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.

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 \((m_r, m_i)\) which are related to a series of measurable quantities \( \lambda_q \) (intensities):

\[
\lambda_q = \lambda(s_q; m_r, m_i)
\]

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 \( |\lambda_q - \lambda| \leq \varepsilon_q \), where \( \lambda_q \) is the observed value, \( \lambda \) is the calculated value, and \( \varepsilon_q \) is the upper bound for accuracy. (The values \( \varepsilon_q \) can be different for each \( q \).)

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

\[
S(s_q; m_r, m_i) = \sum_q \left[ \frac{\lambda_q - \lambda}{d\lambda q} \right]^2
\]

(1)

where \( d\lambda q \) 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 \( \lambda_q \). 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".
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 successfully 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:

3. Requests for further information may be directed to:
   Technology Utilization Officer
   NASA Pasadena Office
   4800 Oak Grove Drive
   Pasadena, California 91103
   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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