A. E. K. Risø

Risø-M- 1279

Risø-M- 1279

Title and author(s)

A FORTRAN IV Version of the Sum-of-Exponential Least-Squares Code EXPOSUM

by

Peter Kirkegaard

Date September 1970

Department or group

Reactor Physics Department

Group's own registration number(s)

56 pages + 0 tables + 1 illustrations

Abstract

An improved version of the computer program AEK P-513 EXPOSUM is described. The program carries out a least-squares fitting of the parameters in a sum-of-exponentials to given table values.

The new EXPOSUM code is written in FORTRAN IV and replaces the old GIER-ALGOL III version.

Copies to

Standard distribution

150 copies

Abstract to

Standard distribution

Available on request from the Library of the Danish Atomic Energy Commission (Atomenergikommissionens Bibliotek), Risø, Roskilde, Denmark.
Telephone: (03) 35 51 01, ext. 334, telex: 5072.

Fi 25-204

ISBN 87 550 0021 5

CONTENTS

1. INTRODUCTION

An earlier report [6] has described a GIER-ALGOL III computer program EXPOSUM which carried out a least-squares fitting of the parameters in a linear combination of exponentials to a given sample of data points.

It was at that time planned to translate the code to FORTRAN IV to extend its utility. In the meantime, however, some shortcomings of the program were revealed, and for this reason a new and considerably improved EXPOSUM model was set up and programmed in FORTRAN IV.

This report has the aim to give a self-contained exposition of the revised model and to supply the user with practical instructions.

2. STATEMENT OF THE PROBLEM

Let a sample of n data points (x_i, y_i) be given, x_i being the independent and y_i the dependent variable. We wish to represent this sample by a linear combination of exponentials

$$y = a_o + \sum_{j=1}^{k} a_j \exp(\omega_j x) \tag{1}$$

Inclusion of the constant term should be optional.

Such an exponential fitting problem is encountered at a variety of places. In radiology and reactor physics it is often required to analyse the decay curves from multi-component radioactive substances; in this case x_i are times and y_i count rates (and $\omega_j < 0$). The growth of certain quantities in economics and insurance may also show a sum-of-exponential behaviour.

One could arrive at the form (1) either because it merely is mathematically convenient, or, alternatively, because one is led to this form by physical reasonings or theoretical predictions.

Determination of the parameters in (1) may be accomplished in many ways. Decay curves have often been resolved by graphical means: one utilizes that for large x_i a single component dominates; its parameters are estimated from a semi-logarithmic plot of the data sample. By subtraction of the component from the sample, a reduced sample is obtained.

The procedure is repeated until all components have been estimated. This method, known as the peel-off method[4], has several limitations: it is subjective, it works only if the ω_j are clearly different; and, finally, it yields no estimate of the variance of the parameters.

For the case of equidistant abscissas, Prony[2] has developed a simple method, which involves the solution of an algebraic equation of degree k; its roots are just the ω_j in (1). Sometimes the roots turn out to be complex corresponding to an oscillating approximation; this restricts the utility of Prony's method.

Finally, the parameters could be estimated by some least-squares method*. Such methods are objective, their resolution power is good, they permit weighting of the data, and they provide an estimation of the statistical distribution of the parameters. Their main disadvantage is the need of an iterative technique when the model as (1) is nonlinear.

We have, in fact, chosen a least-squares method for our solution; in the following, such methods will be described in general terms.

3. THE LEAST-SQUARES PRINCIPLE

Let some general model be given,

$$y = f(x;\ b) \tag{2}$$

where x and y are the independent and dependent variable, resp., and b is a parameter vector with k components,

$$b = (b_1, \ldots, b_k)^T \tag{3}$$

Some or all of the components may enter nonlinearly in (2). Further, let a data sample (x_i, y_i) (cf. sec. 2) be given. According to the least-squares principle, we try to find b such that

$$\emptyset = \sum_{i=1}^{n} w_i (y_i - f(x_i; b))^2 \tag{4}$$

---

*A code EXPALS[12] has appeared quite recently. It is basicly of the Prony type but works according to the least-squares principle applied to the original data sample.

is minimized. The w_i are the weights of the data points; weighting will be discussed in sec. 4, but here we simply assume that the weights are fixed numbers accompanying our sample.

Of course, if some of the b_j occur symmetrically in (2), several permuted b-solutions may exist. On the other hand, it may happen that no minimum solution at all exists for finite b. Or, a local minimum could exist without being a global one. It seems difficult to state conditions for the existence of minimum solutions. Here, we disregard these complications and postulate that a usable solution b to our problem will be determined by the k equations

$$\frac{\partial \varnothing}{\partial b_j} = 0 , \qquad j = 1, \ldots, k \tag{5}$$

(4) and (5) yield

$$\sum_{i=1}^{n} w_i (y_i - f_i) \frac{\partial f_i}{\partial b_j} = 0 , \qquad j = 1, \ldots, k \tag{6}$$

where f_i has been written for $f(x_i; b)$. These "normal equations" are in general nonlinear and must be solved iteratively. How this is done, is upset until sec. 5. At this point, we assume that a solution b is already obtained, and next we proceed to examine its statistical behaviour.

4. STATISTICAL ANALYSIS OF THE LEAST-SQUARES SOLUTION

Often the y_i are the results of measurements and hence subject to statistical fluctuations, while the x_i (and w_i) may be regarded as fixed. The solution of the normal equations (6) for the parameter vector b will also be a random variable with a distribution that can be found under certain restrictive assumptions.

At the first place we shall assume that the y_i display only small fluctuations around their means η_i. Let the solution of (6) corresponding to the sample (x_i, η_i, w_i) be b_o, and that corresponding to an arbitrary sample (x_i, y_i, w_i) be b. Then $b-b_o$ is small, and we may assume that our model (2) is locally linear in b in a domaine S including both b and b_o:

$$f(x_i;b) = f(x_i;b_o) + \sum_{j=1}^{k} \frac{\partial f_i}{\partial b_j} (b_j - b_j^o) \tag{7}$$

where the $\frac{\partial f_i}{\partial b_j}$ may be regarded as constants in S. We next assume that (2) is an ideal model of our sample, i. e.

$$f(x_i;b_o) = \eta_i \tag{8}$$

Then the normal equations (6) form a linear system of the order k with $\delta b = b - b_o$ as unknown:

$$P^T W P \,\delta b = \delta v \tag{9}$$

where $p_{ij} = \frac{\partial f_i}{\partial b_j}$, W is the diagonal matrix

$$W = \begin{bmatrix} w_1 & & \theta \\ & \cdots & \\ \theta & & w_n \end{bmatrix} \tag{10}$$

and

$$\delta v_j = \sum_{i=1}^{n} w_i (y_i - \eta_i) \frac{\partial f_i}{\partial b_j} \tag{11}$$

Introduction of the vector $\delta y = (y_1 - \eta_1, \ldots, y_n - \eta_n)^T$ yields

$$\delta v = P^T W \,\delta y \tag{12}$$

and

$$\delta b = K \,\delta y \tag{13}$$

with

$$K = (P^T W P)^{-1} P^T W \tag{14}$$

Hence δb is related to δy simply by a linear transformation. As δy has zero mean, so has δb, i. e. b is an unbiased estimate of b_o. Further, the moment matrix[8] M of b (or δb) is connected with the moment matrix V of y (or δy) by the equation

$$M = K V K^T \tag{15}$$

In particular, if y has a multi-normal distribution, so has b.

Let us now assume that the y_i are independent. Then V is diagonal

$$V = \begin{bmatrix} \sigma_1^2 & & \theta \\ & \cdots & \\ \theta & & \sigma_n^2 \end{bmatrix} \tag{16}$$

Let us further assume that we know the standard deviation σ_i at each sample point, at least apart from a constant factor σ, i. e.

$$\sigma_i = \sigma \cdot h_i \tag{17}$$

where the h_i are known, whereas σ may or may not be known. With this knowledge one should, as Moore and Zeigler[1] point out, choose the weight as

$$w_i = \frac{1}{h_i^2} \tag{18}$$

This "statistical weighting" has a double advantage. It assures that the points with the largest variances will have small influence on the fit and vice versa. Further, a simple expression of M is obtained: from (14), (15), and the relation

$$V = \sigma^2 W^{-1} \tag{19}$$

we obtain

$$M = A^{-1} P^T W \sigma^2 W^{-1} W P A^{-1}, \quad \text{or}$$

$$M = \sigma^2 A^{-1} \tag{20}$$

where A has been written for $P^T W P$.

If σ is not known in advance, we must estimate it. For this purpose, the minimal $\varnothing$ (cf. (4)), $\varnothing_{min}$, is used. We shall assume that the y_i have normal distributions. This assumption is not very restrictive in practice; when the y_i for instance are count numbers of a reasonable size, their Poisson-distribution will be close to normal. Under the assumption of a locally linear model we shall find the distribution of $\varnothing_{min}/\sigma^2$. If b is the solution of (6), we have

$$\varnothing_{min} = \sum_{i=1}^{n} w_i(y_i - \eta_i - \sum_{j=1}^{k} \frac{\partial f_i}{\partial b_j} (b_j - b_j^o))^2 \tag{21}$$

or, in matrix notation

$$\varnothing_{min} = (\delta y - P\ \delta b)^T\ W(\delta y - P\ \delta b) \tag{22}$$

By (13) and (14) $\varnothing_{min}$ becomes a quadratic form in δy:

$$\varnothing_{min} = \delta y^T\ B\ \delta y \tag{23}$$

where B after an easy calculation is found to

$$B = W - W\ P(P^T\ W\ P)^{-1}\ P^T\ W \tag{24}$$

At this point we introduce the substitution

$$\delta y_i = \sigma_i\ u_i = \sigma w_i^{-1/2}\ u_i \tag{25}$$

Then $\varnothing_{min}$ can be expressed as a quadratic form in terms of u:

$$\varnothing_{min} = \sigma^2\ u^T\ C\ u \tag{26}$$

with

$$C = W^{-1/2}\ B\ W^{-1/2} = I - W^{1/2}\ P(P^T\ W P)^{-1}\ P^T\ W^{1/2} \equiv I - M \tag{27}$$

Clearly, the matrix M is of rank k. Furthermore, all its k eigenvalues $\neq 0$

are unity, as is easily verified by premultiplying $Mx = \lambda x$ by $P^T W^{1/2}$. Hence, an orthogonal substitution $u = V \cdot z$ exists which transforms $\varnothing_{min}/\sigma^2$ into a sum of n-k squares

$$\sum_{1}^{n-k} z_i^2 ,$$

showing[8,9] that $\varnothing_{min}/\sigma^2$ has a χ^2-distribution with n-k degrees of freedom; its mean and variance are n-k and 2(n-k), resp. Then we have shown that the quantity

$$s^2 = \frac{\varnothing_{min}}{n-k} \qquad (28)$$

is an unbiased estimate of σ^2.

If, on the other hand, σ is known in advance, we can compare $\varnothing_{min}/\sigma^2$ with n-k. If the former exceeds the latter by several standard deviations, some of our assumptions will probably be invalid; in practice the normal distribution of y_i will as a rule be sufficiently well approximated, so it becomes most probable that (8) is not satisfied, meaning that our model is insufficient to describe the data sample.

An important special case occurs when $\sigma_i = \sigma$ for all i. Then $h_i = 1$, and (18) leads to equally weighted data, $w_i = 1$. In this case (28) gives that s^2 is an unbiased estimate of the constant variance σ^2 at each point, and, as before, s^2 may be used either to estimate σ^2 or to check the model. In the case $w_i = 1$, s^2 is denoted the "variance of the fit"[1].

5. MARQUARDT'S PRINCIPLE

We now describe the iterative method which was applied in this work to the solution of the normal equations (6) of the least-squares problem. This method* is known as Marquardt's principle[3], and is an efficient combination of two classical iterative least-squares solution methods, which will be mentioned first.

In the Taylor-series method (Gauss-Newton method) one expands the model $f(x;b)$ from a guessed or previously iterated value b_o through the linear terms as in (7). Then $\varnothing$ in (4) is replaced by a linearized form

---

*Marquardt's results[3] assume $w_i = 1$ but are easily generalized to arbitrary w_i.

$$\langle \emptyset \rangle = \sum_{i=1}^{n} w_i \left(y_i - f_i - \sum_{j=1}^{k} \frac{\partial f_i}{\partial b_j} \delta b_j\right)^2 , \qquad j = 1, \ldots, k \tag{29}$$

where $\delta b_j = b_j - b_j^o$ are the components of the Taylor-series method correction vector δ_t, $f_i = f(x_i; b_o)$, and $\partial f_i / \partial b_j$ are evaluated at b_o. $\langle \emptyset \rangle$ is minimized by

$$A \, \delta_t = g \tag{30}$$

where $A = P^T W P$ as defined in sec. 4, and

$$g_j = \sum_{i=1}^{n} w_i (y_i - f_i) \frac{\partial f_i}{\partial b_j} \tag{31}$$

Then $b_o + \delta_t$ replaces b_o as the new iterate. This method often tends to diverge, in particular when the guess is bad. Variants with reduced step length $||\delta_t||$ (so-called damped versions) behave somewhat better in this respect and have been applied to the sum-of-exponential problem * by Späth [7].

The other classical method is the gradient method where the correction vector δg is chosen as

$$\delta g = -\left(\frac{\partial \emptyset}{\partial b_1} , \ldots , \frac{\partial \emptyset}{\partial b_k} \right)^T \tag{32}$$

apart from a constant factor. This method has often an extremely slow rate of convergence. As pointed out by Marquardt [3], this is coupled to the fact that the contour surface of $\emptyset$ is greatly attenuated in some directions and elongated in others so that the minimum lies at the bottom of a long curved trough; this causes further the angle between δ_t from (30) and δg from (32) to be near 90^o.

