ARGONNE NATIONAL LABORATORY
9700 South Cass Avenue
Argonne, Illinois 60440

THE ANALYSIS OF COMPLEX GAMMA-RAY SPECTRA

by

William J. Snow

Applied Mathematics Division

July 1964

Operated by The University of Chicago
under
Contract W-31-109-eng-38
with the
U. S. Atomic Energy Commission

DISCLAIMER

This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency Thereof, nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.

DISCLAIMER

Portions of this document may be illegible in electronic image products. Images are produced from the best available original document.

TABLE OF CONTENTS

	<u>Page</u>
ABSTRACT	3
I. INTRODUCTION.	3
II. PHYSICAL PROBLEM.	3
III. MATHEMATICAL METHOD.	6
IV. PROGRAM DESCRIPTION	10
A. Introduction.	10
B. Input	13
C. Output	14
D. Sample Test Case.	15
ACKNOWLEDGEMENTS	19
APPENDIX	21

THE ANALYSIS OF COMPLEX GAMMA-RAY SPECTRA

by

William J. Snow

ABSTRACT

An IBM-704 program has been written to increase the precision of the determination of the relative intensities and energies of gamma rays in a complex spectrum observed following neutron capture in neutron resonances. The quantity chi-square is formed for the complex spectrum in as many as ten resonances and minimized simultaneously with respect to all unknown intensities as well as the unknown gamma-ray energies. This simultaneous treatment makes use of the wide Porter-Thomas fluctuations in the intensities of the gamma ray to fix the gamma-ray energies.

I. INTRODUCTION

The analysis of gamma-ray spectra has received considerable interest in the literature.¹⁻⁴ However, the wide variety of experimental conditions under which the data are obtained, as well as the many different types of experiments which may be performed, indicates that no overall general procedure exists. Also, scintillation detectors are somewhat limited by resolution due to light collection and the numerous nonunique response curves from monoenergetic photons. The present work consists of the adaptation of the method of minimum chi-square to the analysis of neutron-resonance capture gamma-ray spectra.

II. PHYSICAL PROBLEM

Consider the radiative de-excitation of unbound nuclear states, which are excited by the capture of neutrons in neutron resonances.^{5,6} The

¹James F. Mollenauer, A Computer Analysis for Complex Sodium Iodide Spectra, UCRL-9748 (1961).

²R. O. Chester, "Preliminary Studies of Computer Processing of Gamma Spectra," Proceedings of the Total Absorption Gamma Ray Spectrometry Symposium, May 1960.

³R. L. Heath, "Data Processing Techniques for Routine Application of Gamma Ray Scintillation Spectrometry," ibid.

⁴W. R. Burrus, "Nonlinear Methods in Spectrum Unscrambling," ibid.

⁵L. M. Bollinger, R. E. Coté, and J. P. Marion, Distribution of Partial Radiation Widths, Phys. Rev., **132**, 1640-1662 (1963).

⁶Raymond T. Capenter, The Electric-Dipole Gamma Ray Strength Function for Heavy Even-Even Nuclei, ANL-6589 (Aug 1962).

excitation energy of such a state equals the neutron binding energy plus the kinetic energy of the incident neutron. However, the maximum variation in the neutron energy in a given experiment is typically no greater than 10^{-4} of the excitation energy, so that, within the accuracy of any available techniques, the energy of the gamma-ray transitions from all resonances to a given final state may be considered constant. Moreover, spectra from all resonances to be considered in the analysis are obtained at the same time during the same run, so the energy calibration is necessarily the same for all spectra.

Experimental data are obtained as in the following example. Bursts of neutrons from the Argonne fast chopper strike the target after drifting a distance of 25 m. The capture gamma rays produced are detected by a large sodium iodide crystal located near the target. The pulse height of detected gamma rays and the neutron time-of-flight, measured as the time between a photocell pulse immediately preceding the burst of neutrons and the gamma-ray pulse, are recorded digitally on magnetic tape. In this way, all detected gamma rays are recorded together with a measure of the energy of the neutron which produced each gamma ray. After the run, the magnetic tapes are removed to a separate search station where the data are sorted to produce the gamma-ray spectra associated with all desired neutron energies. Off-resonance regions provide background spectra.

