EUR 4959 e

COMMISSION OF THE EUROPEAN COMMUNITIES

AN ALGORITHM FOR NON LINEAR DATA FIT BY THE LEAST SQUARES METHOD

by

E. VAN DER VOORT and J.P. HALLEUX

1973

Joint Nuclear Research Centre
Ispra Establishment — Italy

Materials Division

LEGAL NOTICE

This report is on sale at the addresses listed on cover page 4

at the price of B.Fr. 85.—

Commission of the
European Communities
D.G. XIII - C.I.D.
29, rue Aldringen
L u x e m b o u r g

April 1973

EUR 4959 e

AN ALGORITHM FOR NON LINEAR DATA FIT BY THE LEAST SQUARES METHOD by E. VAN DER VOORT and J.P. HALLEUX

Commission of the European Communities
Joint Nuclear Research Centre - Ispra Establishment (Italy)
Materials Division
Luxembourg, April 1973 - 64 Pages - B.Fr. 85.—

In this work the least squares estimation of the parameters of a non linear curve is accomplished by using the Taylor's series of the summed squares of the residues (Φ) and retaining all the components up to the second order term. The advantage of this method over other methods lies in the fact that the Hessian matrix of the function, Φ, is calculated without any approximation. This procedure allows the rapid localization of the optimal parameters using known second order methods. Moreover, a brief statistical analysis is given that is based on the exact evaluation of the above mentioned Hessian matrix evaluated at the optimal point in the parameter space. Finally, a complete listing of a computer program together with a workout example and its output is included.

EUR 4959 e

AN ALGORITHM FOR NON LINEAR DATA FIT BY THE LEAST SQUARES METHOD by E. VAN DER VOORT and J.P. HALLEUX

Commission of the European Communities
Joint Nuclear Research Centre - Ispra Establishment (Italy)
Materials Division
Luxembourg, April 1973 - 64 Pages - B.Fr. 85.—

In this work the least squares estimation of the parameters of a non linear curve is accomplished by using the Taylor's series of the summed squares of the residues (Φ) and retaining all the components up to the second order term. The advantage of this method over other methods lies in the fact that the Hessian matrix of the function, Φ, is calculated without any approximation. This procedure allows the rapid localization of the optimal parameters using known second order methods. Moreover, a brief statistical analysis is given that is based on the exact evaluation of the above mentioned Hessian matrix evaluated at the optimal point in the parameter space. Finally, a complete listing of a computer program together with a workout example and its output is included.

EUR 4959 e

AN ALGORITHM FOR NON LINEAR DATA FIT BY THE LEAST SQUARES METHOD by E. VAN DER VOORT and J.P. HALLEUX

Commission of the European Communities
Joint Nuclear Research Centre - Ispra Establishment (Italy)
Materials Division
Luxembourg, April 1973 - 64 Pages - B.Fr. 85.—

In this work the least squares estimation of the parameters of a non linear curve is accomplished by using the Taylor's series of the summed squares of the residues (Φ) and retaining all the components up to the second order term. The advantage of this method over other methods lies in the fact that the Hessian matrix of the function, Φ, is calculated without any approximation. This procedure allows the rapid localization of the optimal parameters using known second order methods. Moreover, a brief statistical analysis is given that is based on the exact evaluation of the above mentioned Hessian matrix evaluated at the optimal point in the parameter space. Finally, a complete listing of a computer program together with a workout example and its output is included.

EUR 4959 e

COMMISSION OF THE EUROPEAN COMMUNITIES

AN ALGORITHM FOR NON LINEAR DATA FIT BY THE LEAST SQUARES METHOD

by

E. VAN DER VOORT and J.P. HALLEUX

1973

Joint Nuclear Research Centre
Ispra Establishment — Italy

Materials Division

ABSTRACT

In this work the least squares estimation of the parameters of a non linear curve is accomplished by using the Taylor's series of the summed squares of the residues (Φ) and retaining all the components up to the second order term. The advantage of this method over other methods lies in the fact that the Hessian matrix of the function, Φ, is calculated without any approximation. This procedure allows the rapid localization of the optimal parameters using known second order methods. Moreover, a brief statistical analysis is given that is based on the exact evaluation of the above mentioned Hessian matrix evaluated at the optimal point in the parameter space. Finally, a complete listing of a computer program together with a workout example and its output is included.

KEYWORDS

NON LINEAR PROBLEMS
MATHEMATICAL MODELS
LEAST SQUARE FIT
STATISTICS
ITERATIVE METHODS
D CODES
COMPUTER CALCULATIONS

AN ALGORITHM FOR NON LINEAR DATA FIT BY THE LEAST SQUARES METHOD

E. Van der Voort and J. P. Halleux
Materials Division - C. C. R. Euratom, Ispra

1. INTRODUCTION

Most algorithms for the least squares estimation of the parameters of a regression curve are based on the linearization of the proposed model [1-4]. The quadraturization of the model, however, leads to an exact evaluation of the matrix of the second partial derivatives of the function of the summed squares of the residues. This quadraturization process presents some advantages in that the optimal parameters can be rapidly localized. Furthermore this complete second order information yields a better statistical analysis of the problem.

2. STATEMENT OF THE PROBLEM AND ITS SOLUTION

We are given a set of n_d experimental points $\left\{ y_i, \vec{x}_i \right\}$, each of a given weight w_i, where each value y_i is related to a n_v-dimensional vector $\vec{x}_i$. The quest of the experimentator becomes to find an adequate model that describes the above relation functionally: $y_i \simeq F(\vec{x}_i, \vec{\Theta})$. The n_p-dimensional vector $\vec{\Theta}$ of the free parameters now may be optimized in the weighted least squares sense, so that the expression

$$\Phi(\vec{\Theta}) = \sum_{i=1}^{n_d} w_i \left[y_i - F(\vec{x}_i, \vec{\Theta}) \right]^2 \tag{1}$$

is a minimum in the parameter space. Let this minimum be denoted by $\vec{\Theta}_m$, then $\vec{\Theta}_m$ must be the solution of the system:

$$\vec{\text{grad}}_{\vec{\Theta}} \, \Phi(\vec{\Theta}_m) = 0 \tag{2}$$

The search of $\vec{\Theta}_m$ is performed by an iterative procedure (subroutine MINIM 1) working essentially with second order methods described in [5]. For each iteration j, the function value $\Phi(\vec{\Theta}_j)$, the local gradient

$$\vec{g}_j = \vec{\mathrm{grad}}_{\vec{\Theta}} \left[\Phi (\vec{\Theta}_j) \right] \tag{3}$$

and the matrix of the second partial derivatives (Hessian)

$$\hat{H}_j = \hat{H}_{\vec{\Theta}} \left[\Phi (\vec{\Theta}_j) \right] \tag{4}$$

are required. Postulating a model $F(\vec{x}, \vec{\Theta})$ it can be easily derived that:

$$(\vec{g})_k \equiv \frac{\partial \Phi(\vec{\Theta})}{\partial \Theta_k} = - 2 \sum_{i=1}^{n_d} w_i \left[y_i - F(\vec{x}_i, \vec{\Theta}) \right] \frac{\partial F(\vec{x}_i, \vec{\Theta})}{\partial \Theta_k} \tag{5}$$

and that

$$(\hat{H})_{k\ell} \equiv \frac{\partial^2 \Phi(\vec{\Theta})}{\partial \Theta_k \partial \Theta_\ell} = (\hat{A})_{k\ell} + (\hat{B})_{k\ell} \tag{6}$$

where the matrices $\hat{A}$ and $\hat{B}$ have the elements:

$$(\hat{A})_{k\ell} = 2 \sum_{i=1}^{n_d} w_i \frac{\partial F(\vec{x}_i, \vec{\Theta})}{\partial \Theta_k} \cdot \frac{\partial F(\vec{x}_i, \vec{\Theta})}{\partial \Theta_\ell} \tag{7}$$

$$(\hat{B})_{k\ell} = -2 \sum_{i=1}^{n_d} w_i \left[y_i - F(\vec{x}_i, \vec{\Theta}) \right] \frac{\partial^2 F(\vec{x}_i, \vec{\Theta})}{\partial \Theta_k \partial \Theta_\ell} \tag{8}$$

In the past the contribution of $\hat{B}$ in $\hat{H}$ was not taken into account. This was due to the linearization of the model $F(\vec{x}, \vec{\Theta})$ around the optimal value $\vec{\Theta}_m$. In this paper second order terms are used in F and full account is given of the matrix $\hat{B}$ in the calculation of $\hat{H}$:

$$F(\vec{x}, \vec{\Theta}) = F(\vec{x}, \vec{\Theta}_m) + \sum_{k=1}^{n_p} (\vec{\Theta} - \vec{\Theta}_m)_k \frac{\partial F(\vec{x}, \vec{\Theta}_m)}{\partial \Theta_k}$$

$$+ \frac{1}{2} \sum_{k=1}^{n_p} \sum_{\ell=1}^{n_p} (\vec{\Theta} - \vec{\Theta}_m)_k (\vec{\Theta} - \vec{\Theta}_m)_\ell \frac{\partial^2 F(\vec{x}, \vec{\Theta}_m)}{\partial \Theta_k \partial \Theta_\ell} + O(\vec{\Theta} - \vec{\Theta}_m)^3 \tag{9}$$

With the input given by a MAIN-programme, and the model by the specific subroutine MØDEL (both to be programmed by the user), the subroutine DATFIT, described in this paper, localizes the optimal parameters $\vec{\Theta}_m$ and gives a short statistical analysis of the results.

It must be said, however, that if the model $F(\vec{x}, \vec{\Theta})$ is well chosen to describe the set of the experimental points $\{y_i, \vec{x}_i\}$, and if the guess for $\vec{\Theta}_m$ approximates the optimal value, then $\hat{A}$ is a good estimator for $\hat{H}$ and there is no need to go beyond the linearization of the model.

The method presented in this paper has the advantage to reach the minimum of $\Phi(\vec{\Theta})$ even if the initial guess of the parameters is badly chosen. Since other methods let $\hat{B} = 0$, they end up working with an approximation of the Hessian matrix that differs substantially from the analytical expression.

3. STATISTICAL ANALYSIS OF THE RESULTS

a) The goodness of the localization of the minimum $\vec{\Theta}_m$ may be appreciated by the smallness of the components of $\vec{g}(\vec{\Theta}_m)$. The minimizing subroutine MINIM1 asks for the following threshold values. First, the variation of the function value (EPSF) from one iteration to the next. Secondly, the variation of the norm of the argument (EPSX) also from one iteration to the next and, thirdly, on the norm of the gradient (EPSG). These threshold values should be adapted by the user so that return from MINIM1 is caused by EPSG (see argument list of MINIM1).

b) The minimum value of $\Phi(\vec{\Theta})$ at $\vec{\Theta}_m$:

$$\Phi(\vec{\Theta}_m) = \sum_{i=1}^{n_d} w_i \left[y_i - F(\vec{x}_i, \vec{\Theta}_m) \right]^2 \tag{10}$$

and the modified standard error of estimate

$$s = \sqrt{\Phi(\vec{\Theta}_m)/(n_d - n_p)} \tag{11}$$

evaluate the scatter of the experimental values y_i against the analytical values prescribed by the optimized model $F(\vec{x}_i, \vec{\Theta}_m)$.

c) Given a confidence level α, the confidence region of the parameters is bounded by the ellipsoid in parameter space:

$$\Phi(\vec{\Theta}_m) + \frac{1}{2}\left[(\vec{\Theta}-\vec{\Theta}_m),\ \hat{H}(\vec{\Theta}_m)(\vec{\Theta}-\vec{\Theta}_m)\right] = \Phi(\vec{\Theta}_m)\left[1+\Delta\right] \tag{12}$$

where Δ is given by:

$$\Delta = \frac{n_p}{n_d - n_p} F(1-\alpha,\ n_p,\ n_d - n_p) \tag{13}$$

The variance ratio statistic $F(1-\alpha, \nu_1, \nu_2)$ must be provided by the user. This confidence region means that there is a risk of about $100\,\alpha$ percent that the physical optimal $\vec{\Theta}$ lies outside this ellipsoid centered about $\vec{\Theta}_m$. The excentricities of this ellipsoid and its inclination with the axes in parameter space (correlation) are contained in $\hat{H}(\vec{\Theta}_m)$. Not all the properties of this ellipsoid are calculated but only the extreme values $(\vec{\Theta}_m \pm \delta\vec{\Theta})_k$ that each parameter Θ_k may reach and the piercing points $(\vec{\Theta}_m \pm \delta\vec{\Theta}')_k$ of the axis. It may be shown that:

$$\delta\Theta_k = \sqrt{2(\widehat{H^{-1}})_{kk} \cdot \Phi(\vec{\Theta}_m)} \cdot \sqrt{\Delta} \tag{14}$$

and

$$\delta'\Theta_k = \sqrt{2(\hat{H})^{-1}_{kk} \cdot \Phi(\vec{\Theta}_m)} \cdot \sqrt{\Delta} \tag{15}$$

where $(\widehat{H^{-1}})_{kk}$ and $(\hat{H})_{kk}$ are the diagonal elements of the matrices $\widehat{H^{-1}}$ and $\hat{H}$, respectively. The values $\delta\Theta_k$ are most significant to determine the confidence intervals of each parameter, Θ_k, separately about $(\vec{\Theta}_m)_k$. These $\delta\Theta_k$ contain two factors: the first is controlled by the goodness of the fit of the optimized model to the experimental data and the second is determined by the confidence level itself. The values $\delta'\Theta_k$ can be used to check the validity of the quadraturization of $\Phi(\vec{\Theta})$ around the minimizing $\vec{\Theta}_m$. Indeed the l.h.m. of equation (12) is only a Taylor series development of $\Phi(\vec{\Theta})$ up to the second order and at the piercing points $(\vec{\Theta}_m \pm \delta'\vec{\Theta})_k$ some discrepancy

may be expected between $\Phi(\vec{\Theta})$ and $\Phi(\vec{\Theta}_m) + \frac{1}{2}\left[(\vec{\Theta}-\vec{\Theta}_m), \hat{H}(\vec{\Theta}_m)(\vec{\Theta}-\vec{\Theta}_m)\right]$.
In these points we evaluate a virtual delta given by:

$$\Delta_v = \left[\Phi(\vec{\Theta}) - \Phi(\vec{\Theta}_m)\right]/\Phi(\vec{\Theta}_m) \tag{16}$$

that should be close to the Δ given by the variance ratio statistic (see equation 13) if the quadraturization of $\Phi(\vec{\Theta})$ is a satisfactory approximation. If this should not be the case, the confidence region would be a distorted ellipsoid and some caution should be taken as to the exact meaning of the confidence intervals of the single parameters.

d) An estimator for the variance-covariance matrix between the parameters $\vec{\Theta}$ is the inverse of the Hessian $\hat{H}$ of $\Phi(\vec{\Theta})$ at $\vec{\Theta}_m$. The correlation between two parameters, Θ_k and Θ_ℓ, is then given by:

$$\frac{(\widehat{H^{-1}})_{k\ell}}{\left[(\widehat{H^{-1}})_{kk}(\widehat{H^{-1}})_{\ell\ell}\right]^{1/2}}$$

The combination between all pairs (k, ℓ) generates a symmetric matrix, known as the correlation matrix. The lower triangular part of the variance-covariance matrix and of the parameter correlation matrix are given in the output produced by DATFIT.

e) Analysis of the residues. It is assumed that the residues:

$$\varepsilon_i = y_i - F(\vec{x}_i, \vec{\Theta}_m) \quad ; i = 1, n_d \tag{17}$$

are Gauss-distributed with a zero mean and some constant variance σ. In an actual case this hypothesis is only partially true and should be tested.

e1) Therefore, first, an overall plot is made of the residues ε_i against the analytical values $F(\vec{x}_i, \vec{\Theta}_m)$ predicted by the optimized model. To this end the plot area is divided into subareas (rectangles) so as to allow for 50 discrete zones for the residues ε_i and for 120 discrete zones for the values given by $F(\vec{x}_i, \vec{\Theta}_m)$. To each subarea a number is associated that is equal to the sum of the weights of the experimental points i for which the pair $\left[\varepsilon_i, F(\vec{x}_i, \vec{\Theta}_m)\right]$ falls in this subarea. The ensemble of these numbers is then scalled from 0 to 9. The printer fills then each subarea with the corresponding digit. When a subarea contains no experimental point, a blank is "printed". The line of zero residue is indicated by dashes. With the plot are also printed the extreme values of the residues and of the analytical values given by the model. If this model is well suited to describe the experimental data and if the residues are indeed Gauss-distributed with a zero mean, the plot should have the following standard shape (Fig. 1):

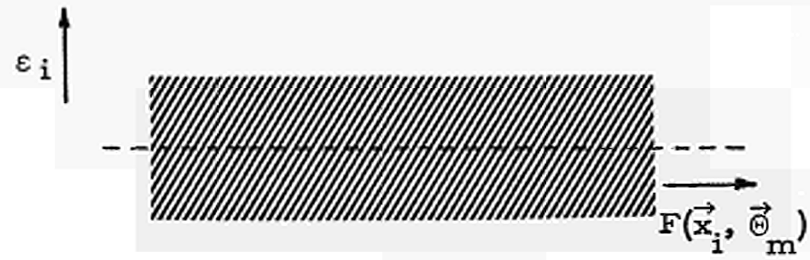


Fig. 1

i. e. the experimental points are randomly scattered around the curve prescribed by the model and are independent from the magnitude of these analytical values. Deviations in this ideal behaviour may be observed. They may have the following particular shapes:

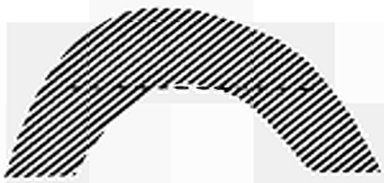


Fig. 2a

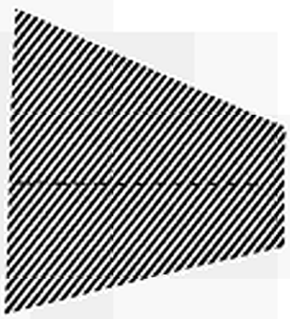


Fig. 2b

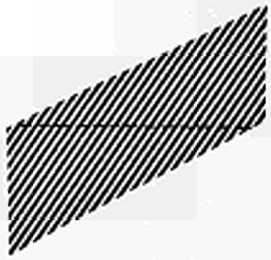


Fig. 2c

According to Draper [3] these abnormalities would indicate that:

- (fig. 2a) the model has a different analytical form - need for extra terms or need for a preliminary transformation on the experimental y_i;
- (fig. 2b) the variance is not constant - need for other weights (if this could

be compatible with the experimental set-up) or need for a preliminary transformation on the y_i;

- (fig. 2c) systematic error in the model - probable need for an additional constant term Θ_o in the model.

Always according to Draper [3], the expressions that are a measure of these abnormalities are:

$$T_{12} = \sum_{i=1}^{n_d} \varepsilon_i \left[F(\vec{x}_i, \vec{\Theta}_m) \right]^2 \qquad \text{for the case of fig. 2a}$$

$$T_{21} = \sum_{i=1}^{n_d} \varepsilon_i^2 \cdot F(\vec{x}_i, \vec{\Theta}_m) \qquad \text{for the case of fig. 2b}$$

$$T_{11} = \sum_{i=1}^{n_d} \varepsilon_i \cdot F(\vec{x}_i, \vec{\Theta}_m) \qquad \text{for the case of fig. 2c}$$

The values of these expressions are also given with the plot; they should always be compared with the mean value of the residues.

e2) Finally the normality of the residues is tested comparing their weighted integrated distribution density to the corresponding area under the normal curve. To this end the residues ε_i are reduced to:

$$\varepsilon_i^* = \frac{1}{\sigma} (\varepsilon_i - \bar{\varepsilon})$$

where $\bar{\varepsilon} = \frac{1}{n_d} \sum_{i=1}^{n_d} \varepsilon_i$

and $\sigma^2 = \frac{1}{n_d} \sum_{i=1}^{n_d} (\varepsilon_i - \bar{\varepsilon})^2$

Many other plots and tests may be imagined on the residues to fulfill their statistical analysis. These have not been included in the program for they require a specific knowledge of the problem. The user may achieve this analysis, if he so wishes in the MAIN program.

4. GENERAL DESCRIPTION OF THE DATFIT-SUBROUTINE

The program, named DATFIT, produces a non linear data fit by the least squares method.

The experimental points $\left\{ y_i, \vec{x}_i, w_i \right\}$; i = 1, n_d should be generated in the MAIN-program that calls DATFIT and transferred to it by a CØMMØN-statement:

CØMMØN/A/ND, NV, YEXP(1000), WGHT(1000), X(ND, NV)

where ND is the number of the experimental points: n_d
NV the dimension of the independent variable: n_v
YEXP the computervector containing $\left\{ y_i \right\}$; i= 1, n_d
WGHT the computervector containing $\left\{ w_i \right\}$; i=1, n_d
X the computervector containing $\left\{ \vec{x}_i \right\}$; i=1, n_d

The storage of the independent variables $\left\{ \vec{x}_i \right\}$ is made as follows:

((X(i, j), j=1, NV), i=1, ND)

The CØMMØN/A/-statement in DATFIT is used with variable dimension; therefore the calling MAIN-program should specify the dimensions of YEXP(i) and of WGHT(i) as 1000 single-precision words; the dimensions of X(i, j) must be specified with their exact length, i.e.: $n_d \cdot n_v$ single-precision-words. It must be noted that DATFIT renorms the vector WGHT(i) on entry so that their sum becomes equal to n_d; if all $w_i = 0$, then DATFIT sets them all $w_i = 1$.

Given an initial guess for $\vec{\Theta}_m$, the DATFIT subroutine finds the optimal $\vec{\Theta}_m$ (see calling sequence of DATFIT), minimizing the function $\Phi(\vec{\Theta})$ defined in (1). This minimization occurs by a subroutine MINIM1 delivered with the deck. This last subroutine is an adapted version of subroutine MINIM that is extensively described in [5]. It is an iterative minimumfinder that needs the convergence thresholds EPSF, EPSX, EPSG, IMAX and NIT as well as a write option IRIT. These data should be given to DATFIT by means of a CØMMØN-statement:

CØMMØN/B/EPSF, EPSX, EPSG, IMAX, NIT, IRIT

where EPSF is the convergence threshold on the function $\Phi(\vec{\Theta}_j)$ from one iteration to the next,

EPSX the convergence threshold on the argument Θ_j from one iteration to the next,

EPSG the absolute convergence threshold on the norm of $\vec{g}_j$,

IMAX the maximum number of iterations made by MINIM1 ,

NIT the iteration number after which the steepest descent method is avoided,

IRIT an option to produce writings by MINIM1 .

