RPN70

RADIATION PROJECT INTERNAL REPORT NUMBER 10

INVERSION OF CONTINUOUS ABSORPTION SPECTRA

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18 November 1968

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The fundamental equation of an absorption spectrometer is

$$S(x) = \int M(E,x)\ R\sigma\ dE,$$

where M is the transmission at photon energy E through thickness x, R is the detector response, and σ is the spectral intensity. The assumption that $R\sigma$ is continuous implies that we can, to whatever approximation is necessary, divide up the spectrum into regions in which $R\sigma$ is constant so that

$$S(x) = \sum_k \int_{E_k-\frac{1}{2}E_o}^{E_k+\frac{1}{2}E_o} M(E,x)\ R\sigma\ dE \equiv \sum_k \langle M(E,k)\rangle_{E_k-\frac{1}{2}E_o}^{E_k+\frac{1}{2}E_o} (R\sigma)_k,$$

where $\langle M\rangle$ is the average transmission of the absorber of thickness x at mean energy E_k. This procedure averages over photoelectric edges in the absorber. If we identify a given absorber with index m, then this equation becomes

$$S_m = \sum_k M_{mk}(R\sigma)_k.$$

These simultaneous equations admit, in principle, of arbitrary approximation to the original integral equation; thus any remarks made relative to the solution of this set apply to the problem in general.

There is a great deal of data available for the preparation of the transmission matrix M. Using this data, a matrix has been set up for a 10-channel absorption spectrometer using lead and copper. The thicknesses were adjusted to provide roughly e-fold absorption at the center of each of ten bands separated by 50 keV. In the study of this matrix partial determinants were evaluated in which the diagonals consisted of successively longer segments of the main diagonal of M, starting from the 11 position. The value of the determinant of rank r was found to be rather well fitted by the expression

$$D(r) = e^{-0.33(r^2-1)},$$

where D is the absolute value of the determinant. The value for r=10 is exceedingly small, and the question is naturally raised as to what meaning the solution vector has for a problem which is so nearly degenerate.

From this expression we can estimate with how many parameters we can justifiably simulate the spectrum. Thus if we solve an equation having a matrix of rank r, the errors in the solution are

$$\delta\sigma = \sum_m \delta S_m \mu^{(r-1)}/D(r);$$

so that on the assumption that the errors are uncorrelated,

$$|\delta\sigma| \sim r^{\frac{1}{2}}(\delta S_m)_{rms}\left[\mu^{(r-1)}\right]_{rms}/D(r),$$

if $\mu(r-1)$ is the minor of rank r-1. The minors should be of the order of D(r-1); therefore

$$|\delta\sigma| \sim r^{\frac{1}{3}}|\delta S|D(r-1)/D(r) = r^{\frac{1}{3}}e^{0.33(2r-1)}|\delta S|$$

for the present case. The solutions are of order unity for this problem, so the rank r must be substantially less than the solution of

$$r^{\frac{1}{3}}e^{0.33(2r-1)} = 1/|\delta S|.$$

r	$\|\delta S\|$
1	0.719
2	0.262
3	0.111
4	0.050
5	0.023

Thus if $|\delta S| \sim 0.05$. the number of parameters <4 if direct inversion is contemplated. For larger numbers of channels direct inversion is valueless because of near degeneracy. We have chosen the alternative method of varying one $k\sigma$ at a time while keeping the total energy constant so as to minimize the error $\Sigma(S-\tilde{S})^2$ at each step. Due to the degeneracy this error can only be relaxed so far before the convergence gets very slow, but generally this point is reached after the error has fallen below what would be expected due to errors in the data. It is unwise to carry convergence beyond the last-mentioned point, since data errors will begin to manifest themselves if such an attempt is made. By using different initial approximations one will get different spectra corresponding to the same final error. With the given information there is no way to select among these various answers, and the choice has to be made on the basis of other constraints not appearing in the original equations.

In our case, we have chosen to vary the four lowest components, knowing that these have the greatest effect on the spectrum, and have chosen initial spectra which should be close to the final one.

These general remarks hold regardless of the particular method of approximation used. The least-squares approach has the advantage of guaranteed convergence independent of the form of the matrix, though the rate may be very slow if degeneracy is approached. A method such as Gold's[1] can diverge for certain types of matrix, while its convergence also becomes very slow if the matrix is nearly degenerate (as indeed it must).

REFERENCES

1. R. Gold, ANL-6984 (1964).