At this point we introduce Marquardt's correction vector δ_m, defined by the equation

---

* It has not been possible to compare Späth's algorithm to EXPOSUM due to numerical or code-conversion problems.

$$(A + \lambda D^2)\ \delta_m = g \tag{33}$$

As before, $A = P^T W P$, and g is defined in (31), whereas D is a diagonal matrix with $D_j = \sqrt{a_{jj}}$. As we shall see the parameter λ provides for interpolation between the Taylor-series method and a gradient-like method. The former method is obtained by setting $\lambda = 0$ (cf. (30)). On the other hand, for $\lambda \to \infty$ we obtain a solution vector proportional to $D^{-2} g$. As g itself is proportional to δ_g (cf. (31) and (32)), the limiting correction vector (apart from a constant) will be

$$\delta_m^\infty = D^{-2}\ \delta_g \tag{34}$$

δ_m^∞ may be regarded as a scaled form of δ_g; although it does not have the steepest-descent direction, it shares with δ_g the property that $\emptyset$ certainly does decrease initially along the correction vector (provided we are not already at the minimum). The interpolation is based on three theorems, which are generalized versions* of those given by Marquardt [3] and are proved in the same way.

Theorem 1: Let $\lambda \geq 0$ be arbitrary and let δ_m satisfy (33). Then δ_m minimizes $\langle \emptyset \rangle$ (cf. (29)) on the ellipsoid $||D\delta|| = ||D\ \delta_m||$.

Theorem 2: Let $\delta_m(\lambda)$ be the solution of (33). Then the norm $||D\,\delta_m(\lambda)||$ is a continuous decreasing function of λ tending to zero when $\lambda \to \infty$.

Theorem 3: The angle between $D\ \delta_m$ and $D\ \delta_m^\infty$ is a continuous decreasing function of λ tending to zero when $\lambda \to \infty$.

These theorems lead directly to the algorithm. The equation to be solved at iteration no. r reads

$$(A^{(r)} + \lambda^{(r)}\ D^{2(r)})\ \delta_m^{(r)} = g^{(r)} \tag{35}$$

From its solution $\delta_m^{(r)}$ we calculate

$$b^{(r+1)} = b^{(r)} + \delta_m^{(r)} \tag{36}$$

---

*Marquardt has in his exposition the unit matrix I instead of D. At a later stage, however, he introduces a scaling of the method, and his scaled algorithm is in fact equivalent to (33).

and a new $\emptyset$-value, $\emptyset^{(r+1)}$. Now it is essential that $\lambda^{(r)}$ is so chosen that

$$\emptyset^{(r+1)} \leq \emptyset^{(r)} \tag{37}$$

If we are not already at the minimum, it is always possible to satisfy (37) by selecting a sufficiently large $\lambda^{(r)}$, and so we avoid the divergence problems from the Taylor-series method. However, $\lambda^{(r)}$ should not be chosen unnecessarily large, because we then (cf. theorem 3) approaches the gradient method with its slow convergence. When $\emptyset$ approaches the minimum value, $\lambda^{(r)}$ decreases steadily. Then the method approaches the Taylor-series method, which shows a very fast (quadratic) rate of convergence near the minimum. Marquardt recommends the following strategy:

Let $\nu > 1$. Let $\lambda^{(r-1)}$ be the λ-value from the previous iteration; we choose as $\lambda^{(0)}$ a suitable value, e. g. 0.01. Compute $\emptyset(\lambda^{(r-1)})$ and $\emptyset(\lambda^{(r-1)}/\nu)$.

i. If $\emptyset\left(\frac{\lambda^{(r-1)}}{\nu}\right) \leq \emptyset^{(r)}$, let $\lambda^{(r)} = \frac{\lambda^{(r-1)}}{\nu}$

ii. If $\left[\emptyset\left(\frac{\lambda^{(r-1)}}{\nu}\right) > \emptyset^{(r)} \wedge \emptyset(\lambda^{(r-1)}) \leq \emptyset^{(r)}\right]$, let $\lambda^{(r)} = \lambda^{(r-1)}$

iii. If $\left[\emptyset\left(\frac{\lambda^{(r-1)}}{\nu}\right) > \emptyset^{(r)} \wedge \emptyset(\lambda^{(r-1)}) > \emptyset^{(r)}\right]$, increase λ by successive multiplication by ν until for some smallest w, $\emptyset(\lambda^{(r-1)}\nu^{w}) \leq \emptyset^{(r)}$. Let $\lambda^{(r)} = \lambda^{(r-1)}\nu^{w}$

The iteration is theoretically converged when $\delta_m = 0$. Then also $g = 0$ (eq. (33)) and the normal equations (6) are satisfied. In practice, however, a suitable convergence criterion is chosen, like

$$\frac{|\delta_{mj}^{(r)}|}{\tau + |b_j^{(r)}|} < \epsilon \tag{38}$$

for all j, for some suitably small $\epsilon > 0$, say $3 \cdot 10^{-5}$ and some suitable τ, say 10^{-3}. The choice $\nu = 10$ is recommended.

6. SEMI-LINEAR EXPOSUM METHOD

We now turn to apply the ideas discussed above to the sum-of-exponential problem.

At this point we draw the attention to two modifications from the earlier to the present EXPOSUM version.

First, experience with the old version indicated that it was not worthwhile to retain its particular search option [5, 6, 11)] that replaced the procedure of guessing an initial b.

Next, the new version takes advantage of the fact that the sum-of-exponential problem (1) is only partially nonlinear. According to (1) we partition the b-vector in the linear component a and the nonlinear component ω:

$$b = (a, \omega) \tag{39}$$

Here a is of dimension $k1 = k + h$ (the option integer h is 1 if the a_o-term is present, otherwise $h = 0$), ω is of dimension k, so b has the dimension $k + k1$ ($= 2k$ or $2k+1$). The new EXPOSUM iterates in the ω-space instead of the b-space and has as a result gained considerably in efficiency. The implementation of this modification caused some additional problems which were surmounted in the way outlined below. We consider a general linear-nonlinear model

$$y = f(x; \alpha_1, \ldots, \alpha_{k1}; \beta_1, \ldots, \beta_k) \equiv f(x; \alpha; \beta) \tag{40}$$

where f is supposed to be linear in α and nonlinear in β. i.e. f is of the type

$$f(x; \alpha; \beta) = \sum_{j=1}^{k1} \alpha_j \, \varphi_j(x; \beta) \tag{41}$$

When β is fixed so is also α through the standard solution of

$$\emptyset \equiv \sum_{i=1}^{n} w_i (y_i - \sum_{j=1}^{k1} \alpha_j \, \varphi_j(x_i; \beta))^2 = \min. \quad , \tag{42}$$

so we have

$$\alpha = \alpha(\beta) \tag{43}$$

Iterations take place in the β-space and are governed by the linear Marquardt system

$$(A + \lambda D^2)\ \delta_m \beta = g \tag{44}$$

of order k. As in sec. 5, $A = P^T W P$ with $p_{ij} = \partial f_i / \partial \beta_j$, D is diagonal with

$$D_j = \sqrt{a_{jj}}, \text{ and } g_j = \sum_{i=1}^{n} w_i (y_i - f_i) \frac{\partial f_i}{\partial \beta_j}.$$

The derivative $\partial f_i / \partial \beta_j$ takes, according to (41) and (43), the form

$$\frac{\partial f_i}{\partial \beta_j} = \sum_{j1=1}^{k1} \left[\frac{\partial \alpha_{j1}}{\partial \beta_j} \varphi_{j1}(x_i; \beta) + \alpha_{j1} \frac{\partial \varphi_{j1}(x_i; \beta)}{\partial \beta_j} \right], \quad j = 1, \ldots, k) \tag{45}$$

Hence, it becomes a central problem to evaluate, in some way, the quantities $\partial \alpha_{j1} / \partial \beta_j$. We first made an attempt to find them by numerical means, using the difference-quotient approximation, but with ill success. Fortunately, it turned out that they could instead be exactly evaluated by a simple linear-algebraic method. To see this, let us first develop the solution α of (42) obtained by the usual conditions $\partial \varnothing / \partial \alpha_j = 0$:

$$\sum_{j1=1}^{k1} \sum_{i=1}^{n} w_i \varphi_j(x_i; \beta) \varphi_{j1}(x_i; \beta) \alpha_{j1} = \sum_{i=1}^{n} w_i y_i \varphi_j(x_i; \beta), \quad (j = 1, \ldots, k1) \tag{46}$$

By taking the derivative of both members of (46) with respect to $\beta_{j'}$ ($j' = 1, \ldots, k$), one finds

$$\sum_{j1=1}^{k1} \sum_{i=1}^{n} w_i \varphi_j \varphi_{j1} \frac{\partial \alpha_{j1}}{\partial \beta_{j'}} + \sum_{j1=1}^{k1} \sum_{i=1}^{n} w_i \left[\varphi_j \frac{\partial \varphi_{j1}}{\partial \beta_{j'}} + \frac{\partial \varphi_j}{\partial \beta_{j'}} \varphi_{j1} \right] \alpha_{j'}$$
$$= \sum_{i=1}^{n} w_i y_i \frac{\partial \varphi_j}{\partial \beta_{j'}} \qquad (j = 1, \ldots, k1;\ j' = 1, \ldots, k) \tag{47}$$

Expressed in matrix notation, (46) and (47) read

$$C\alpha = \gamma \tag{48}$$

and

$$Cd_{j'} = t \tag{49}$$

where

$$c_{j,j1} = \sum_{i=1}^{n} w_i \varphi_j \varphi_{j1}, \quad \gamma_j = \sum_{i=1}^{n} w_i y_i \varphi_j, \quad d_{j'} = \left(\frac{\partial \alpha_1}{\partial \beta_{j'}}, \ldots, \frac{\partial \alpha_{k1}}{\partial \beta_{j'}}\right)^T,$$

and

$$t_j = \sum_{i=1}^{n} w_i \left[y_i \frac{\partial \varphi_j}{\partial \beta_{j'}} - \sum_{j1=1}^{k1} \left(\varphi_j \frac{\partial \varphi_{j1}}{\partial \beta_{j'}} + \frac{\partial \varphi_j}{\partial \beta_{j'}} \varphi_{j1}\right) \alpha_{j1} \right].$$

Note that it is the same matrix C occurring in the systems (48) and (49).

These results are now applied to the sum-of-exponential model (1), where a plays the role of α* and ω that of β (cf. (39)). We find

$$\varphi_j = \exp(\omega_j x_i) \equiv u_{ij}, \quad j = 1, \ldots, k; \text{ and, if } h = 1, \ \varphi_{k1} = 1 \equiv u_{i,k1}, \tag{50}$$

$$\frac{\partial \varphi_j}{\partial \omega_{j'}} = \delta_{jj'} x_i u_{ij}, \quad (j = 1, \ldots, k1;\ j' = 1, \ldots, k) \tag{51}$$

($\delta_{jj'}$ is the Kronecker-delta)

$$\frac{\partial f_i}{\partial \omega_j} = a_j x_i u_{ij} + \sum_{j1=1}^{k1} u_{i,j1} \frac{\partial a_{j1}}{\partial \omega_j}, \quad (j = 1, \ldots, k) \tag{52}$$

$$c_{j,j1} = \sum_{i=1}^{n} w_i u_{ij} u_{i,j1}, \quad (j = 1, \ldots, k1;\ j1 = 1, \ldots, k1) \tag{53}$$

---

* In this analysis the constant term a_o in (1) (if present) is denoted a_{k1}.

$$t_j = -a_{j'} \sum_{i=1}^{n} w_i\, x_i\, u_{ij}\, u_{ij'} \quad \text{for} \quad j \neq j' \tag{54}$$

and

$$t_{j'} = \sum_{i=1}^{n} w_i\, x_i\, u_{ij'} (y_i - a_{j'}\, u_{ij'} - \sum_{j1=1}^{k1} u_{i,j1}\, a_{j1}) \tag{55}$$

7. EXPOSUM WITH EXAMPLES OF APPLICATION

7.1. Some Features of the Code

The EXPOSUM code is written in FORTRAN IV. It is registered in the Risö Computer Library as AEK P-513 Fortran Version. A print-out is given in Appendix III.

EXPOSUM in its present form is intended for use on the IBM 7094 at the NEUCC center in Lyngby, Denmark. However, it should not be difficult to adapt it for other computing installations. The symbolic nos. of the input and output units are 5 and 6 for the IBM 7094 at NEUCC. Only the statements

```
NIN  = 5
NOUT = 6
```

(at the beginning of the print-out) should be changed to fit other conventions. Another conversion problem may occur in the solution of the linear equations and will be mentioned in Appendix IV.

EXPOSUM is divided into main program and subprograms according to the list below:

Main program	EXPSUM
Subroutine	LIPHIF
Subroutine	COLDEC
Subroutine	COLSL
Subroutine	IMPRUV
Subroutine	SING

EXPSUM contains the I/O-part and the nonlinear-iterative and statistical computations. LIPHIF carries out 3 jobs:

a) computes the elements of the matrices $A^{(r)}$ and $g^{(r)}$ in eq. (35),

b) carries out the linear-least-squares calculation (43) of the linear parameters as functions of the nonlinear,

c) evaluates Ø according to (4). This evaluation is carried out in double precision, and for this the same comments as stated in connection with eq. (64), Appendix IV, are pertinent.

The remaining four subroutines refer to solution of linear equations; this topic is discussed in Appendix IV.

7.2. Preparation of Input Data

Input data for EXPOSUM is prepared according to the data sheets given in Appendix I. The sheets contain data for 5 sample problems, separated by full-drawn lines. Data formats are of the types I 10 for integers and E 10.5 for reals. The data for each problem are composed of five data blocks (separated by dashed lines), to be discussed below.

Block a) contains only a problem no. A negative problem no. signals that no more problems are to be solved in our data badge.