The experimental data thus consist of a set of spectra for which it is known that the energies and response functions are the same for each gamma-ray line present. Examples of the sort of data that may be obtained in a favorable case is shown in Fig. 1, for nine observed resonances in the $\text{Pt}^{195}(n,\gamma)\text{Pt}^{196}$ reaction. The neutron energy at which each spectrum was observed is indicated at the left of the corresponding spectrum. The intensity scale is arbitrary and is included only to show that the plot is logarithmic. The scale at the bottom of the graph gives the energy of the detected gamma ray in MeV. The scale at the top gives the energy of the final state involved in the transition. Notice that there are indications of final states with excitations as high as about 1.8 MeV. Above approximately this energy the density of final states becomes so high that all the spectra are approximately the same, and no individual transitions are resolved.

In the present work we are concerned with the analysis of only those spectral regions where each gamma-ray line present is at least partially resolved in at least one resonance. A further restriction of the spectral region which may be reliably analyzed arises from the difficulty of determining accurately the response function over a wide energy range. The response function is determined by observing some set of strong lines with the same experimental arrangement used in the measurement of the resonance capture spectra and correcting the resulting spectrum for any

109-4092 Rev.

Fig. 1. Capture Gamma-ray Spectra Obtained in Spin 1⁺ Neutron Resonances in Platinum-195 ^{5,6}

weaker lines present and for background. The particular lines used depend on the energies of the lines to be analyzed. However, because of uncertainties in the background and in the intensities of the various weaker lines present in the spectrum, the response function is known only poorly at energies more than about 1.2 MeV below the photo peak. Therefore, we may only consider transitions with energies which are less than the highest energy transition in any of the spectra by no more than about 1.2 MeV. For a typical nucleus, this means perhaps four or five transitions may be considered.

III. MATHEMATICAL METHOD

A complex gamma-ray spectrum consists of a linear superposition of a number of response functions each with a certain intensity and a certain position or energy; that is, we can always write for a particular spectrum

$$n_i = \sum_{\ell=1}^L a_{\ell} R(E_i, E_{\ell}), \quad (1)$$

where

n_i = Number of counts in channel i , corresponding to energy E_i ;

a_{ℓ} = Relative intensity of the ℓ th line in the spectrum;

$R(E_i, E_{\ell})$ = Number of counts in channel i due to a monoenergetic gamma ray of unit intensity having energy E_{ℓ} .

The sum is over all lines of which the spectrum is composed.

Experimentally, one obtains a set of numbers $\{N_i\}$ which differs from the above $\{n_i\}$ because of counting statistics. The analysis of the spectrum then consists of extracting the quantities $\{a_{\ell}\}$ and $\{E_{\ell}\}$ from the spectrum $\{N_i\}$.

If the set of energies $\{E_{\ell}\}$ of the gamma rays being considered and the response function $R(E_i, E_{\ell})$ are known by some means, the analysis is quite simple and straightforward. One minimized the expression

$$\sum_i [n_i - \sum_{\ell} a_{\ell} R(E_i, E_{\ell})]^2 (\Delta n_i)^{-2} \quad (2)$$

with respect to the unknown $\{a_\ell\}$. The response function $R(E_i, E_\ell)$ can be determined quite accurately by various means. One method is the graphical interpolation scheme;⁷ another is a theoretical method⁸ employing the Monte Carlo technique.

For gamma rays with energies in the range from above 4 to 10 MeV, the response function may be determined quite accurately by observing one or more of a set of strong lines from various different sources. However, the set of energies $\{E_\ell\}$ is in general either unknown or known only poorly and must, therefore, be obtained from the data.

Now it is possible to obtain an indication of the line positions from the data using individual spectra. The above expression, evaluated by the derived least-squares values for the intensities, is χ^2 . One may evaluate χ^2 for different values of ℓ_i and determine the value of ℓ_i which corresponds to minimum χ^2 . For spectra with well-resolved lines, values of ℓ_i may be determined by this technique well enough so as to introduce uncertainties in the intensities of only about 1%. With spectra containing unresolved lines, the same is true of the sum of the intensities. However, the intensities of the individual lines may vary by an order of magnitude or more while the sum is varying only a few percent. This is because there are many ways in which the individual unresolved lines may be superposed to fit the spectrum with an acceptable value of χ^2 .

This difficulty may be largely overcome by making use of the characteristics of the spectra mentioned earlier. Because of the fluctuations of intensities, different lines are strong or weak in different spectra, and all the spectra must be fit with the same set of line positions. Thus, whereas there are a large number of ways in which the individual lines may add up to fit a particular spectrum, this number of ways is greatly reduced if the same lines must add up, to be sure with different intensities, to fit several spectra. A further restriction on the line positions is that their differences must be consistent with whatever is known of the energies of the final states in the nuclides involved.

