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Minimization Search Method For Data Inversion

In the physical, biological, or social sciences, an experimenter often makes a series of measurements of a dependent variable as correspond to values of a selected subset of the independent variables occurring in a known mathematical formulation. For instance, if X = f(a,b,c,d), measurements of X might be made at a selected value of a and at $b = b_1, b_2, b_3, \ldots$ etc. The remaining unknowns, independent variables c and d, may be of primary interest, but their values cannot generally be determined analytically from the known relationship. Instead, one must take successive guesses for c and d, until values of c and d are found that give a value of X sufficiently close to the measured X (at all the values of b for which measurements are taken).

Several methods, such as least-squares techniques, are known for finding the values of such variables. However, the required computation time using a new technique, the minimization search method, increases with the 1st power of the number of variables. This is in contrast with classical minimization methods for which the computational time increases with the 3d power of the number of variables.

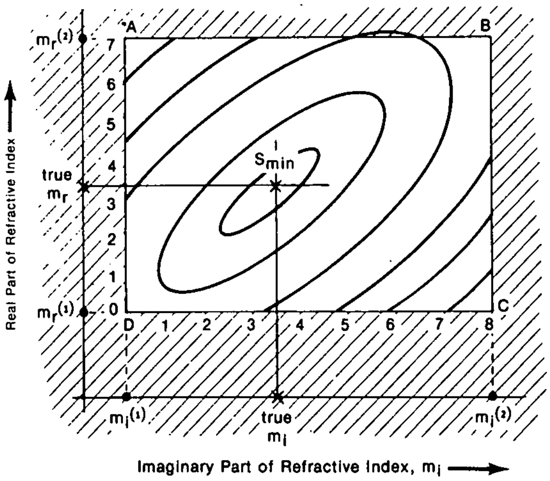


Figure 1. Meaningful Values of m_i and m_r. The "Contour Lines" Represent Lines of Equal Value of the Function S.

The new method was developed to calculate refractive indices from measurements taken by a spectrometer described in NASA Tech Brief B75-10335. In that case it was desired to determine the values of the independent real and complex terms of the refractive index (m_r and m_i) which are related to a series of measurable quantities I_q (intensities):

$$I_q \equiv I(s_q; m_r, m_i)$$

where s_q represents one or more independent variables with known values. The problem is to find for any and all q the particular couple (m_r, m_i) such that $|\overline{I_q} - I_q| \leqslant \varepsilon_q$, where $\overline{I_q}$ is the observed value, I_q is the calculated value, and ε_q is the upper bound for accuracy. (The values ε_q can be different for each q.)

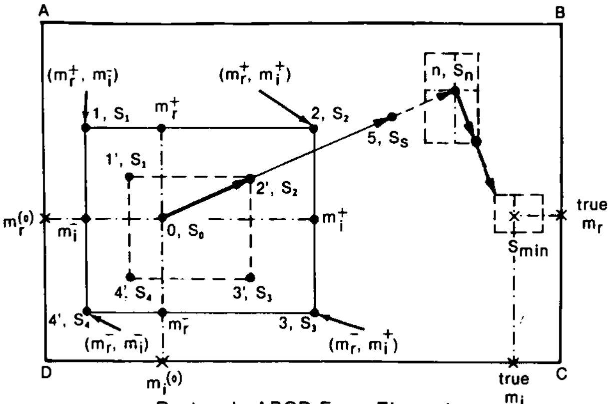
To find the values of m_i and m_r, a surface is defined

$$S(s_q;\, m_r,\, m_i) = \sum_q \left[\frac{\overline{I_q} - I_q}{d_q I_q} \right]^2 \qquad (1)$$

where d_q is a statistical weighting factor related to the manner in which the values of s_q (at which measurements are taken) are chosen and to the weights accorded the individual measurements $\overline{I_q}$. Such a surface is shown in Figure 1. The minimum of the surface S_{min}, corresponds to the values of m_i and m_r within the required accuracy. The minimization search method can be used to find the point.

The first step is to apply any physical or theoretical information which limits the range of values for the minimum. In Figure 1 the rectangle ABCD represents the region of possible physically meaningful values of m_i and m_r. Then an initial guess, $m_r^{(0)}$ and $m_i^{(0)}$, is made and defines point 0 that serves as an "origin"

(continued overleaf)



Rectangle ABCD From Figure 1

Figure 2. Minimization Search Method

(see Figure 2). Next a rectangle is constructed parallel to ABCD and containing 0 (the rectangle need not be centered around 0). It is obtained after perturbing m_i and m_r both positively and negatively. (The magnitudes of these perturbations need not be equal — neither in the positive nor negative directions nor for each dependent variable). The value of S (equation 1) is computed for the origin (S_0) and, when interrogated, the points at each corner of the rectangle and the additional four points on the rectangle sides corresponding to null perturbations in one of the two dependent variables. A random number generator (RNG) subroutine is attached to this set of eight possible improvements on the guess. Subsets of this set are then interrogated sequentially. The interrogation of any subset is carried out only if that of the subset previously generated by the RNG subroutine was unsuccessful in determining a better approximation to the solution.

If none of the S values of the various subsets is smaller than S_0, none of the eight points is closer to the minimum than S_0; and a new, smaller, rectangle should be drawn at 0. If a point belonging to any of these subsets or to a subset of the new rectangle (say 2') corresponds to an S smaller than S_0, then it is closer to the minimum.

The direction from 0 to 2' is taken as the direction along which S decreases. A new point (5 in Figure 2) is chosen by moving along the line (0, 2') according to the formula $5 = 2' + c(2' - 0)$ where c is a constant and the corresponding value of S, that is S_5, is computed. If $S_5 < S_{2'}$, successive similar steps are taken along the line (0, 2') until point n at which $S_n > S_{n-1}$. If $S_n > S_{n-1}$, c is decreased in a limited number of steps until a point at which $S_n < S_{n-1}$ is found; and that point becomes the origin for a new rectangle. The entire process is then reiterated.

Usually, only a few iterations are required to find S_{min}. One way of testing for uniqueness is to repeat the search, starting at other widely differing points. A unique minimum requires that the same S_{min} be found each time.

This method has also been applied successfuly to a considerably larger number of unknowns. The rectangle is then replaced by a multidimensional figure in the parameter-space of the dependent variables.

Notes:

1. A spectrophotometer which uses the method described here to determine the refractive index of particles suspended in a gas or a liquid is described in NASA Tech Brief B75-10335: Developments in Spectrophotometry III: Multiple-Field-of-View Spectrometer To Determine Particle-Size Distribution and Refractive Index
2. Further discussion may be found in:
   a. "Satellite Determination of Nature and Microstructure of Atmospheric Aerosols," by A. L. Fymat in Satellites For Meteorology and Earth Resources, ed. Rassegna, Rome, Italy, vol. 14, March 1974, p. 327
   b. "Inverse Multiple Scattering Problems: II," by A. L. Fymat and R. E. Kalaba, Journal of Quantitative Spectroscopy and Radiative Transfer, vol. 14, March 1974, p. 919
3. Requests for further information may be directed to:

   Technology Utilization Officer
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   Reference: TSP75-10338

Patent status:

This invention is owned by NASA, and a patent application has been filed. Inquiries concerning nonexclusive or exclusive license for its development should be addressed to:

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