Block b) contains five integers, I1, I2, I3, I4, I5. These are options governing calculations, print-out, etc., according to the following rules:

I1 concerns weighting	I1=1 means $w_i = 1$ (equally weighted data) I1=2 means that weights are added as input I1=3 means $w_i = 1/y_i$ (Poisson-weighting*)
I2 concerns iteration print-out	I2=0 means that only the final parameter estimates are printed I2=1 means that, in addition, current iteration estimates are given
I3 concerns statistics (illustrative examples are given in 7.3)	I3=0 means that no statistical analysis is given I3=1 means statistical analysis with unknown σ I3=2 means statistical Poisson-analysis with known σ

*We shall always assume that our Poisson-distributions are close to normal, so the statistical analysis in sec. 4 becomes valid.

I4 concerns the constant term a_o (cf. (1). I4 = h (sec. 6)	I4=0 means that a_o is not included I4=1 means that a_o is included
I5 concerns table print-out	I5=0 means no table print-out I5=1 means print-out of the sample data and the deviations (fit minus data)

When options are unchanged from the previous problem, one replaces block b) with a zero-card, i.e. a card with zero in col. 10.

Block c) begins with the number n of data points. Then the data sample follows, in the form (x_i, y_i) or (x_i, y_i, w_i) according to whether I1 $\neq$ 2 or I1 = 2.

As before, a zero-card indicates that the data sample is unaltered from the previous problem.

Block d) begins with the number k of exponential terms in the sum. The next card contains k guess values of the parameters. A zero-card may be used in the usual way.

Block e) concerns the control of the Marquardt iterations. Here, use of the zero-card is the normal course of action. This causes the following standard values for the control data to be applied (cf. sec. 5):

r_{max} (max. number of iterations)	= 25
$\lambda^{(0)}$ (initial value of $\lambda^{(r)}$ in (35))	= 0.01
ν	= 10.0
τ (cf. (38))	= 10^{-3}
ϵ (cf. (38))	= $3 \cdot 10^{-5}$
ϵ_1 (the tolerable relative violation of (37))	= $3 \cdot 10^{-7}$

If non-standard values are desired, these are supplied as input instead of the zero-card, as in problem no. 4 where $\epsilon = 10^{-5}$ and $\epsilon_1 = 10^{-7}$.

7.3. Discussion of Solution for Sample Problems

The output from the computer run of the five sample problems is shown in Appendix II. Some comments to the solution will be given here.

Problem no. 1 concerns the analysis of the decay curve for a Cu-Al mixture activated in the neutron flux of the DR 1 reactor. The sample contains 23 points (x_i, y_i, w_i); y_i is the count rate at time x_i, and the weights w_i are here added as input data*. A three-term analysis with a constant term (background) was required. For the resulting vector $(\omega_1, \omega_2, \omega_3)$, the components ω_1 and ω_2 are easily identified: by conversion to half life $T = \ln 2/\omega$ one gets $(T_1, T_2) = (2.42$ min, 5.39 min$)$. In view of the stated deviations for ω_1 and ω_2 of about 10-15%, this is consistent with the half lives 2.3 min and 5.1 min taken from the isotope chart for Al-28 and Cu-66. The third term could not be identified.

Our computer run showed an underflow; this is harmless and may safely be ignored.

At the end of each iteration print-out, a single-letter message is given which defines the character of that iteration according to the following rule:

A: Entrance into test i (sec. 5)

B: Entrance into test ii

C: Entrance into test iii

D: Exceptional case where test iii cannot be passed for a reasonable λ; this case is treated as outlined by Marquardt [3].

The statistical part of the output consists of estimated standard deviations of the parameters, the matrix of correlations between the parameters and the inverse of the variance-covariance matrix; the latter is coupled with the distribution of probability mass around the minimum-estimate of the parameters and will be discussed in connection with problem no. 4. The derivative matrix refers to the quantities $\partial \alpha_{j1}/\partial \beta_j$ defined in sec. 5.

Finally a table print-out is given, containing the sets (x_i, y_i, δ_i) where δ_i = fit ordinate - data ordinate y_i.

Problem no. 2 is an example taken from Späth [7]. Our computations resulted in a parameter vector and a minimum Ø close to Späth's values. Notice the extremely high correlations between some of the parameters. The "variance of the fit" is given here, because we have equally weighted data (I1=1), and statistics on (I3=1).

Problem no. 3 treats the same data with the number of exponential terms increased from 2 to 3. It is clear that this problem severely taxes the capability of EXPOSUM. Yet, convergence was obtained after 24 iterations. On the other hand, Späth [7] reports convergence after 17 iterations,

---

*This choice (IWG = 2) was made for illustrative purposes, although Poisson-weighting (IWG = 3) is the standard choice for counting problems like this.

but his minimum Ø exceeds ours by some 9%, perhaps indicating some shortcoming in his method. The third term in our result has very extreme parameters, and probably for this reason a statistical analysis was impossible (due to overflow conditions). In any case, the conclusion must be that the data sample does not contain sufficient information to permit a reasonable three-term analysis.

Problem no. 4 is a synthetical case constructed to illustrate the significance of the inverse variance-covariance matrix M^{-1} (cf. eq. (20)). We noticed in sec. 4 that the parameter vector b under certain conditions had a multi-normal distribution with mean b_o and the moment matrix M. Then the equiprobability surfaces in the parameter space are ellipsoides around b_o. Now, we may replace this distribution by another having the same mean and moment matrix, but with a uniform probability density inside a certain ellipsoid and zero density outside. This ellipsoid, called the concentration ellipsoid, has the equation [8)]

$$(b - b_o)^T M^{-1} (b - b_o) = k + 2 \tag{56}$$

where k here denotes the dimension of b. In the case of problem no. 4, $k = 2$, so we may write $y = ae^{\omega x}$, and (56) becomes an ellipse:

$$A(\omega - \omega_o)^2 + B(a - a_o)^2 + 2C(\omega - \omega_o)(a - a_o) = 4 \tag{57}$$

with $A = 0.106 \cdot 10^{10}$, $B = 0.460 \cdot 10^7$, $C = 0.581 \cdot 10^8$, and $b - b_o = \begin{Bmatrix} \omega - \omega_o \\ a - a_o \end{Bmatrix}$

The concentration ellipse (57) is shown in fig. 1. Now, what happens to a, if ω is given a small displacement from ω_o and we still require that a should be a (conditional) least-squares solution? The answer is that $\partial a/\partial\omega$ is given by the slope of the line of regression [8)] of a on ω. Conversely, $\partial\omega/\partial a$ is determined by the line of regression of ω on a. Both these lines are obtained by differentiating (57); if we write $\Delta\omega$ for $\omega - \omega_o$ and Δa for $a - a_o$, we get

$$(A\,\Delta\omega + C\,\Delta a)\, d\omega + (B\Delta a + C\Delta\omega)\, da = 0 \tag{58}$$

The first regression line is obtained by setting $d\omega = 0$, the second by setting $da = 0$. In this way, the slope of the line of regression of a on ω is calculated to $\partial a/\partial\omega = - C/B = -12.6$. An independent check of this result is obtained from the print-out of the derivative matrix, here the single number $\partial a/\partial \omega$, found by the analysis outlined in sec. 6.

For more than two parameters, things are of course more complicated, but the principal features of the statistical analysis are the same.

The last two examples are Rossi-α experiments, performed at the DR 1 reactor. A multi-channel analyser gives number of counts for a serial of equidistant times. Hence the output in each channel (y_i) may be expected to have a Poisson distribution. The time distance between neighbour counts is 90 μs, and this will be chosen as the unit for the x_i, so that $x_{i+1} - x_i = 1$.

The output for problem no. 5 shows a condensed print-out; neither the progress of iterations, the statistical analysis, nor the table print-out is given.

On the contrary, problem no. 6 is solved with all print-out options active.

We notice that the statistical option I3 has been set equal to 3; this means Poisson statistics with known σ (sec. 4). In fact, eq. (17) takes here the form

$$\sigma_i = \frac{1}{E(y_i)} \qquad (59)$$

When the y_i are not too small, as we shall assume, (59) is safely replaced by

$$\sigma_i = \frac{1}{y_i} \qquad (60)$$

corresponding to $\sigma = 1$ and $h_i = 1/y_i$ in eq. (17). Here we have operated with count numbers as the y_i, in contrary to count rates. In the latter case one would replace (60) by

$$\sigma_i = \frac{\sigma}{y_i} \qquad (61)$$

where σ had to be estimated from the sample; this would be accomplished by setting I3 = 2. In the case I3 = 3, better estimates of variances etc. are obtained than for I3 = 2. As pointed out in sec. 4 we have further for I3 = 3 through the weighted sum-of-squared-errors Ø a χ^2-test of the validity of our model. This is illustrated by the print-out for problem no. 6. It turns out that Ø for this problem is many standard deviations larger than predicted by the model. Our conclusion is then (cf. sec. 4) that the model is insufficient to describe the data sample. A study of the print-out table reveals in this case the reason for this shortcoming. Let us consider the signs of the deviations throughout the table. We consider the two first signs as one set which may be (+,+), (+,-), (-,+), or (-,-). The same is done for the points 3 and 4, and so on. A comparison of the number of (+,-) to the number of (-,+) showed that the latter number exceeded the former by a very significant amount. This anomali was traced back to a fault in a multi-vibrator in the electronic equipment.

8. SUMMARY AND CONCLUSIONS

The present report has discussed a FORTRAN IV code EXPOSUM which replaces an earlier ALGOL version. The code carries out a least-squares fit of the parameters in a sum-of-exponential to a given data sample, and analyses the fit statistically.

The EXPOSUM code uses a Marquardt iteration scheme. However, a new model has been developed, according to which iterations principally are confined to the space of the nonlinear parameters.

Illustrative examples of the practical use of EXPOSUM has been given.

It seems justable to conclude that EXPOSUM solves the sum-of-exponential fitting problem very efficiently for a majority of practical cases. Further, it is most possible that its underlying principles may be used successfully also for other types of non-linear fitting problems.

9. ACKNOWLEDGEMENT

The author wishes to thank P. Skjerk Christensen who supplied all the experimental data samples used as examples.

10. REFERENCES

1) R. H. Moore and R. K. Zeigler, The Solution of the General Least Squares Problem with Special Reference to High-Speed Computers. Los Alamos Scientific Laboratory, LA-2367 (1960).

2) R. A. Buckingham, Numerical Methods (Pitman and Sons, London, 1957) 329.

3) D. W. Marquardt, An Algorithm for Least-Squares Estimation of Nonlinear Parameters, J. SIAM 11, No. 2 (1963) 431-441.

4) E. L. Bell et al., Fitting Multi-Component Exponential Decay Curves by Digital Computer, USAF-AD 477451 (1965).

5) P. Kirkegaard, Tilpasning af et tabelmateriale til en sum af exponentialudtryk. Conference paper, Nord DATA-68, Helsingfors/Otnäs 6-8.6.1968, vol. I, 197-217.

6) P. Kirkegaard, Description of AEK Programme no. 513, EXPOSUM. Risø-M-812 (1968).

7) H. Späth, FORTRAN-IV Programs for Fitting Data to one or more Exponentials. Kernforschungszentrum Karlsruhe, KFK 707 (1968).

8) H. Cramer, Mathematical Methods of Statistics (Princeton, 1946).

9) A. Hald, Statistical Theory with Engineering Applications (Wiley and Sons, New York, 1952).

10) G. E. Forsythe and C. B. Moler, Computer Solutions of Linear Algebraic Systems (Prentice-Hall, Englewood Cliffs, 1967).

11) Yu. A. Shreider et al., The Monte Carlo Method (Pergamon Press, 1966) 131-132.

12) C. D. Gardner, EXPALS: FORTRAN Code for Exponential Approximation by Least Squares. California Univ., Livermore. Lawrence Radiation Lab., UCRL-14541 (1970).

13) G. H. Golub, Matrix Decompositions and Statistical Calculations. Proceedings of a Conference Held at The University of Wisconsin, Madison, Wisconsin, April 28-30, 1969 (Statistical Computation, Academic Press, New York, 1969) 365-397.