To make use of this, we sum the above expression also over all the resonances observed in a particular nuclide and minimize the resulting expression simultaneously with respect to all the a_ℓ 's and the E_ℓ 's.

The specific mathematical problem to be solved is the minimization of the function

⁷Russell L. Heath, Digital Analysis of Pulse-height Spectra, Nucleonics, 20(5), 67-69 (May 1962).

⁸W. F. Miller and William J. Snow, Energy Loss Spectrum for Gamma Rays in NaI, Rev. Sci. Instr., 31, 39-45 (1960).

$$F(a_{\ell,j}, E_{\ell}) = \sum_{j=1}^S \sum_{i=i_1}^{i_1+n} (\Delta x)_{i,j}^{-2} \left[\chi_{i,j} - \sum_{\ell=1}^L a_{\ell,j} Z_i(E_{\ell}) \right]^2 \quad (3)$$

with respect to the parameters $a_{\ell,j}$ and E_{ℓ} . The subscript j refers to the particular complex spectrum and the subscript ℓ refers to the lines of which the spectra are composed, where $j = 1, 2, \dots, S$ and $\ell = 1, 2, \dots, L$. The $a_{\ell,j}$ are the relative intensities and the E_{ℓ} are the line positions or the energy value of various contributors at their photopeak. Thus, $a_{\ell,j} Z_i(E_{\ell})$ is the contribution to point i from a line whose photopeak is at E_{ℓ} . Also, S is the number of complex gamma-ray spectra to be considered, and on each experimental spectrum there are n points $\chi_{i,j}$ with corresponding uncertainties $(\Delta \chi)_{i,j}$. Further, L is the number of lines assumed in these complex spectra.

We begin by supplying spectra resulting from monoenergetic sources at various energies throughout the energy range under consideration. These spectra are called reference spectra. The reference spectra $R_i(E)$ is supplied as a tabular function of i for various energies E at the photopeak, since they cannot be represented as closed algebraic functions of E . As in most minimization techniques, it is necessary to supply initial guesses of the parameters under consideration; in this problem guesses are made only of the line positions E_{ℓ} and the number of contributors L to the complex spectra. Although it is assumed that the shape of the line spectrum is a function of the energy value of the photopeak, we assume that the change in shape from one reference spectrum to another is linear. Using the initial guesses as to the line positions, we are, therefore, able to generate through linear interpolation the corresponding simple spectra $Z_i(E_{\ell})$, that is, the spectra which would result from monoenergetic sources with these corresponding energies. We treat a number of complex spectra obtained from the same energy source simultaneously to improve the statistical reliability of the resulting decomposition.

The minimization of F is a twofold iterative procedure. Using the simple spectra $Z_i(E_{\ell})$ generated from the initial guesses of line positions, we solve for the corresponding best sets $a_{\ell,j}$ of relative intensities by the method of least squares. Since with respect to the relative intensities the various complex spectra are independent, and since the relative intensities occur only linearly in F , we just solve a system of linear equations to obtain the best $a_{\ell,j}$ for a given set of line positions. We call these sets $\bar{a}_j(E_1, \dots, E_L)$. We now use the variable metric minimization technique⁹ to determine better values of line positions $(E_1, E_2, \dots, E_L)$, better in the sense that the value of $G(E_{\ell}) = F(\bar{a}_{\ell,j}, E_{\ell})$ is decreased. The

⁹W. C. Davidon, Variable Metric Method for Minimization, ANL-5990 (1959).

variable metric method requires subroutines to evaluate the function to be minimized, in our case G , and to evaluate the various partial derivatives $\frac{\partial G}{\partial E_\ell}$, since

$$\frac{\partial G}{\partial E_\ell} = \frac{\partial F}{\partial E_\ell} + \sum_{p=1} \sum_{q=1} \frac{\partial F(\bar{a}_{\ell,j}, E_\ell)}{\partial a_{p,q}} \frac{\partial \bar{a}_{p,q}}{\partial E_\ell} \quad (4)$$

and since, by definition of $\bar{a}_{\ell,j}$, $\frac{\partial F(\bar{a}_{\ell,j}, E_\ell)}{\partial a_{p,q}}$ is zero for all p and q , $\frac{\partial G}{\partial E_\ell} = \frac{\partial F}{\partial E_\ell}$. Because all spectra are available only tabularly, all derivatives are obtained by numerical methods. With the new $E_1, E_2, \dots, E_\ell$ we generate the necessary simple spectra, again through linear interpolation and solve the corresponding $\bar{a}_{\ell,j}$. This process is repeated until the change in F is less than the desired tolerance ϵ .