When EPSF, EPSX, EPSG and IMAX are put zero, MINIM1 works as if EPSF = EPSX = EPSG = 10^{-8} and IMAX = 40. When NIT is set less than zero, MINIM 1 works with the standard NIT = $2.\sqrt[3]{n_p}$. These standards have been found satisfactory for many examples; however, in some cases they must be fixed differently. The user should adapt these values so that return from MINIM 1 is caused by the EPSG threshold.

The computation of $\Phi(\vec{\Theta})$, its gradient and its Hessian is made by a subroutine NØNLIN that is also furnished with the deck. This subroutine NØNLIN, as well as DATFIT itself, call for a subroutine MØDEL that has to be programmed by the user entirely in double precision. For each vectors $\vec{x}$ and $\vec{\Theta}$ as input, MØDEL should produce the function $F(\vec{x}, \vec{\Theta})$, its gradient in $\vec{\Theta}$ and its Hessian in $\vec{\Theta}$.

5. CALLING SEQUENCE OF DATFIT

SUBRØUTINE DATFIT (NP, TH, PHI, YANAL, FF)

NP number of parameters n_p (dimension of $\vec{\Theta}$)

TH computervector containing the parameters forming $\vec{\Theta}_m$; initial guess of $\vec{\Theta}_m$ on entry, optimal values on return (double precision)

PHI sum of the squared residues: $\Phi(\vec{\Theta}_m)$ (double precision)

YANAL computervector containing the analytical values of the dependent variable produced by the fit: $\left\{F(\vec{x}_i, \vec{\Theta}_m)\right\}$; i=1, n_d (double precision)

FF variance ratio statistic $F(1-\alpha, n_p, n_d-n_p)$ (single precision)

The arguments needed on entry are NP, TH and FF. The produced arguments on return are TH, PHI and YANAL.

6. CALLING SEQUENCE FOR MØDEL

SUBRØUTINE MØDEL (X, TH, F, G, H, NØHESS, NØGRAD)

X computervector containing the values of the independent variables forming an $\vec{x}$ (double precision)

TH computervector containing the parameters forming a $\vec{\Theta}$ (double precision)

F value of $F(\vec{x},\vec{\Theta})$ (double precision)

G computervector containing $\left\{\frac{\partial F(\vec{x},\vec{\Theta})}{\partial \Theta_k}\right\}$; k=1, n_p (double precision)

H computervector containing $\left\{\frac{\partial^2 F(\vec{x},\vec{\Theta})}{\partial \Theta_k \, \partial \Theta_\ell}\right\}$; k=1, ℓ and ℓ=1, n_p (double precision)

Only the lower triangular part of this (symmetric) Hessian must be stored in the following sequence:

$$H(1) = \partial^2 F/\partial\Theta_1 \partial\Theta_1 \; ; \; H(2) = \partial^2 F/\partial\Theta_1 \partial\Theta_2 \; ; \; H(3) = \partial^2 F/\partial\Theta_2 \partial\Theta_2$$

$$H(4) = \partial^2 F/\partial\Theta_1 \partial\Theta_3 \; ; \; H(5) = \partial^2 F/\partial\Theta_2 \partial\Theta_3 \; ; \; \text{etc. } \ldots$$

NØHESS if this equals 1, nothing may be changed to the original content of the computervector H

NØGRAD if this equals 1, nothing may be changed to the original content of the computervector G

The arguments needed on entry are X, TH, NØHESS and NØGRAD. The produced arguments on return are F, G and H.

7. SOME SHORT EXAMPLES

a) With the model: $\Theta_1 \exp(\Theta_2 x) + \Theta_3 \exp(-\Theta_4 x)$ and with experimental data obtained from rounded-off values in a sinh(x) table, the optimal $\vec{\Theta}$ is found to be $\vec{\Theta}_m = \{0.5, 1, -0.5, 1\}$ as expected. The same result is obtained for every initial guess of $\vec{\Theta}$, even if it is very far from $\vec{\Theta}_m$ (see annex).

b) With the same model and experimental data obtained from rounded-off values in an exp(x) table, the optimal Θ is found to be $\vec{\Theta}_m = \{1, -1, \ldots, \ldots\}$ or $\{\ldots, \ldots, 1, +1\}$. The values of the remaining parameters are indetermined but they always generate a vanishing contribution of their corresponding term in the model. This indeterminancy is reflected by the ill-conditioning of the Hessian of $\Phi(\Theta)$ (see [3] p. 59). A statistical analysis of this problem obviously makes no sense.

c) With the model proposed in the REEP-program [2]: $\Theta_1 \exp(\Theta_2 x) + \Theta_3 \log x$ and the experimental data used there, the optimal parameters $\{1.98, 0.51, -1.09\}$ are retrieved in 7 iterations starting from the initial guess $\{1, 1, -2\}$. Starting from a worse initial guess, the REEP-program fails to converge. DATFIT finds the optimal parameters from the initial guess $\{10, 10, 10\}$ and $\{30, 30, 30\}$. In both cases convergence is soon reached but this test has permitted us to localize another optimal $\vec{\Theta}_m$, namely $\{16.86, -1.637, 5.94\}$ with a corresponding $\Phi(\Theta_m)$ that is somewhat less than the one corresponding to the minimum $\{1.98, 0.51, -1.09\}$. This gives the enormous advantage that one may expect from DATFIT compared with REEP: one is much more free in the choice of the initial guess.

d) A linear model is treated with the function:

$$F(\vec{x}, \vec{\Theta}) = \Big[\Theta_1 \sin x_1 + \Theta_2 \sin 2x_1 + \Theta_3 \sin 3x_1 + \Theta_4 \sin 4x_1 + \Theta_5 \sin 5x_1 + \Theta_6 \sin x_2 + \Theta_7 \sin 2x_2 + \Theta_8 \sin 3x_2 + \Theta_9 \sin 4x_2 + \Theta_{10} \sin 5x_2 + \Theta_{11} \sin x_3 + \Theta_{12} \sin 2x_3 + \Theta_{13} \sin 3x_3 + \Theta_{14} \sin 4x_3 + \Theta_{15} \sin 5x_3 + \Theta_{16} \sin x_4 + \Theta_{17} \sin 2x_4 + \Theta_{18} \sin 3x_4 + \Theta_{19} \sin 4x_4 + \Theta_{20} \sin 5x_4\Big] \pm 100$$

and with synthetic data obtained with some $\vec{\Theta}_{synth}$ and with a random set of values $\left\{\vec{x}_i\right\}$. One Newton-Raphson iteration in MINIM1 is sufficient to reach convergence (this may be proved analytically) and to find $\vec{\Theta}_m = \vec{\Theta}_{synth}$ starting from an initial guess $\vec{\Theta}_m = 0$.

e) Many other practical examples were worked through with very satisfactory results.

BIBLIOGRAPHY

[1] D. W. MARQUARDT; "An Algorithm for Least-Squares Estimation of Non Linear Parameters"; SIAM - Journal 11, 431 (1963)

[2] D. F. SHANNO; "REEP-Non Linear Estimation of Package". Share Program Library SDA 3493 (1967)

[3] N. R. DRAPER; "Applied Regression Analysis". John Wiley & Sons, Inc., New York (1967)

[4] D. DUMAS de RAULY; "L'estimation Statistique". Gauthier-Villars, Paris (1966)

[5] E. VAN DER VOORT and B. DORPEMA; "A New Algorithm to Minimize Functions", EUR-4777e (1972)