11. APPENDIX I: EXPOSUM Data Sheet

IBM

IBM Data Centre
Punching Instructions

NAME: PK

Date: 19/8 1970 — Page 1 of 5

APPLICATION: Data P-513 EXPOSUM

Col. 1–10	Col. 11–20	Col. 21–30	Col. 31–40	Col. 41–50	Col. 51–80
1					
2	1	1	1	1	
23					
0.5	17796.	0.56			
1.5	13863.	1.93			
2.5	11430.	0.87			
3.5	9396.	1.05			
4.5	7500.	1.31			
5.5	6372.	1.54			
6.5	5190.	1.89			
8.	4038.	4.82			
10.	3048.	6.34			
12.	2270.	12.62			
14.	1836.	20.58			
17.5	1246.	44.31			
20.5	996.	54.35			
24.	835.	63.63			
28.	691.	112.64			
36.	561.	89.69			
46.	471.	155.44			
56.	474.	206.36			
66.	452.	267.86			
86.	421.	453.69			
106.	414.5	459.55			

D 2023

IBM

IBM Data Centre
Punching Instructions

NAME PK
Date 19/8 1970 | Page 2 of 5
APPLICATION Data P-513 EXPOSUM

1–10	11–20	21–30	31–40	41–50	51–60	61–70	71–80
146.	392.	480.48					
176.	389.	483.38					
3							
-0.30	-0.136	-0.073					
0							
2							
1	1	1	1	1			
24							
0.05	2.51						
0.10	2.04						
0.15	1.67						
0.20	1.37						
0.25	1.12						
0.30	0.93						
0.35	0.77						
0.40	0.64						
0.45	0.53						
0.50	0.45						
0.55	0.38						
0.60	0.32						
0.65	0.27						
0.70	0.23						
0.75	0.20						
0.80	0.17						

IBM

IBM Data Centre

Punching Instructions

NAME PK

Date 19/8 1970 | Page 3 of 5

APPLICATION Data P-513 EXPOSUM

1–10	11–20	21–30	31–40	41–50
0.85	0.15			
0.90	0.13			
0.95	0.11			
1.00	0.10			
1.05	0.09			
1.10	0.08			
1.15	0.07			
1.20	0.06			
2				
-4.0	-2.0			
0				
3				
1	1	0	1	1
0				
3				
-7.0	-4.0	-0.2		
0				
4				
1	1	1	0	1
10				
1.	2.895			
2.	2.619			
3.	2.370			
4.	2.143			

D 2023

IBM

IBM Data Centre
Punching Instructions

NAME: PK
Date: 19/8 1970 | Page 4 of 5

APPLICATION: Data P-513 EXPOSUM

1–10	11–20	21–30	31–40	41–50	51–80
5.	1.940				
6.	1.757				
7.	1.590				
8.	1.438				
9.	1.301				
10.	1.176				
1					
-0.15					
25					
0.02	10.	0.001	0.00001	1.E-7	
5					
3	0	0	0	0	
252					
1.	14501 }				
---	} 252 punched cards converted from paper-tape output of multi-channel analyser				
253.	2834. }				
2					
-0.01	-0.03				
0					
6					
3	1	2	1	1	
255					
1.	9482. }				
	} 255 punched cards converted from paper-tape output of multi-channel analyser				
255.	8174. }				

D 2023

IBM

IBM Data Centre

Punching Instructions

NAME PK

Date 19/8 1970 | Page 5 of 5

APPLICATION Data P-513 EXPOSUM

Columns 1–10
1
-0.0025
0
-1

D 2023

12: APPENDIX II. RESULTS FOR SAMPLE PROBLEMS

```
PROBLEM NO   1

FIT WITH CONSTANT TERM
NUMBER OF EXPONENTIAL  TERMS =  3
NUMBER OF DATA POINTS = 23

GUESS  FOR OMEGAS
    -0.3C0CC00E C0    -C.136C0C0E C0    -0.7300000E-01

CONTROL PARAMETERS
LAM =    0.2C00E-C1
NY  =    0.1000E C2
TAU =    0.1C00E-C2
EPS =    0.3C00E-C4
EPS1=    0.3C00E-C6
RMAX =   25

FLOATING POINT TRAP AT LOCATION *** 22240
UNDERFLOW
IN MULTIPLIER-QUOTIENT REGISTER

ITERATION NO   1
OMEGAS
    -0.3000C00E C0    -C.136C0C0E C0    -0.7300000E-01
COEFFICIENTS
     0.1320644E C5     C.5131076E 04     0.1221563E 04
CONSTANT
     0.4119918E C3
PHI =     0.1498C644E C7
LAM =     0.2C00E-01
B
C
A

ITERATION NO   2
OMEGAS
    -0.3122368E C0    -C.1778916E C0    -0.3291236E-01
COEFFICIENTS
     0.7051685E C4     C.1133768E 05     0.5614736E 03
CONSTANT
     0.3874023E C3
PHI =     0.8158C880E C6
LAM =     0.2000E C0
A

ITERATION NO   3
OMEGAS
    -0.3207900E C0    -C.1475235E CC    -0.2967251E-01
COEFFICIENTS
     0.1076902E C5     C.8329966E C4     0.3635943E 03
CONSTANT
     0.3919960E C3
PHI =     0.44478227E C6
LAM =     0.2C0CE-C1
A
```

```
ITERATION NO   4
OMEGAS
    -0.2865236E C0     -C.1318673E C0     -0.1972045E-01
COEFFICIENTS
     0.1264258E C5      C.6354365E C4      0.2457422E 03
CONSTANT
     0.3802245E C3
PHI =      0.39056614E C6
LAM =      0.2000E-02
A

ITERATION NO   5
OMEGAS
    -0.2864703E C0     -C.1284321E C0     -0.1825540E-01
COEFFICIENTS
     0.1294863E 05      0.6117142E 04      0.2239034E 03
CONSTANT
     0.3788361E C3
PHI =      0.38524559E C6
LAM =      0.2000E-03
A

ITERATION NO   6
OMEGAS
    -0.2864990E C0     -C.1285049E C0     -0.1818243E-01
COEFFICIENTS
     0.1293862E C5      0.6126106E C4      0.2237236E 03
CONSTANT
     0.3786485E C3
PHI =      0.38522932E C6
LAM =      0.2000E-04
A

ITERATION NO   7
OMEGAS
    -0.2865089E C0     -C.1285128E C0     -0.1818616E-01
COEFFICIENTS
     0.1293781E C5      C.6126922E 04      0.2237621E 03
CONSTANT
     0.3786543E C3
PHI =      0.38522923E C6
LAM =      0.2000E-05
A
CONVERGENCE OBTAINED AFTER    7 ITERATIONS

WEIGHTEC SUM OF SQUARED ERRORS      0.38522933E 06

FINAL ESTIMATES OF PARAMETERS
OMEGAS
    -0.2865099E C0     -C.1285134E 00     -0.1818629E-01
STANDARC DEVIATIONS
     0.2620120E-C1      C.1777428E-01      0.8380155E-02
COEFFICIENTS
     0.1293773E C5      C.6127001E 04      0.2237637E 03
STANDARC DEVIATIONS
     0.1963259E C4      C.2005333E 04      0.8558162E 02
CONSTANT
     0.3786545E C3
STANDARC DEVIATION
     0.1494939E C2
```

MATRIX OF CORRELATIONS BETWEEN THE PARAMETERS

1.0000	0.9085	0.5291	0.9429	-0.9704	-0.6279	-0.3998
0.9085	1.0000	0.7496	0.9828	-0.9734	-0.8535	-0.5859
0.5291	0.7496	1.0000	0.6533	-0.6160	-0.9379	-0.9241
0.9429	0.9828	0.6533	1.0000	-0.9937	-0.7613	-0.5009
-0.9704	-0.9734	-0.6160	-0.9937	1.0000	0.7256	0.4678
-0.6279	-0.8535	-0.9379	-0.7613	0.7256	1.0000	0.7567
-0.3998	-0.5859	-0.9241	-0.5009	0.4678	0.7567	1.0000

INVERSE OF VARIANCE-COVARIANCE MATRIX

0.137E 06	0.275E 06	0.421E 05	0.222E 01	0.579E 01	0.164E 02	0.204E 02
0.275E 06	0.117E 07	0.404E 06	0.274E 01	0.141E 02	0.885E 02	0.130E 03
0.421E 05	0.404E 06	0.142E 07	0.284E 00	0.323E 01	0.108E 03	0.396E 03
0.222E 01	0.274E 01	0.284E 00	0.697E-04	0.113E-03	0.198E-03	0.223E-03
0.579E 01	0.141E 02	0.323E 01	0.113E-03	0.280E-03	0.967E-03	0.129E-02
0.164E 02	0.885E 02	0.108E 03	0.198E-03	0.967E-03	0.120E-01	0.293E-01
0.204E 02	0.130E 03	0.396E 03	0.223E-03	0.129E-02	0.293E-01	0.121E 00

DERIVATIVE MATRIX DCOEF(ROW)/DOMEGA(COLUMN)

0.130E 05	0.102E 06	-0.305E 05
-0.293E 05	-0.813E 05	0.303E 05
0.118E 04	-0.368E 04	-0.567E 04
-0.166E 03	0.491E 03	-0.215E 04

X	Y	DEVIATION
0.50000E 00	0.17796E 05	0.23895E 03
0.15000E 01	0.13863E 05	-0.20425E 03
0.25000E 01	0.11430E 05	0.73146E 02
0.35000E 01	0.93960E 04	0.15355E 03
0.45000E 01	0.75000E 04	-0.85027E 02
0.55000E 01	0.63720E 04	0.92939E 02
0.65000E 01	0.51900E 04	-0.54319E 02
0.80000E 01	0.40380E 04	-0.33083E 02
0.10000E 02	0.30480E 04	0.50819E 02
0.12000E 02	0.22700E 04	-0.14850E 02
0.14000E 02	0.18360E 04	0.35932E 02
0.17500E 02	0.12460E 04	-0.27829E 02
0.20500E 02	0.99600E 03	-0.12808E 02
0.24000E 02	0.83500E 03	0.17994E 02
0.28000E 02	0.69100E 03	0.59418E 01
0.36000E 02	0.56100E 03	0.56721E 01
0.46000E 02	0.47100E 03	-0.21203E 02
0.56000E 02	0.47400E 03	0.99403E 01
0.66000E 02	0.45200E 03	0.46996E 01
0.86000E 02	0.42100E 03	-0.45837E 01
0.10600E 03	0.41450E 03	0.32859E 01
0.14600E 03	0.39200E 03	-0.23817E 01
0.17600E 03	0.38900E 03	0.12316E 01

```
PROBLEM NO  2

FIT WITH CONSTANT TERM
NUMBER OF EXPONENTIAL TERMS =  2
NUMBER OF DATA POINTS = 24

GUESS FOR OMEGAS
    -0.4C0CC00E C1    -C.2CCCCC0E 01

CONTROL PARAMETERS
LAM =    0.2C00E-C1
NY  =    0.1C00E C2
TAU =    0.1C00E-C2
EPS =    0.3C00E-C4
EPS1=    0.3C00E-C6
RMAX =   25


ITERATION NO  1
OMEGAS
    -0.4C0C000E C1    -C.2CCCCC0E 01
COEFFICIENTS
     0.3052739E C1    -C.7C27091E-01
CONSTANT
     0.5511866E-C1
PHI =     0.16172681E-C2
LAM =     0.2000E-01
A

ITERATION NO  2
OMEGAS
    -0.4612884E C1    -C.1469180E 01
COEFFICIENTS
     0.2692387E C1     0.4311534E C0
CONSTANT
    -0.2641907E-C1
PHI =     0.20593709E-C3
LAM =     0.200CE-02
A

ITERATION NO  3
OMEGAS
    -0.4670061E C1    -C.2224297E C1
COEFFICIENTS
     0.2481180E C1     C.5940280E C0
CONSTANT
     0.1214341E-C1
PHI =     0.11044285E-C3
LAM =     0.2C00E-03
A

ITERATION NO  4
OMEGAS
    -0.4801812E C1    -C.2524314E 01
COEFFICIENTS
     0.2281814E C1     C.7859138E C0
CONSTANT
     0.1749616E-C1
PHI =     0.10909728E-C3
LAM =     0.200CE-04
A
```

```
ITERATION NO   5
OMEGAS
   -0.4828423E 01    -0.2522515E 01
COEFFICIENTS
     0.2266087E 01     0.8083650E 00
CONSTANT
    0.1642617E-01
PHI =     0.10764015E-03
LAM =     0.2000E-05
A

ITERATION NO   6
OMEGAS
   -0.4828738E 01    -0.2523062E 01
COEFFICIENTS
     0.2265632E 01     0.8088156E 00
CONSTANT
     0.1643447E-01
PHI =     0.10764010E-03
LAM =     0.2000E-06
A
CONVERGENCE OBTAINED AFTER    6 ITERATIONS

WEIGHTED SUM OF SQUARED ERRORS      0.10764000E-03

FINAL ESTIMATES OF PARAMETERS
OMEGAS
   -0.4828759E 01    -0.2523101E 01
STANDARD DEVIATIONS
     0.3346409E 00     0.6136175E 00
COEFFICIENTS
     0.2265603E 01     0.8088447E 00
STANDARD DEVIATIONS
     0.4941647E 00     0.4879240E 00
CONSTANT
     0.1643526E-01
STANDARD DEVIATION
     0.1075764E-01

VARIANCE OF THE FIT =   0.56653E-05

MATRIX OF CORRELATIONS BETWEEN THE PARAMETERS

  1.0000  0.9867  0.9952 -0.9963 -0.9316

  0.9867  1.0000  0.9975 -0.9967 -0.9755

  0.9952  0.9975  1.0000 -0.9999 -0.9586

 -0.9963 -0.9967 -0.9999  1.0000  0.9555

 -0.9316 -0.9755 -0.9586  0.9555  1.0000

INVERSE OF VARIANCE-COVARIANCE MATRIX

 0.402E 05 0.324E 05 0.841E 05 0.146E 06 0.335E 06

 0.324E 05 0.340E 05 0.522E 05 0.110E 06 0.365E 06

 0.841E 05 0.522E 05 0.284E 06 0.397E 06 0.644E 06

 0.146E 06 0.110E 06 0.397E 06 0.614E 06 0.125E 07

 0.335E 06 0.365E 06 0.644E 06 0.125E 07 0.424E 07
```

CERIVATIVE MATRIX DCOEF(ROW)/DOMEGA(COLUMN)

0.615E 00 C.473E 0C

-0.712E C0-C.409E 0C

0.375E-01-0.373E-01

X	Y	DEVIATION
0.50000E-01	C.2510CE 01	C.96029E-03
0.10000E 00	C.2040CE 01	-C.28021E-02
0.15000E 00	C.1670CE 01	C.15371E-02
0.20000E C0	C.1370CE 01	C.27290E-02
0.25C00E C0	C.1120CE C1	-C.43834E-02
0.30000E C0	C.93C0CE C0	C.19593E-02
0.35000E C0	C.77C0CE C0	C.10827E-02
0.40000E 00	C.64C0CE CC	C.39010E-03
0.45000E C0	C.53C0CE C0	-0.42345E-02
0.50000E C0	C.45C00E C0	0.18915E-02
0.55000E 00	C.38C0CE C0	C.24995E-02
0.60000E 00	C.32C0CE C0	C.56792E-03
0.65000E C0	C.27C0CE C0	-C.15224E-02
0.70000E C0	C.23C0CE C0	-0.18647E-02
0.75000E C0	C.20C0CE C0	C.10712E-02
0.80000E 00	C.17C0CE CC	-C.14845E-02
0.85000E 00	C.15C0CE C0	0.14598E-02
0.90000E 00	C.13C0CE C0	C.70491E-03
0.95000E C0	C.11C0CE CC	-C.31CC5E-02
0.10000E 01	C.10C0CE C0	C.57012E-03
0.10500E 01	C.90C0CE-01	C.21457E-02
0.11000E C1	C.80C0CE-01	0.19762E-02
0.11500E 01	C.70C0CE-01	C.34871E-03
0.12000E C1	C.60C0CE-01	-0.25013E-02