IV. PROGRAM DESCRIPTION

A. Introduction

The subprogram called FCN is used in conjunction with the Variable Metric Minimization program (see Appendix) and performs the following functions (see Fig. 2):

1. Reads input data (experimental data, reference spectra, weights, program parameters, etc.); see section B (INPUT).
2. Determines the shape of each simple spectrum, $Z_i(E_\ell)$, for each ℓ .
3. Minimizes F by the method of least squares to determine the $a_{\ell,j}$'s as follows:

To calculate $a_{\ell,j}$'s, minimize F' with respect to the variations of the $a_{\ell,j}$'s for each j separately:

$$F = \sum_{j=1}^S \sum_{i=i_1}^{i_1+n} (\Delta X)_{i,j}^{-2} \left[X_{i,j} - \sum_{\ell=1}^L a_{\ell,j} Z_i(E_\ell) \right]^2; \quad (5)$$

$$F' = \sum_{i=i_1}^{i_1+n} (\Delta X)_i^{-2} \left[X_i - \sum_{\ell=1}^L a_\ell Z_i(E_\ell) \right]^2; \quad (6)$$

$$\frac{\partial F'}{\partial a_r} = 0 = 2 \sum_{i=i_1}^{i_1+n} (\Delta X)_i^{-2} \left[X_i - \sum_{\ell=1}^L a_\ell Z_i(E_\ell) \right] Z_i(E_r), \quad (7)$$

where a_r is any a_ℓ . Rearrangement of Eq. (7) gives

$$\sum_{\ell=1}^L \left\{ \left[\sum_{i=i_1}^{i_1+n} (\Delta X)_i^{-2} Z_i(E_\ell) Z_i(E_r) \right] a_\ell \right\} = \sum_{i=i_1}^{i_1+n} (\Delta X)_i^{-2} Z_i(E_r) X_i. \quad (8)$$

The normal equations corresponding to $\partial F' / \partial a_r = 0$ can be written:

$$\begin{aligned} A_{11}a_1 + A_{12}a_2 + \dots + A_{1L}a_L &= B_1 \\ A_{21}a_1 + A_{22}a_2 + \dots + A_{2L}a_L &= B_2 \\ \cdot & \quad \cdot \quad \cdot \quad \cdot \quad \cdot \\ \cdot & \quad \cdot \quad \cdot \quad \cdot \quad \cdot \\ \cdot & \quad \cdot \quad \cdot \quad \cdot \quad \cdot \\ A_{L1}a_1 + A_{L2}a_2 + \dots + A_{LL}a_L &= B_L, \end{aligned} \quad (9)$$

Fig. 2. Schematic Flow Diagram of Analysis Program

where

$$A_{pq} = \sum_{i=i_1}^{i_1+n} Z_i(E_p) Z_i(E_q) (\Delta X)_i^{-2} \quad (10)$$

and

$$B_p = \sum_{i=i_1}^{i_1+n} Z_i(E_p) X_i (\Delta X)_i^{-2}; \quad (11)$$

then $a = A^{-1}B$ and the standard deviations of the a_ℓ 's are

$$\left(A_{\ell,\ell}^{-1} \times \frac{F_\ell}{n-L-1} \right)^{1/2}, \quad \ell = 1, \dots, L. \quad (12)$$

4. Evaluates $F(a_{\ell,j}, E_\ell)$ and ∂F with respect to the E_ℓ 's, where

$$\frac{\partial F}{\partial a_{\ell,j}} = \frac{F(a_{\ell,j}, E_\ell + \Delta E_\ell) - F(a_{\ell,j}, E_\ell - \Delta E_\ell)}{2\Delta}, \quad (13)$$

and transfers control to the Variable Metric Minimization Program.