ANNEXES

1. Listing of DATFIT, MINIM 1 and NØNLIN with a MAIN-program and a MØDEL as working example (see 7a).
2. Corresponding output.

```
0001                 SUBROUTINE  D A T F I T  (NP,TH,PHI,YANAL,FF)
                C
                C    ..............................................................
                C
                C    NON LINEAR DATA FIT BY THE LEAST SQUARES METHOD
                C
                C    ..............................................................
                C
                C
                C
                C    THE CALLING SEQUENCE CONTAINS
                C
0002                 INTEGER*4 NP
0003                 REAL*8 TH(1),PHI,YANAL(1)
0004                 REAL*4 FF
                C
                C    WHERE
                C         NP            NUMBER OF PARAMETERS TO OPTIMIZE BY  D A T F I T
                C                       IN THE LEAST SQUARES SENSE
                C         TH(K)         VECTOR OF THESE PARAMETERS CONTAINING AN INITIAL
                C         K=1,NP        GUESS ON ENTRY AND THE OPTIMAL VALUES ON RETURN
                C         PHI           VALUE OF THE SUM OF THE SQUARED RESIDUES
                C         YANAL(I)      VECTOR OF DEPENDENT VARIABLES PREDICTED BY THE
                C         I=1,ND        MODEL WITH THE OPTIMAL PARAMETERS
                C                       EACH RESIDUE(I) IS YEXP(I)-YANAL(I)
                C         FF            VARIANCE RATIO STATISTIC F(1-A,NP,ND-NP)
                C
                C    ..............................................................
                C
                C    EXPERIMENTAL DATA (SINGLE PRECISION) SHOULD BE PRODUCED BY THE
                C    CALLING PROGRAM AND TRANSFERRED TO  D A T F I T  BY A
0005                 COMMON/A/ND,NV,YEXP(1000),WGHT(1000),X(1)
                C
                C    WHERE
                C         ND            NUMBER OF EXPERIMENTAL POINTS (MAX 1000)
                C         NV            NUMBER OF INDEPENDENT VARIABLES (MAX 20)
                C         YEXP(I)       VECTOR OF DEPENDENT VARIABLES (I=1,ND)
                C         WGHT(I)       VECTOR OF CORRESPONDING WEIGHTS (I=1,ND)
                C                       D A T F I T  RENORMS THESE WEIGHTS SO THAT
                C                       THERE SUM IS ND. IF THEY ARE ALL ZERO ON ENTRY,
                C                       THEY RETURN WITH A VALUE 1.0E0
                C         X(I,J)        MATRIX OF THE INDEPENDENT VARIABLES (I=1,ND AND
                C                       J=1,NV) -USED HERE WITH VARIABLE DIMENSION
                C                       THE PROGRAM CALLING  D A T F I T  SHOULD SPECIFY
                C                       EXACTLY THESE DIMENSIONS WITH MAXIMA ND=1000
                C                       AND NV=20
                C
                C    ..............................................................
                C
                C    M E T H O D
                C
                C    THE COMPUTATION OF FUNCTION PHI IS MADE BY A SUBROUTINE NONLIN
                C    (DELIVERED WITH THE DECK). THE OPTIMIZATION OF THE PARAMETERS TH
```

```
      C      IS DONE BY MINIMIZING THE FUNCTION PHI. THIS IS PERFORMED BY A
      C      SUBROUTINE MINIM1 (ALSO DELIVERED WITH THE DECK AND HAVING ITS OWN
      C      DESCRIPTION). THE CONVERGENCE THRESHOLDS EPSX,EPSF,EPSG,IMAX AND
      C      NIT AND THE WRITE OPTION IRIT, ALL NEEDED BY MINIM1, MUST BE GIVEN
      C      BY THE PROGRAM THAT CALLS  D A T F I T  AND MUST BE TRANSFERRED
      C      TO IT BY A
0006         COMMON/B/EPSF,EPSX,EPSG,IMAX,NIT,IRIT
      C
      C      .................................................................
      C
      C      THE MODEL F(XI,TH) TO FIT EXPERIMENTAL DATA SHOULD BE PROGRAMMED
      C      BY THE  D A T F I T -USER ENTIRELY IN DOUBLE PRECISION BY A
      C      SUBROUTINE MODEL (XI,TH,FI,GI,HI,NOHESS,NOGRAD)
      C
      C            FOR GIVEN VECTORS XI(J),J=1,NV AND TH(K),K=1,NP THIS MODEL
      C            SHOULD COMPUTE THE FUNCTION FI=F(XI,TH),ITS GRADIENT GI(K),
      C            K=1,NP AND ALSO ITS MATRIX OF SECOND PARTIAL DERIVATIVES
      C            (HESSIAN). THIS SYMMETRIC MATRIX MUST BE STORED AS A VECTOR
      C            HI(1)=HI(1,1) HI(2)=HI(2,1) HI(3)=HI(2,2) HI(4)=HI(3,1)...
      C            IF NOHESS AND/OR NOGRAD ARE EQUAL TO ONE, NOTHING MAY BE
      C            CHANGED TO THE CONTENTS OF HI AND/OR GI
      C
      C      .................................................................
      C
0007         REAL*8 G(100),H(5050),XI(20),YMOD,TH1(100),PHI1,DELTH1,DELTH2,
            1       LOW1(100),UPP1(100),LOW2(100),UPP2(100)
0008         DIMENSION RES(1000),COEF1(100),COEF2(100),HD(100),XE(20),
            1          DELVRL(100),DELVRU(100),Z(51,121),ZSYMB(50,120),ZZ(13),
            2          AREA(10),NRES(1000),NY(1000),NAREA(10),THRES(10)
0009         DATA THRES/ 1.959964 , 1.644854 , 1.281552 , 1.036433 , 0.841621 ,
            1          0.674490 , 0.524401 , 0.385320 , 0.153347 , 0.125661 /
0010         DATA ZZ/'0','1','2','3','4','5','6','7','8','9',' ','-','*'/
0011         EXTERNAL NONLIN
      C
      C
      C      .................................................................
      C
      C      WRITE INPUT
      C
0012         M=NP*(NP+1)/2
0013         WRITE(6,302) NP,ND,NV
0014         WRITE(6,304) FF
0015         WRITE(6,306)
0016         WRITE(6,308)(TH(I),I=1,NP)
0017         DO 12 I=1,ND
0018         IF(WGHT(I)) 16,12,16
0019      12 CONTINUE
0020         DO 14 I=1,ND
0021      14 WGHT(I)=1.D0
0022         GO TO 22
0023      16 SWGHT=0.
0024         DO 18 I=1,ND
0025      18 SWGHT=SWGHT+WGHT(I)
```

```
0026              SWGHT=SWGHT/ND                                                  DATF1070
0027              DO 20 I=1,ND                                                    DATF1080
0028           20 WGHT(I)=WGHT(I)/SWGHT                                           DATF1090
0029           22 J2=50                                                           DATF1100
0030              IF(NV.GT.4) J2=25                                               DATF1110
0031              IF(NV.GT.8) J2=16                                               DATF1120
0032              IF(NV.GT.12) J2=12                                              DATF1130
0033              IF(NV.GT.16) J2=10                                              DATF1140
0034              IPAGE=0                                                         DATF1150
0035              I2=0                                                            DATF1160
0036           24 IPAGE=IPAGE+1                                                   DATF1170
0037              WRITE(6,310)                                                    DATF1180
0038              I1=I2+1                                                         DATF1190
0039              I2=I2+J2                                                        DATF1200
0040              DO 28 I=I1,I2                                                   DATF1210
0041              DO 26 J=1,NV                                                    DATF1220
0042              K=(J-1)*ND+I                                                    DATF1230
0043           26 XE(J)=X(K)                                                      DATF1240
0044              WRITE(6,312)(XE(J),J=1,NV)                                      DATF1250
0045              WRITE(6,314) YEXP(I),WGHT(I),I                                  DATF1260
0046              IF(I.GE.ND) GC TO 30                                            DATF1270
0047           28 CONTINUE                                                        DATF1280
0048              GO TO 24                                                        DATF1290
            C                                                                     DATF1300
            C     FIND AND WRITE OPTIMAL PARAMETERS                               DATF1310
            C                                                                     DATF1320
0049           30 CALL MINIM1(NCNLIN,PHI,TH,G,H,NP,M,IRIT,EPSF,EPSX,EPSG,IMAX,NIT,0)DATF1330
0050              WRITE(6,316)                                                    DATF1340
0051              WRITE(6,308)(TH(I),I=1,NP)                                      DATF1350
0052              WRITE(6,318)                                                    DATF1360
0053              WRITE(6,308)(G(I),I=1,NP)                                       DATF1370
0054              WRITE(6,320) PHI                                                DATF1380
            C                                                                     DATF1390
            C     MODIFIED STANDARD ERROR OF ESTIMATE                             DATF1400
            C                                                                     DATF1410
0055              STERMO=DSQRT(PHI/(ND-NP))                                       DATF1420
0056              WRITE(6,322) STERMO                                             DATF1430
            C                                                                     DATF1440
            C     PARAMETER ELLIPSOID WITH UNITARY DELTA                          DATF1450
            C                                                                     DATF1460
0057              DO 32 J=1,NP                                                    DATF1470
0058              L=J*(J+1)/2                                                     DATF1480
0059           32 COEF1(J)=DSQRT(2.D0/H(L)*PHI)                                   DATF1490
0060              CALL MINIM1(NONLIN,PHI,TH,G,H,NP,M,IRIT,EPSF,EPSX,EPSG,IMAX,NIT,1)DATF1500
0061              DO 34 J=1,NP                                                    DATF1510
0062              L=J*(J+1)/2                                                     DATF1520
0063           34 COEF2(J)=DSQRT(2.D0*H(L)*PHI)                                   DATF1530
0064              DO 36 J=1,NP                                                    DATF1540
0065              IF(MOD(J,50).EQ.1) WRITE(6,324)                                 DATF1550
0066           36 WRITE(6,326) J,TH(J),COEF1(J),COEF2(J)                          DATF1560
            C                                                                     DATF1570
            C     SIGNIFICANT LCWER AND UPPER BOUNDS FCR THE PARAMETERS           DATF1580
            C                                                                     DATF1590
```

```
0067         DELTA=FF*NP/(ND-NP)
0068         WRITE(6,328) DELTA
0069         SQDEL= SQRT(DELTA)
0070         DO 38 I=1,NP
0071      38 TH1(I)=TH(I)
0072         DO 40 I=1,NP
0073         DELTH1=COEF1(I)*SQDEL
0074         DELTH2=COEF2(I)*SQDEL
0075         LOW1(I)=TH(I)-DELTH1
0076         UPP1(I)=TH(I)+DELTH1
0077         TH1(I)=LOW1(I)
0078         CALL NONLIN(NP,TH1,PHI1,G,H,1,1)
0079         DELVRL(I)=(PHI1-PHI)/PHI
0080         TH1(I)=UPP1(I)
0081         CALL NONLIN(NP,TH1,PHI1,G,H,1,1)
0082         DELVRU(I)=(PHI1-PHI)/PHI
0083         TH1(I)=TH(I)
0084         LOW2(I)=TH(I)-DELTH2
0085      40 UPP2(I)=TH(I)+DELTH2
0086         DO 42 I=1,NP
0087         IF(MOD(I,50).EQ.1) WRITE(6,330)
0088      42 WRITE(6,332) I,TH(I),LOW1(I),DELVRL(I),UPP1(I),DELVRU(I),LOW2(I),
            1UPP2(I)
       C
       C     WRITE INVERSE OF HESSIAN MATRIX OF PHI
       C
0089         WRITE(6,334)
0090         I=0
0091         J2=0
0092      44 J1=J2+1
0093         I=I+1
0094         J2=J2+I
0095         WRITE(6,336)(H(K),K=J1,J2)
0096         WRITE(6,338) I
0097         IF(J2.LT.M) GO TO 044
       C
       C     PARAMETER CORRELATION MATRIX
       C
0098         I=0
0099         DO 46 J=1,NP
0100         I=J+I
0101      46 HD(J)=DSQRT(H(I))
0102         DO 52 K=1,M
0103         J=0
0104         KK=K
0105      48 J=J+1
0106         KK=KK-J
0107         IF(KK.GT.0) GO TO 48
0108         I=K-J*(J-1)/2
0109      52 H(K)=H(K)/(HD(I)*HD(J))
0110         WRITE(6,340)
0111         I=0
0112         J2=0
```

```
0113         54 J1=J2+1                                                DATF2130
0114            I=I+1                                                  DATF2140
0115            J2=J2+I                                                DATF2150
0116            WRITE(6,336)(H(K),K=J1,J2)                             DATF2160
0117            WRITE(6,338) I                                         DATF2170
0118            IF(J2.LT.M) GO TO 54                                   DATF2180
          C                                                            DATF2190
          C     FIND AND WRITE RESIDUES                                DATF2200
          C                                                            DATF2210
0119            I1=1                                                   DATF2220
0120            I2=I1+49                                               DATF2230
0121         56 WRITE(6,342)                                           DATF2240
0122            DO 60 I=I1,I2                                          DATF2250
0123            DO 58 J=1,NV                                           DATF2260
0124            K=(J-1)*ND+I                                           DATF2270
0125         58 XI(J)=X(K)                                             DATF2280
0126            CALL MODEL (XI,TH,YMOD,G;H,1,1)                        DATF2290
0127            YANAL(I)=YMOD                                          DATF2300
0128            RES(I)=YEXP(I)-YMOD                                    DATF2310
0129            WRITE(6,344) I,YEXP(I),YMOD,RES(I)                     DATF2320
0130            IF(I.EQ.ND) GO TO 62                                   DATF2330
0131         60 CONTINUE                                               DATF2340
0132            I1=I2+1                                                DATF2350
0133            I2=I1+49                                               DATF2360
0134            GO TO 56                                               DATF2370
          C                                                            DATF2380
          C     OVERALL PLOT OF THE RESIDUES AGAINST FIT (YANAL)       DATF2390
          C                                                            DATF2400
0135         62 WRITE(6,346)                                           DATF2410
0136            YMA=YANAL(1)                                           DATF2420
0137            YMI=YMA                                                DATF2430
0138            RESMA=RES(1)                                           DATF2440
0139            RESMI=RESMA                                            DATF2450
0140            DO 64 I=2,ND                                           DATF2460
0141            P=YANAL(I)                                             DATF2470
0142            YMA=AMAX1(YMA,P)                                       DATF2480
0143            YMI=AMIN1(YMI,P)                                       DATF2490
0144            RESMA=AMAX1(RESMA,RES(I))                              DATF2500
0145         64 RESMI=AMIN1(RESMI,RES(I))                              DATF2510
0146            DELRES=(RESMA-RESMI)/49.                               DATF2520
0147            DELY=(YMA-YMI)/119.                                    DATF2530
0148            DO 66 I=1,ND                                           DATF2540
0149            P=(RESMA-RES(I))/DELRES                                DATF2550
0150            NRES(I)=IFIX(P+0.499999)+1                             DATF2560
0151            P=(YANAL(I)-YMI)/DELY                                  DATF2570
0152         66 NY(I)=IFIX(P+0.499999)+1                               DATF2580
0153            P=RESMA/DELRES                                         DATF2590
0154            NULRES=IFIX(P+0.499999)+1                              DATF2600
0155            DO 68 I=1,50                                           DATF2610
0156            DO 68 J=1,120                                          DATF2620
0157         68 Z(I,J)=0.                                              DATF2630
0158            DO 70 I=1,50                                           DATF2640
0159            DO 70 J=1,120                                          DATF2650
```

```
      DO 70 K=1,ND
      IF ((NRES(K).EQ.I).AND.(NY(K).EQ.J)) Z(I,J)=Z(I,J)+WGHT(K)
   70 CONTINUE
      ZMA=Z(1,1)
      DO 72 I=1,50
      DO 72 J=1,120
   72 ZMA=AMAX1(ZMA,Z(I,J))
      IF(ZMA.LT.10.) GO TO 76
      DELZ=ZMA/10.
      DO 74 I=1,50
      DO 74 J=1,120
   74 Z(I,J)=Z(I,J)/DELZ
   76 DO 78 I=1,50
      DO 78 J=1,120
      ZSYMB(I,J)=ZZ(11)
      IF (I.EQ.1) ZSYMB(I,J)=ZZ(13)
      IF (I.EQ.50) ZSYMB(I,J)=ZZ(13)
      IF (J.EQ.1) ZSYMB(I,J)=ZZ(13)
      IF (J.EQ.120) ZSYMB(I,J)=ZZ(13)
      IF (I.EQ.NULRES) ZSYMB(I,J)=ZZ(12)
      P=Z(I,J)
      DO 78 K=1,10
      IF((P.GE.(K-1)).AND.(P.NE.0)) ZSYMB(I,J)=ZZ(K)
   78 CONTINUE
      WRITE(6,348)((ZSYMB(I,J),J=1,120),I=1,50)
      WRITE(6,350) RESMA,RESMI,YMA,YMI
C
C     VALUES TO ESTIMATE DEFECTS IN PLOT
C
      T11=0.
      T12=0.
      T21=0.
      DO 80 J=1,ND
      P=RES(J)*YANAL(J)
      T11=T11+P
      T12=T12+P*YANAL(J)
      T21=T21+P*RES(J)
   80 CONTINUE
      WRITE(6,352) T11,T12,T21
C
C     NORMALITY OF THE DEVIATES
C
      S=0.
      DO 82 J=1,ND
   82 S=S+RES(J)*WGHT(J)
      S=S/ND
      STER=0.
      DO 84 J=1,ND
      P=RES(J)-S
   84 STER=STER+P*P*WGHT(J)
      STER= SQRT(STER/ND)
      DO 86 J=1,ND
   86 RES(J)=(RES(J)-S)/STER
```

```
0207            DO 88 I=1,10
0208         88 AREA(I)=0.
0209            DO 90 J=1,ND
0210            P=ABS(RES(J))
0211            DO 90 I=1,10
0212            IF(P.LE.THRES(I)) AREA(I)=AREA(I)+WGHT(J)
0213         90 CONTINUE
0214            DO 92 I=1,10
0215         92 NAREA(I)=IFIX(AREA(I)*1000./ND)
0216            WRITE(6,354) S,STER
0217            WRITE(6,356) NAREA
          C
          C     ..................................................................
          C
0218            RETURN
          C
          C     ..................................................................
          C
0219       302  FORMAT (1H1,'NUMBER OF PARAMETERS',T22,I4/
               1              1H ,'NUMBER OF DATA',T22,I4/
               2              1H ,'NUMBER OF IND. VAR.',T22,I4//)
0220       304  FORMAT (1H0,'VARIANCE RATIO STATISTIC  F(1-A),NP,ND-NP) = ',E10.3/
               1/)
0221       306  FORMAT (1H0,'THE INITIAL VALUES OF THE PARAMETERS ARE'/)
0222       308  FORMAT (1H0,6D20.10)
0223       310  FORMAT (1H1,T10,'EXPERIMENTAL DATA',T42,'X(I,J),J=1,NV',T91,'YEXP(
               1I)',T111,'WGHT(I)',T129,'I'/1H0,T9,73('-'),T88,13('-'),T108,13('-'
               2),T128,3('-')//)
0224       312  FORMAT (1H ,4E20.6)
0225       314  FORMAT (1H+,T81,2E20.6,T127,I4)
0226       316  FORMAT (1H1,'THE FINAL VALUES OF THE PARAMETERS ARE'////)
0227       318  FORMAT (1H1,'THE VALUES OF THE GRADIENT ARE'////)
0228       320  FORMAT (1H1,'THE VALUE OF THE FUNCTION PHI IS',E23.10////)
0229       322  FORMAT (1H0,'MODIFIED STANDARD ERROR OF ESTIMATE',E20.6)
0230       324  FORMAT (1H1,T6,'PARAMETER VARIATICNS CORRESPCNCING TO A UNITARY DE
               1LTA'/1H0,T7,'K',T20,'PARAMETER',T40,'MAXIMUM VARIATION ON THE AXIS
               2',T80,'EXTREME VARIATION'/)
0231       326  FORMAT (1H ,T5,I3,T10,D20.6,T40,E20.6,T75,E20.6)
0232       328  FORMAT (1H1,'THE VARIANCE RATIO STATISTIC GIVES A DELTA',E20.6)
0233       330  FORMAT (1H1,T4,'K',T8,'PARAMETER',T45,'MAXIMUM VALUES ON THE AXIS'
               1,T105,'EXTREME VALUES'/1H0,T27,'LOWER',T41,'VIRT. DELTA',T64,'UPPE
               2R',T78,'VIRT. DELTA',T102,'LOWER',T119,'UPPER'/)
0234       332  FORMAT (1H ,I3,T6,D13.6,T23,D14.7,T40,E13.6,T60,D14.7,T77,E13.6,T9
               18,D14.7,T115,D14.7)
0235       334  FORMAT (1H1,'INVERSE OF HESSIAN MATRIX OF FUNCTICN PHI'//)
0236       336  FORMAT (1H ,6D20.6)
0237       338  FORMAT (1H+,T121,I10/)
0238       340  FORMAT (1H1,'PARAMETER CORRELATION MATRIX'//)
0239       342  FORMAT (1H1,T10,'DATA PT.',T23,'EXPERIMENTAL',T43,'ANALYTICAL',T63
               1,'RESIDUE'/1H0,T10,8('-'),T23,12('-'),T43,10('-'),T63,7('-')//)
0240       344  FORMAT (1H ,I14,E19.6,D19.6,E19.6)
0241       346  FORMAT (1H1,'OVERALL PLOT OF THE RESIDUES AGAINST THE VALUES PREDI
               1CTED BY THE FIT (YANAL)'///)
```

```
 0242          348 FORMAT (1H ,T5,120A1)
 0243          350 FORMAT (//1H0,'EXTREME VALUES OF THE RESIDUES',2E16.6,T73,'EXTREME
                  1 VALUES OF YANAL',2E16.6)
 0244          352 FORMAT (1H0,'T11 = ',E13.6,30X,'T12 = ',E13.6,30X,'T21 = ',E13.6)
 0245          354 FORMAT (1H1,'THE MEAN VALUE OF THE RESIDUES IS',T41,E13.6/1H0,'THE
                  1IR STANDARD DEVIATION IS',T41,E13.6////)
 0246          356 FORMAT (1H0,'THEORETICAL AREAS UNDER THE NORMAL CURVE (1/1000)',T6
                  15,'  950  900  800  700  600  500  400  300  200  100'/1H0,'COMPAR
                  1ATIVE AREAS FOR THE WEIGHTED REDUCED RESIDUES',T65,10I5)
             C
             C        ....................................................................
             C
 0247              END
```

```
0001          SUBROUTINE MINIM1 (FUN,FM,X,G,H,N,M,IRIT,EPSF,EPSX,EPSG,IMAX,NIT,
             1INVERT)
        C
        C     ..................................................................
        C
        C     PROGRAM CALCULATES MINIMUM OF FUNCTION FM=FM(X(I)) I=1,N
        C
        C     ..................................................................
        C     DESCRIPTION CALLING SEQUENCE OF MINIM1
        C     FUN    NAME OF FUNCTION TO BE MINIMISED
        C     X(I)    VECTOR OF INDEPENDENT VARIABLES
        C     G(I)    VECTOR OF FIRST DERIVATIVES (GRADIENT)
        C     H(J)       MATRIX ( IN VECTOR FORM ) OF SECOND DERIVATIVES (HESSIAN)
        C     N       NUMBER CF ELEMENTS X(I),G(I)  (MAXIMUM 100)
        C     M       NUMBER OF ELEMENTS H(J),MUST BE PUT EQUAL N*(N+1)/2
        C     IRIT=0   NO PRINTING IN MINIM1
        C     IRIT=1   PRINTING OF ESSENTIAL DATA OF EACH ITERATION
        C     IRIT=2   XOLD AND XNEW ARE ALSO PRINTED
        C     IRIT=3   G,S AND D  VECTORS ARE ALSO PRINTED
        C     EPSF DESIRED ACCURACY IN FM (FUNCTION)
        C     EPSX DESIRED ACCURACY IN X(I) (INDEPENDENT VARIABLES)
        C     EPSG DESIRED ACCURACY IN G (NORM OF GRADIENT)
        C     IMAX DESIRED MAXIMUM NUMBER OF ITERATIONS
        C     NIT  ITERATION NUMBER AFTER WHICH GRADIENT METHCD IS AVOIDED
        C     INVERT  AS MINIM1 CONTAINS AN IMPLICIT MATRIX INVERTER,THE MATRIX
        C     H(I,J) IS INVERTED IF INVERT=1, THE CTHER VARIABLES IN THE
        C     CALLING SEQUENCE REMAIN UNCHANGED
        C     WHEN EPSF,EPSX,EPSG OR IMAX ARE PUT ZERO,MINIM1 SETS THESE VALUES
        C     TO   1.-8 1.-8 1.-8      40
        C     WHEN NIT IS LESS THAN ZERO,MINIM1 SETS THIS VALUE TO THE STANDARD
        C          2*N**(1/3)
0002                                                                    CONTINUE
        C     ..................................................................
        C     THE MAIN PROGRAM THAT CALLS MINIM1 MUST PROVIDE THE SUBROUTINE
        C     WITH THESE PARAMETERS AND MUST DEFINE THE DIMENSICNS OF X,G AND H
        C
        C     ..................................................................
        C
        C     SPECIFICATION OF FUNCTION TO BE MINIMISED
        C     CALLING SUBROUTINE FUN(N,X,FM,G,H,L)
        C     FUN IS NAME
        C     N NUMBER OF VARIABLES               DELIVERED BY MINIM1
        C     X(I) VARIABLES                      DELIVERED BY MINIM1
        C     FM FUNCTION                         CALCULATED IN FUN
        C     G(I) GRADIENT                       CALCULATED IN FUN
        C     H(J) HESSIAN                        CALCULATED IN FUN
        C     L OPTION SWITCH                     DELIVERED BY MINIM1
        C     FOR L=0 FUN MUST CALCULATE H(J)
        C     FOR L=1 FUN MUST NOT CALCULATE H(J)
        C     H(J) MATRIX IS STORED AS A VECTOR IN FOLLOWING MANNER,
        C     H(1) = H(1,1)
        C     H(2) = H(2,1)
        C     H(3) = H(2,2)
```

```
              C      H(4) = H(3,1)
              C      ETC
              C
              C      ..................................................................
              C
0003                 IMPLICIT REAL*8 (A-H,O-Z)
0004                 REAL*4 EPSF,EPSX,EPSG
0005                 DIMENSION D(100),G1(100),S(100),XOLD(100),A(100)
0006                 DIMENSION ALFA(4),BETA(3),X(N),G(N),H(M)
0007                 DATA ALFA /8HMODIFIED,8H NEWTON ,8HRAPHSON ,8HGRADIENT/
0008                 DATA BLANK /8H        /
              C
              C      ..................................................................
              C
0009                 IF (INVERT.EQ.1) GO TO 23
              C
              C      INITIALIZING,START VALUE,LENGTH OF GRADIENT
              C
0010                 FPSF=EPSF
0011                 FPSX=EPSX
0012                 FPSG=EPSG
0013                 IMAC=IMAX
0014                 NYT=NIT
0015                 IF (FPSX.LE.0.0D0) FPSX=1.0D-8
0016                 IF (FPSF.LE.0.0D0) FPSF=1.0D-8
0017                 IF (FPSG.LE.0.0D0) FPSG=1.0D-8
0018                 IF (IMAC.LE.0) IMAC=40
0019                 FN=N
0020                 IF (NYT.LT.0) NYT=2.0*FN**0.333333
              C
0021                 CALL FUN(N,X,FM,G,H,0,0)
0022                 GG=0.0D0
0023                 DO 12 I=1,N
0024              12 GG=GG+G(I)**2
0025                 GNORM=DSQRT(GG)
0026                 ITR=0
              C
              C      BEGIN NEW ITERATION
              C
0027              14 ITR=ITR+1
0028                 I5=1
0029                 I6=1
              C
              C      SAFE X AND COMPUTE GHG
              C
0030                 FL=FM
0031                 GHG=0.0D0
0032                 II=0
0033                 DO 22 I=1,N
0034                 XOLD(I)=X(I)
0035                 HGI=0.0D0
0036                 II=II+I-1
0037                 JJ=II
```

```
0038          DO 20 J=1,N                                          MINI1070
0039          IF (J-I)16,16,18                                     MINI1080
0040       16 IJ=II+J                                              MINI1090
0041          GO TO 20                                             MINI1100
0042       18 JJ=JJ+J-1                                            MINI1110
0043          IJ=JJ+I                                              MINI1120
0044       20 HGI=HGI+H(IJ)*G(J)                                   MINI1130
0045       22 GHG=GHG+G(I)*HGI                                     MINI1140
        C                                                          MINI1150
        C     DEVELOP H IN L*D*LT,STORE L IN H                     MINI1160
        C     SEARCH FOR LOWEST AND SMALLEST ELEMENT OF D          MINI1170
        C                                                          MINI1180
0046       23 II=0                                                 MINI1190
0047          DO 34 I=1,N                                          MINI1200
0048          IME=I-1                                              MINI1210
0049          JJ=II                                                MINI1220
0050          II=II+IME                                            MINI1230
0051          DO 32 J=I,N                                          MINI1240
0052          JJ=JJ+J-1                                            MINI1250
0053          IJ=JJ+I                                              MINI1260
0054          AIJ=0.0D0                                            MINI1270
0055          IF (I.EQ.1) GC TO 26                                 MINI1280
0056          DO 24 K=1,IME                                        MINI1290
0057          KI=II+K                                              MINI1300
0058          KJ=JJ+K                                              MINI1310
0059       24 AIJ=AIJ+H(KI)*H(KJ)*D(K)                             MINI1320
0060       26 IF (J-I)32,28,30                                     MINI1330
0061       28 D(I)=H(IJ)-AIJ                                       MINI1340
0062          H(IJ)=1.0D0                                          MINI1350
0063          GO TO 32                                             MINI1360
0064       30 H(IJ)=(H(IJ)-AIJ)/D(I)                               MINI1370
0065       32 CONTINUE                                             MINI1380
0066       34 CONTINUE                                             MINI1390
0067          IF (INVERT.EQ.1) GO TO 44                            MINI1400
        C                                                          MINI1410
0068          ILW=1                                                MINI1420
0069          ISM=1                                                MINI1430
0070          DO 36 I=2,N                                          MINI1440
0071          IF (D(I).LT.D(ILW)) ILW=I                            MINI1450
0072          IF (DABS(D(I)).LT.DABS(D(ISM))) ISM=I                MINI1460
0073       36 CONTINUE                                             MINI1470
        C                                                          MINI1480
        C     DETERMINE WHETHER H IS POSITIVE DEFINITE OR NOT      MINI1490
        C     DEFINE VECTOR A,SEARCH NUMBER OF NEGATIVE ELEMENTS IN D  MINI1500
        C                                                          MINI1510
0074          NNEG=0                                               MINI1520
0075          DO 38 I=1,N                                          MINI1530
0076          A(I)=0.0D0                                           MINI1540
0077          IF (D(I).GT.0.0D0) GO TO 38                          MINI1550
0078          NNEG=NNEG+1                                          MINI1560
0079          A(I)=1.0D0                                           MINI1570
0080       38 CONTINUE                                             MINI1580
0081          I7=0                                                 MINI1590
```

```
0082             IF (NNEG.GT.0) I7=1                                        MINI1600
           C                                                                MINI1610
           C     WHEN HESSLAN NOT POS-DEF USE STEEPEST DESCENT METHOD FOR   MINI1620
           C     FIRST 2*N**(1/3) ITERATIONS                                MINI1630
           C     THE S-DIRECTION IS GIVEN BY    S=-G                        MINI1640
           C                                                                MINI1650
0083             IF (I7.EQ.0.OR.ITR.GT.NYT) GO TO 44                        MINI1660
0084             DO 40 I=1,N                                                MINI1670
0085          40 S(I)=-G(I)                                                 MINI1680
0086             I6=0                                                       MINI1690
0087             GO TO 70                                                   MINI1700
           C                                                                MINI1710
           C     INVERT LOWER TRIANGULAR MATRIX L AND STORE IN H            MINI1720
           C                                                                MINI1730
0088          44 JJ=0                                                       MINI1740
0089             DO 48 J=2,N                                                MINI1750
0090             JME=J-1                                                    MINI1760
0091             JJ=JJ+JME                                                  MINI1770
0092             II=0                                                       MINI1780
0093             DO 48 I=1,JME                                              MINI1790
0094             IME=I+1                                                    MINI1800
0095             II=II+I-1                                                  MINI1810
0096             IJ=JJ+I                                                    MINI1820
0097             AIJ=0.0D0                                                  MINI1830
0098             IF ((J-I).EQ.1) GO TO 48                                   MINI1840
0099             KK=II                                                      MINI1850
0100             DO 46 K=IME,JME                                            MINI1860
0101             KK=KK+K-1                                                  MINI1870
0102             IK=KK+I                                                    MINI1880
0103             KJ=JJ+K                                                    MINI1890
0104          46 AIJ=AIJ+H(IK)*H(KJ)                                        MINI1900
0105          48 H(IJ)=-H(IJ)-AIJ                                           MINI1910
0106             IF (INVERT.EQ.1) GO TO 56                                  MINI1920
           C                                                                MINI1930
           C     IF H NOT POS-DEF DETERMINE S-DIRECTION SATISFYING          MINI1940
           C     THE EQUATION    LT.S=A                                     MINI1950
           C                                                                MINI1960
0107             IF (I7.EQ.0) GO TO 56                                      MINI1970
0108             I5=1                                                       MINI1980
0109             II=0                                                       MINI1990
0110             DO 54 I=1,N                                                MINI2000
0111             AI=0.0D0                                                   MINI2010
0112             II=II+I-1                                                  MINI2020
0113             IF (I.EQ.N) GO TO 54                                       MINI2030
0114             IPE=I+1                                                    MINI2040
0115             JJ=II                                                      MINI2050
0116             DO 52 J=IPE,N                                              MINI2060
0117             JJ=JJ+J-1                                                  MINI2070
0118             IJ=JJ+I                                                    MINI2080
0119          52 AI=AI+H(IJ)*A(J)                                           MINI2090
0120          54 S(I)=A(I)+AI                                               MINI2100
0121             GO TO 70                                                   MINI2110
           C                                                                MINI2120
```

```
C     IF H IS POS-DEF COMPUTE INVERTED HESSIAN AND STORE IN H
C     H(-1)=L(-1)*D*LT(-1)
C
   56 I5=0
      II=0
      DO 60 I=1,N
      JJ=II
      II=II+I-1
      DO 60 J=I,N
      JJ=JJ+J-1
      IJ=JJ+I
      AIJ=0.0D0
      IF (J.EQ.N) GO TO 60
      JPE=J+1
      KK=JJ
      DO 58 K=JPE,N
      KK=KK+K-1
      IK=KK+I
      JK=KK+J
   58 AIJ=AIJ+H(IK)*H(JK)/D(K)
   60 H(IJ)=H(IJ)/D(J)+AIJ
      IF (INVERT.EQ.1) RETURN
C
C     DETERMINE S-DIRECTION SATISFYING THE EQUATION  H*S=-G
C
      II=0
      DO 66 I=1,N
      S(I)=0.0D0
      II=II+I-1
      JJ=II
      DO 66 J=1,N
      IF (J-I)62,62,64
   62 IJ=II+J
      GO TO 66
   64 JJ=JJ+J-1
      IJ=JJ+I
   66 S(I)=S(I)-H(IJ)*G(J)
C
C     COMPUTE GS,SHS,NORM OF S
C
   70 GS=0.0D0
      SS=0.0D0
      SHS=0.0D0
      DO 72 I=1,N
      IF (D(I).LT.0.0D0) SHS=SHS+D(I)
      GS=GS+G(I)*S(I)
   72 SS=SS+S(I)**2
      SNORM=DSQRT(SS)
C
      IF (I5.EQ.0) SHS=-GS
      IF (I6.EQ.0) SHS=GHG
      IF (GS.LT.0.0D0) GO TO 80
      DO 74 I=1,N
```

```
0165         74 S(I)=-S(I)                                              MINI2660
0166            GS=-GS                                                  MINI2670
          C                                                             MINI2680
          C                                                             MINI2690
          C     APPROXIMATE NEW FUNCTION MINIMUM IN THE S-DIRECTION    MINI2700
          C     LAMBDA IS DETERMINED BY DAVIDON METHOD                  MINI2710
          C                                                             MINI2720
0167         80 K1=0                                                    MINI2730
0168            K2=0                                                    MINI2740
0169            YA=0.0D0                                                MINI2750
0170            FA=FL                                                   MINI2760
0171            GSA=GS                                                  MINI2770
0172            YB=-GS/DABS(SHS)                                        MINI2780
0173            IF (I5.NE.0) YB=DMIN1(YB,1.0D0/SNORM)                   MINI2790
0174            YM=YB                                                   MINI2800
0175         82 DO 84 I=1,N                                             MINI2810
0176         84 X(I)=XOLD(I)+YB*S(I)                                    MINI2820
0177            K1=K1+1                                                 MINI2830
0178         86 CALL FUN(N,X,FB,G1,H,I7,0)                              MINI2840
0179            FM=FB                                                   MINI2850
0180            GSB=0.0D0                                               MINI2860
0181            DO 88 I=1,N                                             MINI2870
0182         88 GSB=GSB+G1(I)*S(I)                                      MINI2880
0183            IF (FB.GT.FA+FPSF) GO TO 90                             MINI2890
0184            IF (I5.EQ.0) GO TO 110                                  MINI2900
0185            IF (GSB.GT.0.0D0) GO TO 90                              MINI2910
0186            YA=YB                                                   MINI2920
0187            FA=FB                                                   MINI2930
0188            GSA=GSB                                                 MINI2940
0189            YB=YB+YB                                                MINI2950
0190            GO TO 82                                                MINI2960
          C                                                             MINI2970
0191         90 IF (YA.EQ.YB)    WRITE (6,330)                          MINI2980
0192            Z=3.0D0*(FA-FB)/(YB-YA)+GSA+GSB                         MINI2990
0193            W=DSQRT(Z*Z-GSA*GSB)                                    MINI3000
0194            YM=YB-(GSB+W-Z)*(YB-YA)/(GSB-GSA+W+W)                   MINI3010
0195            YMS=YA+(YB-YA)*0.25D0                                   MINI3020
0196            ISAF=0                                                  MINI3030
0197            IF (YM.LT.YMS) ISAF=1                                   MINI3040
0198            IF (ISAF.EQ.1) YM=YMS                                   MINI3050
0199            DO 92 I=1,N                                             MINI3060
0200         92 X(I)=XOLD(I)+YM*S(I)                                    MINI3070
0201            K2=K2+1                                                 MINI3080
0202            CALL FUN(N,X,FM,G1,H,0,0)                               MINI3090
0203            GIS=0.0D0                                               MINI3100
0204            DO 94 I=1,N                                             MINI3110
0205         94 GIS=GIS+G1(I)*S(I)                                      MINI3120
          C                                                             MINI3130
          C     TEST ON CORRECT LAMBDA                                  MINI3140
          C                                                             MINI3150
0206            IF (ISAF.EQ.1) GO TO 110                                MINI3160
0207            IF (FM-FA-FPSF) 98,98,96                                MINI3170
0208         96 YB=YM                                                   MINI3180
```

```
0209            FB=FM
0210            GSB=GIS
0211            GO TO 90
0212         98 IF (FM-FB-FPSF) 110,110,100
0213        100 YA=YM
0214            FA=FM
0215            GSA=GIS
0216            GO TO 90
          C
0217        110 YL=YM
0218            DAX=YL*SNORM
0219            GG=0.0D0
0220            DO 112 I=1,N
0221            G(I)=G1(I)
0222        112 GG=GG+G(I)**2
0223            GNORM=DSQRT(GG)
          C
          C     PRINTING
          C
0224            IF (IRIT.EQ.0) GO TO 116
0225            IPAG=50
0226            NVF=(N+4)/5
0227            IBL=7
0228            IF (IRIT.EQ.2) IBL=8+NVF*2
0229            IF (IRIT.EQ.3) IBL=9+NVF*5
0230            ILN=MAX0 (1,(IPAG-2)/IBL)
0231            IF (MOD(ITR,ILN).NE.1.AND.ILN.NE.1)  GO TO 114
0232            WRITE (6,320) FPSX,FPSF,FPSG,IMAC,NYT
0233        114 BETA(1)=BLANK
0234            BETA(2)=BLANK
0235            BETA(3)=ALFA(4)
0236            IF (I6.EQ.0) GO TO 118
0237            BETA(2)=ALFA(2)
0238            BETA(3)=ALFA(3)
0239            IF (I7.EQ.1)  BETA(1)=ALFA(1)
0240        118 WRITE (6,302) ITR,BETA,K1,K2,NNEG,I6,I7
0241            WRITE (6,304) FL,GS,SHS,GHG
0242            WRITE (6,306) FM,GNORM,SNORM,DAX
0243            WRITE (6,308) D(ILW),D(ISM),YL
0244            IF (IRIT.EQ.1) GO TO 116
0245            WRITE (6,310) (XOLD(I),I=1,N)
0246            WRITE (6,312) (X(I),I=1,N)
0247            IF (IRIT.EQ.2) GO TO 116
0248            WRITE (6,314) (G(I),I=1,N)
0249            WRITE (6,316) (S(I),I=1,N)
0250            WRITE (6,318) (D(I),I=1,N)
0251        116 CONTINUE
          C
          C     TEST QUALITY OF ITERATION
          C
0252            IF (ITR.GE.IMAC) GO TO 120
0253            IF (DAX.LT.FPSX) GO TO 120
0254            IF (DABS(FL-FM).LT.FPSF) GO TO 120
```

```
0255          IF (GNORM.GT.EPSG) GO TO 14                                         MINI3720
0256      120 RETURN                                                              MINI3730
        C                                                                         MINI3740
        C     ..................................................................MINI3750
        C                                                                         MINI3760
0257      302 FORMAT (1H0/1H ,10HITERATION=I3,2X3A8,8H METHCD ,6X17HEXTERNAL SUBMINI3770
         1 ITR=I2,4X17HINTERNAL SUB ITR=I2,5X6HNEG-D=I3,10X2I2)                   MINI3780
0258      304 FORMAT (1H0,8H F(OLD)=D22.15,5X4HG*S=D22.15,4X6HS*H*S=D22.15,3X6HGMINI3790
         1*H*G=D22.15)                                                           MINI3800
0259      306 FORMAT (1H ,8H F(NEW)=D22.15,3X6HGNCRM=D22.15,4X6HSNORM=D22.15,4X5MINI3810
         1HDAX =D22.15)                                                          MINI3820
0260      308 FORMAT (1H ,8H D(LOW)=D22.15,2X7HD(SML)=D22.15,3X7HLAMBDA=D22.15)  MINI3830
0261      310 FORMAT (1H0,8HXOLD(I)=D17.10,4D20.10/(D26.10,4D20.10))             MINI3840
0262      312 FORMAT (1H ,8HXNEW(I)=D17.10,4D20.10/(D26.10,4D20.10))             MINI3850
0263      314 FORMAT (1H0,6X2HG=D17.10,4D20.10/(D26.10,4D20.1C))                 MINI3860
0264      316 FORMAT (1H ,6X2HS=D17.10,4D20.10/(D26.10,4D20.10))                 MINI3870
0265      318 FORMAT (1H ,6X2HD=D17.10,4D20.10/(D26.10,4D20.10))                 MINI3880
0266      320 FORMAT (1H1,5HMINIM,9X5HEPSX=D11.4,5X5HEPSF=D11.4,5X5HEPSG=D11.4,  MINI3890
         15X5HIMAX=I3,6X4HNIT=I2,9X5HMINIM)                                      MINI3900
0267      330 FORMAT (1H0,45HERROR MESSAGE FROM MINIM,CHECK SUBROUTINE FUN)      MINI3910
        C                                                                         MINI3920
        C     ..................................................................MINI3930
        C                                                                         MINI3940
0268          END                                                                 MINI3950
```

```
0001            SUBROUTINE NONLIN (NP,TH,PHI,G,H,NOHESS,NOGRAD)
          C
          C     ..................................................................
          C
0002            REAL*8 TH(1),PHI,G(1),H(1),XI(20),FI,GI(100),HI(5050),DEI,AID1,
               1AID2
0003            REAL*4 YEXP(1000),WGHT(1000),X(1)
0004            INTEGER*4 ND,NV,NP,NOHESS,NOGRAD,M,I,J,JJ,KK,JI
0005            COMMON/A/ND,NV,YEXP,WGHT,X
          C
          C     ..................................................................
          C
0006            M=NP*(NP+1)/2
0007            PHI=0.D0
0008            IF (NOGRAD.EQ.1) GO TO 14
0009            DO 12 J=1,NP
0010         12 G(J)=0.D0
0011         14 IF (NOHESS.EQ.1) GO TO 18
0012            DO 16 J=1,M
0013         16 H(J)=0.D0
0014         18 DO 30 I=1,ND
0015            DO 20 J=1,NV
0016            K=(J-1)*ND+I
0017         20 XI(J)=X(K)
0018            CALL MODEL (XI,TH,FI,GI,HI,NOHESS,NOGRAD)
0019            DEI=(YEXP(I)-FI)*WGHT(I)
0020            IF(DABS(DEI).LT.1.0D-30) DEI=0.0D0
0021            PHI=PHI+DEI*(YEXP(I)-FI)
0022            IF(NOGRAD.EQ.1) GO TO 24
0023            DO 22 J=1,NP
0024            IF(DABS(GI(J)).LT.1.0D-30) GI(J)=0.0D0
0025            AID1=DEI*GI(J)
0026         22 G(J)=G(J)-AID1-AID1
0027         24 IF(NOHESS.EQ.1) GO TO 30
0028            DO 28 J=1,M
0029            IF(DABS(HI(J)).LT.1.0D-30) HI(J)=0.0D0
0030            JJ=0
0031            KK=J
0032         26 JJ=JJ+1
0033            KK=KK-JJ
0034            IF(KK.GT.0) GO TO 26
0035            JI=J-JJ*(JJ-1)/2
0036            AID1=DEI*HI(J)
0037            AID2=WGHT(I)*GI(JI)*GI(JJ)
0038         28 H(J)=H(J)-AID1-AID1+AID2+AID2
0039         30 CONTINUE
0040            RETURN
          C
          C     ..................................................................
          C
0041            END
```

```
          C      MAIN PROGRAM
          C
0001             REAL*8 TH(4),PHI,YANAL(1000)
0002             COMMON/A/ND,NV,YEXP(1000),WGHT(1000),X(500,1)
0003             COMMON/B/EPSF,EPSX,EPSG,IMAX,NIT,IRIT
          C
0004             EPSF=0.
0005             EPSX=0.
0006             EPSG=0.
0007             IMAX=0
0008             NIT=-1
0009             IRIT=3
0010             IXR=169703951
0011             IXG=841978415
0012             AM=0.
0013             S=0.25
0014             ND=500
0015             NV=1
0016             NP=4
0017             FF=2.37
0018             DO 12 I=1,ND
0019             CALL RANDU(IXR,IXR,XI)
          C      XI IS NOW A RANDOM NUMBER WITH HOMOGENEOUS DISTRIBUTION BETWEEN
          C      0 AND 1
0020             XI=XI*10.-5.
0021          12 X(I,1)=XI
0022             DO 18 I=1,ND
0023             CALL GAUSZ(IXG,S,AM,V)
          C      V IS NOW A RANDOM NUMBER HAVING GAUSS DISTRIBUTICN WITH A MEAN
          C      'AM' AND A VARIANCE 'S'
0024             YEXP(I)=SINH(X(I,1))+V
0025          18 WGHT(I)=1.
0026             DO 20 K=1,NP
0027          20 TH(K)=3.0
0028             CALL DATFIT(NP,TH,PHI,YANAL,FF)
          C
0029             STOP
0030             END
```

```
0001            SUBROUTINE MODEL (XI,TH,FI,GI,HI,NOHESS,NOGRAD)
          C
          C     THIS SUBROUTINE MUST BE PROGRAMMED IN DOUBLE PRECISION
          C
0002            REAL*8 XI(1),TH(1),FI,GI(1),HI(1),GP(4)
          C
0003            GP(1)=DEXP(TH(2)*XI(1))
0004            GP(2)=TH(1)*GP(1)
0005            GP(3)=DEXP(-TH(4)*XI(1))
0006            GP(4)=TH(3)*GP(3)
0007            FI=GP(2)+GP(4)
0008            IF(NOGRAD.EQ.1) GO TO 5000
0009            GI(1)=GP(1)
0010            GI(2)=XI(1)*GP(2)
0011            GI(3)=GP(3)
0012            GI(4)=-XI(1)*GP(4)
0013       5000 IF(NOHESS.EQ.1) GO TO 4000
0014            DO3000 I=1,10
0015       3000 HI(I)=0.D0
0016            HI(2)=XI(1)*GI(1)
0017            HI(3)=XI(1)*GI(2)
0018            HI(9)=-XI(1)*GI(3)
0019            HI(10)=-XI(1)*GI(4)
0020       4000 RETURN
          C
0021            END
```