PROBLEM NO 3

FIT WITH CONSTANT TERM
NUMBER OF EXPONENTIAL TERMS = 3
NUMBER OF DATA POINTS = 24

GUESS FOR OMEGAS
-0.7000C00E C1   -C.4CCCCC0E 01   -0.2000000E 00

CONTROL PARAMETERS
LAM = C.2C00E-C1
NY = 0.1C00E C2
TAU = 0.1C00E-C2
EPS = 0.3C00E-C4
EPS1= 0.3C00E-06
RMAX = 25

```
ITERATION NO   1
OMEGAS
   -0.7000000E C1    -0.4CCC0C0E 01    -0.2000000E 00
COEFFICIENTS
     0.3586476E C0     C.2617343E 01     0.3613377E 00
CONSTANT
   -0.2442264E C0
PHI =     0.10561C23E-C3
LAM =     0.2000E-01
B
A

ITERATION NO   2
OMEGAS
   -0.7103588E C1    -0.3926617E 01     0.1785018E 00
COEFFICIENTS
     0.4020145E C0     C.26C1066E 01    -0.2255798E 00
CONSTANT
     0.3178871E C0
PHI =     0.10485941E-C3
LAM =     0.200CE-01
B
A

ITERATION NO   3
OMEGAS
   -0.6878016E C1    -C.3870219E 01     0.6315185E 00
COEFFICIENTS
     0.4662877E C0     C.2550860E C1    -0.3606816E-01
CONSTANT
     0.1140376E C0
PHI =     0.10468474E-C3
LAM =     0.2000E-01
B
A

ITERATION NO   4
OMEGAS
   -0.6649102E C1    -C.38C2611E 01     0.1153062E 01
COEFFICIENTS
     0.5516310E C0     0.2477615E 01    -0.1011026E-01
CONSTANT
     0.7596381E-C1
PHI =     0.10447252E-C3
LAM =     0.200CE-01
B
A

ITERATION NO   5
OMBGAS
   -0.6424518E 01    -C.3727080E 01     0.1837942E 01
COEFFICIENTS
     0.6550341E C0     0.2384344E 01    -0.2684380E-02
CONSTANT
     0.5841142E-C1
PHI =     0.10417930E-C3
LAM =     0.200CE-01
B
A
```

```
 ITERATION NO  6
OMEGAS
    -0.6206938E C1    -C.3642391E 01     0.2805120E 01
COEFFICIENTS
     0.7786101E C0     0.2269096E 01    -0.5404841E-03
CONSTANT
     0.4797727E-C1
PHI =     0.10374197E-C3
LAM =     0.2000E-01
B
A

 ITERATION NO  7
OMEGAS
    -0.5994115E C1    -0.3546741E 01     0.4281088E 01
COEFFICIENTS
     0.9255660E C0     C.2128770E 01    -0.6167621E-04
CONSTANT
     0.4091730E-C1
PHI =     0.10303019E-C3
LAM =     0.2000E-01
B
A

 ITERATION NO  8
OMEGAS
    -0.5783770E C1    -0.3438330E 01     0.6757913E 01
COEFFICIENTS
     0.1098535E 01     0.1960912E 01    -0.2241265E-05
CONSTANT
     0.3576248E-C1
PHI =     0.10177649E-C3
LAM =     0.2000E-01
B
A

 ITERATION NO  9
OMEGAS
    -0.5580967E C1    -C.3319603E 01     0.1130556E 02
COEFFICIENTS
     0.1291275E C1     C.1771848E C1    -0.7536772E-08
CONSTANT
     0.3191185E-C1
PHI =     0.99647566E-C4
LAM =     0.2000E-01
B
A

 ITERATION NO 10
OMEGAS
    -0.5414492E C1    -C.3209719E 01     0.1943607E 02
COEFFICIENTS
     0.1467591E C1     C.1597688E C1    -0.3917843E-12
CONSTANT
     0.2927C99E-C1
PHI =     0.97338518E-C4
LAM =     0.2000E-01
B
A
```

```
ITERATION NO 11
OMEGAS
    -0.5318267E 01    -0.3140664E 01     0.2913798E 02
COEFFICIENTS
     0.1575741E 01     0.1490353E 01    -0.3281126E-17
CONSTANT
     0.2790922E-01
PHI =     0.96563710E-04
LAM =     0.2000E-01
A

ITERATION NO 12
OMEGAS
    -0.5195572E 01    -0.3052181E 01     0.3332303E 02
COEFFICIENTS
     0.1715201E 01     0.1350924E 01    -0.2083591E-19
CONSTANT
     0.2673610E-01
PHI =     0.96483443E-04
LAM =     0.2000E-02
A

ITERATION NO 13
OMEGAS
    -0.5202094E 01    -0.3050599E 01     0.3073425E 02
COEFFICIENTS
     0.1713217E 01     0.1353401E 01    -0.4564920E-18
CONSTANT
     0.2657619E-01
PHI =     0.96414974E-04
LAM =     0.2000E-03
A

ITERATION NO 14
OMEGAS
    -0.5186352E 01    -0.3035295E 01     0.3339283E 02
COEFFICIENTS
     0.1734139E 01     0.1332694E 01    -0.1851794E-19
CONSTANT
     0.2628586E-01
PHI =     0.96414522E-04
LAM =     0.2000E-04
B
C
C
C
A

ITERATION NO 15
OMEGAS
    -0.5190177E 01    -0.3039954E 01     0.3124871E 02
COEFFICIENTS
     0.1728388E 01     0.1338324E 01    -0.2443478E-18
CONSTANT
     0.2640664E-01
PHI =     0.96413398E-04
LAM =     0.2000E-01
A
```

```
ITERATION NO 16
OMEGAS
    -0.5190556E C1    -0.3039229E 01     0.3287477E 02
COEFFICIENTS
     0.1728668E C1     0.1338121E 01    -0.3459368E-19
CONSTANT
     0.2635404E-C1
PHI =     0.96412C61E-C4
LAM =     0.2000E-02
B
C
A

ITERATION NO 17
OMEGAS
    -0.5192692E C1    -0.3041988E 01     0.3155506E 02
COEFFICIENTS
     0.1725334E C1     0.1341375E 01    -0.1693193E-18
CONSTANT
     0.2642924E-C1
PHI =     0.96411602E-C4
LAM =     0.2000E-01
A

ITERATION NO 18
OMEGAS
    -0.5192520E C1    -0.3041180E 01     0.3256416E 02
COEFFICIENTS
     0.1726023E C1     0.1340737E 01    -0.5031731E-19
CONSTANT
     0.2639126E-C1
PHI =     0.96411157E-C4
LAM =     0.2000E-02
B
C
A

ITERATION NO 19
OMEGAS
    -0.5193819E C1    -0.3042861E 01     0.3174591E 02
COEFFICIENTS
     0.1723992E C1     0.1342719E 01    -0.1346893E-18
CONSTANT
     0.2643729E-C1
PHI =     0.9641C701E-C4
LAM =     0.2000E-01
A

ITERATION NO 20
OMEGAS
    -0.5193633E C1    -0.3042289E 01     0.3237134E 02
COEFFICIENTS
     0.1724523E C1     0.1342220E C1    -0.6348969E-19
CONSTANT
     0.2641283E-C1
PHI =     0.96410680E-C4
LAM =     0.2000E-02
B
A
```

```
ITERATION NO 21
OMEGAS
    -0.5196432E C1     -0.3045133E 01      0.3175268E 02
COEFFICIENTS
     0.1720716E C1      0.1345980E 01     -0.1338051E-18
CONSTANT
     0.2647113E-C1
PHI =     0.96410668E-C4
LAM =     0.2000E-02
A

ITERATION NO 22
OMEGAS
    -0.5193523E C1     -C.3C42199E C1      0.3237189E 02
COEFFICIENTS
     0.1724657E C1      C.1342086E 01     -0.6344559E-19
CONSTANT
     0.2641167E-C1
PHI =     0.9641C551E-C4
LAM =     0.2000E-03
B
C
C
A

ITERATION NO 23
OMEGAS
    -0.5194359E C1     -0.3C43257E C1      0.3186724E 02
COEFFICIENTS
     0.1723370E C1      C.1343344E 01     -0.1164494E-18
CONSTANT
     0.2644C36E-C1
PHI =     0.9641C536E-C4
LAM =     0.2000E-01
A

ITERATION NO 24
OMEGAS
    -0.5194302E C1     -0.3C42956E C1      0.3224861E 02
COEFFICIENTS
     0.1723626E C1      C.1343108E C1     -0.7361793E-19
CONSTANT
     0.2642616E-C1
PHI =     0.9641C413E-C4
LAM =     0.2000E-02
B
C
C
C
C
C
C
C
C
C
C
C
C
C
A
CONVERGENCE OBTAINEC AFTER   24 ITERATIONS
```

```
WEIGHTED SUM OF SQUARED ERRORS      0.96410407E-04

FINAL ESTIMATES OF PARAMETERS
OMEGAS
    -0.5194302E 01    -0.3042956E 01      0.3224861E 02
COEFFICIENTS
     0.1723626E 01     0.1343108E 01    -0.7361795E-19
CONSTANT
     0.2642616E-01
```

```
PROBLEM NO   4

FIT WITHOUT CONSTANT TERM
NUMBER OF EXPONENTIAL TERMS =  1
NUMBER OF DATA POINTS = 10

GUESS FOR OMEGAS
    -0.1500000E 00

CONTROL PARAMETERS
LAM =    0.2000E-01
NY  =    0.1000E 02
TAU =    0.1000E-02
EPS =    0.1000E-04
EPS1=    0.1000E-06
RMAX =   25


ITERATION NO   1
OMEGAS
    -0.1500000E 00
COEFFICIENTS
     0.3806774E 01
PHI =     0.61285987E 00
LAM =     0.2000E-01
A

ITERATION NO   2
OMEGAS
    -0.9788765E-01
COEFFICIENTS
     0.3172482E 01
PHI =     0.11946196E-02
LAM =     0.2000E-02
A
```

```
ITERATION NO   3
OMEGAS
    -0.9996744E-C1
COEFFICIENTS
     0.3198807E C1
PHI =     0.68017587E-C5
LAM =     0.2000E-03
A

ITERATION NO   4
OMEGAS
    -0.9997176E-C1
COEFFICIENTS
     0.3198862E C1
PHI =     0.67965559E-C5
LAM =     0.200CE-04
B
C
A
CONVERGENCE OBTAINED AFTER    4 ITERATIONS

WEIGHTED SUM OF SQUARED ERRORS      0.67965559E-05

FINAL ESTIMATES OF PARAMETERS
OMEGAS
    -0.9997176E-C1
STANDARD DEVIATIONS
     0.5584172E-C4
COEFFICIENTS
     0.3198862E C1
STANDARD DEVIATIONS
     0.8460578E-C3

VARIANCE OF THE FIT =  0.84957E-C6

MATRIX OF CORRELATIONS BETWEEN THE PARAMETERS

  1.0000 -0.8344

 -0.8344  1.00CC

INVERSE OF VARIANCE-COVARIANCE MATRIX

 0.106E 10 C.581E 08

 0.581E 08 C.46CE 07

DERIVATIVE MATRIX DCOEF(ROW)/DOMEGA(COLUMN)

-0.126E 02
```