5. Repeats steps 2, 3, and 4 until convergence on E_ℓ (line positions) is obtained.

6. Calculates the standard deviations of the E_ℓ 's:

$$\left(2H_{\ell,\ell} \times \frac{F_\ell}{S_n - L + N_c} \right)^{1/2}, \quad \ell = 1, 2, \dots, L, \quad (14)$$

where

$H_{\ell,\ell}$ are the elements of the final error matrix in the Variable Metric Minimization Routine

S is the total number of complex spectra

n is the total number of data points in one complex spectra

L is the number of lines

N_c is the number of linear constraints.

$$V_i^1 = \sum_{\ell=1}^L a_\ell Z_i(E_\ell) = Y_i. \quad (15)$$

$$V_i^2 = X_i - Y_i = D_i. \quad (16)$$

$$V_i^3 = D_i^2 / (\Delta X)_i^2. \quad (17)$$

7. Prints results, see section C (OUTPUT).

B. Input

There are two sets of input data: the first set is peculiar to the control program (Variable Matrix Minimization, see Appendix); the second set is used by subprogram FCN and is as follows:

Input is from cards. The order is as follows.

Card 1	Column No.	Quantity	FORMAT
	1-5	Experiment number	I5
	6-7	KT = number of reference spectra	I2
	8	If 0, print $Z_i(E_\ell)$, $\ell = 1, 2, \dots, L$	I1
	9	If 0, print V_i^1 , $i = i_1, i_1+1, i_1+2, \dots, i_1+n$	I1
	10	If 0, print V_i^2 , $i = i_1, i_1+1, i_1+2, \dots, i_1+n$	I1
	11	If 0, print V_i^3 , $i = i_1, i_1+1, i_1+2, \dots, i_1+n$	I1
	12-13	$MP = \sum_{\ell=1}^{MP} a_{\ell,j}$ $j = 1, 2, \dots, S$	I2
Card 2	1-4	Channel number of reference spectrum photopeak (1)	I4
	5-8	" (2)	I4
	9-12	" (3)	I4
	13-16	" (4)	I4
	17-20	" (5)	I4

The latter format consists of 4 digits, in which a decimal point is assumed between the third and fourth digit.

Card 3	Column No.	Quantity	FORMAT
	1-6	Channel number of first and last entry of reference spectra DATA (1)	I3,I3
	7-12	" (2)	"
	13-18	" (3)	"
	19-24	" (4)	"
	25-30	" (5)	"

Card 4	1-6	Channel number of first and last entry for all complex spectra calculations, (i,i ₁ +n)	I3,I3
	7-8	S = total number of complex spectra	I2
	9-13	Δ = first partial derivative step width (channels)	F5.2
	14-19	Channel number of first and last entry for all complex spectra to be read, ($\bar{i}_1, \bar{i}_1+\bar{n}$)	I3,I3
	20-22	Number of linear constraints on the line positions	I3

Card 5 Identifying labels: $(Res)_j$, where $j=1,2,\dots,10$, having a format of 10A6.

Cards 6,7,...,N contain data in the following order:

- A. All complex spectra $(X_{i,j})$ in their respective order and having a format of F8.2, with 9 elements per card.
- B. The latter's associated errors $(\Delta X_{i,j})$ in their respective order and having a format of F8.2, with 9 elements per card.
- C. Reference spectrums $R_i(E_n)$, $n = 1,2,\dots,5$, in their respective order and having a format of F8.2, with 9 elements per card.

C. Output

The output of AN Z013 (Variable Metric Minimization) is followed by the following additional quantities on logical tape unit 1 (see section D).

1. The standard deviation of each of the fitted parameters σ_{E_ℓ} labeled "SIGMA" on the printed output.

2. The experiment number.
3. The number of reference spectra used.
4. The number of complex spectra used.
5. First partial derivative step width (see Eq. 13, ΔE_ℓ), labeled DEL.
6. The final value of the function F.
7. The relative intensities $a_{\ell,j}$ and their associated errors $\sigma_{a_{\ell,j}}$.
8. The quantity R_j labeled REPLACEMENT for each j is an indicator which means the following:
 if $F'/n-L-1$ (Eq. 12) > 1 , $F'/n-L-1$ is set = 1 and $R_j = 1$;
 if $F'/n-L-1$ (Eq. 12) ≤ 1 , $F'/n-L-1 \equiv F'/n-L-1$ and $R_j = 0$.
9. The quantity MP.
10. The quantities labeled SUM = $\sum_{\ell=1}^{MP} a_{\ell,j}$ for each j.
11. The quantities labeled VARIANCE = $\sigma_{\sum_{\ell} a_{\ell,j}}^2$ for each j, where