NUMBER OF PARAMETERS 4
NUMBER OF DATA 500
NUMBER OF IND. VAR. 1

VARIANCE RATIO STATISTIC F(1-A),NP,ND-NP) = 0.237E 01

THE INITIAL VALUES OF THE PARAMETERS ARE

0.3000000000D 01 0.3000000000D 01 0.3000000000D 01 0.3000000000D 01

EXPERIMENTAL DATA X(I,J),J=1,NV	YEXP(I)	WGHT(I)	I
-0.243240E 01	-0.554337E 01	0.100000E 01	1
0.133401E 01	0.201142E 01	0.100000E 01	2
-0.258965E 01	-0.694325E 01	0.100000E 01	3
0.242887E 00	-0.197423E 00	0.100000E 01	4
-0.255322E 01	-0.630987E 01	0.100000E 01	5
0.102700E 01	0.172460E 01	0.100000E 01	6
0.367767E 01	0.201085E 02	0.100000E 01	7
0.379743E 01	0.220056E 02	0.100000E 01	8
-0.177368E 00	0.757754E-01	0.100000E 01	9
-0.401436E 01	-0.280714E 02	0.100000E 01	10
-0.111991E 01	-0.132387E 01	0.100000E 01	11
0.381364E 01	0.225253E 02	0.100000E 01	12
-0.477211E 01	-0.591323E 02	0.100000E 01	13
-0.404950E 01	-0.293943E 02	0.100000E 01	14
0.217691E 01	0.404915E 01	0.100000E 01	15
-0.537528E 00	0.950556E-01	0.100000E 01	16
-0.237605E 01	-0.553698E 01	0.100000E 01	17
-0.128882E 01	-0.148650E 01	0.100000E 01	18
-0.244011E 01	-0.589898E 01	0.100000E 01	19
0.275928E 00	0.439964E 00	0.100000E 01	20
-0.132670E 01	-0.146950E 01	0.100000E 01	21
-0.372673E 01	-0.210305E 02	0.100000E 01	22
0.214913E 01	0.440362E 01	0.100000E 01	23
-0.381300E 00	-0.449046E 00	0.100000E 01	24
-0.400359E 01	-0.269237E 02	0.100000E 01	25
0.282225E 01	0.862647E 01	0.100000E 01	26
-0.215160E 01	-0.449002E 01	0.100000E 01	27
0.183175E 01	0.256297E 01	0.100000E 01	28
-0.837125E 00	-0.944424E 00	0.100000E 01	29
0.323419E 01	0.127348E 02	0.100000E 01	30
0.109694E 00	0.393398E 00	0.100000E 01	31
0.179771E 01	0.331243E 01	0.100000E 01	32
-0.283295E 01	-0.886194E 01	0.100000E 01	33
0.683398E 00	0.119255E 01	0.100000E 01	34
-0.244265E 01	-0.559712E 01	0.100000E 01	35
-0.432179E 01	-0.382027E 02	0.100000E 01	36
0.113798E 01	0.127318E 01	0.100000E 01	37
0.349691E 01	0.166081E 02	0.100000E 01	38
-0.377860E 01	-0.217050E 02	0.100000E 01	39
0.157306E 01	0.270395E 01	0.100000E 01	40
-0.396623E 01	-0.264315E 02	0.100000E 01	41
-0.419415E 01	-0.331045E 02	0.100000E 01	42
0.213033E 01	0.409532E 01	0.100000E 01	43
-0.114870E 01	-0.184481E 01	0.100000E 01	44
-0.492973E 01	-0.690826E 02	0.100000E 01	45
-0.225634E 01	-0.461605E 01	0.100000E 01	46
-0.398673E 01	-0.268654E 02	0.100000E 01	47
0.490410E 01	0.679730E 02	0.100000E 01	48
0.634153E 00	0.279759E 00	0.100000E 01	49
-0.305875E 01	-0.104375E 02	0.100000E 01	50

EXPERIMENTAL DATA X(I,J),J=1,NV	YEXP(I)	WGHT(I)	I
0.386149E 01	0.237091E 02	0.100000E 01	51
-0.193039E 01	-0.324556E 01	0.100000E 01	52
-0.456959E 01	-0.480780E 02	0.100000E 01	53
0.426896E 01	0.363323E 02	0.100000E 01	54
-0.290071E 01	-0.918810E 01	0.100000E 01	55
-0.452038E 01	-0.456447E 02	0.100000E 01	56
-0.238584E 01	-0.560207E 01	0.100000E 01	57
0.117544E 01	0.163781E 01	0.100000E 01	58
-0.388568E 01	-0.248900E 02	0.100000E 01	59
0.457811E 01	0.486432E 02	0.100000E 01	60
0.365686E 01	0.191473E 02	0.100000E 01	61
-0.242661E 01	-0.550736E 01	0.100000E 01	62
0.897160E 00	0.138233E 01	0.100000E 01	63
-0.293832E 01	-0.927564E 01	0.100000E 01	64
0.269690E 01	0.773859E 01	0.100000E 01	65
-0.977818E 00	-0.756522E 00	0.100000E 01	66
0.254040E 01	0.618953E 01	0.100000E 01	67
0.399188E 01	0.269518E 02	0.100000E 01	68
-0.387543E 01	-0.238516E 02	0.100000E 01	69
0.195734E 01	0.339115E 01	0.100000E 01	70
-0.652975E 00	-0.806147E 00	0.100000E 01	71
0.829331E 00	0.122890E 01	0.100000E 01	72
-0.384861E 01	-0.231651E 02	0.100000E 01	73
-0.428308E 01	-0.366237E 02	0.100000E 01	74
0.129816E 01	0.152797E 01	0.100000E 01	75
0.113986E 01	0.159801E 01	0.100000E 01	76
-0.288620E 01	-0.875321E 01	0.100000E 01	77
0.114744E 00	0.381137E 00	0.100000E 01	78
-0.336974E 01	-0.147786E 02	0.100000E 01	79
-0.227764E 01	-0.475103E 01	0.100000E 01	80
0.326129E 01	0.129588E 02	0.100000E 01	81
-0.268948E 01	-0.760733E 01	0.100000E 01	82
0.427159E 01	0.355468E 02	0.100000E 01	83
-0.913715E-01	0.570740E 00	0.100000E 01	84
-0.322119E 01	-0.128532E 02	0.100000E 01	85
-0.327315E 01	-0.131988E 02	0.100000E 01	86
-0.411182E 01	-0.304904E 02	0.100000E 01	87
-0.421496E 01	-0.339475E 02	0.100000E 01	88
-0.206341E 00	-0.429806E 00	0.100000E 01	89
0.176305E 01	0.259742E 01	0.100000E 01	90
0.128904E 01	0.184329E 01	0.100000E 01	91
-0.191389E 01	-0.341254E 01	0.100000E 01	92
0.411664E 01	0.304961E 02	0.100000E 01	93
-0.294405E 01	-0.969667E 01	0.100000E 01	94
0.940834E 00	0.111043E 01	0.100000E 01	95
0.250991E 01	0.566641E 01	0.100000E 01	96
0.246770E 01	0.602068E 01	0.100000E 01	97
-0.496252E 01	-0.713307E 02	0.100000E 01	98
-0.658081E 00	-0.636079E 00	0.100000E 01	99
-0.279463E 01	-0.823633E 01	0.100000E 01	100

EXPERIMENTAL DATA X(I,J),J=1,NV	YEXP(I)	WGHT(I)	I
0.493586E 01	0.695800E 02	0.100000E 01	101
0.539155E 00	0.800329E 00	0.100000E 01	102
0.300572E 01	0.993192E 01	0.100000E 01	103
0.218147E 01	0.462196E 01	0.100000E 01	104
0.442353E 01	0.415154E 02	0.100000E 01	105
0.219347E 01	0.454618E 01	0.100000E 01	106
-0.319650E 01	-0.121832E 02	0.100000E 01	107
-0.261170E 01	-0.696987E 01	0.100000E 01	108
0.482529E 01	0.623572E 02	0.100000E 01	109
-0.617883E 00	-0.832492E 00	0.100000E 01	110
0.241654E 01	0.534337E 01	0.100000E 01	111
-0.178001E 01	-0.335358E 01	0.100000E 01	112
-0.430910E 01	-0.373172E 02	0.100000E 01	113
0.348112E 01	0.163286E 02	0.100000E 01	114
0.264762E 01	0.723510E 01	0.100000E 01	115
-0.281054E 01	-0.820358E 01	0.100000E 01	116
-0.287719E 01	-0.904902E 01	0.100000E 01	117
0.215280E 01	0.437898E 01	0.100000E 01	118
-0.465803E 01	-0.527666E 02	0.100000E 01	119
0.525205E 00	0.620485E 00	0.100000E 01	120
-0.134204E 01	-0.178000E 01	0.100000E 01	121
-0.456531E 01	-0.481923E 02	0.100000E 01	122
0.667477E 00	0.681623E 00	0.100000E 01	123
-0.156026E 01	-0.218160E 01	0.100000E 01	124
-0.411597E 01	-0.307295E 02	0.100000E 01	125
0.237523E 01	0.569818E 01	0.100000E 01	126
-0.449561E 01	-0.447158E 02	0.100000E 01	127
-0.217988E 01	-0.443049E 01	0.100000E 01	128
-0.145999E 01	-0.218810E 01	0.100000E 01	129
-0.303361E 01	-0.105860E 02	0.100000E 01	130
-0.130568E 01	-0.148400E 01	0.100000E 01	131
-0.390983E 01	-0.248347E 02	0.100000E 01	132
0.385113E 01	0.231913E 02	0.100000E 01	133
0.212321E 01	0.423763E 01	0.100000E 01	134
0.898647E 00	0.634402E 00	0.100000E 01	135
0.499471E 01	0.736140E 02	0.100000E 01	136
-0.115175E 01	-0.154560E 01	0.100000E 01	137
0.460103E 00	0.879084E 00	0.100000E 01	138
0.281627E 01	0.839522E 01	0.100000E 01	139
0.305562E 01	0.110590E 02	0.100000E 01	140
-0.457847E 01	-0.489248E 02	0.100000E 01	141
0.614135E 00	0.499565E 00	0.100000E 01	142
-0.448921E 01	-0.445087E 02	0.100000E 01	143
-0.455029E 01	-0.473483E 02	0.100000E 01	144
0.165853E 01	0.307295E 01	0.100000E 01	145
-0.213487E 01	-0.404096E 01	0.100000E 01	146
-0.340299E 01	-0.153235E 02	0.100000E 01	147
0.586014E-01	0.239680E 00	0.100000E 01	148
0.461668E 01	0.502534E 02	0.100000E 01	149
-0.219732E 01	-0.480721E 01	0.100000E 01	150