X	Y	DEVIATION
0.10000E C1	C.2895CE C1	C.46843E-03
0.20000E C1	C.2619CE 01	-C.15447E-03
0.30000E C1	C.2370CE C1	C.2414CE-04
0.40000E 01	C.2143CE 01	-C.15C34E-02
0.50000E 01	C.1940CE C1	-C.48169E-C3
0.60000E 01	C.1757CE C1	C.113C0E-02
0.70000E C1	C.1590CE C1	C.11782E-02
0.80000E 01	C.1438CE 01	C.334C2E-03
0.90000E 01	C.13C1CE C1	C.1093CE-03
0.10000E 02	C.1176CE C1	-C.11278E-02

```
PROBLEM NO   5

FIT WITHOUT CONSTANT TERM
NUMBER OF EXPONENTIAL TERMS =  2
NUMBER OF DATA POINTS =252

GUESS FOR OMEGAS
    -0.1000000E-01    -0.3000000E-01

CONTROL PARAMETERS
LAM =    0.2000E-01
NY  =    0.1000E 02
TAU =    0.1000E-02
EPS =    0.3000E-04
EPS1=    0.3000E-06
RMAX =   25

CONVERGENCE OBTAINED AFTER    8 ITERATIONS

WEIGHTED SUM OF SQUARED ERRORS      0.82410743E 03

FINAL ESTIMATES OF PARAMETERS
OMEGAS
    -0.5640193E-02    -0.3911065E-01
COEFFICIENTS
      0.1185816E 05     0.3459731E 04




PROBLEM NO   6

FIT WITH CONSTANT TERM
NUMBER OF EXPONENTIAL TERMS =  1
NUMBER OF DATA POINTS =255

GUESS FOR OMEGAS
    -0.2500000E-02

CONTROL PARAMETERS
LAM =    0.2000E-01
NY  =    0.1000E 02
TAU =    0.1000E-02
EPS =    0.3000E-04
EPS1=    0.3000E-06
RMAX =   25
```

```
ITERATION NO  1
OMEGAS
   -0.2500000E-02
COEFFICIENTS
    0.2050123E C4
CONSTANT
    0.6948171E C4
PHI =     0.16161343E C4
LAM =     0.2000E-01
A

ITERATION NO  2
OMEGAS
   -0.1657433E-C1
COEFFICIENTS
    0.1351147E 04
CONSTANT
    0.8153695E C4
PHI =     0.61935490E C3
LAM =     0.2000E-02
A

ITERATION NO  3
OMEGAS
   -0.2563036E-01
COEFFICIENTS
    0.1535206E C4
CONSTANT
    0.8235171E 04
PHI =     0.46136856E C3
LAM =     0.2000E-03
A

ITERATION NO  4
OMEGAS
   -0.2666336E-C1
COEFFICIENTS
    0.1554997E C4
CONSTANT
    0.8241317E C4
PHI =     0.46032807E C3
LAM =     0.2000E-04
A

ITERATION NO  5
OMEGAS
   -0.2653476E-C1
COEFFICIENTS
    0.1552556E C4
CONSTANT
    0.8240574E C4
PHI =     0.46031308E C3
LAM =     0.2000E-05
A
```

```
ITERATION NO  6
OMEGAS
   -0.2655302E-01
COEFFICIENTS
     0.1552906E 04
CONSTANT
     0.8240680E 04
PHI =     0.46031276E 03
LAM =     0.2000E-06
A

ITERATION NO  7
OMEGAS
   -0.2655046E-01
COEFFICIENTS
     0.1552855E 04
CONSTANT
     0.8240665E 04
PHI =     0.46031273E 03
LAM =     0.2000E-07
A
CONVERGENCE OBTAINED AFTER    7 ITERATIONS

WEIGHTED SUM OF SQUARED ERRORS      0.46031277E 03
THIS SHOULD BE APPROXIMATELY DISTRIBUTED AS CHI-SQUARE
WITH 252 DEGREES OF FREEDOM


FINAL ESTIMATES OF PARAMETERS
OMEGAS
   -0.2655082E-01
STANDARD DEVIATIONS
     0.9691019E-03
COEFFICIENTS
     0.1552864E 04
STANDARD DEVIATIONS
     0.3231000E 02
CONSTANT
     0.8240667E 04
STANDARD DEVIATION
     0.8827682E 01

MATRIX OF CORRELATIONS BETWEEN THE PARAMETERS

  1.0000 -0.5697 -0.6363

 -0.5697  1.0000  0.0240

 -0.6363  0.0240  1.0000

INVERSE OF VARIANCE-COVARIANCE MATRIX

 0.370E 07 0.616E 02 0.253E 03

 0.616E 02 0.198E-02 0.413E-02

 0.253E 03 0.413E-02 0.302E-01

DERIVATIVE MATRIX DCOEF(ROW)/DOMEGA(COLUMN)

-0.190E 05

-0.580E 04
```

X	Y	DEVIATION
0.10000E 01	0.94820E 04	-0.27084E 03
0.20000E 01	0.97500E 04	0.36777E 02
0.30000E 01	0.96170E 04	-0.57639E 02
0.40000E 01	0.94930E 04	-0.14407E 03
0.50000E 01	0.94600E 04	-0.14048E 03
0.60000E 01	0.95460E 04	-0.18850E 02
0.70000E 01	0.93570E 04	-0.17316E 03
0.80000E 01	0.95080E 04	0.11631E 02
0.90000E 01	0.95630E 04	0.99533E 02
0.10000E 02	0.94240E 04	-0.74282E 01
0.11000E 02	0.93980E 04	-0.22285E 01
0.12000E 02	0.93860E 04	0.16154E 02
0.13000E 02	0.92860E 04	-0.54260E 02
0.14000E 02	0.95050E 04	0.19355E 03
0.15000E 02	0.92390E 04	-0.44393E 02
0.16000E 02	0.93990E 04	0.14293E 03
0.17000E 02	0.92620E 04	0.32533E 02
0.18000E 02	0.92630E 04	0.59441E 02
0.19000E 02	0.94040E 04	0.22567E 03
0.20000E 02	0.91960E 04	0.42238E 02
0.21000E 02	0.89930E 04	-0.13684E 03
0.22000E 02	0.91420E 04	0.35460E 02
0.23000E 02	0.91310E 04	0.47147E 02
0.24000E 02	0.93030E 04	0.24124E 03
0.25000E 02	0.90000E 04	-0.40246E 02
0.26000E 02	0.92560E 04	0.23670E 03
0.27000E 02	0.92040E 04	0.20510E 03
0.28000E 02	0.90050E 04	0.25972E 02
0.29000E 02	0.90970E 04	0.13732E 03
0.30000E 02	0.89320E 04	-0.88429E 01
0.31000E 02	0.89360E 04	0.13503E 02
0.32000E 02	0.89250E 04	0.20368E 02
0.33000E 02	0.89540E 04	0.66765E 02
0.34000E 02	0.87420E 04	-0.12829E 03
0.35000E 02	0.87310E 04	-0.12280E 03
0.36000E 02	0.88650E 04	0.27268E 02
0.37000E 02	0.87180E 04	-0.10409E 03
0.38000E 02	0.89880E 04	0.18115E 03
0.39000E 02	0.89820E 04	0.18998E 03
0.40000E 02	0.89310E 04	0.15343E 03
0.41000E 02	0.88040E 04	0.40495E 02
0.42000E 02	0.88280E 04	0.78194E 02
0.43000E 02	0.85470E 04	-0.18947E 03
0.44000E 02	0.85040E 04	-0.21948E 03
0.45000E 02	0.85550E 04	-0.15583E 03
0.46000E 02	0.89800E 04	0.28149E 03
0.47000E 02	0.86880E 04	0.14896E 01
0.48000E 02	0.90520E 04	0.37717E 03
0.49000E 02	0.87910E 04	0.12755E 03
0.50000E 02	0.88970E 04	0.24462E 03
0.51000E 02	0.84270E 04	-0.20459E 03
0.52000E 02	0.85950E 04	-0.36083E 02
0.53000E 02	0.85440E 04	-0.76854E 02
0.54000E 02	0.87110E 04	0.10011E 03
0.55000E 02	0.85960E 04	-0.51919E 01
0.56000E 02	0.85710E 04	-0.20746E 02
0.57000E 02	0.83830E 04	-0.19955E 03
0.58000E 02	0.85620E 04	-0.11589E 02
0.59000E 02	0.84560E 04	-0.10887E 03
0.60000E 02	0.85610E 04	0.46284E 01
0.61000E 02	0.82950E 04	-0.25310E 03
0.62000E 02	0.85360E 04	-0.40444E 01
0.63000E 02	0.81730E 04	-0.35920E 03

0.64000E 02	0.85530E 04	0.28438E 02
0.65000E 02	0.85120E 04	-0.51233E 01
0.66000E 02	0.85060E 04	-0.38798E 01
0.67000E 02	0.84820E 04	-0.20826E 02
0.68000E 02	0.84810E 04	-0.14957E 02
0.69000E 02	0.83030E 04	-0.18627E 03
0.70000E 02	0.85040E 04	0.21246E 02
0.71000E 02	0.84170E 04	-0.59411E 02
0.72000E 02	0.85970E 04	0.12677E 03
0.73000E 02	0.84540E 04	-0.10219E 02
0.74000E 02	0.83920E 04	-0.66362E 02
0.75000E 02	0.85200E 04	0.67342E 02
0.76000E 02	0.83930E 04	-0.54104E 02
0.77000E 02	0.83460E 04	-0.95695E 02
0.78000E 02	0.85180E 04	0.81573E 02
0.79000E 02	0.83420E 04	-0.89298E 02
0.80000E 02	0.85320E 04	0.10570E 03
0.81000E 02	0.84420E 04	0.20560E 02
0.82000E 02	0.84930E 04	0.76297E 02
0.83000E 02	0.83730E 04	-0.39091E 02
0.84000E 02	0.83900E 04	-0.17599E 02
0.85000E 02	0.83020E 04	-0.10123E 03
0.86000E 02	0.85030E 04	0.10403E 03
0.87000E 02	0.83030E 04	-0.91818E 02
0.88000E 02	0.84750E 04	0.84221E 02
0.89000E 02	0.83210E 04	-0.65846E 02
0.90000E 02	0.82450E 04	-0.13802E 03
0.91000E 02	0.82000E 04	-0.17929E 03
0.92000E 02	0.83420E 04	-0.33654E 02
0.93000E 02	0.84870E 04	0.11488E 03
0.94000E 02	0.85190E 04	0.15033E 03
0.95000E 02	0.81370E 04	-0.22832E 03
0.96000E 02	0.82720E 04	-0.90053E 02
0.97000E 02	0.82380E 04	-0.12087E 03
0.98000E 02	0.85960E 04	0.24022E 03
0.99000E 02	0.81010E 04	-0.25176E 03
0.10000E 03	0.82720E 04	-0.77823E 02
0.10100E 03	0.82300E 04	-0.11696E 03
0.10200E 03	0.83770E 04	0.32823E 02
0.10300E 03	0.82190E 04	-0.12247E 03
0.10400E 03	0.85030E 04	0.16418E 03
0.10500E 03	0.83690E 04	0.32748E 02
0.10600E 03	0.83660E 04	0.32252E 02
0.10700E 03	0.81850E 04	-0.14631E 03
0.10800E 03	0.82990E 04	-0.29934E 02
0.10900E 03	0.81740E 04	-0.15262E 03
0.11000E 03	0.83540E 04	0.29631E 02
0.11100E 03	0.83340E 04	0.11824E 02
0.11200E 03	0.85960E 04	0.27596E 03
0.11300E 03	0.83160E 04	-0.19607E 01
0.11400E 03	0.84610E 04	0.14506E 03
0.11500E 03	0.81180E 04	-0.19596E 03
0.11600E 03	0.84160E 04	0.10396E 03
0.11700E 03	0.81610E 04	-0.14917E 03
0.11800E 03	0.83730E 04	0.64648E 02
0.11900E 03	0.83030E 04	-0.35781E 01
0.12000E 03	0.83370E 04	0.32149E 02
0.12100E 03	0.82060E 04	-0.97169E 02
0.12200E 03	0.82620E 04	-0.39532E 02
0.12300E 03	0.83590E 04	0.59063E 02
0.12400E 03	0.83460E 04	0.47616E 02
0.12500E 03	0.81070E 04	-0.18987E 03
0.12600E 03	0.82820E 04	-0.13399E 02
0.12700E 03	0.82360E 04	-0.57965E 02

0.12800E 03	0.82400E 04	-0.52569E 02
0.12900E 03	C.8174CE 04	-0.11721E 03
0.13000E 03	C.83160E 04	C.26116E 02
0.13100E 03	C.84C5CE 04	C.11641E 03
0.13200E 03	C.8288CE 04	C.66089E 00
0.13300E 03	C.8172CE 04	-C.11412E 03
0.13400E 03	C.84C70E 04	0.122C7E 03
0.13500E 03	C.8276CE 04	-C.77657E 01
0.13600E 03	C.8362CE 04	0.79364E 02
0.13700E 03	C.8159CE 04	-0.82537E 02
0.13800E 03	C.8293CE 04	0.12534E 02
0.13900E 03	C.8293CE 04	0.13577E 02
0.14000E 03	C.8175CE 04	-C.10341E 03
0.14100E 03	C.82400E 04	-C.37419E 02
0.14200E 03	C.8312CE 04	0.35544E 02
0.14300E 03	C.8195CE 04	-C.80518E 02
0.14400E 03	C.8571CE 04	0.29640E 03
0.14500E 03	C.8233CE 04	-0.40716E 02
0.14600E 03	C.80250E 04	-C.24785E 03
0.14700E 03	C.8237CE 04	-0.350C7E 02
0.14800E 03	C.8276CE 04	C.48145E 01
0.14900E 03	C.8073CE 04	-C.19739E 03
0.15000E 03	C.82780E 04	C.83928E 01
0.15100E 03	C.8052CE 04	-C.21685E 03
0.15200E 03	C.8572CE 04	C.30389E 03
0.15300E 03	C.8134CE 04	-C.13339E 03
0.15400E 03	C.8396CE 04	0.12931E 03
0.15500E 03	C.81720E 04	-0.94CC9E 02
0.15600E 03	C.8243CE 04	-0.22345E 02
0.15700E 03	C.8212CE 04	-0.52699E 02
0.15800E 03	0.8325CE 04	0.60931E 02
0.15900E 03	C.8159CE 04	-0.10446E 03
0.16000E 03	0.8289CE 04	0.26141E 02
0.16100E 03	C.82630E 04	0.72266E 00
0.16200E 03	C.83330E 04	C.71289E 02
0.16300E 03	C.8256CE 04	-0.51597E 01
0.16400E 03	C.8272CE 04	C.11377E 02
0.16500E 03	C.8426CE 04	0.16590E 03
0.16600E 03	C.84C2CE 04	C.14241E 03
0.16700E 03	C.8246CE 04	-C.13095E 02
0.16800E 03	C.8450CE 04	C.19139E 03
0.16900E 03	C.81730E 04	-0.85142E 02
0.17000E 03	C.8372CE 04	C.11432E 03
0.17100E 03	C.8230CE 04	-0.27238E 02
0.17200E 03	C.8245CE 04	-C.11804E 02
0.17300E 03	C.8128CE 04	-0.12838E 03
0.17400E 03	C.8157CE 04	-C.98969E 02
0.17500E 03	C.8211CE 04	-0.44568E 02
0.17600E 03	C.8590CE 04	C.33482E 03
0.17700E 03	C.8080CE 04	-C.17480E 03
0.17800E 03	C.8375CE 04	C.12057E 03
0.17900E 03	C.8152CE 04	-0.102C7E 03
0.18000E 03	C.8352CE 04	0.98284E 02
0.18100E 03	C.8301CE 04	C.47626E 02
0.18200E 03	C.82430E 04	-0.10041E 02
0.18300E 03	C.8345CE 04	0.92283E 02
0.18400E 03	C.85310E 04	0.27860E 03
0.18500E 03	C.80700E 04	-0.182C9E 03
0.18600E 03	C.82380E 04	-C.13794E 02
0.18700E 03	C.83240E 04	C.72497E 02
0.18800E 03	C.8267CE 04	0.15781E 02
0.18900E 03	C.8218CE 04	-C.32942E 02
0.19000E 03	0.8296CE 04	0.45327E 02
0.19100E 03	C.8267CE 04	C.16589E 02