$$\sigma_{\sum_{\ell} a_{\ell}}^2 = \frac{F'}{n-L-1} \left[\sum_{\ell=1}^{MP} C_{\ell,\ell} + 2 \sum_{\ell=1}^{MP-1} C_{\ell,\ell+1} \right].$$
12. $Z_i(E_\ell)$, where $i = \bar{i}_1, \bar{i}_1+1, \bar{i}_1+2, \dots, \bar{i}_1+\bar{n}$, and $\ell = 1, 2, \dots, L$.
13. V_i^1, V_i^2 , (Eqs. 15 and 16), where $i = \bar{i}_1, \bar{i}_1+1, \bar{i}_1+2, \dots, \bar{i}_1+\bar{n}$.
14. V_i^3 (Eq. 17), where $i = i_1, i_1+1, i_1+2, \dots, i_1+n$.
15. The quantities labeled SUMS = $\sum_{i=i_1}^{i_1+n} V_i^3$.

D. Sample Test Case

The test case presented herein contains three lines with seven resonances for platinum-195, 68, 112, 120, 140, 151, 155, and 189 eV, treated simultaneously. The experimental data points and the resultant curve from this case are shown in Fig. 1. The total running time on the IBM-704 for this test case was approximately 3 min.

1. Input parameters used:

a. Variable Metric Minimization

$N = 3$
 $K = 2$
 $NC = 2$
 $FAC = 0.1$
 $MI = 10$
 $X_i = 175.03, 182.86, 191.74$
 $\Delta = 1$
 $E = 10$
 $P = 5$
 $C(I, 1) = -10^6, 0, 10^6$
 $C(I, 2) = 0, -10^6, 10^6$

b. FCN

Experiment No. = 00002
 $KT = 1$
 $MP = 3$
 Channel no. of reference spectrum photopeak(1) = 195.7
 Channel nos. of 1st and last entry of reference spectra =
 138, 206
 $i_1 = 173$
 $i_1 + n = 197$
 $S = 7$
 $DEL = 0.1$
 $\bar{i}_1 = 140$
 $\bar{i}_1 + \bar{n} = 202$
 $(Res)_j = 68\text{eV}, 112\text{eV}, 120\text{eV}, 140\text{eV}, 151\text{eV}, 155\text{eV}, 189\text{eV}$

The distribution of counts follows the multinomial distribution so that the standard deviation is given by $(\Delta X)_i = (X_i)^{1/2}$. One reference spectrum $R(E_i, E_\ell)$ was used (see Fig. 3).