EXPERIMENTAL DATA

X(I,J),J=1,NV	YEXP(I)	WGHT(I)	I
-0.396317E 01	-0.263745E 02	0.100000E 01	151
-0.155966E 01	-0.238545E 01	0.100000E 01	152
0.408010E 01	0.295902E 02	0.100000E 01	153
0.178997E 01	0.263739E 01	0.100000E 01	154
-0.470544E 01	-0.551155E 02	0.100000E 01	155
0.472987E 00	0.356572E 00	0.100000E 01	156
-0.194918E 01	-0.356636E 01	0.100000E 01	157
0.297458E 01	0.922031E 01	0.100000E 01	158
0.360150E 01	0.186816E 02	0.100000E 01	159
0.142005E 01	0.154157E 01	0.100000E 01	160
-0.327564E 01	-0.129932E 02	0.100000E 01	161
0.159604E 01	0.221246E 01	0.100000E 01	162
-0.491996E 01	-0.685807E 02	0.100000E 01	163
0.167763E 00	0.431187E 00	0.100000E 01	164
0.289969E 01	0.918328E 01	0.100000E 01	165
-0.165963E 01	-0.214809E 01	0.100000E 01	166
0.476986E 00	0.962471E 00	0.100000E 01	167
-0.261570E 01	-0.677800E 01	0.100000E 01	168
0.117359E 01	0.121901E 01	0.100000E 01	169
0.449143E 01	0.446338E 02	0.100000E 01	170
-0.274361E 01	-0.794895E 01	0.100000E 01	171
0.235079E 01	0.493912E 01	0.100000E 01	172
-0.130684E 00	-0.288285E-01	0.100000E 01	173
-0.237084E 01	-0.541598E 01	0.100000E 01	174
0.180168E 01	0.317983E 01	0.100000E 01	175
-0.278572E 01	-0.809091E 01	0.100000E 01	176
-0.550264E 00	-0.336569E 00	0.100000E 01	177
0.162468E 01	0.231881E 01	0.100000E 01	178
-0.252284E 01	-0.621371E 01	0.100000E 01	179
-0.258747E 01	-0.681986E 01	0.100000E 01	180
0.116475E 01	0.128755E 01	0.100000E 01	181
-0.317663E 00	-0.265830E 00	0.100000E 01	182
0.229894E 01	0.547974E 01	0.100000E 01	183
-0.297932E 01	-0.990692E 01	0.100000E 01	184
-0.316857E 00	-0.421533E 00	0.100000E 01	185
-0.821499E 00	-0.953394E 00	0.100000E 01	186
-0.347967E-01	0.140981E-01	0.100000E 01	187
-0.223018E 01	-0.431397E 01	0.100000E 01	188
0.345881E 01	0.156316E 02	0.100000E 01	189
-0.295264E 01	-0.970468E 01	0.100000E 01	190
-0.200416E 01	-0.371952E 01	0.100000E 01	191
0.487431E 00	0.349096E 00	0.100000E 01	192
-0.341870E 01	-0.151628E 02	0.100000E 01	193
0.446352E 01	0.430591E 02	0.100000E 01	194
-0.326852E 01	-0.131682E 02	0.100000E 01	195
-0.229036E 01	-0.492837E 01	0.100000E 01	196
-0.413917E 01	-0.319743E 02	0.100000E 01	197
-0.428508E 00	-0.343587E 00	0.100000E 01	198
0.294191E 01	0.969053E 01	0.100000E 01	199
-0.378455E 01	-0.220201E 02	0.100000E 01	200

EXPERIMENTAL DATA X(I,J),J=1,NV	YEXP(I)	WGHT(I)	I
-0.310241E 01	-0.110788E 02	0.100000E 01	201
-0.298794E 01	-0.987907E 01	0.100000E 01	202
0.179379E 01	0.317238E 01	0.100000E 01	203
-0.176721E 01	-0.290132E 01	0.100000E 01	204
0.288545E 01	0.883908E 01	0.100000E 01	205
0.299554E 01	0.999437E 01	0.100000E 01	206
0.927882E 00	0.827548E 00	0.100000E 01	207
0.664110E-01	-0.701111E-01	0.100000E 01	208
-0.999470E-01	-0.530404E 00	0.100000E 01	209
0.467188E 01	0.536059E 02	0.100000E 01	210
0.395504E 00	0.302704E 00	0.100000E 01	211
-0.310228E 01	-0.111349E 02	0.100000E 01	212
0.242129E 01	0.543849E 01	0.100000E 01	213
0.254764E 01	0.655295E 01	0.100000E 01	214
0.220447E 01	0.434355E 01	0.100000E 01	215
0.250646E 01	0.602376E 01	0.100000E 01	216
0.284012E 01	0.822849E 01	0.100000E 01	217
0.469989E 01	0.550862E 02	0.100000E 01	218
0.322434E 01	0.125108E 02	0.100000E 01	219
0.266424E 01	0.730141E 01	0.100000E 01	220
-0.130022E 01	-0.156633E 01	0.100000E 01	221
0.153694E 01	0.207491E 01	0.100000E 01	222
-0.479892E 01	-0.606199E 02	0.100000E 01	223
0.950000E 00	0.159270E 01	0.100000E 01	224
0.142138E 01	0.196500E 01	0.100000E 01	225
-0.144047E 00	-0.341568E 00	0.100000E 01	226
-0.436891E 01	-0.395804E 02	0.100000E 01	227
-0.426272E 01	-0.359885E 02	0.100000E 01	228
0.263853E 00	0.557501E 00	0.100000E 01	229
0.494744E 01	0.707221E 02	0.100000E 01	230
0.324458E 01	0.125496E 02	0.100000E 01	231
-0.289658E 01	-0.905612E 01	0.100000E 01	232
-0.473169E 01	-0.567456E 02	0.100000E 01	233
-0.503390E 00	-0.300107E 00	0.100000E 01	234
0.184839E 01	0.335378E 01	0.100000E 01	235
0.241062E 01	0.540537E 01	0.100000E 01	236
0.293672E 01	0.889244E 01	0.100000E 01	237
-0.196834E 01	-0.345877E 01	0.100000E 01	238
-0.372193E 01	-0.205016E 02	0.100000E 01	239
-0.691150E 00	-0.320702E 00	0.100000E 01	240
-0.160497E 01	-0.239871E 01	0.100000E 01	241
-0.433117E 01	-0.379719E 02	0.100000E 01	242
0.420946E 01	0.339081E 02	0.100000E 01	243
0.491068E 01	0.681344E 02	0.100000E 01	244
-0.220939E 01	-0.447329E 01	0.100000E 01	245
-0.955629E-01	-0.456176E 00	0.100000E 01	246
-0.242042E 01	-0.588684E 01	0.100000E 01	247
-0.112081E 00	-0.750074E-01	0.100000E 01	248
0.467409E 01	0.535423E 02	0.100000E 01	249
0.420374E 01	0.334785E 02	0.100000E 01	250

EXPERIMENTAL DATA X(I,J),J=1,NV	YEXP(I)	WGHT(I)	I
-0.263313E 01	-0.696656E 01	0.100000E 01	251
-0.375977E 01	-0.214054E 02	0.100000E 01	252
0.411555E 01	0.309448E 02	0.100000E 01	253
0.213667E 01	0.397371E 01	0.100000E 01	254
-0.451912E 01	-0.457627E 02	0.100000E 01	255
-0.251451E 01	-0.603031E 01	0.100000E 01	256
-0.169485E 01	-0.256484E 01	0.100000E 01	257
0.810442E 00	0.714845E 00	0.100000E 01	258
-0.248874E 01	-0.567504E 01	0.100000E 01	259
0.221643E-01	-0.515722E 00	0.100000E 01	260
-0.261195E 01	-0.714418E 01	0.100000E 01	261
0.234906E 01	0.505066E 01	0.100000E 01	262
0.861807E-01	0.373876E 00	0.100000E 01	263
0.441343E 01	0.415939E 02	0.100000E 01	264
-0.716218E 00	-0.802063E 00	0.100000E 01	265
0.216968E 01	0.426816E 01	0.100000E 01	266
-0.340990E 01	-0.152369E 02	0.100000E 01	267
-0.465675E 01	-0.525215E 02	0.100000E 01	268
0.223993E 01	0.455030E 01	0.100000E 01	269
0.280585E 01	0.828195E 01	0.100000E 01	270
0.499091E 01	0.732698E 02	0.100000E 01	271
-0.100567E 01	-0.947337E 00	0.100000E 01	272
0.387022E 01	0.242804E 02	0.100000E 01	273
0.202763E 01	0.405386E 01	0.100000E 01	274
0.152646E 01	0.205837E 01	0.100000E 01	275
-0.340213E 01	-0.152274E 02	0.100000E 01	276
0.427010E 00	0.366140E 00	0.100000E 01	277
0.400860E 01	0.274530E 02	0.100000E 01	278
0.400046E 01	0.278971E 02	0.100000E 01	279
0.290529E 01	0.938576E 01	0.100000E 01	280
0.580854E-01	0.114014E 00	0.100000E 01	281
0.228967E 01	0.509465E 01	0.100000E 01	282
-0.156226E 01	-0.193707E 01	0.100000E 01	283
-0.166824E 01	-0.277791E 01	0.100000E 01	284
0.379790E 01	0.218959E 02	0.100000E 01	285
0.328992E 01	0.136313E 02	0.100000E 01	286
0.284893E 01	0.897149E 01	0.100000E 01	287
0.352164E 01	0.166586E 02	0.100000E 01	288
-0.195686E 01	-0.341368E 01	0.100000E 01	289
-0.885901E 00	-0.996076E 00	0.100000E 01	290
0.185443E 01	0.287016E 01	0.100000E 01	291
-0.491422E 01	-0.682112E 02	0.100000E 01	292
0.226272E 01	0.473207E 01	0.100000E 01	293
-0.159278E 01	-0.257177E 01	0.100000E 01	294
-0.408212E 01	-0.296916E 02	0.100000E 01	295
0.126071E 01	0.146637E 01	0.100000E 01	296
-0.430793E 01	-0.373499E 02	0.100000E 01	297
0.400588E 01	0.271996E 02	0.100000E 01	298
-0.106115E 01	-0.134990E 01	0.100000E 01	299
-0.376032E 01	-0.214951E 02	0.100000E 01	300

EXPERIMENTAL DATA X(I,J),J=1,NV	YEXP(I)	WGHT(I)	I
-0.323813E 01	-0.130041E 02	0.100000E 01	301
-0.386352E 01	-0.237495E 02	0.100000E 01	302
-0.204492E 01	-0.348715E 01	0.100000E 01	303
0.192558E 01	0.296209E 01	0.100000E 01	304
-0.988833E 00	-0.180190E 01	0.100000E 01	305
-0.895863E-01	-0.265581E 00	0.100000E 01	306
-0.129608E 01	-0.164896E 01	0.100000E 01	307
-0.414421E 01	-0.310045E 02	0.100000E 01	308
-0.276522E 01	-0.779713E 01	0.100000E 01	309
-0.413402E 01	-0.310767E 02	0.100000E 01	310
0.793268E 00	0.509542E 00	0.100000E 01	311
0.404880E 01	0.283736E 02	0.100000E 01	312
-0.238484E 01	-0.539270E 01	0.100000E 01	313
0.230729E 01	0.523467E 01	0.100000E 01	314
-0.376814E 01	-0.217030E 02	0.100000E 01	315
-0.247718E 01	-0.601074E 01	0.100000E 01	316
-0.441136E 01	-0.408600E 02	0.100000E 01	317
-0.180997E 01	-0.300624E 01	0.100000E 01	318
-0.493111E 01	-0.691148E 02	0.100000E 01	319
0.123618E 01	0.156369E 01	0.100000E 01	320
-0.480408E 01	-0.609587E 02	0.100000E 01	321
-0.469597E 01	-0.540395E 02	0.100000E 01	322
0.189303E 01	0.329277E 01	0.100000E 01	323
0.419962E 01	0.334290E 02	0.100000E 01	324
0.366716E 01	0.192033E 02	0.100000E 01	325
-0.149722E 01	-0.246710E 01	0.100000E 01	326
-0.305916E 01	-0.106316E 02	0.100000E 01	327
-0.489491E 00	-0.664239E 00	0.100000E 01	328
0.499120E 01	0.732888E 02	0.100000E 01	329
0.272982E 01	0.782339E 01	0.100000E 01	330
-0.443543E 01	-0.417354E 02	0.100000E 01	331
0.305888E 01	0.111330E 02	0.100000E 01	332
-0.378065E 01	-0.224203E 02	0.100000E 01	333
-0.440808E 01	-0.408924E 02	0.100000E 01	334
-0.190752E 00	-0.248227E 00	0.100000E 01	335
-0.344663E 00	-0.584310E-02	0.100000E 01	336
0.253416E 00	0.433757E 00	0.100000E 01	337
0.422927E 01	0.344346E 02	0.100000E 01	338
-0.415075E 01	-0.318882E 02	0.100000E 01	339
-0.466909E 01	-0.532056E 02	0.100000E 01	340
-0.113179E 01	-0.124009E 01	0.100000E 01	341
-0.476756E 01	-0.587531E 02	0.100000E 01	342
0.103418E 01	0.134247E 01	0.100000E 01	343
0.455869E 01	0.481442E 02	0.100000E 01	344
-0.281629E 00	0.587996E-01	0.100000E 01	345
-0.364379E 01	-0.191207E 02	0.100000E 01	346
0.429416E 01	0.366736E 02	0.100000E 01	347
0.114740E 01	0.139661E 01	0.100000E 01	348
0.107955E 01	0.133864E 01	0.100000E 01	349
-0.121962E 01	-0.172318E 01	0.100000E 01	350

EXPERIMENTAL DATA X(I,J),J=1,NV	YEXP(I)	WGHT(I)	I
0.365443E 01	0.193288E 02	0.100000E 01	351
0.155684E 01	0.214114E 01	0.100000E 01	352
-0.192597E 01	-0.327028E 01	0.100000E 01	353
-0.133265E 01	-0.154449E 01	0.100000E 01	354
0.460946E 01	0.502108E 02	0.100000E 01	355
-0.614845E 00	-0.735534E 00	0.100000E 01	356
0.413067E 01	0.310450E 02	0.100000E 01	357
-0.323339E 01	-0.128789E 02	0.100000E 01	358
0.310625E 01	0.114391E 02	0.100000E 01	359
-0.221947E 00	0.165501E 00	0.100000E 01	360
0.142924E 01	0.210396E 01	0.100000E 01	361
0.481611E 01	0.615744E 02	0.100000E 01	362
-0.311283E 01	-0.111872E 02	0.100000E 01	363
0.250984E 01	0.613433E 01	0.100000E 01	364
0.407915E 01	0.300730E 02	0.100000E 01	365
-0.250948E 01	-0.645164E 01	0.100000E 01	366
-0.105791E 01	-0.132213E 01	0.100000E 01	367
0.248634E 01	0.598689E 01	0.100000E 01	368
-0.221749E 01	-0.469641E 01	0.100000E 01	369
-0.135367E 01	-0.157022E 01	0.100000E 01	370
-0.318011E 01	-0.121665E 02	0.100000E 01	371
-0.358027E 01	-0.176400E 02	0.100000E 01	372
-0.268385E 00	-0.423265E 00	0.100000E 01	373
0.613834E 00	0.930450E 00	0.100000E 01	374
0.154937E 01	0.210543E 01	0.100000E 01	375
0.442519E 01	0.414557E 02	0.100000E 01	376
0.249075E 01	0.567498E 01	0.100000E 01	377
-0.471397E 01	-0.557997E 02	0.100000E 01	378
-0.804567E-01	0.405326E 00	0.100000E 01	379
-0.471051E 01	-0.554705E 02	0.100000E 01	380
-0.438756E 01	-0.404137E 02	0.100000E 01	381
-0.424568E 01	-0.347873E 02	0.100000E 01	382
0.386924E 01	0.242329E 02	0.100000E 01	383
0.416136E 01	0.320484E 02	0.100000E 01	384
-0.126199E 01	-0.161627E 01	0.100000E 01	385
-0.275884E 01	-0.825370E 01	0.100000E 01	386
0.736156E 00	0.728979E 00	0.100000E 01	387
0.141388E 01	0.182639E 01	0.100000E 01	388
-0.674648E-01	-0.132912E 00	0.100000E 01	389
-0.392046E 01	-0.252183E 02	0.100000E 01	390
-0.188473E 01	-0.333890E 01	0.100000E 01	391
0.142858E 01	0.200590E 01	0.100000E 01	392
0.300422E 01	0.986084E 01	0.100000E 01	393
-0.451064E 01	-0.452362E 02	0.100000E 01	394
-0.292342E 01	-0.930094E 01	0.100000E 01	395
0.515394E-01	-0.104874E 00	0.100000E 01	396
-0.244192E 01	-0.579263E 01	0.100000E 01	397
-0.309936E 01	-0.112013E 02	0.100000E 01	398
-0.250773E 01	-0.622055E 01	0.100000E 01	399
-0.528686E 00	-0.863089E 00	0.100000E 01	400

EXPERIMENTAL DATA X(I,J),J=1,NV	YEXP(I)	WGHT(I)	I
-0.446599E 01	-0.433382E 02	0.100000E 01	401
-0.442632E 01	-0.420343E 02	0.100000E 01	402
-0.776752E 00	-0.102476E 01	0.100000E 01	403
-0.731275E 00	-0.621044E 00	0.100000E 01	404
-0.202072E 01	-0.368319E 01	0.100000E 01	405
-0.733971E 00	-0.703811E 00	0.100000E 01	406
0.291501E 01	0.937096E 01	0.100000E 01	407
0.238855E 01	0.601404E 01	0.100000E 01	408
-0.419465E 01	-0.335940E 02	0.100000E 01	409
-0.130364E 01	-0.175707E 01	0.100000E 01	410
0.415295E 01	0.318722E 02	0.100000E 01	411
0.478306E 01	0.594913E 02	0.100000E 01	412
-0.172089E 01	-0.302268E 01	0.100000E 01	413
-0.144479E 01	-0.211775E 01	0.100000E 01	414
0.472697E 01	0.562470E 02	0.100000E 01	415
-0.252252E 01	-0.658325E 01	0.100000E 01	416
0.299840E 01	0.103668E 02	0.100000E 01	417
-0.218742E 01	-0.397055E 01	0.100000E 01	418
0.475554E 01	0.579904E 02	0.100000E 01	419
-0.192731E 00	-0.105574E 00	0.100000E 01	420
0.110207E 01	0.127118E 01	0.100000E 01	421
-0.192754E 01	-0.354766E 01	0.100000E 01	422
-0.580930E 00	-0.798274E 00	0.100000E 01	423
0.257732E 01	0.640065E 01	0.100000E 01	424
0.146421E 01	0.183770E 01	0.100000E 01	425
-0.127582E 01	-0.141267E 01	0.100000E 01	426
0.405271E 01	0.291086E 02	0.100000E 01	427
-0.107029E 00	-0.799800E-01	0.100000E 01	428
-0.237707E 01	-0.540438E 01	0.100000E 01	429
-0.235936E 01	-0.539198E 01	0.100000E 01	430
0.134847E 01	0.160046E 01	0.100000E 01	431
-0.158700E 01	-0.242205E 01	0.100000E 01	432
0.119345E 01	0.119265E 01	0.100000E 01	433
-0.382656E 01	-0.229161E 02	0.100000E 01	434
0.441676E 01	0.412999E 02	0.100000E 01	435
0.277438E 01	0.805409E 01	0.100000E 01	436
-0.448450E 01	-0.443266E 02	0.100000E 01	437
-0.280512E 01	-0.840145E 01	0.100000E 01	438
-0.542727E 00	-0.444930E 00	0.100000E 01	439
-0.406102E 01	-0.290335E 02	0.100000E 01	440
0.328522E 01	0.131425E 02	0.100000E 01	441
0.493682E 01	0.697235E 02	0.100000E 01	442
0.178929E 01	0.276748E 01	0.100000E 01	443
0.321210E 01	0.127329E 02	0.100000E 01	444
0.192134E 01	0.358327E 01	0.100000E 01	445
-0.462359E 01	-0.509573E 02	0.100000E 01	446
-0.100870E 01	-0.653039E 00	0.100000E 01	447
-0.131708E 01	-0.190563E 01	0.100000E 01	448
0.415771E 00	0.397817E 00	0.100000E 01	449
-0.408129E 01	-0.300986E 02	0.100000E 01	450

