum are treated as zero after confirmation.

Errors

Experimental errors of the input data may be specified via an attached error analyzer; by default statistical errors (square root of the observed counting rates) are assumed. An error analysis for the deconvoluted spectrum is performed if the ERRANL-keyword (with an analyzer name as argument) is specified.

The familiar law of quadratic propagation of errors is not applicable since correlations between the variables involved (original spectrum elements $y(k)$ and the elements of the previous iteration $f_{i-1}(k)$) are neglected.

An estimate for the error $\Delta f(k)$ of a channel contents $f(k)$ is given by varying $f(k)$ holding all other channel contents constant until X^2 increases by 1.0 (i.e. one standard deviation). This means, the X^2-equation is solved for $\Delta f(k)$ after replacing $f(k)$ by $f(k)+\Delta f(k)$; the procedure is repeated throughout the whole spectrum.

Problems

The proper execution of deconvolution is strongly dependent on the input data. The following difficulties may occur.

- The iterative method used here not able to unfold response functions with nearly tridiagonal-matrices. This case arises for instance when the Gaussian-like resolution spreads only over one neighbour channel in each direction. In this case it should be considered if unfolding is really necessary at all.
- In some cases the value of chi-square increases so that the iteration is aborted after a few steps. The reason may be a bad selection of the displayed input data. Generally the noise counts in low channels should be excluded unless considered by the response matrix. If the first channels of the original spectrum contain no counts they should be cut off too.
- A bad agreement between input and check spectrum may be caused by an insufficient number of iterations. It may be improved simply be decreasing the accuracy parameter or increasing the maximum number of iterations, a wrong or not completely appropriate response matrix. This may be tested by deconvoluting a calibration spectrum with the matrix derived from it. The unfolded spectrum should consist of a “δ-function” and the check should reproduce the calibration spectrum.

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[1] J. Mollenauer, UCRL-9748 (1961)
[2] R. God, An Iterative Unfolding Method for Response Matrices, ANL-6984 (1964), Argonne
[3] M. Krämer, Diplomarbeit TH Darmstadt (1982)