Fig. 3

Reference Spectrum
 $R(E_i, E_\ell)^{5,6}$

2. Computer Output

VARIABLE METRIC MINIMIZATION

PHY 222

PT 1-2-61 FIRST THREE LEVELS CONSTRAINTS ON ALL THREE SET OF SEVEN

N= 3 K= 2 E= 1.00000E 01 P= 5.00000E 00 DELTA= 1.00000E 00

X= 1.75030E 02 1.82860E 02 1.91740E 02

H

10.00000E-02	0.	0.
0.	10.00000E-02	0.
0.	0.	10.00000E-02

IT 0 STEP 0 F= 3.25191E 02

X= 1.75030E 02 1.82860E 02 1.91740E 02

- - - - -

COLINEAR

IT 1 STEP 0 F= 1.49700E 02 GS= -9.29267E 03

X= 1.75627E 02 1.83457E 02 1.92337E 02

DELTA= 3.39265E-02

- - - - -

RANDOM STEP 1 GS= -4.79145E-01

IT 0 STEP 1 F= 1.59467E 02

X= 1.75459E 02 1.83289E 02 1.92169E 02

- - - - -

COLINEAR

IT 1 STEP 1 F= 1.52424E 02 GS= -1.49607E 01

X= 1.75616E 02 1.83446E 02 1.92326E 02

DELTA= 3.93959E-02

- - - - -

RANDOM STEP 2 GS= -9.05645E-01

IT 0 STEP 2 F= 1.65385E 02

X= 1.75797E 02 1.83627E 02 1.92507E 02

- - - - -

COLINEAR

IT 1 STEP 2 F= 1.52424E 02 GS= -3.24317E 01

X= 1.75619E 02 1.83449E 02 1.92329E 02

DELTA= 3.27929E-02

- - - - -

FINAL VALUES

ERROR MATRIX

1.09310E-03 1.09310E-03 1.09310E-03

1.09310E-03 1.09310E-03 1.09310E-03

1.09310E-03 1.09310E-03 1.09310E-03

F= 1.52424E 02 GS= -7.53851E-01

X= 1.75619E 02 1.83449E 02 1.92329E 02

G= 2.26611E 01 -3.45221E 01 -1.44002E 01

SIGMA= 4.34943E-02 4.34943E-02 4.34943E-02

BEST VALUES FOR MINIMUM F

F= 1.49700E 02

X= 1.75627E 02 1.83457E 02 1.92337E 02

SIGMA= 4.34943E-02 4.34943E-02 4.34943E-02

1129 - PHY 222

EXPERIMENT NO. 2

NUMBER OF REFERENCE SPECTRUMS = 1

NUMBER OF COMPLEX SPECTRUMS = 7

DEL = 0.10

F = 149.70042

RELATIVE INTENSITIES A(L,J)

	68 EV	112 EV	120 EV	140 EV	151 EV	155 EV	189 EV
175.6	0.0070	0.0406	0.0872	0.2160	0.0046	0.0075	0.0491
183.5	0.1286	0.0776	0.0237	0.0195	0.0043	0.0008	0.0060
192.3	0.1457	0.0639	0.2727	0.0238	0.0150	0.0103	0.0366

STANDARD DEVIATIONS E(L,J)

0.0051	0.0050	0.0080	0.0047	0.0025	0.0019	0.0040
0.0053	0.0046	0.0070	0.0024	0.0023	0.0015	0.0029
0.0037	0.0029	0.0063	0.0015	0.0017	0.0011	0.0022

REPLACEMENTS R(J)

1.0000	1.0000	0.	1.0000	0.	1.0000	1.0000
--------	--------	----	--------	----	--------	--------

NO. OF RELATIVE INTENSITIES IN SUM (I) = 3

SUM(I)	0.2813	0.1821	0.3836	0.2593	0.0238	0.0186	0.0916
--------	--------	--------	--------	--------	--------	--------	--------

VARIANCE	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000
----------	--------	--------	--------	--------	--------	--------	--------

ACKNOWLEDGEMENTS

I wish to acknowledge the invaluable assistance of Dr. Raymond T. Carpenter, especially in connection with the physical problem which was written by him. I would also like to acknowledge the assistance of Dr. L. Wos in the preparation of this report and his contribution in both the mathematical and programming aspects.

APPENDIX

VARIABLE METRIC MINIMIZATION (AN Z013 Fortran II)

Kenneth E. Hillstrom - July 1, 1960

Revision: Burton S. Garbow - March 13, 1961

Argonne National Laboratory, Argonne, Illinois

PURPOSE

This FORTRAN routine determines local minima of differentiable functions of N variables when linear constraints may be imposed on the variables.

In addition to the output of the initial estimates, there is an intermediate output of terms which indicate the path followed, the value of the function at each iteration, and the improvement that had been predicted in the function for that iteration. The final output includes the error matrix $H^{\mu\nu}$, the coordinates of the point of minimization X^μ , the function F at this point, the expected improvement GS if the next iteration were taken, and the gradient $G^\mu(\mu, \nu = 1, \dots, N)$.

Optional output includes: (1) an intermediate output of the coordinates of the point X^μ and of the determinant Δ of the error matrix $H^{\mu\nu}$, (2) a final output, punched on cards, of the coordinates of the point of minimization X^μ , the error matrix $H^{\mu\nu}$, the determinant of the $H^{\mu\nu}$ matrix Δ , the minimization epsilon E , and the random step-size control P . This card output can then be used as the initial estimates for a run to improve the minimum.

METHOD

The program employs the variable metric method for minimization. In the process of locating each minimum, a matrix $H^{\mu\nu}$, which characterizes the behavior of the function about the minimum, is determined. For a region in which the function depends quadratically on the variables, no more than N iterations are required, where N is the number of variables. By suitable choice of starting values and without modification of the procedure, linear constraints can be imposed upon the variables.

A necessary condition that the function be a minimum is that the partial derivatives of the function with respect to the parameters be equal to zero.

After a relative minimum has been found, a random step is taken such that the value of the function is increased by about $0.5P^2$, where P is an input parameter. After the step has been taken, the routine again seeks a relative minimum. The number of such steps is determined by an input integer K , which may be specified as zero.