EXPERIMENTAL DATA X(I,J),J=1,NV	YEXP(I)	WGHT(I)	I
0.490002E 01	0.673277E 02	0.100000E 01	451
0.283682E 01	0.832154E 01	0.100000E 01	452
0.141855E 01	0.194283E 01	0.100000E 01	453
0.312621E 01	0.114658E 02	0.100000E 01	454
-0.178117E 01	-0.271349E 01	0.100000E 01	455
0.895023E-01	-0.337666E-02	0.100000E 01	456
0.230723E 01	0.489474E 01	0.100000E 01	457
-0.275482E 01	-0.745760E 01	0.100000E 01	458
-0.514505E 00	-0.594274E 00	0.100000E 01	459
0.499312E 01	0.738312E 02	0.100000E 01	460
-0.100950E 01	-0.127028E 01	0.100000E 01	461
0.227887E 01	0.450569E 01	0.100000E 01	462
0.149355E 00	-0.311281E 00	0.100000E 01	463
-0.413586E 01	-0.312424E 02	0.100000E 01	464
-0.380362E 01	-0.226604E 02	0.100000E 01	465
0.357717E 00	0.676181E 00	0.100000E 01	466
-0.249217E 01	-0.592276E 01	0.100000E 01	467
0.458319E 01	0.491892E 02	0.100000E 01	468
-0.200542E 01	-0.385186E 01	0.100000E 01	469
-0.843749E 00	-0.902797E 00	0.100000E 01	470
-0.747674E 00	-0.545539E 00	0.100000E 01	471
0.131673E 01	0.208181E 01	0.100000E 01	472
0.230341E 01	0.466832E 01	0.100000E 01	473
0.110701E 01	0.948851E 00	0.100000E 01	474
0.137350E 01	0.201331E 01	0.100000E 01	475
0.291059E 01	0.927796E 01	0.100000E 01	476
0.313095E 01	0.112168E 02	0.100000E 01	477
0.316127E 01	0.119469E 02	0.100000E 01	478
0.317591E 01	0.120877E 02	0.100000E 01	479
0.370543E 01	0.200208E 02	0.100000E 01	480
0.430065E 01	0.370029E 02	0.100000E 01	481
-0.415334E 01	-0.316739E 02	0.100000E 01	482
0.315204E 01	0.115672E 02	0.100000E 01	483
-0.247600E 01	-0.575475E 01	0.100000E 01	484
-0.158870E 01	-0.240087E 01	0.100000E 01	485
0.371663E 00	0.510537E 00	0.100000E 01	486
-0.534282E 00	-0.805686E 00	0.100000E 01	487
-0.419626E 00	-0.182469E 00	0.100000E 01	488
0.478134E 01	0.593804E 02	0.100000E 01	489
0.252696E 01	0.617216E 01	0.100000E 01	490
-0.120515E 01	-0.167372E 01	0.100000E 01	491
-0.293904E 01	-0.943684E 01	0.100000E 01	492
0.127589E 00	-0.196805E 00	0.100000E 01	493
0.213371E 01	0.430789E 01	0.100000E 01	494
-0.271640E 01	-0.788723E 01	0.100000E 01	495
-0.287255E 01	-0.900640E 01	0.100000E 01	496
-0.427165E 01	-0.356456E 02	0.100000E 01	497
-0.321138E 01	-0.121960E 02	0.100000E 01	498
-0.264610E 01	-0.730739E 01	0.100000E 01	499
0.109162E 01	0.942934E 00	0.100000E 01	500

```
MINIM          EPSX= 0.1000D-07     EPSF= 0.1000D-07     EPSG= 0.1000D-07     IMAX= 40      NIT= 3         MINIM

ITERATION=  1                    GRADIENT METHOD      EXTERNAL SUB ITR= 6    INTERNAL SUB ITR= 4     NEG-D=  2          0 1

 F(OLD)= 0.167072533303515D 16     G*S=-0.137942791343867D 33     S*H*S= 0.119186394224327D 50   G*H*G= 0.119186394224327D 50
 F(NEW)= 0.183021548563025D 07   GNORM= 0.746219429839031D 07     SNORM= 0.117449049099542D 17     DAX = 0.428566660939949D 01
 D(LOW)=-0.962444174738219D 17  D(SML)= 0.146836835166925D 15   LAMBDA= 0.364895811609955D-15

XOLD(I)= 0.3000000000D 01      0.3000000000D 01     0.3000000000D 01     0.3000000000D 01
XNEW(I)= 0.2754314891D 01     -0.5993328474D 00     0.2839257527D 01     0.6922864075D 00

      G= 0.3466160080D 06     -0.4041859604D 07     0.5146677152D 06     0.6242010027D 07
      S=-0.6733020804D 15     -0.9864001539D 16    -0.4405160824D 15    -0.6324308252D 16
      D= 0.2244363105D 15     -0.9624441747D 17     0.1468368352D 15    -0.6043845751D 17

ITERATION=  2                    GRADIENT METHOD      EXTERNAL SUB ITR= 5    INTERNAL SUB ITR= 4     NEG-D=  2          0 1

 F(OLD)= 0.183021548563025D 07     G*S=-0.556843437469289D 14     S*H*S= 0.229068323262996D 22   G*H*G= 0.229068323262996D 22
 F(NEW)= 0.173713374337898D 06   GNORM= 0.283204247822698D 05     SNORM= 0.746219429839031D 07     DAX = 0.152341886636118D 01
 D(LOW)=-0.103559914315928D 09  D(SML)= 0.359055274208586D 05   LAMBDA= 0.204151594751399D-06

XOLD(I)= 0.2754314891D 01     -0.5993328474D 00     0.2839257527D 01     0.6922864075D 00
XNEW(I)= 0.2683552680D 01      0.2258192366D 00     0.2734187292D 01    -0.5820298939D 00

      G= 0.8842587156D 04     -0.1279668280D 05     0.1014418472D 05    -0.2138213128D 05
      S=-0.3466160080D 06      0.4041859604D 07    -0.5146677152D 06    -0.6242010027D 07
      D= 0.3590552742D 05     -0.7574702379D 08     0.6159739319D 05    -0.1035599143D 09

ITERATION=  3                    GRADIENT METHOD      EXTERNAL SUB ITR= 2    INTERNAL SUB ITR= 1     NEG-D=  1          0 1

 F(OLD)= 0.173713374337898D 06     G*S=-0.802046459848202D 09     S*H*S= 0.149137146711136D 16   G*H*G= 0.149137146711136D 16
 F(NEW)= 0.173486345473600D 06   GNORM= 0.330099923548388D 05     SNORM= 0.283204247822698D 05     DAX = 0.190380942465764D-01
 D(LOW)=-0.444839133201076D 06  D(SML)= 0.196902812169111D 04   LAMBDA= 0.672239007463450D-06

XOLD(I)= 0.2683552680D 01      0.2258192366D 00     0.2734187292D 01    -0.5820298939D 00
XNEW(I)= 0.2677608348D 01      0.2344216660D 00     0.2727367975D 01    -0.5676559912D 00

      G= 0.7904749089D 04     -0.2119886906D 05     0.6285985367D 04     0.2320062231D 05
      S=-0.8842587156D 04      0.1279668280D 05    -0.1014418472D 05     0.2138213128D 05
      D= 0.1969028122D 04      0.3073768177D 06     0.2044035442D 04    -0.4448391332D 06
```

```
MINIM         EPSX= 0.1000D-07     EPSF= 0.1000D-07     EPSG= 0.1000D-07     IMAX= 40     NIT= 3          MINIM

ITERATION=  4  MODIFIED NEWTON RAPHSON  METHOD       EXTERNAL SUB ITR= 5   INTERNAL SUB ITR= 2    NEG-D=  1          1 1

 F(OLD)= 0.173486345473600D 06     G*S=-0.111096366467890D 05     S*H*S=-0.103600960104796D 04   G*H*G= 0.240639588490676D 16
 F(NEW)= 0.144349889029756D 06   GNORM= 0.158054469864013D 07     SNORM= 0.275665340280052D 01    DAX = 0.949594205531327D 01
 D(LOW)=-0.103600960104796D 04  D(SML)=-0.103600960104796D 04   LAMBDA= 0.344473557889658D 01

XOLD(I)= 0.2677608348D 01     0.2344216660D 00     0.2727367975D 01    -0.5676559912D 00
XNEW(I)=-0.6159096635D 01    -0.2339343380D 00     0.6172103554D 01    -0.5676559912D 00

      G= 0.1250748908D 05     0.2018545664D 06     0.6360621728D 05    -0.1566261182D 07
      S=-0.2565278170D 01    -0.1359628317D 00     0.1000000000D 01     0.0
      D= 0.2068707314D 04     0.2897034822D 06    -0.1036009601D 04     0.1761116761D 06

ITERATION=  5  MODIFIED NEWTON RAPHSON  METHOD       EXTERNAL SUB ITR= 4   INTERNAL SUB ITR= 1    NEG-D=  2          1 1

 F(OLD)= 0.144349889029756D 06     G*S=-0.613975210306322D 06     S*H*S=-0.898786175964675D 07   G*H*G= 0.571510606864031D 20
 F(NEW)= 0.741840167058295D 05   GNORM= 0.356229326729319D 06     SNORM= 0.393486885252030D 02    DAX = 0.500000000000000D 01
 D(LOW)=-0.854288661742431D 07  D(SML)= 0.234957895809745D 04   LAMBDA= 0.127069038064572D 00

XOLD(I)=-0.6159096635D 01    -0.2339343380D 00     0.6172103554D 01    -0.5676559912D 00
XNEW(I)=-0.4214705751D 01    -0.2759699997D 00     0.1567602435D 01    -0.6947250293D 00

      G= 0.1229804001D 05     0.2638346562D 06    -0.3218183526D 05     0.2368621858D 06
      S= 0.1530184626D 02    -0.3308096322D 00    -0.3623621607D 02    -0.1000000000D 01
      D= 0.2349578958D 04    -0.4449751422D 06     0.2498668413D 05    -0.8542886617D 07

ITERATION=  6  MODIFIED NEWTON RAPHSON  METHOD       EXTERNAL SUB ITR= 2   INTERNAL SUB ITR= 1    NEG-D=  1          1 1

 F(OLD)= 0.741840167058295D 05     G*S=-0.345450124305755D 06     S*H*S=-0.555936074196765D 06   G*H*G= 0.121486242044293D 18
 F(NEW)= 0.291980874834586D 05   GNORM= 0.246620115372809D 06     SNORM= 0.671137989894252D 01    DAX = 0.125000000000000D 01
 D(LOW)=-0.555936074196765D 06  D(SML)= 0.306308694233977D 04   LAMBDA= 0.186250818583069D 00

XOLD(I)=-0.4214705751D 01    -0.2759699997D 00     0.1567602435D 01    -0.6947250293D 00
XNEW(I)=-0.5450752122D 01    -0.4622208183D 00     0.1567602435D 01    -0.6947250293D 00

      G=-0.9626347372D 04    -0.1032458915D 06    -0.3110053450D 05     0.2215893891D 06
      S=-0.6636461418D 01    -0.1000000000D 01     0.0                  0.0
      D= 0.3063086942D 04    -0.5559360742D 06     0.7051865249D 05     0.7199554711D 06
```

```
MINIM         EPSX= 0.1000D-07     EPSF= 0.1000D-07     EPSG= 0.1000D-07     IMAX= 40     NIT= 3          MINIM

ITERATION=  7  MODIFIED NEWTON RAPHSON  METHOD        EXTERNAL SUB ITR= 3    INTERNAL SUB ITR= 1     NEG-D=  1          1 1

 F(OLD)= 0.291980874834586D 05      G*S=-0.117205431849394D 06     S*H*S=-0.258299402412452D 06    G*H*G= 0.178629615298427D 18
 F(NEW)= 0.179979204649912D 05    GNORM= 0.241169470413729D 06     SNORM= 0.229226506620760D 02     DAX = 0.264301499238050D 01
 D(LOW)=-0.258299402412452D 06  D(SML)= 0.118809275650328D 05    LAMBDA= 0.115301455810833D 00

XOLD(I)=-0.5450752122D 01    -0.4622208183D 00    0.1567602435D 01    -0.6947250293D 00
XNEW(I)=-0.2810253339D 01    -0.5775222741D 00    0.1567602435D 01    -0.6947250293D 00

      G= 0.5971888507D 04     0.1180775127D 06   -0.2751339822D 05     0.2083932914D 06
      S= 0.2290082779D 02    -0.1000000000D 01    0.0                  0.0
      D= 0.1188092757D 05    -0.2582994024D 06    0.7690683083D 05     0.6653728275D 06

ITERATION=  8           NEWTON RAPHSON  METHOD        EXTERNAL SUB ITR= 1    INTERNAL SUB ITR= 0     NEG-D=  0          1 0

 F(OLD)= 0.179979204649912D 05      G*S=-0.266877721954030D 05     S*H*S= 0.266877721954030D 05    G*H*G= 0.159019356139823D 18
 F(NEW)= 0.864447448432081D 04    GNORM= 0.218758645986766D 06     SNORM= 0.109902609732055D 01     DAX = 0.109902609732055D 01
 D(LOW)= 0.299947543458397D 05  D(SML)= 0.299947543458397D 05    LAMBDA= 0.100000000000000D 01

XOLD(I)=-0.2810253339D 01    -0.5775222741D 00    0.1567602435D 01    -0.6947250293D 00
XNEW(I)=-0.1742451320D 01    -0.7021973540D 00    0.1369893516D 01    -0.8088500451D 00

      G= 0.6289308193D 04     0.7261073557D 05    0.3619208487D 05    -0.2030605916D 06
      S= 0.1067802019D 01    -0.1246750799D 00   -0.1977089192D 00    -0.1141250159D 00
      D= 0.2999475435D 05     0.4334750193D 06    0.7103258761D 05     0.6401552480D 06

ITERATION=  9  MODIFIED NEWTON RAPHSON  METHOD        EXTERNAL SUB ITR= 2    INTERNAL SUB ITR= 1     NEG-D=  1          1 1

 F(OLD)= 0.864447448432081D 04      G*S=-0.473504993837432D 05     S*H*S=-0.919528387914794D 06    G*H*G= 0.381870100899534D 18
 F(NEW)= 0.424204088465262D 04    GNORM= 0.759597025984163D 05     SNORM= 0.696631880520692D 01     DAX = 0.553460416499691D 00
 D(LOW)=-0.919528387914794D 06  D(SML)= 0.851572589458487D 05    LAMBDA= 0.794480459444392D-01

XOLD(I)=-0.1742451320D 01    -0.7021973540D 00    0.1369893516D 01    -0.8088500451D 00
XNEW(I)=-0.1684120764D 01    -0.7098099237D 00    0.8253331104D 00    -0.8882980911D 00

      G= 0.6374444310D 04     0.7373110246D 05   -0.2711563817D 04     0.1690014290D 05
      S= 0.7341974966D 00    -0.9581821183D-01   -0.6854295777D 01    -0.1000000000D 01
      D= 0.8515725895D 05     0.3063086926D 06    0.1945035802D 06    -0.9195283879D 06
```

```
MINIM          EPSX= 0.1000D-07     EPSF= 0.1000D-07     EPSG= 0.1000D-07     IMAX= 40      NIT= 3          MINIM

ITERATION= 10             NEWTON RAPHSON  METHOD        EXTERNAL SUB ITR= 1    INTERNAL SUB ITR= 0     NEG-D=  0            1 0

  F(OLD)= 0.4242040884652620D 04      G*S=-0.4010420704848880D 04      S*H*S= 0.4010420704848880D 04    G*H*G= 0.2613293588505520D 17
  F(NEW)= 0.2167043403963720D 04    GNORM= 0.9979232388527530D 05      SNORM= 0.6561570151704430D 00     DAX = 0.6561570151704430D 00
  D(LOW)= 0.9085697324520510D 05   D(SML)= 0.9085697324520510D 05     LAMBDA= 0.1000000000000000D 01

XOLD(I)=-0.1684120764D 01     -0.7098099237D 00     0.8253331104D 00     -0.8882980911D 00
XNEW(I)=-0.1077206688D 01     -0.8107262534D 00     0.6056326702D 00     -0.9494940354D 00

      G= 0.1459979801D 05      0.8367941666D 05    -0.1701287436D 05      0.4953454490D 05
      S= 0.6069140762D 00     -0.1009163297D 00    -0.2197004402D 00     -0.6119594429D-01
      D= 0.9085697325D 05      0.3160651967D 06     0.3961933691D 06      0.1329454830D 06

ITERATION= 11             NEWTON RAPHSON  METHOD        EXTERNAL SUB ITR= 1    INTERNAL SUB ITR= 0     NEG-D=  0            1 0

  F(OLD)= 0.2167043403963720D 04      G*S=-0.2641223531594450D 04      S*H*S= 0.2641223531594450D 04    G*H*G= 0.4884544596136500D 17
  F(NEW)= 0.6867812414414690D 03    GNORM= 0.6071585661325790D 04      SNORM= 0.1855272278013560D 00     DAX = 0.1855272278013560D 00
  D(LOW)= 0.2164681834116010D 06   D(SML)= 0.2164681834116010D 06     LAMBDA= 0.1000000000000000D 01

XOLD(I)=-0.1077206688D 01     -0.8107262534D 00     0.6056326702D 00     -0.9494940354D 00
XNEW(I)=-0.9028657317D 00     -0.8667255292D 00     0.5820149781D 00     -0.9677113093D 00

      G=-0.1356092631D 04      0.5046979381D 04     0.1633333190D 04     -0.2624002103D 04
      S= 0.1743409559D 00     -0.5599927577D-01    -0.2361769208D-01     -0.1821727389D-01
      D= 0.2164681834D 06      0.3684707640D 06     0.6895318265D 06      0.2726126285D 06

ITERATION= 12             NEWTON RAPHSON  METHOD        EXTERNAL SUB ITR= 1    INTERNAL SUB ITR= 1     NEG-D=  0            1 0

  F(OLD)= 0.6867812414414690D 03      G*S=-0.1545387157186080D 04      S*H*S= 0.1545387157186080D 04    G*H*G= 0.1831887664332600D 15
  F(NEW)= 0.4631487641160260D 03    GNORM= 0.6090551753237880D 05      SNORM= 0.5888513802321440D 00     DAX = 0.2665580505795620D 00
  D(LOW)= 0.5559173888590400D 05   D(SML)= 0.5559173888590400D 05     LAMBDA= 0.4526745788971000D 00

XOLD(I)=-0.9028657317D 00     -0.8667255292D 00     0.5820149781D 00     -0.9677113093D 00
XNEW(I)=-0.6510941720D 00     -0.9302107335D 00     0.5254479086D 00     -0.9885456926D 00

      G= 0.1851510609D 05      0.5780002897D 05    -0.1753961881D 04      0.4770029425D 04
      S= 0.5561866547D 00     -0.1402446863D 00    -0.1249618869D 00     -0.4602507915D-01
      D= 0.3527163678D 06      0.7615641318D 05     0.8135523195D 06      0.5559173889D 05
```

```
MINIM   .     EPSX= 0.1000D-07     EPSF= 0.1000D-07     EPSG= 0.1000D-07     IMAX= 40     NIT= 3          MINIM

ITERATION= 13            NEWTON RAPHSON  METHOD       EXTERNAL SUB ITR= 1    INTERNAL SUB ITR= 0     NEG-D=  0            1 0

 F(OLD)= 0.463148764116026D 03     G*S=-0.742925894766403D 03     S*H*S= 0.742925894766403D 03   G*H*G= 0.203083465622430D 17
 F(NEW)= 0.893500890480312D 02    GNORM= 0.370345423477093D 04     SNORM= 0.478389294193340D-01    DAX = 0.478389294193340D-01
 D(LOW)= 0.901025353994276D 05  D(SML)= 0.901025353994276D 05    LAMBDA= 0.100000000000000D 01

XOLD(I)=-0.6510941720D 00    -0.9302107335D 00     0.5254479086D 00    -0.9885456926D 00
XNEW(I)=-0.6133744984D 00    -0.9550264112D 00     0.5111374230D 00    -0.9952674135D 00

      G=-0.2161973861D 04    -0.2972411544D 04    -0.1362535556D 03     0.4331822672D 03
      S= 0.3771967360D-01    -0.2481567775D-01    -0.1431048558D-01    -0.6721720873D-02
      D= 0.6163455843D 06     0.2933553860D 06     0.9839542963D 06     0.9010253540D 05

ITERATION= 14            NEWTON RAPHSON  METHOD       EXTERNAL SUB ITR= 1    INTERNAL SUB ITR= 1     NEG-D=  0            1 0

 F(OLD)= 0.893500890480312D 02     G*S=-0.175737068940713D 03     S*H*S= 0.175737068940713D 03   G*H*G= 0.824866160241155D 14
 F(NEW)= 0.399008827995078D 02    GNORM= 0.913984851717824D 04     SNORM= 0.171465061215198D 00    DAX = 0.803721718046543D-01
 D(LOW)= 0.504301926123845D 05  D(SML)= 0.504301926123845D 05    LAMBDA= 0.468737894676880D 00

XOLD(I)=-0.6133744984D 00    -0.9550264112D 00     0.5111374230D 00    -0.9952674135D 00
XNEW(I)=-0.5379622292D 00    -0.9822493615D 00     0.5059698270D 00    -0.9974770696D 00

      G= 0.3198553691D 04     0.8555992691D 04    -0.1009615320D 03     0.3014648311D 03
      S= 0.1608836625D 00    -0.5807712707D-01    -0.1102448955D-01    -0.4714054749D-02
      D= 0.7675357457D 06     0.5043019261D 05     0.1046084765D 07     0.7129857836D 05

ITERATION= 15            NEWTON RAPHSON  METHOD       EXTERNAL SUB ITR= 1    INTERNAL SUB ITR= 0     NEG-D=  0            1 0

 F(OLD)= 0.399008827995078D 02     G*S=-0.197977528940376D 02     S*H*S= 0.197977528940376D 02   G*H*G= 0.547527670559511D 15
 F(NEW)= 0.289561755910604D 02    GNORM= 0.750437348092376D 03     SNORM= 0.218224102316449D-01    DAX = 0.218224102316449D-01
 D(LOW)= 0.710746900222725D 05  D(SML)= 0.710746900222725D 05    LAMBDA= 0.100000000000000D 01

XOLD(I)=-0.5379622292D 00    -0.9822493615D 00     0.5059698270D 00    -0.9974770696D 00
XNEW(I)=-0.5185917290D 00    -0.9917935864D 00     0.5030933020D 00    -0.9987556179D 00

      G= 0.1960186529D 03     0.7240528800D 03    -0.8119107216D 01     0.2035701902D 02
      S= 0.1937050018D-01    -0.9544224928D-02    -0.2876524949D-02    -0.1278548355D-02
      D= 0.9770711211D 06     0.1018595287D 06     0.1067513043D 07     0.7107469002D 05
```

```
MINIM          EPSX= 0.1000D-07     EPSF= 0.1000D-07     EPSG= 0.1000D-07     IMAX= 40       NIT= 3          MINIM

ITERATION= 16            NEWTON RAPHSON  METHOD       EXTERNAL SUB ITR= 1    INTERNAL SUB ITR= 0     NEG-D=  0              1 0

 F(OLD)= 0.289561755910604D 02     G*S=-0.110864332554301D 01     S*H*S= 0.110864332554301D 01    G*H*G= 0.373459958530580D 13
 F(NEW)= 0.283881280223563D 02   GNORM= 0.198238801099036D 03     SNORM= 0.972453975496087D-02     DAX = 0.972453975496087D-02
 D(LOW)= 0.694104370167826D 05  D(SML)= 0.694104370167826D 05    LAMBDA= 0.100000000000000D 01

XOLD(I)=-0.5185917290D 00    -0.9917935864D 00     0.5030933020D 00    -0.9987556179D 00
XNEW(I)=-0.5097118150D 00    -0.9957283113D 00     0.5026518337D 00    -0.9989475705D 00

      G= 0.7668355463D 02     0.1828054409D 03    -0.2275402594D 00     0.6113354542D 00
      S= 0.8879914060D-02    -0.3934724854D-02    -0.4414682846D-03    -0.1919526192D-03
      D= 0.1063535487D 07     0.6941043702D 05     0.1080034472D 07     0.6988321798D 05

ITERATION= 17            NEWTON RAPHSON  METHOD       EXTERNAL SUB ITR= 1    INTERNAL SUB ITR= 0     NEG-D=  0              1 0

 F(OLD)= 0.283881280223563D 02     G*S=-0.655278172223445D-02     S*H*S= 0.655278172223445D-02    G*H*G= 0.267696776570367D 12
 F(NEW)= 0.283848480168340D 02   GNORM= 0.895937121449538D-01     SNORM= 0.270673881574149D-03     DAX = 0.270673881574149D-03
 D(LOW)= 0.674252034551892D 05  D(SML)= 0.674252034551892D 05    LAMBDA= 0.100000000000000D 01

XOLD(I)=-0.5097118150D 00    -0.9957283113D 00     0.5026518337D 00    -0.9989475705D 00
XNEW(I)=-0.5094771086D 00    -0.9958626097D 00     0.5026409410D 00    -0.9989523172D 00

      G= 0.4981528868D-02     0.8945402364D-01    -0.1536179916D-03     0.4143456832D-03
      S= 0.2347064175D-03    -0.1342984142D-03    -0.1089276870D-04    -0.4746712794D-05
      D= 0.1101399129D 07     0.6742520346D 05     0.1081931175D 07     0.6981028706D 05

ITERATION= 18            NEWTON RAPHSON  METHOD       EXTERNAL SUB ITR= 1    INTERNAL SUB ITR= 0     NEG-D=  0              1 0

 F(OLD)= 0.283848480168340D 02     G*S=-0.918909541263904D-07     S*H*S= 0.918909541263904D-07    G*H*G= 0.480698336991940D 05
 F(NEW)= 0.283848479709884D 02   GNORM= 0.183747505783269D-04     SNORM= 0.290905963420095D-05     DAX = 0.290905963420095D-05
 D(LOW)= 0.666529430963253D 05  D(SML)= 0.666529430963253D 05    LAMBDA= 0.100000000000000D 01

XOLD(I)=-0.5094771086D 00    -0.9958626097D 00     0.5026409410D 00    -0.9989523172D 00
XNEW(I)=-0.5094744507D 00    -0.9958637849D 00     0.5026408197D 00    -0.9989523691D 00

      G= 0.7348338286D-05     0.1684133997D-04    -0.1804319716D-07     0.4822517688D-07
      S= 0.2657836747D-05    -0.1175220324D-05    -0.1212461068D-06    -0.5184931939D-07
      D= 0.1102715279D 07     0.6665294310D 05     0.1081977350D 07     0.6980607838D 05
```

```
MINIM        EPSX= 0.1000D-07     EPSF= 0.1000D-07     EPSG= 0.1000D-07     IMAX= 40      NIT= 3          MINIM

ITERATION= 19           NEWTON RAPHSON  METHOD       EXTERNAL SUB ITR= 1    INTERNAL SUB ITR= 0     NEG-D=  0            1 0

 F(OLD)= 0.283848479708884D 02      G*S=-0.495394380717392D-16     S*H*S= 0.495394380717392D-16   G*H*G= 0.230174902542005D-02
 F(NEW)= 0.283848479708885D 02    GNORM= 0.104989277317143D-09     SNORM= 0.292743519627740D-11    DAX = 0.292743519627740D-11
 D(LOW)= 0.666526586412853D 05  D(SML)= 0.666526586412853D 05    LAMBDA= 0.100000000000000D 01

XOLD(I)=-0.5094744507D 00   -0.9958637849D 00     0.5026408197D 00    -0.9989523691D 00
XNEW(I)=-0.5094744507D 00   -0.9958637849D 00     0.5026408197D 00    -0.9989523691D 00

      G= 0.2926869858D-10    0.6864300794D-10    -0.2952527112D-10     0.6769407257D-10
      S=-0.3289221236D-13   -0.2927168724D-11     0.2176626824D-13     0.2102644811D-14
      D= 0.1102726803D 07    0.6665265864D 05     0.1081977863D 07     0.6980608111D 05
```