0.19200E 03	0.83990E 04	0.14884E 03
0.19300E 03	0.82380E 04	-0.11907E 02
0.19400E 03	0.83790E 04	0.12934E 03
0.19500E 03	0.81000E 04	-0.14943E 03
0.19600E 03	0.82760E 04	0.26800E 02
0.19700E 03	0.81430E 04	-0.10598E 03
0.19800E 03	0.83700E 04	0.12124E 03
0.19900E 03	0.81970E 04	-0.51546E 02
0.20000E 03	0.81750E 04	-0.73340E 02
0.20100E 03	0.82590E 04	0.10861E 02
0.20200E 03	0.82090E 04	-0.38943E 02
0.21300E 03	0.81320E 04	-0.11410E 03
0.20300E 03	0.81580E 04	-0.89752E 02
0.20400E 03	0.79970E 04	-0.25057E 03
0.20500E 03	0.80860E 04	-0.16139E 03
0.20600E 03	0.81770E 04	-0.70210E 02
0.20700E 03	0.82110E 04	-0.36038E 02
0.20800E 03	0.83420E 04	0.95129E 02
0.20900E 03	0.82020E 04	-0.44709E 02
0.21000E 03	0.82690E 04	0.22449E 02
0.21100E 03	0.82430E 04	-0.33965E 01
0.21200E 03	0.82700E 04	0.23754E 02
0.21400E 03	0.83820E 04	0.13604E 03
0.21500E 03	0.83050E 04	0.59181E 02
0.21600E 03	0.83230E 04	0.77316E 02
0.21700E 03	0.81630E 04	-0.82553E 02
0.21800E 03	0.83420E 04	0.96575E 02
0.21900E 03	0.84140E 04	0.16870E 03
0.22000E 03	0.82740E 04	0.28821E 02
0.22100E 03	0.81600E 04	-0.85060E 02
0.22200E 03	0.82460E 04	0.10547E 01
0.22300E 03	0.82550E 04	0.10167E 02
0.22400E 03	0.81610E 04	-0.83724E 02
0.22500E 03	0.83410E 04	0.96382E 02
0.22600E 03	0.82400E 04	-0.45143E 01
0.22700E 03	0.83200E 04	0.75587E 02
0.22800E 03	0.79580E 04	-0.28632E 03
0.22900E 03	0.83000E 04	0.55780E 02
0.23000E 03	0.82820E 04	0.37873E 02
0.23100E 03	0.81900E 04	-0.54036E 02
0.23200E 03	0.85100E 04	0.26605E 03
0.23300E 03	0.83860E 04	0.14214E 03
0.23400E 03	0.82530E 04	0.92220E 01
0.23500E 03	0.80940E 04	-0.14970E 03
0.23600E 03	0.81890E 04	-0.54617E 02
0.23700E 03	0.81620E 04	-0.81540E 02
0.23800E 03	0.83490E 04	0.10554E 03
0.23900E 03	0.83040E 04	0.60609E 02
0.24000E 03	0.86500E 04	0.40668E 03
0.24100E 03	0.83350E 04	0.91750E 02
0.24200E 03	0.84770E 04	0.23382E 03
0.24300E 03	0.83330E 04	0.89883E 02
0.24400E 03	0.82530E 04	0.99475E 01
0.24500E 03	0.81500E 04	-0.92990E 02
0.24600E 03	0.82960E 04	0.53071E 02
0.24700E 03	0.83200E 04	0.77130E 02
0.24800E 03	0.82530E 04	0.10188E 02
0.24900E 03	0.81540E 04	-0.88756E 02
0.25000E 03	0.83120E 04	0.69299E 02
0.25100E 03	0.82630E 04	0.20352E 02
0.25200E 03	0.83610E 04	0.11840E 03
0.25300E 03	0.80930E 04	-0.14955E 03
0.25400E 03	0.83220E 04	0.79504E 02
0.25500E 03	0.81740E 04	-0.68448E 02

13 APPENDIX III: COMPUTER CODE PRINT-OUT

```
      COMMON K,K1,IOPT,N,X(800),Y(800),W(800),F(800),U(800,6),
     1A(6),B(6),G(12,12),AR(12,12),RHS(12),PHI
      DIMENSION A1(6),B1(6),DEL(12),SCALE(6),GG(6),DJM(6),
     1DIJ(800,6),DAB(6,6),AA(12,12),AK(12,12),GS(6)
     2,DEVI(12),VARCOV(12,12)
      NIN=5
      NOUT=6
  200 FORMAT(8I10)
  201 FORMAT(8E10.5)
   86 READ(NIN,200)IPNO
      IF(IPNO.LT.0)STOP
      READ(NIN,200)I1,I2,I3,I4,I5
      IF(I1.EQ.0)GO TO 600
      IWG=I1
      IPR1=I2
      ISTA=I3
      IOPT=I4
      IPR2=I5
  600 READ(NIN,200)I1
      IF(I1.EQ.0)GO TO 601
      N=I1
      DO 602 I=1,N
      READ(NIN,201)X(I),Y(I),W(I)
      IF(IWG.EQ.1)W(I)=1.
  602 IF(IWG.EQ.3)W(I)=1./Y(I)
  601 READ(NIN,200)I1
      IF(I1.EQ.0)GO TO 603
      K=I1
      READ(NIN,201)(B(J),J=1,K)
      KM1=K-1
  603 K1=K+IOPT
      K2=K+K1
      IRMAX=25
      RLAM=0.02
      RNY=10.
      TAU=0.001
      EPS=0.00003
      EPS1=3.E-7
      READ(NIN,200)I1
      IF(I1.EQ.0)GO TO 604
      READ(NIN,201)RLAM,RNY,TAU,EPS,EPS1
  604 WRITE(NOUT,101)IPNO
  101 FORMAT(1H1,10HPROBLEM NO,I3)
      IF(IOPT.EQ.1)GO TO 36
      WRITE(NOUT,102)
      GOTO 37
   36 WRITE(NOUT,103)
  102 FORMAT(1H0,25HFIT WITHOUT CONSTANT TERM)
```

```
103 FORMAT(1HO,22HFIT WITH CONSTANT TERM)
 37 WRITE(NOUT,104)K
104 FORMAT(1H ,29HNUMBER OF EXPONENTIAL TERMS =,I3)
    WRITE(NOUT,105)N
105 FORMAT(1H ,23HNUMBER OF DATA POINTS =,I3)
    WRITE(NOUT,142)
142 FORMAT(1HO,16HGUESS FOR OMEGAS)
    WRITE(NOUT,114)(B(J),J=1,K)
    WRITE(NOUT,106)
106 FORMAT(1HO,18HCONTROL PARAMETERS)
    WRITE(NOUT,107)RLAM
107 FORMAT(1H ,5HLAM =,E13.4)
    WRITE(NOUT,108)RNY
108 FORMAT(1H ,5HNY  =,E13.4)
    WRITE(NOUT,109)TAU
109 FORMAT(1H ,5HTAU =,E13.4)
    WRITE(NOUT,110)EPS
110 FORMAT(1H ,5HEPS =,E13.4)
    WRITE(NOUT,129)EPS1
129 FORMAT(1H ,5HEPS1=,E13.4)
    WRITE(NOUT,111)IRMAX
111 FORMAT(1H ,6HRMAX =,I4///)
    OEPS1=1.+EPS1
    IF(IOPT)47,47,48
 48 DO 49 I=1,N
 49 U(I,K1)=1.
 47 CALL LIPHIF
    PHIR=PHI
    RLAMO=RLAM
    IR=0
 82 IR=IR+1
    IF(IPR1.EQ.0)GOTO4
    WRITE(NOUT,112)IR
112 FORMAT(1HO,12HITERATION NO,I3)
    WRITE(NOUT,115)
115 FORMAT(1H ,6HOMEGAS)
    WRITE(NOUT,114)(B(J),J=1,K)
114 FORMAT(1H ,6E18.7)
    WRITE(NOUT,113)
113 FORMAT(1H ,12HCOEFFICIENTS)
    WRITE(NOUT,114)(A(J),J=1,K)
    IF(IOPT.EQ.0)GOTO5
    WRITE(NOUT,116)
116 FORMAT(1H ,8HCONSTANT)
    WRITE(NOUT,114)A(K1)
  5 WRITE(NOUT,117)PHIR
117 FORMAT(1H ,5HPHI =,E18.8)
    WRITE(NOUT,119)RLAM
119 FORMAT(1H ,5HLAM =,E14.4)
  4 RLAM1=RLAM
    DO 39 JM=1,K
    AJM=A(JM)
    B1(JM)=B(JM)
    DO 40 J=1,K1
    H1=0.
    IF(J-JM)41,42,41
```

```
41 DO 43 I=1,N
43 H1=H1+W(I)*X(I)*U(I,J)*U(I,JM)
   RHS(J)=-AJM*H1
   GOTO 40
42 DO 44 I=1,N
   H3=U(I,JM)
   H4=AJM*H3
   H2=0.
   DO 45 J1=1,K1
45 H2=H2+U(I,J1)*A(J1)
44 H1=H1+W(I)*X(I)*H3*(Y(I)-H4-H2)
   RHS(J)=H1
40 CONTINUE
   CALL  COLSL(K1,G,RHS,DJM)
   CALL  IMPRUV(K1,AR,G,RHS,DJM)
   DO 46 J=1,K1
46 DAB(J,JM)=DJM(J)
39 CONTINUE
   DO 10 I=1,N
   DO 10 J=1,K
   H1=A(J)*X(I)*U(I,J)
   DO 11 J1=1,K1
11 H1=H1+DAB(J1,J)*U(I,J1)
10 DIJ(I,J)=H1
   DO 12 J=1,K
   DO 12 J1=J,K
   H1=0.
   DO 13 I=1,N
13 H1=H1+DIJ(I,J)*DIJ(I,J1)*W(I)
12 AA(J1,J)=H1
   DO 14 J=1,K
14 SCALE(J)=SQRT(AA(J,J))
   DO 15 J=1,K
   H1=0.
   DO 16 I=1,N
16 H1=H1+(Y(I)-F(I))*DIJ(I,J)*W(I)
   GG(J)=H1
15 GS(J)=H1/SCALE(J)
   DO 17 J=1,KM1
   JP1=J+1
   DO 17 J1=JP1,K
17 AK(J1,J)=AA(J1,J)/SCALE(J)/SCALE(J1)
   IF(RLAM.GT.2.E-9)RLAM=RLAM1/RNY
19 DO 34 J=1,K
34 AK(J,J)=1.+RLAM
   CALL  COLDEC(K,AK,G)
   CALL  COLSL(K,G,GS,DEL)
   CALL  IMPRUV(K,AK,G,GS,DEL)
   DO 21 J=1,K
   DEL(J)=DEL(J)/SCALE(J)
21 B(J)=B1(J)+DEL(J)
   CALL LIPHIF
   H1=PHI
   IF(H1/PHIR.GT.DEPS1)GOTO22
23 PHIR=H1
   IF(IPR1.EQ.1)WRITE(NOUT,120)
```

```
 120 FORMAT(1H ,1HA)
     GOTO24
  22 IF(RLAM-RLAM1)25,26,26
  25 RLAM=RLAM1
     IF(IPR1.EQ.1)WRITE(NOUT,121)
 121 FORMAT(1H ,1HB)
     GOTO19
  26 H1=0.
     H2=0.
     H3=0.
     DO 27 J=1,K
     H1=H1+DEL(J)*GG(J)
     H2=H2+DEL(J)**2
  27 H3=H3+GG(J)**2
     IF(H1**2/H2/H3-0.5)28,29,29
  28 RLAM=RLAM*RNY
     IF(IPR1.EQ.1)WRITE(NOUT,122)
 122 FORMAT(1H ,1HC)
     GOTO19
  29 IF(IPR1.EQ.1)WRITE(NOUT,123)
 123 FORMAT(1H ,1HD)
  30 DO 31 J=1,K
     DEL(J)=DEL(J)/2.
  31 B(J)=B1(J)+DEL(J)
     CALL LIPHIF
     H1=PHI
     IF(DEPS1-H1/PHIR)30,30,23
  24 DO 32 J=1,K
     H1=ABS(DEL(J))/(TAU+ABS(B(J)))
     IF(H1.GE.EPS.AND.IR.LT.IRMAX)GOTO82
  32 CONTINUE
     IF(IR.EQ.IRMAX)WRITE(NOUT,124)IRMAX
 124 FORMAT(1H ,30HCONVERGENCE NOT OBTAINED AFTER,I4,11H ITERATIONS)
     IF(IR.LT.IRMAX)WRITE(NOUT,140)IR
 140 FORMAT(1H ,26HCONVERGENCE OBTAINED AFTER,I4,11H ITERATIONS)
     WRITE(NOUT,126)PHIR
 126 FORMAT(1H0,30HWEIGHTED SUM OF SQUARED ERRORS,E19.8)
     IF(ISTA.EQ.0)GOTO605
     NMIK2=N-K2
     IF(ISTA.EQ.2)WRITE(NOUT,141)NMIK2
 141 FORMAT(1H ,59HTHIS SHOULD BE APPROXIMATELY DISTRIBUTED AS CHI-SQUA
    1RE WITH,I4,19H DEGREES OF FREEDOM)
     COEF=1.
     IF(ISTA.EQ.1)COEF=PHIR/FLOAT(NMIK2)
     DO 238 JM=1,K
     DO 238 JM1=JM,K
     H1=0.
     DO 239 I=1,N
 239 H1=H1+W(I)*(X(I))**2*U(I,JM)*U(I,JM1)
 238 AA(JM1,JM)=A(JM)*A(JM1)*H1/COEF
     DO 240 J=1,K1
     J2=J+K
     DO 240 JM=1,K
     H1=0.
     DO 241 I=1,N
 241 H1=H1+W(I)*X(I)*U(I,JM)*U(I,J)
```

```
240 AA(J2,JM)=A(JM)*H1/COEF
    DO 242 J=1,K1
    J2=J+K
    DO 242 J1=J,K1
    J3=J1+K
    H1=0.
    DO 243 I=1,N
243 H1=H1+W(I)*U(I,J1)*U(I,J)
242 AA(J3,J2)=H1/COEF
    CALL COLDEC(K2,AA,G)
    DO 244 J=1,K2
    DO 245 J1=1,K2
245 RHS(J1)=0.
    RHS(J)=1.
    CALL COLSL(K2,G,RHS,DEL)
    CALL IMPRUV(K2,AA,G,RHS,DEL)
    DO 246 J1=1,K2
246 VARCOV(J1,J)=DEL(J1)
244 DEVI(J)=SQRT(VARCOV(J,J))
605 WRITE(NOUT,125)
125 FORMAT(1H0,29HFINAL ESTIMATES OF PARAMETERS)
    WRITE(NOUT,115)
    WRITE(NOUT,114)(B(J),J=1,K)
    IF(ISTA.GT.0)WRITE(NOUT,137)
137 FORMAT(1H ,19HSTANDARD DEVIATIONS)
    IF(ISTA.GT.0)WRITE(NOUT,114)(DEVI(J),J=1,K)
    WRITE(NOUT,113)
    WRITE(NOUT,114)(A(J),J=1,K)
    IF(ISTA.GT.0)WRITE(NOUT,137)
    KLOW=K+1
    KUPP=2*K
    IF(ISTA.GT.0)WRITE(NOUT,114)(DEVI(J),J=KLOW,KUPP)
    IF(IOPT.EQ.0)GOTO33
    WRITE(NOUT,116)
    WRITE(NOUT,114)A(K1)
    IF(ISTA.GT.0)WRITE(NOUT,130)
130 FORMAT(1H ,18HSTANDARD DEVIATION)
    IF(ISTA.GT.0)WRITE(NOUT,114)DEVI(K2)
 33 IF(ISTA.EQ.0)GOTO86
    IF(ISTA.EQ.1.AND.IWG.EQ.1)WRITE(NOUT,131)COEF
131 FORMAT(1H0,21HVARIANCE OF THE FIT =,E13.5)
    DO 606 J=1,K2
    DO 606 J1=1,K2
606 VARCOV(J,J1)=VARCOV(J,J1)/DEVI(J)/DEVI(J1)
    WRITE(NOUT,132)
132 FORMAT(1H0,45HMATRIX OF CORRELATIONS BETWEEN THE PARAMETERS/)
    DO 134 J=1,K2
134 WRITE(NOUT,118)(VARCOV(J,J1),J1=1,K2)
118 FORMAT(1H0,12F8.4)
133 FORMAT(1H0,12E10.3)
    WRITE(NOUT,135)
135 FORMAT(1H0,37HINVERSE OF VARIANCE-COVARIANCE MATRIX)
    DO 136 J=1,K2
136 WRITE(NOUT,133)(AA(J,J1),J1=1,K2)
    WRITE(NOUT,138)
138 FORMAT(1H0,43HDERIVATIVE MATRIX DCOEF(ROW)/DOMEGA(COLUMN))
```

```
      DO 139 J=1,K1
139   WRITE(NOUT,133)(DAB(J,JM),JM=1,K)
      IF(IPR2.EQ.0)GOTO86
      WRITE(NOUT,127)
127   FORMAT(1H0,38H          X                 Y            DEVIATION)
      DO 35 I=1,N
      H1=Y(I)-F(I)
 35   WRITE(NOUT,128)X(I),Y(I),H1
128   FORMAT(1H ,3E13.5)
      GOTO86
      END
```

```
      SUBROUTINE LIPHIF
      COMMON K,K1,IOPT,N,X(800),Y(800),W(800),F(800),U(800,6),
     1A(6),B(6),G(12,12),AR(12,12),RHS(12),PHI
      DO 7 J=1,K
      DO 7 I=1,N
    7 U(I,J)=EXP(B(J)*X(I))
      DO 1 J=1,K1
      DO 2 J1=J,K1
      H1=0.
      DO 3 I=1,N
    3 H1=H1+W(I)*U(I,J)*U(I,J1)
    2 AR(J1,J)=H1
      H1=0.
      DO 4 I=1,N
    4 H1=H1+W(I)*U(I,J)*Y(I)
    1 RHS(J)=H1
      CALL COLDEC(K1,AR,G)
      CALL COLSL(K1,G,RHS,A)
      CALL IMPRUV(K1,AR,G,RHS,A)
      OPT=IOPT
      DOUBLE PRECISION SUM
      SUM=0.
      DO 5 I=1,N
      H1=OPT*A(K1)
      DO 6 J=1,K
    6 H1=H1+A(J)*U(I,J)
      F(I)=H1
      H2=Y(I)-H1
      H3=W(I)*H2
    5 SUM=SUM+H2*H3
      PHI=SUM
      RETURN
      END
```

```
      SUBROUTINE COLDEC(N,A,G)
      DIMENSION A(12,12),G(12,12)
      H1=A(1,1)
      IF(H1)6,6,7
    7 G(1,1)=SQRT(H1)
      IF(N.EQ.1)RETURN
      DO 1 I=2,N
    1 G(I,1)=A(I,1)/G(1,1)
      DO 2 J=2,N
      SUM=0.
      JM1=J-1
      DO 3 K=1,JM1
    3 SUM=SUM+G(J,K)**2
      H1=A(J,J)-SUM
      IF(H1)6,6,8
    8 G(J,J)=SQRT(H1)
      IF(J.EQ.N)RETURN
      JP1=J+1
      DO 4 I=JP1,N
      SUM=0.
      DO 5 K=1,JM1
    5 SUM=SUM+G(I,K)*G(J,K)
    4 G(I,J)=(A(I,J)-SUM)/G(J,J)
    2 CONTINUE
    6 CALL SING(1)
      RETURN
      END
```

```
      SUBROUTINE COLSL(N,G,B,X)
      DIMENSION G(12,12),B(12),X(12)
      IF(N.EQ.1)GOTO5
      X(1)=B(1)/G(1,1)
      DO 2 I=2,N
      IM1=I-1
      SUM=0.
      DO 1 J=1,IM1
    1 SUM=SUM+G(I,J)*X(J)
    2 X(I)=(B(I)-SUM)/G(I,I)
      X(N)=X(N)/G(N,N)
      NP1=N+1
      DO 4 IBACK=2,N
      I=NP1-IBACK
      IP1=I+1
      SUM=0.
      DO 3 J=IP1,N
    3 SUM=SUM+G(J,I)*X(J)
    4 X(I)=(X(I)-SUM)/G(I,I)
      RETURN
    5 X(1)=B(1)/(G(1,1))**2
      RETURN
      END
```

```
      SUBROUTINE IMPRUV(N,A,G,B,X)
      DIMENSION A(12,12),G(12,12),B(12),X(12),R(12),DX(12)
      DOUBLE PRECISION SUM
      EPS=1.E-8
      ITMAX=16
      XNORM=0.
      DO 2 I=1,N
      DO 2 J=I,N
    2 A(I,J)=A(J,I)
      DO 1 I=1,N
    1 XNORM=AMAX1(XNORM,ABS(X(I)))
      IF(XNORM)3,10,3
    3 DO 9 ITER=1,ITMAX
      DO 5 I=1,N
      SUM=0.
      DO 4 J=1,N
    4 SUM=SUM+A(I,J)*X(J)
      SUM=B(I)-SUM
    5 R(I)=SUM
      CALL COLSL(N,G,R,DX)
      DXNORM=0.
      DO 6 I=1,N
      T=X(I)
      X(I)=X(I)+DX(I)
    6 DXNORM=AMAX1(DXNORM,ABS(X(I)-T))
      IF(DXNORM-EPS*XNORM)10,10,9
    9 CONTINUE
      CALL SING(2)
   10 RETURN
      END
```

```
      SUBROUTINE SING(IWHY)
   11 FORMAT(30HCMATRIX NOT POSITIVE-DEFINITE.)
   12 FORMAT(54HCNO CONVERGENCE IN IMPROVE. MATRIX IS NEARLY SINGULAR.)
      NOUT=6
      GOTO(1,2),IWHY
    1 WRITE(NOUT,11)
      RETURN
    2 WRITE(NOUT,12)
      RETURN
      END
```