If there is an accumulator or quotient overflow, $H^{\mu\nu}$, F , X^μ , and G^μ are printed and, if sense switch 2 is down, X^μ , $H^{\mu\nu}$, Δ , E , and P are punched on cards. The machine then comes to overflow stop HPR 66666_S.

USAGE

FCN Subprogram:

AN Z013 is a general FORTRAN routine which requires a FORTRAN subprogram called FCN. This subroutine must compute the function F and the gradient vector G^μ (i.e., the vector whose elements are the first partial derivatives of F with respect to the parameters), given the coordinates of the point X^μ . The function F must minimize to some non-negative value. In the case of functions which naturally minimize to a negative value, a positive constant should be added to the function to insure positive minimization.

A counter $M1$ is set equal to 1 by the general routine at the first entry into FCN; it is set equal to 2 for subsequent entries up to the final entry, and it is set equal to 3 for the final entry. This makes allowance for special input and output on the initial and final entries.

It is often necessary to impose boundary conditions on the parameters. Whenever the FCN program is given values of the parameters (i.e., the values of the coordinates of X^μ) which exceed these bounds, FCN should double the previously computed value of the function F and return to the main program. In particular, at the outset or immediately after taking a random step, AN Z013 sets F to zero just before calling FCN, and if zero (or any negative number) is returned for F from FCN, the program immediately takes the next random step. Similarly, FCN can use receipt of zero for F as a signal to take some possibly special action before returning to AN Z013.

Storage:

The storage allotments are such that $N \leq 40$, where N is the dimension (i.e., the number of parameters).

Input deck:

The input deck consists of the AN Z013 binary deck, the FCN binary deck, a transfer card, and the data cards.

Tapes used:

Logical tape 1 is used for printed output.

Sense Switch Settings:

- 1 Up x^μ , Δ is not printed
- 1 Down x^μ , Δ printed at the end of every iteration
- 2 Up $>$ Cards not punched as part of final and overflow output
- 2 Down Cards punched as part of final and overflow output

Input:

- N - the number of parameters.
 - K - the number of random steps.
 - NC - the number of linear constraints on the parameters.
 - FAC - a number which if positive signals that, instead of expecting cards for H(I,J), the program is to initialize H to FAC times the identity matrix; and which is ignored if zero or negative.
 - MI - the maximum number of iterations to be performed.
 - X(I) - the initial estimate of the parameters (i.e., of the coordinates of X^μ).
 - H(I,J) - a non-negative symmetric matrix whose diagonal elements are the squares of the errors in the estimates of the parameters. If FAC is nonpositive, H is input in upper triangular form beginning with the diagonal element of each row.
 - Δ - the determinant of H(I,J).
 - E - the minimization epsilon. Convergence is attained for each random step when the expected improvement GS in F satisfies $GS \leq E$ (more literally, when $GS + E \geq 0$, since GS, when interpreted correctly as the expected change in F, is a negative number).
 - P - the random step size control.
 - C(I,J)
 - if NC $>$ 0 - the linear constraint coefficients as an N x NC array.
- If the jth constraint is written $\sum_{i=1}^N c_{ij}x_i = d_j$, the c_{ij} are input here - the parameter guesses imply the value(s) of d_j . NOTE: A constraint c is considered already ignored if $c^T H c > E$; thus coefficient upscaling may be necessary.

Input is from cards on-line. The order is as follows:

<u>Quantity</u>	<u>Format</u>
Message 1	Blank + message up to 71 characters in length
Message 2	Blank + message up to 71 characters in length
N,K,NC,FAC,MI	3I6,F6.0,I2
X(I)	6E12.5
H(I,J)	6E12.5
Δ ,E,P	6E12.5
C(I,J)	6E12.5

Data required by FCN subroutine.

NOTE: Rows (columns) of H and columns of C always begin on new cards.

Additional Information:

The random number-generating program present on Argonne's library tape and used by this program returns at each entry the next in a chain of pseudo-random numbers in the interval (0,1). Although an argument is formally required in calling the program, no use is made of it.

Stops:

Overflow Stop: HPR 66666₈
Normal Stop: HPR 77777₈

NOTE: After either stop, a return to the beginning of the program can be effected by pressing START.

CODING INFORMATION

The FORTRAN subprogram must have the name:

SUBROUTINE FCN (N,G,F,X,M1), where

N is the number of variables
G is the gradient vector
F is the function
X is the coordinate vector
M1 is the counter set by the general routine