THE FINAL VALUES OF THE PARAMETERS ARE

```
   -0.5094744507D 00   -0.9958637849D 00    0.5026408197D 00   -0.9989523691D 00
```

THE VALUES OF THE GRADIENT ARE

```
    0.2926869858D-10    0.6864300794D-10   -0.2952527112D-10    0.6769407257D-10
```

THE VALUE OF THE FUNCTION PHI IS   0.2838484797D 02

MODIFIED STANDARD ERROR OF ESTIMATE   0.239223E 00

PARAMETER VARIATIONS CORRESPONDING TO A UNITARY DELTA

K	PARAMETER	MAXIMUM VARIATION ON THE AXIS	EXTREME VARIATION
1	-0.509474D 00	0.717504E-02	0.665697E-01
2	-0.995864D 00	0.314888E-02	0.292143E-01
3	0.502641D 00	0.724327E-02	0.658679E-01
4	-0.998952D 00	0.313606E-02	0.285175E-01

THE VARIANCE RATIO STATISTIC GIVES A DELTA 0.191129E-01

K	PARAMETER	MAXIMUM VALUES ON THE AXIS				EXTREME VALUES	
		LOWER	VIRT. DELTA	UPPER	VIRT. DELTA	LOWER	UPPER
1	-0.509474D 00	-0.5104664D 00	0.191129E-01	-0.5084825D 00	0.191129E-01	-0.5186777D 00	-0.5002712D 00
2	-0.995864D 00	-0.9962991D 00	0.191507E-01	-0.9954285D 00	0.190752E-01	-0.9999026D 00	-0.9918249D 00
3	0.502641D 00	0.5016394D 00	0.191129E-01	0.5036422D 00	0.191129E-01	0.4935346D 00	0.5117470D 00
4	-0.998952D 00	-0.9993859D 00	0.191516E-01	-0.9985188D 00	0.190743E-01	-0.1002895D 01	-0.9950098D 00

INVERSE OF HESSIAN MATRIX OF FUNCTION PHI

0.780616D-04				1
-0.340579D-04	0.150340D-04			2
-0.354114D-05	0.153151D-05	0.764243D-04		3
-0.151233D-05	0.653961D-06	0.328872D-04	0.143254D-04	4

PARAMETER CORRELATION MATRIX

0.100000D 01				1
-0.994175D 00	0.100000D 01			2
-0.458468D-01	0.451822D-01	0.100000D 01		3
-0.452247D-01	0.445617D-01	0.993935D 00	0.100000D 01	4

DATA PT.	EXPERIMENTAL	ANALYTICAL	RESIDUE
1	-0.554337E 01	-0.569865D 01	0.155287E 00
2	0.201142E 01	0.177054D 01	0.240882E 00
3	-0.694325E 01	-0.667867D 01	-0.264583E 00
4	-0.197423E 00	0.240653D 00	-0.438076E 00
5	-0.630987E 01	-0.643794D 01	0.128066E 00
6	0.172460E 01	0.121900D 01	0.505600E 00
7	0.201085E 02	0.197919D 02	0.316588E 00
8	0.220056E 02	0.223105D 02	-0.304822E 00
9	0.757754E-01	-0.186877D 00	0.262652E 00
10	-0.280714E 02	-0.277449D 02	-0.326511E 00
11	-0.132387E 01	-0.138991D 01	0.660326E-01
12	0.225253E 02	0.226750D 02	-0.149694E 00
13	-0.591323E 02	-0.590227D 02	-0.109537E 00
14	-0.293943E 02	-0.287337D 02	-0.660616E 00
15	0.404915E 01	0.436439D 01	-0.315243E 00
16	0.950556E-01	-0.576363D 00	0.671419E 00
17	-0.553698E 01	-0.538270D 01	-0.154284E 00
18	-0.148650E 01	-0.170009D 01	0.213592E 00
19	-0.589898E 01	-0.574327D 01	-0.155714E 00
20	0.439964E 00	0.275099D 00	0.164865E 00
21	-0.146950E 01	-0.177592D 01	0.306425E 00
22	-0.210305E 02	-0.208292D 02	-0.201363E 00
23	0.440362E 01	0.424174D 01	0.161874E 00
24	-0.449046E 00	-0.401363D 00	-0.476827E-01
25	-0.269237E 02	-0.274487D 02	0.524937E 00
26	0.862647E 01	0.839611D 01	0.230359E 00
27	-0.449002E 01	-0.428338D 01	-0.206637E 00
28	0.256297E 01	0.305066D 01	-0.487695E 00
29	-0.944424E 00	-0.954863D 00	0.104391E-01
30	0.127348E 02	0.126964D 02	0.383975E-01
31	0.393398E 00	0.104099D 00	0.289299E 00
32	0.331243E 01	0.294308D 01	0.369344E 00
33	-0.886194E 01	-0.852829D 01	-0.333653E 00
34	0.119255E 01	0.100344D 01	0.189110E 00
35	-0.559712E 01	-0.575800D 01	0.160878E 00
36	-0.382027E 02	-0.376887D 02	-0.513982E 00
37	0.127318E 01	0.140256D 01	-0.129382E 00
38	0.166081E 02	0.165175D 02	0.905744E-01
39	-0.217050E 02	-0.219347D 02	0.229776E 00
40	0.270395E 01	0.231308D 01	0.390866E 00
41	-0.264315E 02	-0.264455D 02	0.140177E-01
42	-0.331045E 02	-0.331884D 02	0.839218E-01
43	0.409532E 01	0.416056D 01	-0.652434E-01
44	-0.184481E 01	-0.143976D 01	-0.405048E 00
45	-0.690826E 02	-0.690556D 02	-0.270724E-01
46	-0.461605E 01	-0.476655D 01	0.150497E 00
47	-0.268654E 02	-0.269914D 02	0.126010E 00
48	0.679730E 02	0.674256D 02	0.547335E 00
49	0.279759E 00	0.676135D 00	-0.396376E 00
50	-0.104375E 02	-0.106922D 02	0.254691E 00

DATA PT.	EXPERIMENTAL	ANALYTICAL	RESIDUE
51	0.237091E 02	0.237862D 02	-0.770371E-01
52	-0.324556E 01	-0.341039D 01	0.164839E 00
53	-0.480780E 02	-0.482406D 02	0.162672E 00
54	0.363323E 02	0.357448D 02	0.587494E 00
55	-0.918810E 01	-0.912759D 01	-0.605093E-01
56	-0.456447E 02	-0.459331D 02	0.288427E 00
57	-0.560207E 01	-0.543634D 01	-0.165733E 00
58	0.163781E 01	0.146830D 01	0.169506E 00
59	-0.248900E 02	-0.244056D 02	-0.484440E 00
60	0.486432E 02	0.486827D 02	-0.394445E-01
61	0.191473E 02	0.193842D 02	-0.236861E 00
62	-0.550736E 01	-0.566536D 01	0.157999E 00
63	0.138233E 01	0.102313D 01	0.359192E 00
64	-0.927564E 01	-0.947802D 01	0.202382E 00
65	0.773859E 01	0.740025D 01	0.338346E 00
66	-0.756522E 00	-0.115979D 01	0.403272E 00
67	0.618953E 01	0.631836D 01	-0.128824E 00
68	0.269518E 02	0.270980D 02	-0.146240E 00
69	-0.238516E 02	-0.241574D 02	0.305774E 00
70	0.339115E 01	0.347910D 01	-0.879505E-01
71	-0.806147E 00	-0.714386D 00	-0.917608E-01
72	0.122890E 01	0.927876D 00	0.301025E 00
73	-0.231651E 02	-0.235202D 02	0.355029E 00
74	-0.366237E 02	-0.362629D 02	-0.360738E 00
75	0.152797E 01	0.169859D 01	-0.170621E 00
76	0.159801E 01	0.140581D 01	0.192200E 00
77	-0.875321E 01	-0.899584D 01	0.242629E 00
78	0.381137E 00	0.109227D 00	0.271910E 00
79	-0.147786E 02	-0.145886D 02	-0.189958E 00
80	-0.475103E 01	-0.487098D 01	0.119957E 00
81	0.129588E 02	0.130460D 02	-0.871283E-01
82	-0.760733E 01	-0.738425D 01	-0.223079E 00
83	0.355468E 02	0.358389D 02	-0.292086E 00
84	0.570740E 00	-0.992146D-01	0.669954E 00
85	-0.128532E 02	-0.125772D 02	-0.275986E 00
86	-0.131988E 02	-0.132473D 02	0.485030E-01
87	-0.304904E 02	-0.305745D 02	0.841166E-01
88	-0.339475E 02	-0.338834D 02	-0.641239E-01
89	-0.429806E 00	-0.216683D 00	-0.213124E 00
90	0.259742E 01	0.283706D 01	-0.239644E 00
91	0.184329E 01	0.168064D 01	0.162655E 00
92	-0.341254E 01	-0.335240D 01	-0.601398E-01
93	0.304961E 02	0.306974D 02	-0.201279E 00
94	-0.969667E 01	-0.953258D 01	-0.164095E 00
95	0.111043E 01	0.108693D 01	0.235027E-01
96	0.566641E 01	0.612632D 01	-0.459901E 00
97	0.602068E 01	0.586988D 01	0.150800E 00
98	-0.713307E 02	-0.713480D 02	0.173204E-01
99	-0.636079E 00	-0.720694D 00	0.846150E-01
100	-0.823633E 01	-0.820671D 01	-0.296215E-01

CATA PT.	EXPERIMENTAL	ANALYTICAL	RESIDUE
101	0.695800E 02	0.695992D 02	-0.191962E-01
102	0.800329E 00	0.563510D 00	0.236819E 00
103	0.993192E 01	0.100962D 02	-0.164303E 00
104	0.462196E 01	0.438486D 01	0.237099E 00
105	0.415154E 02	0.417155D 02	-0.200069E 00
106	0.454618E 01	0.443913D 01	0.107050E 00
107	-0.121832E 02	-0.122708D 02	0.875846E-01
108	-0.696987E 01	-0.682856D 01	-0.141304E 00
109	0.623572E 02	0.623205D 02	0.367254E-01
110	-0.832492E 00	-0.671520D 00	-0.160972E 00
111	0.534337E 01	0.557294D 01	-0.229572E 00
112	-0.335358E 01	-0.291407D 01	-0.439514E 00
113	-0.373172E 02	-0.372152D 02	-0.102034E 00
114	0.163286E 02	0.162585D 02	0.701126E-01
115	0.723510E 01	0.704138D 01	0.193714E 00
116	-0.820358E 01	-0.833869D 01	0.135107E 00
117	-0.904902E 01	-0.891504D 01	-0.133978E 00
118	0.437898E 01	0.425775D 01	0.121232E 00
119	-0.527666E 02	-0.526832D 02	-0.833654E-01
120	0.620485E 00	0.547424D 00	0.730612E-01
121	-0.178000E 01	-0.180736D 01	0.273544E-01
122	-0.481923E 02	-0.480355D 02	-0.156875E 00
123	0.681623E 00	0.717035D 00	-0.354121E-01
124	-0.218160E 01	-0.230375D 01	0.122148E 00
125	-0.307295E 02	-0.307011D 02	-0.284346E-01
126	0.569818E 01	0.534384D 01	0.354341E 00
127	-0.447158E 02	-0.448136D 02	0.978078E-01
128	-0.443049E 01	-0.440902D 01	-0.214728E-01
129	-0.218810E 01	-0.206364D 01	-0.124457E 00
130	-0.105860E 02	-0.104266D 02	-0.159425E 00
131	-0.148400E 01	-0.173353D 01	0.249527E 00
132	-0.248347E 02	-0.250001D 02	0.165380E 00
133	0.231913E 02	0.235411D 02	-0.349787E 00
134	0.423763E 01	0.413021D 01	0.107420E 00
135	0.634402E 00	0.102527D 01	-0.390873E 00
136	0.736140E 02	0.738143D 02	-0.200328E 00
137	-0.154560E 01	-0.144511D 01	-0.100489E 00
138	0.879084E 00	0.473716D 00	0.405367E 00
139	0.839522E 01	0.834574D 01	0.494756E-01
140	0.110590E 02	0.106148D 02	0.444145E 00
141	-0.489248E 02	-0.486693D 02	-0.255510E 00
142	0.499565E 00	0.651929D 00	-0.152364E 00
143	-0.445087E 02	-0.445289D 02	0.202261E-01
144	-0.473483E 02	-0.473220D 02	-0.263067E-01
145	0.307295E 01	0.313779D 01	-0.648475E-01
146	-0.404096E 01	-0.421063D 01	0.169666E 00
147	-0.153235E 02	-0.150809D 02	-0.242611E 00
148	0.239680E 00	0.523507D-01	0.187330E 00
149	0.502534E 02	0.505957D 02	-0.342370E 00
150	-0.480721E 01	-0.448826D 01	-0.318951E 00

DATA PT.	EXPERIMENTAL	ANALYTICAL	RESIDUE
151	-0.263745E 02	-0.263649D 02	-0.953374E-02
152	-0.238545E 01	-0.230226D 01	-0.831906E-01
153	0.295902E 02	0.295965D 02	-0.628825E-02
154	0.263739E 01	0.291912D 01	-0.281729E 00
155	-0.551155E 02	-0.552307D 02	0.115252E 00
156	0.356572E 00	0.488134D 00	-0.131562E 00
157	-0.356636E 01	-0.347755D 01	-0.888120E-01
158	0.922031E 01	0.978542D 01	-0.565108E 00
159	0.186816E 02	0.183400D 02	0.341626E 00
160	0.154157E 01	0.195263D 01	-0.411057E 00
161	-0.129932E 02	-0.132803D 02	0.287124E 00
162	0.221246E 01	0.237166D 01	-0.159200E 00
163	-0.685807E 02	-0.683868D 02	-0.193857E 00
164	0.431187E 00	0.163259D 00	0.267928E 00
165	0.918328E 01	0.907616D 01	0.107122E 00
166	-0.214809E 01	-0.256439D 01	0.416301E 00
167	0.962471E 00	0.492625D 00	0.469846E 00
168	-0.677800E 01	-0.685617D 01	0.781690E-01
169	0.121901E 01	0.146500D 01	-0.245993E 00
170	0.446338E 02	0.446439D 02	-0.100712E-01
171	-0.794895E 01	-0.779694D 01	-0.152011E 00
172	0.493912E 01	0.521262D 01	-0.273494E 00
173	-0.288285E-01	-0.139162D 00	0.110333E 00
174	-0.541598E 01	-0.535435D 01	-0.616325E-01
175	0.317983E 01	0.295546D 01	0.224365E 00
176	-0.809091E 01	-0.813364D 01	0.427375E-01
177	-0.336569E 00	-0.591184D 00	0.254615E 00
178	0.231881E 01	0.244645D 01	-0.127636E 00
179	-0.621371E 01	-0.624371D 01	0.299978E-01
180	-0.681986E 01	-0.666403D 01	-0.155831E 00
181	0.128755E 01	0.144933D 01	-0.161779E 00
182	-0.265830E 00	-0.333087D 00	0.672572E-01
183	0.547974E 01	0.494446D 01	0.535285E 00
184	-0.990692E 01	-0.987523D 01	-0.316898E-01
185	-0.421533E 00	-0.332231D 00	-0.893017E-01
186	-0.953394E 00	-0.933329D 00	-0.200645E-01
187	0.140981E-01	-0.419695D-01	0.560676E-01
188	-0.431397E 01	-0.464120D 01	0.327226E 00
189	0.156316E 02	0.158994D 02	-0.267727E 00
190	-0.970468E 01	-0.961493D 01	-0.897467E-01
191	-0.371952E 01	-0.368113D 01	-0.383864E-01
192	0.349096E 00	0.504394D 00	-0.155298E 00
193	-0.151628E 02	-0.153192D 02	0.156396E 00
194	0.430591E 02	0.434160D 02	-0.356874E 00
195	-0.131682E 02	-0.131861D 02	0.179173E-01
196	-0.492837E 01	-0.493439D 01	0.602362E-02
197	-0.319743E 02	-0.314191D 02	-0.555273E 00
198	-0.343587E 00	-0.453033D 00	0.109446E 00
199	0.969053E 01	0.946950D 01	0.221036E 00
200	-0.220201E 02	-0.220651D 02	0.450708E-01

DATA PT.	EXPERIMENTAL	ANALYTICAL	RESIDUE
201	-0.110788E 02	-0.111694D 02	0.906081E-01
202	-0.987907E 01	-0.996077D 01	0.817000E-01
203	0.317238E 01	0.293094D 01	0.241447E 00
204	-0.290132E 01	-0.287498D 01	-0.263396E-01
205	0.883908E 01	0.894713D 01	-0.108054E 00
206	0.999437E 01	0.999364D 01	0.730998E-03
207	0.827548E 00	0.106780D 01	-0.240254E 00
208	-0.701111E-01	0.602480D-01	-0.130359E 00
209	-0.530404E 00	-0.107914D 00	-0.422491E 00
210	0.536059E 02	0.534642D 02	0.141731E 00
211	0.302704E 00	0.402568D 00	-0.998631E-01
212	-0.111349E 02	-0.111679D 02	0.330239E-01
213	0.543849E 01	0.559989D 01	-0.161400E 00
214	0.655295E 01	0.636476D 01	0.188193E 00
215	0.434355E 01	0.448943D 01	-0.145878E 00
216	0.602376E 01	0.610497D 01	-0.812081E-01
217	0.822849E 01	0.854845D 01	-0.319958E 00
218	0.550862E 02	0.549816D 02	0.104614E 00
219	0.125108E 02	0.125717D 02	-0.608402E-01
220	0.730141E 01	0.716046D 01	0.140941E 00
221	-0.156633E 01	-0.172265D 01	0.156317E 00
222	0.207491E 01	0.222343D 01	-0.148519E 00
223	-0.606199E 02	-0.606202D 02	0.297050E-03
224	0.159270E 01	0.110058D 01	0.492118E 00
225	0.196500E 01	0.195555D 01	0.944407E-02
226	-0.341568E 00	-0.152785D 00	-0.188782E 00
227	-0.395804E 02	-0.395002D 02	-0.802191E-01
228	-0.359885E 02	-0.355349D 02	-0.453643E 00
229	0.557501E 00	0.262478D 00	0.295023E 00
230	0.707221E 02	0.704090D 02	0.313186E 00
231	0.125496E 02	0.128293D 02	-0.279777E 00
232	-0.905612E 01	-0.908992D 01	0.338039E-01
233	-0.567456E 02	-0.566939D 02	-0.516571E-01
234	-0.300107E 00	-0.537085D 00	0.236978E 00
235	0.335378E 01	0.310453D 01	0.249251E 00
236	0.540537E 01	0.553953D 01	-0.134158E 00
237	0.889244E 01	0.942026D 01	-0.527816E 00
238	-0.345877E 01	-0.354730D 01	0.885313E-01
239	-0.205016E 02	-0.207298D 02	0.228219E 00
240	-0.320702E 00	-0.762007D 00	0.441305E 00
241	-0.239871E 01	-0.241808D 01	0.193744E-01
242	-0.379719E 02	-0.380427D 02	0.708236E-01
243	0.339081E 02	0.336814D 02	0.226656E 00
244	0.681344E 02	0.678700D 02	0.264321E 00
245	-0.447329E 01	-0.454385D 01	0.705563E-01
246	-0.456176E 00	-0.103466D 00	-0.352711E 00
247	-0.588684E 01	-0.562998D 01	-0.256851E 00
248	-0.750074E-01	-0.120236D 00	0.452284E-01
249	0.535423E 02	0.535824D 02	-0.400182E-01
250	0.334785E 02	0.334894D 02	-0.108797E-01

DATA PT.	EXPERIMENTAL	ANALYTICAL	RESIDUE
251	-0.696656E 01	-0.697744D 01	0.108784E-01
252	-0.214054E 02	-0.215269D 02	0.121422E 00
253	0.309448E 02	0.306637D 02	0.281141E 00
254	0.397371E 01	0.418777D 01	-0.214056E 00
255	-0.457627E 02	-0.458754D 02	0.112723E 00
256	-0.603031E 01	-0.619144D 01	0.161139E 00
257	-0.256484E 01	-0.266268D 01	0.978423E-01
258	0.714845E 00	0.902126D 00	-0.187281E 00
259	-0.567504E 01	-0.603249D 01	0.357446E 00
260	-0.515722E 00	0.155418D-01	-0.531264E 00
261	-0.714418E 01	-0.683031D 01	-0.313864E 00
262	0.505066E 01	0.520346D 01	-0.152804E 00
263	0.373876E 00	0.802577D-01	0.293618E 00
264	0.415939E 02	0.412962D 02	0.297691E 00
265	-0.802063E 00	-0.793873D 00	-0.819030E-02
266	0.426816E 01	0.433214D 01	-0.639808E-01
267	-0.152369E 02	-0.151852D 02	-0.516299E-01
268	-0.525215E 02	-0.526159D 02	0.944704E-01
269	0.455030E 01	0.465532D 01	-0.105018E 00
270	0.828195E 01	0.825867D 01	0.232871E-01
271	0.732698E 02	0.735344D 02	-0.264570E 00
272	-0.947337E 00	-0.120293D 01	0.255596E 00
273	0.242804E 02	0.239948D 02	0.285599E 00
274	0.405386E 01	0.374236D 01	0.311495E 00
275	0.205837E 01	0.219798D 01	-0.139603E 00
276	-0.152274E 02	-0.150680D 02	-0.159490E 00
277	0.366140E 00	0.437039D 00	-0.708985E-01
278	0.274530E 02	0.275548D 02	-0.101765E 00
279	0.278971E 02	0.273316D 02	0.565528E 00
280	0.938576E 01	0.912735D 01	0.258412E 00
281	0.114014E 00	0.518291D-01	0.621852E-01
282	0.509465E 01	0.489794D 01	0.196703E 00
283	-0.193707E 01	-0.230877D 01	0.371698E 00
284	-0.277791E 01	-0.258813D 01	-0.189782E 00
285	0.218959E 02	0.223209D 02	-0.424918E 00
286	0.136313E 02	0.134255D 02	0.205725E 00
287	0.897149E 01	0.862451D 01	0.346984E 00
288	0.166586E 02	0.169314D 02	-0.272741E 00
289	-0.341368E 01	-0.350534D 01	0.916581E-01
290	-0.996076E 00	-0.102359D 01	0.275142E-01
291	0.287016E 01	0.312430D 01	-0.254146E 00
292	-0.682112E 02	-0.679967D 02	-0.214498E 00
293	0.473207E 01	0.476501D 01	-0.329473E-01
294	-0.257177E 01	-0.238645D 01	-0.185320E 00
295	-0.296916E 02	-0.296830D 02	-0.860890E-02
296	0.146637E 01	0.162578D 01	-0.159406E 00
297	-0.373499E 02	-0.371720D 02	-0.177875E 00
298	0.271996E 02	0.274800D 02	-0.280351E 00
299	-0.134990E 01	-0.129163D 01	-0.582685E-01
300	-0.214951E 02	-0.215387D 02	0.435080E-01