14. APPENDIX IV: SOLUTION OF LINEAR EQUATIONS

An essential problem in EXPOSUM is the solution of a linear system

$$Ax = b \tag{62}$$

where A is a symmetric and positive-definite matrix. As A as a rule is ill-conditioned, it is important to choose some good solution technique; here Cholesky's method with iterative improvement is used. In Cholesky's method A is factorized as

$$A = G G^T \tag{63}$$

where G is a lower triangular matrix with positive diagonal elements. A subroutine COLDEC for the decomposition, and a subroutine COLSL for the subsequent solution, have been written along the lines indicated by Forsythe and Moler [10]. The merits of the Colesky decomposition method are discussed intensively by Golub [13].

The iterative improvement is performed by the subroutine IMPRUV, a slightly changed version of the IMPRUV-routine given by Forsythe and Moler [10]. As they point out, it is necessary to compute the residuals to double precision*. Now, on the IBM 7094 the statement (see print-out for IMPRUV)

```
4 SUM = SUM + A(I, J) * X(J)                                    (64)
```

where only SUM is declared in double precision, causes a single-precision multiplication, a double precision addition, and a double precision store; this is exactly what we want. Declaration of additional double precision quantities may be necessary when the program has to be used on another computer.

When A fails to be positive-definite (possibly due to rounding errors alone), or the iterative improvement procedure fails to converge, control is transferred to the emergency routine SING, which prints out a message and thereafter returns control back to the program (this action could easily be modified, if desired).

---

*As noticed in 7.1 quite the same situation occurs in the evaluation of the sum-of-squared-errors Ø.

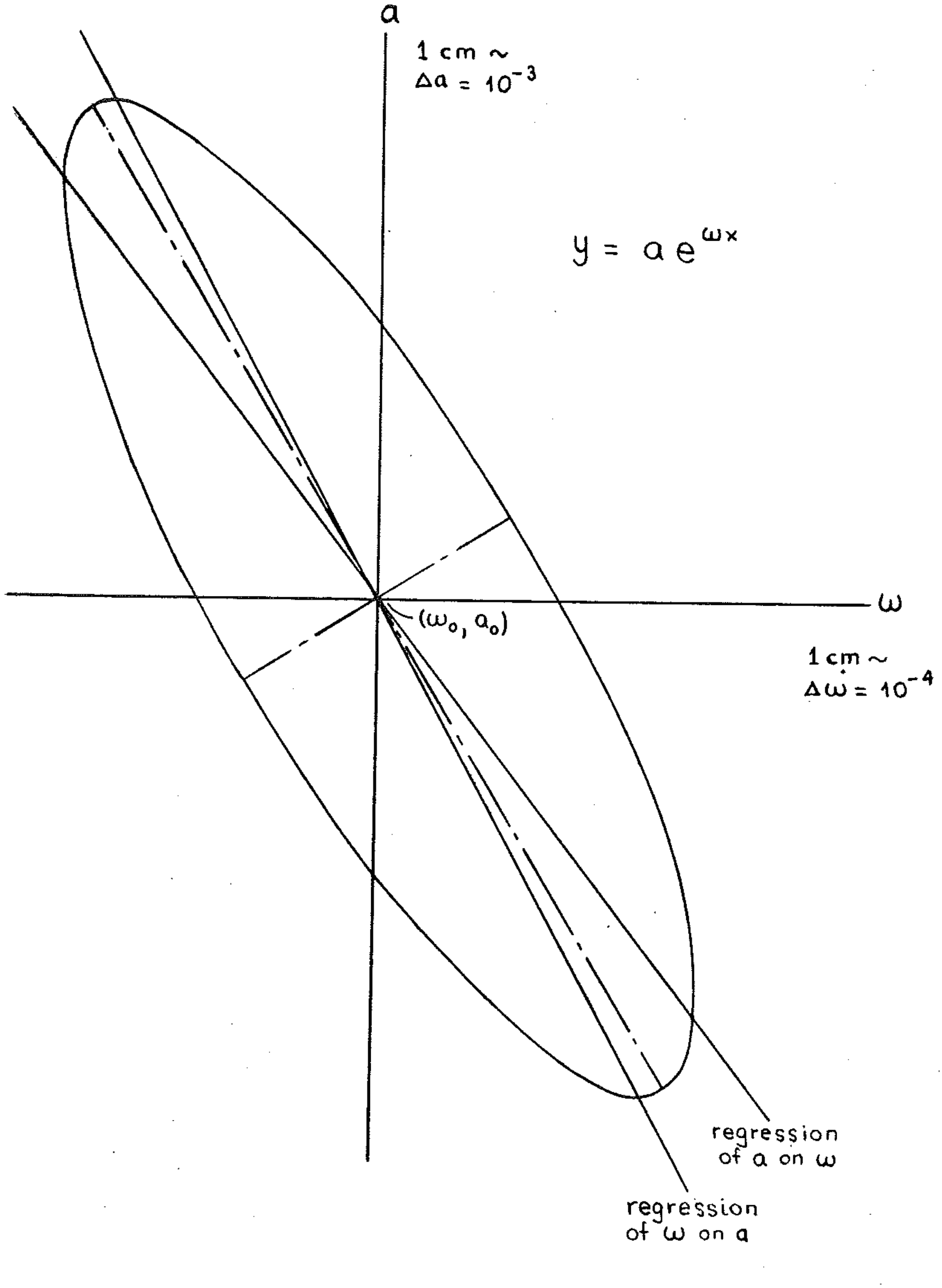

Fig. 1: Concentration ellipse