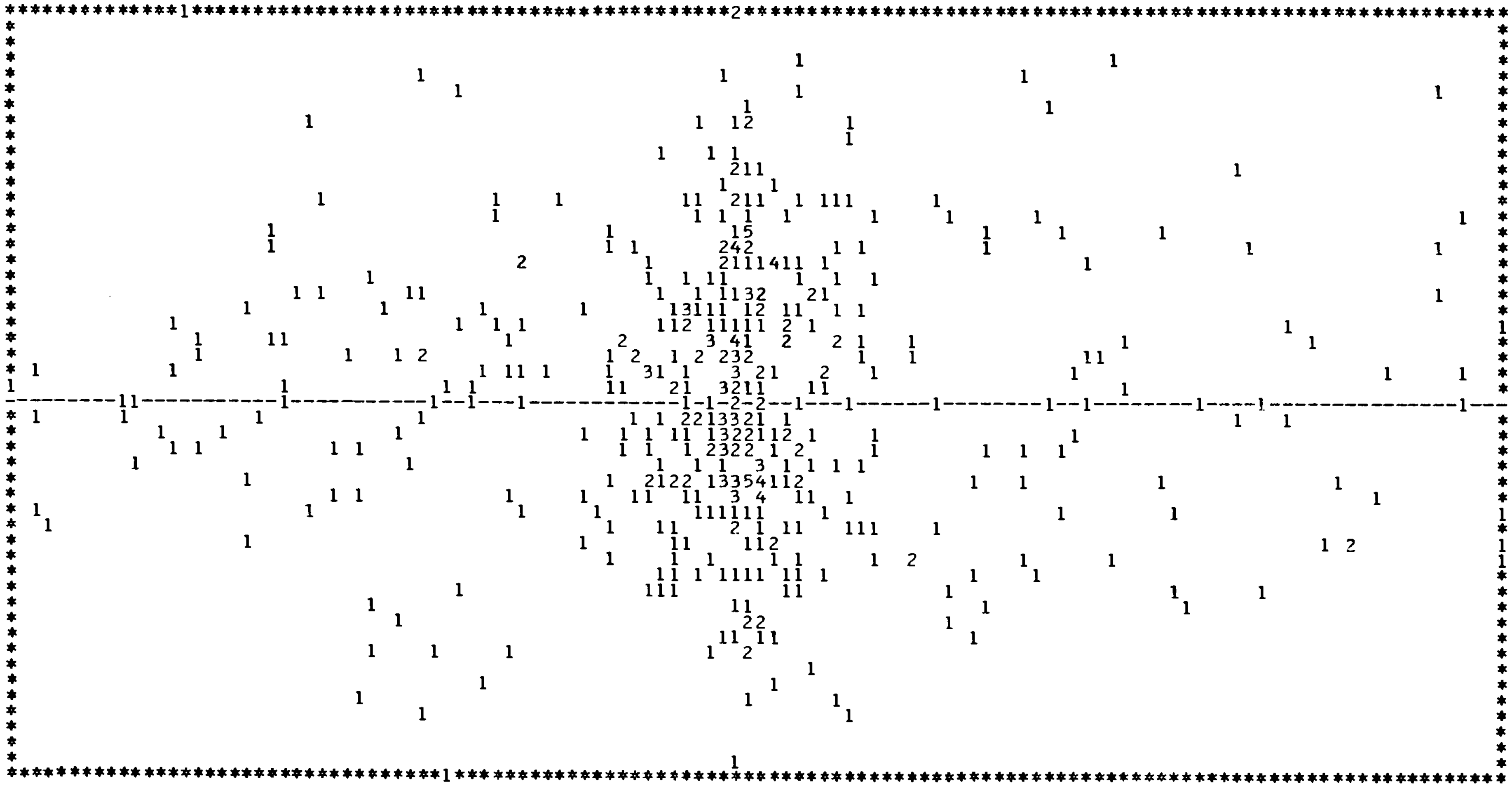
CATA PT.	EXPERIMENTAL	ANALYTICAL	RESIDUE
301	-0.130041E 02	-0.127919D 02	-0.212220E 00
302	-0.237495E 02	-0.238722D 02	0.122757E 00
303	-0.348715E 01	-0.383915D 01	0.351999E 00
304	0.296209E 01	0.336585D 01	-0.403760E 00
305	-0.180190E 01	-0.117675D 01	-0.625150E 00
306	-0.265581E 00	-0.974045D-01	-0.168176E 00
307	-0.164896E 01	-0.171444D 01	0.654786E-01
308	-0.310045E 02	-0.315775D 02	0.572964E 00
309	-0.779713E 01	-0.796800D 01	0.170864E 00
310	-0.310767E 02	-0.312584D 02	0.181745E 00
311	0.509542E 00	0.878994D 00	-0.369452E 00
312	0.283736E 02	0.286847D 02	-0.311048E 00
313	-0.539270E 01	-0.543080D 01	0.381000E-01
314	0.523467E 01	0.498675D 01	0.247927E 00
315	-0.217030E 02	-0.217071D 02	0.407488E-02
316	-0.601074E 01	-0.596246D 01	-0.482764E-01
317	-0.408600E 02	-0.412064D 02	0.346442E 00
318	-0.300624E 01	-0.300738D 01	0.114289E-02
319	-0.691148E 02	-0.691506D 02	0.358033E-01
320	0.156369E 01	0.157931D 01	-0.156226E-01
321	-0.609587E 02	-0.609322D 02	-0.265276E-01
322	-0.540395E 02	-0.547121D 02	0.672597E 00
323	0.329277E 01	0.325330D 01	0.394711E-01
324	0.334290E 02	0.333516D 02	0.773572E-01
325	0.192033E 02	0.195850D 02	-0.381678E 00
326	-0.246710E 01	-0.215026D 01	-0.316844E 00
327	-0.106316E 02	-0.106965D 02	0.649515E-01
328	-0.664239E 00	-0.521273D 00	-0.142966E 00
329	0.732888E 02	0.735559D 02	-0.267146E 00
330	0.782339E 01	0.764990D 01	0.173491E 00
331	-0.417354E 02	-0.422061D 02	0.470699E 00
332	0.111330E 02	0.106496D 02	0.483377E 00
333	-0.224203E 02	-0.219796D 02	-0.440684E 00
334	-0.408924E 02	-0.410717D 02	0.179308E 00
335	-0.248227E 00	-0.200625D 00	-0.476015E-01
336	-0.584310E-02	-0.361877D 00	0.356033E 00
337	0.433757E 00	0.251599D 00	0.182158E 00
338	0.344346E 02	0.343549D 02	0.797251E-01
339	-0.318882E 02	-0.317837D 02	-0.104482E 00
340	-0.532056E 02	-0.532667D 02	0.611550E-01
341	-0.124009E 01	-0.141033D 01	0.170232E 00
342	-0.587531E 02	-0.587560D 02	0.296684E-02
343	0.134247E 01	0.123040D 01	0.112073E 00
344	0.481442E 02	0.477472D 02	0.397033E 00
345	0.587996E-01	-0.295032D 00	0.353832E 00
346	-0.191207E 02	-0.191760D 02	0.552582E-01
347	0.366736E 02	0.366562D 02	0.173197E-01
348	0.139661E 01	0.141891D 01	-0.223030E-01
349	0.133864E 01	0.130391D 01	0.347313E-01
350	-0.172318E 01	-0.156771D 01	-0.155473E 00

DATA PT.	EXPERIMENTAL	ANALYTICAL	RESIDUE
351	0.193288E 02	0.193373D 02	-0.842557E-02
352	0.214114E 01	0.227245D 01	-0.131312E 00
353	-0.327028E 01	-0.339478D 01	0.124502E 00
354	-0.154449E 01	-0.178807D 01	0.243583E 00
355	0.502108E 02	0.502317D 02	-0.209295E-01
356	-0.735534E 00	-0.667849D 00	-0.676860E-01
357	0.310450E 02	0.311306D 02	-0.856366E-01
358	-0.128789E 02	-0.127316D 02	-0.147325E 00
359	0.114391E 02	0.111679D 02	0.271130E 00
360	0.165501E 00	-0.232810D 00	0.398311E 00
361	0.210396E 01	0.197291D 01	0.131050E 00
362	0.615744E 02	0.617513D 02	-0.176905E 00
363	-0.111872E 02	-0.112863D 02	0.991475E-01
364	0.613433E 01	0.612586D 01	0.847308E-02
365	0.300730E 02	0.295683D 02	0.504745E 00
366	-0.645164E 01	-0.616012D 01	-0.291522E 00
367	-0.132213E 01	-0.128636D 01	-0.357726E-01
368	0.598689E 01	0.598179D 01	0.510256E-02
369	-0.469641E 01	-0.458155D 01	-0.114863E 00
370	-0.157022E 01	-0.183147D 01	0.261243E 00
371	-0.121665E 02	-0.120715D 02	-0.950195E-01
372	-0.176400E 02	-0.179988D 02	0.358826E 00
373	-0.423265E 00	-0.281143D 00	-0.142122E 00
374	0.930450E 00	0.651568D 00	0.278882E 00
375	0.210543E 01	0.225396D 01	-0.148524E 00
376	0.414557E 02	0.417847D 02	-0.328990E 00
377	0.567498E 01	0.600859D 01	-0.333611E 00
378	-0.557997E 02	-0.557020D 02	-0.976573E-01
379	0.405326E 00	-0.881523D-01	0.493478E 00
380	-0.554705E 02	-0.555104D 02	0.399139E-01
381	-0.404137E 02	-0.402407D 02	-0.173027E 00
382	-0.347873E 02	-0.349367D 02	0.149399E 00
383	0.242329E 02	0.239712D 02	0.261684E 00
384	0.320484E 02	0.321005D 02	-0.521117E-01
385	-0.161627E 01	-0.164785D 01	0.315778E-01
386	-0.825370E 01	-0.791711D 01	-0.336592E 00
387	0.728979E 00	0.803894D 00	-0.749144E-01
388	0.182639E 01	0.193910D 01	-0.112709E 00
389	-0.132912E 00	-0.749979D-01	-0.579137E-01
390	-0.252183E 02	-0.252662D 02	0.478999E-01
391	-0.333890E 01	-0.325214D 01	-0.867538E-01
392	0.200590E 01	0.197144D 01	0.344601E-01
393	0.986084E 01	0.100811D 02	-0.220279E 00
394	-0.452362E 02	-0.454897D 02	0.253536E 00
395	-0.930094E 01	-0.933768D 01	0.367422E-01
396	-0.104874E 00	0.452125D-01	-0.150086E 00
397	-0.579263E 01	-0.575376D 01	-0.388674E-01
398	-0.112013E 02	-0.111354D 02	-0.659414E-01
399	-0.622055E 01	-0.614923D 01	-0.713149E-01
400	-0.863089E 00	-0.566127D 00	-0.296962E 00

CATA PT.	EXPERIMENTAL	ANALYTICAL	RESIDUE
401	-0.433382E 02	-0.435108D 02	0.172542E 00
402	-0.420343E 02	-0.418249D 02	-0.209390E 00
403	-0.102476E 01	-0.872895D 00	-0.151860E 00
404	-0.621044E 00	-0.813248D 00	0.192204E 00
405	-0.368319E 01	-0.374460D 01	0.614038E-01
406	-0.703811E 00	-0.816736D 00	0.112926E 00
407	0.937096E 01	0.921702D 01	0.153938E 00
408	0.601404E 01	0.541669D 01	0.597348E 00
409	-0.335940E 02	-0.332047D 02	-0.389288E 00
410	-0.175707E 01	-0.172946D 01	-0.276058E-01
411	0.318722E 02	0.318317D 02	0.405039E-01
412	0.594913E 02	0.597455D 02	-0.254138E 00
413	-0.302268E 01	-0.273743D 01	-0.285254E 00
414	-0.211775E 01	-0.202909D 01	-0.886607E-01
415	0.562470E 02	0.564895D 02	-0.242509E 00
416	-0.658325E 01	-0.624171D 01	-0.341543E 00
417	0.103668E 02	0.100224D 02	0.344427E 00
418	-0.397055E 01	-0.444312D 01	0.472569E 00
419	0.579904E 02	0.581251D 02	-0.134749E 00
420	-0.105574E 00	-0.202661D 00	0.970868E-01
421	0.127118E 01	0.134138D 01	-0.701976E-01
422	-0.354766E 01	-0.340032D 01	-0.147349E 00
423	-0.798274E 00	-0.627264D 00	-0.171010E 00
424	0.640065E 01	0.655867D 01	-0.158027E 00
425	0.183770E 01	0.205160D 01	-0.213903E 00
426	-0.141267E 01	-0.167463D 01	0.261961E 00
427	0.291086E 02	0.287971D 02	0.311478E 00
428	-0.799800E-01	-0.115104D 00	0.351238E-01
429	-0.540438E 01	-0.538823D 01	-0.161422E-01
430	-0.539198E 01	-0.529242D 01	-0.995597E-01
431	0.160046E 01	0.180018D 01	-0.199721E 00
432	-0.242205E 01	-0.237157D 01	-0.504795E-01
433	0.119265E 01	0.150063D 01	-0.307988E 00
434	-0.229161E 02	-0.230089D 02	0.928034E-01
435	0.412999E 02	0.414339D 02	-0.133937E 00
436	0.805409E 01	0.800117D 01	0.529259E-01
437	-0.443266E 02	-0.443204D 02	-0.623034E-02
438	-0.840145E 01	-0.829347D 01	-0.107978E 00
439	-0.444930E 00	-0.582401D 00	0.137471E 00
440	-0.290335E 02	-0.290654D 02	0.319046E-01
441	0.131425E 02	0.133626D 02	-0.220067E 00
442	0.697235E 02	0.696662D 02	0.573254E-01
443	0.276748E 01	0.291702D 01	-0.149544E 00
444	0.127329E 02	0.124184D 02	0.314508E 00
445	0.358327E 01	0.335101D 01	0.232261E 00
446	-0.509573E 02	-0.509068D 02	-0.504591E-01
447	-0.653039E 00	-0.120768D 01	0.554636E 00
448	-0.190563E 01	-0.175643D 01	-0.149197E 00
449	0.397817E 00	0.424694D 00	-0.268764E-01
450	-0.300986E 02	-0.296584D 02	-0.440147E 00

DATA PT.	EXPERIMENTAL	ANALYTICAL	RESIDUE
451	0.673277E 02	0.671517D 02	0.176051E 00
452	0.832154E 01	0.852007D 01	-0.198532E 00
453	0.194283E 01	0.194935D 01	-0.651296E-02
454	0.114658E 02	0.113938D 02	0.719564E-01
455	-0.271349E 01	-0.291762D 01	0.204136E 00
456	-0.337666E-02	0.836226D-01	-0.869992E-01
457	0.489474E 01	0.498640D 01	-0.916565E-01
458	-0.745760E 01	-0.788526D 01	0.427665E 00
459	-0.594274E 00	-0.549804D 00	-0.444705E-01
460	0.738312E 02	0.736967D 02	0.134500E 00
461	-0.127028E 01	-0.120893D 01	-0.613531E-01
462	0.450569E 01	0.484425D 01	-0.338563E 00
463	-0.311281E 00	0.144455D 00	-0.455735E 00
464	-0.312424E 02	-0.313158D 02	0.733369E-01
465	-0.226604E 02	-0.224887D 02	-0.171692E 00
466	0.676181E 00	0.361749D 00	0.314432E 00
467	-0.592276E 01	-0.605341D 01	0.130652E 00
468	0.491892E 02	0.489304D 02	0.258804E 00
469	-0.385186E 01	-0.368593D 01	-0.165922E 00
470	-0.902797E 00	-0.964061D 00	0.612638E-01
471	-0.545539E 00	-0.834559D 00	0.289020E 00
472	0.208181E 01	0.173558D 01	0.346235E 00
473	0.466832E 01	0.496703D 01	-0.298709E 00
474	0.948851E 00	0.134970D 01	-0.400849E 00
475	0.201331E 01	0.185240D 01	0.160910E 00
476	0.927796E 01	0.917616D 01	0.101799E 00
477	0.112168E 02	0.114481D 02	-0.231268E 00
478	0.119469E 02	0.118015D 02	0.145366E 00
479	0.120877E 02	0.119759D 02	0.111781E 00
480	0.200208E 02	0.203492D 02	-0.328341E 00
481	0.370029E 02	0.368949D 02	0.107985E 00
482	-0.316739E 02	-0.318658D 02	0.191869E 00
483	0.115672E 02	0.116928D 02	-0.125567E 00
484	-0.575475E 01	-0.595537D 01	0.200620E 00
485	-0.240087E 01	-0.237595D 01	-0.249232E-01
486	0.510537E 00	0.376751D 00	0.133786E 00
487	-0.805686E 00	-0.572600D 00	-0.233086E 00
488	-0.182469E 00	-0.443239D 00	0.260770E 00
489	0.593804E 02	0.596429D 02	-0.262505E 00
490	0.617216E 01	0.623300D 01	-0.608359E-01
491	-0.167372E 01	-0.154099D 01	-0.132736E 00
492	-0.943684E 01	-0.948490D 01	0.480648E-01
493	-0.196805E 00	0.122283D 00	-0.319089E 00
494	0.430789E 01	0.417504D 01	0.132855E 00
495	-0.788723E 01	-0.758678D 01	-0.300453E 00
496	-0.900640E 01	-0.887365D 01	-0.132757E 00
497	-0.356456E 02	-0.358525D 02	0.206893E 00
498	-0.121960E 02	-0.124546D 02	0.258575E 00
499	-0.730739E 01	-0.706915D 01	-0.238246E 00
500	0.942934E 00	0.132392D 01	-0.380986E 00

OVERALL PLOT OF THE RESIDUES AGAINST THE VALUES PREDICTED BY THE FIT (YANAL)



EXTREME VALUES OF THE RESIDUES 0.672597E 00 -0.660616E 00 EXTREME VALUES OF YANAL 0.738143E 02 -0.713480E 02

T11 = -0.231475E-02 T12 = 0.141421E 03 T21 = 0.967468E 01

THE MEAN VALUE OF THE RESIDUES IS 0.480074E-02

THEIR STANDARD DEVIATION IS 0.238207E 00

[redacted] ER THE [redacted]

[redacted] FOR THE [redacted] RESIDUES

950	[redacted] 00	500	40 [redacted] 0	200	100	
948	[redacted] 306	512	38 [redacted] 8	126	90	

NOTICE TO THE READER

All scientific and technical reports published by the Commission of the European Communities are announced in the monthly periodical **"euro-abstracts"**. For subscription (1 year: BF.1025) or free specimen copies please write to:

Office for Official Publications
of the European Communities
Case postale 1003
Luxembourg 1
(Grand-Duchy of Luxembourg)

To disseminate knowledge is to disseminate prosperity — I mean general prosperity and not individual riches — and with prosperity disappears the greater part of the evil which is our heritage from darker times.

Alfred Nobel

SALES OFFICES

The Office for Official Publications sells all documents published by the Commission of the European Communities at the addresses listed below, at the price given on cover. When ordering, specify clearly the exact reference and the title of the document.

UNITED KINGDOM

H.M. Stationery Office
P.O. Box 569
London S.E. 1 — Tel. 01-928 69 77, ext. 365

BELGIUM

Moniteur belge — Belgisch Staatsblad
Rue de Louvain 40-42 — Leuvenseweg 40-42
1000 Bruxelles — 1000 Brussel — Tel. 12 00 26
CCP 50-80 — Postgiro 50-80

Agency :
Librairie européenne — Europese Boekhandel
Rue de la Loi 244 — Wetstraat 244
1040 Bruxelles — 1040 Brussel

DENMARK

J.H. Schultz — Boghandel
Møntergade 19
DK 1116 København K — Tel. 14 11 95

FRANCE

Service de vente en France des publications des Communautés européennes — Journal officiel
26, rue Desaix — 75 732 Paris - Cédex 15e
Tel. (1) 306 51 00 — CCP Paris 23-96

GERMANY (FR)

Verlag Bundesanzeiger
5 Köln 1 — Postfach 108 006
Tel. (0221) 21 03 48
Telex: Anzeiger Bonn 08 882 595
Postscheckkonto 834 00 Köln

GRAND DUCHY OF LUXEMBOURG

Office for Official Publications of the European Communities
Case postale 1003 — Luxembourg
Tel. 4 79 41 — CCP 191-90
Compte courant bancaire: BIL 8-109/6003/200

IRELAND

Stationery Office — The Controller
Beggar's Bush
Dublin 4 — Tel. 6 54 01

ITALY

Libreria dello Stato
Piazza G. Verdi 10
00198 Roma — Tel. (6) 85 08
CCP 1/2640

NETHERLANDS

Staatsdrukkerij- en uitgeverijbedrijf
Christoffel Plantijnstraat
's-Gravenhage — Tel. (070) 81 45 11
Postgiro 42 53 00

UNITED STATES OF AMERICA

European Community Information Service
2100 M Street, N.W.
Suite 707
Washington, D.C., 20 037 — Tel. 296 51 31

SWITZERLAND

Librairie Payot
6, rue Grenus
1211 Genève — Tel. 31 89 50
CCP 12-236 Genève

SWEDEN

Librairie C.E. Fritze
2, Fredsgatan
Stockholm 16
Post Giro 193, Bank Giro 73/4015

SPAIN

Libreria Mundi-Prensa
Castello 37
Madrid 1 — Tel. 275 51 31

OTHER COUNTRIES

Office for Official Publications of the European Communities
Case postale 1003 — Luxembourg
Tel. 4 79 41 — CCP 191-90
Compte courant bancaire: BIL 8-109/6003/200

CDNA04959ENC

OFFICE FOR OFFICIAL PUBLICATIONS OF THE EUROPEAN COMMUNITIES
Case postale 1003 — Luxembourg 6076