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PARAMETER ESTIMATION IN NON-LINEAR DIFFERENTIAL EQUATIONS

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Contents

Preface

This report describes some experiences with the estimation of parameters in nonlinear differential equations. The work was done as part of work in a group on biomathematics and a group on stiff differential equations. The program used is written in ALGOL 60 and has been run on the EL X8 computer of the Mathematical Centre. After an exposition of the method, a detailed description of the procedure is given and a number of solved problems are shown in detail.

1. Introduction

In this report we shall be concerned with a problem which arises from experimental science. In order to predict the behaviour of systems, an experimental scientist not only wants to describe phenomena phenomenologically, but he also wants to construct a model of the process under consideration. Often a mathematical representation of the model will be given by a system of differential equations in which a set of parameters is not known a priori. These parameters have to be determined on the basis of experiments.

Mathematically stated, the problem is this: A set of n differential equations is given *

$$\frac{d}{dt} y = f(t,y,p) \tag{1.1}$$

where p represents an m-vector of parameters. In the process considered, p has the value p^*, but p^* is not known. Some components of the vector y can be measured for different values of t, but these measurements are affected by some random errors. It is assumed that the form of f is known, together with some statistical properties of the measurement errors. The problem is to deduce an estimate $\bar{p}$ of the vector p^*.

With y_i $(1 \leq i \leq N)$ we denote the observed value of some component y at time t_i. Thus the index i identifies an observation and also determines what component of y has been observed. So we have a set of observations $\{y_i\}$, a corresponding set $\{t_i\}$ $(t_1 \leq t_2 \leq \dots \leq t_N)$ and, for some p, we can compute a set of theoretical values $y(t_i,p)$. The problem now seems to be quite simple: we define the N-vector

$$Y(p) = (y(t_i,p) - y_i) \quad 1 \leq i \leq N \tag{1.2}$$

and we define

*) We use vector notation throughout, so $p \in R^m$, $y \in R \times R^m \to R^n$, $f \in R \times R^n \times R^m \to R^n$ etc..

$$S(p) = \|\, Y(p)\|_2^2 = \Sigma_{i=1}^{N}(y(t_i,p)-y_i)^2 \qquad (1.3)$$

the sum of the squares of the discrepancies. Using an integration procedure to solve $y(t_i,p)$, we can solve the problem stated by minimizing $S(p)$ using standard techniques.Even when we assume that the minimum is unique and that the function $S(p)$ is the best one to minimize (this can be justified under certain conditions), the question still remains as to how badly conditioned the problem is. I.e. how small a perturbation in some values of y_i will cause how large a variation in the minimizing vector $\bar{p}$. In relation to this question it is clear that not only an estimate of p^* has to be determined but also an estimate of its reliability.

In this report we will assume that the measurement errors are statistically independent and that they have a Gaussian distribution with zero mean and variance σ^2. Thus the covariance matrix of the vector of errors η is

$$E(\eta\eta^T) = \sigma^2 I \qquad (1.4)$$

and the probability density of η is given by

$$p(\eta) = (2\pi\sigma)^{-N/2} \exp\,(-\,\|\eta\|^2/2\sigma^2).$$

2. The method

2.1. The dependence of $Y(p)$ on p

The solution of the differential equation (1) can be considered to be a function of t as well as a function of p. We consider the difference between two adjacent solutions $y_1(t,p)$ and $y_2(t,p+\delta)$ of equation (1), both starting at $y_1(0,p) = y_2(0,p+\delta) = c$. We compute the perturbation due to this small change in p.

$$\frac{d}{dt}\, y_1 = f(t,y_1,p) \qquad y_1(0) = c \qquad (2.1)$$

$$\frac{d}{dt}\, y_2 = f(t,y_2,p+\delta) \qquad y_2(0) = c \qquad (2.2)$$

Expanding (2.2) in a Taylorseries and keeping only first order terms in δ, we obtain

$$\frac{d}{dt}\, y_2 = f(t,y_1,p) + FY(y_2-y_1) + FP\ \delta \quad (2.3)$$

where

$$FY = \left(\frac{\partial}{\partial y_1}\ f\ (t,y_1,p)\right) \qquad (2.4)$$

is an $n \times n$ matrix and

$$FP = \left(\frac{\partial}{\partial p}\ f\ (t,y_1,p)\right) \qquad (2.5)$$

is an $n \times p$ matrix, both matrices being functions of t,p and y_1, but not of δ or y_2-y_1.

It would be expedient to know how the computable values $y(t_i,p)$ depend upon small variations δ around p. Since equation (2.3) enables us to construct the differential equation which defines

$$YP = \frac{\partial}{\partial p}\ y(t,p), \qquad (2.6)$$

we use (2.3) and write

$$\frac{\partial}{\partial p}\ \frac{d}{dt}\ y(t,p) = FP + FY.\frac{\partial}{\partial p}\ y(t,p) \qquad (2.7)$$

or, in shorthand,

$$\frac{d}{dt}\ YP = FP + FY.YP\ . \qquad (2.8)$$

This is a system of $n \times m$ differential equations. If we solve this system together with system (1.1), we are able to compute

$$A(p) = \frac{\partial}{\partial p}\ y(t_i,p), \qquad (2.9)$$

an $N \times m$ matrix, giving the dependence of $Y(p)$ (see equation (1.2)) upon variations to p.

2.2. Minimizing S(p)

Consider the function $S(p)$ defined by equation (1.3). The value $\bar{p}$ that minimizes $S(p)$ is an estimate of the true value p^*. In equation (1.3) y is a nonlinear function of p. Without some further assumptions the analysis would therefore be too involved to give hope of useful results. This difficulty is dealt with by assuming that p is a reasonably good approximation to $\bar{p}$. Using a generalized Newton-Raphson technique we linearize the nonlinearity for small departures δp from $\bar{p}$.
Suppose that p is a trial vector and δp is the required correction ($p+\delta p = \bar{p}$). The residual vector $Y(p)$ is approximated by a linear function of the parameter

$$Y(p) = Y(\bar{p}-\delta p) = Y(\bar{p}) - A\ \delta p$$

and for the residual function

$$S(\bar{p}) = S(p+\delta p) = ||\ Y(p+\delta p)\ ||^2$$

$$\simeq ||\ Y(p) + A(p)\ \delta p||^2$$

$$= ||Y||^2 + 2\delta p^T A^T Y + \delta p^T A^T A \delta p$$

The approximating function to $S(p)$ has a minimum at the point given by the normal equations

$$A^T(p)A(p)\delta p = -\ A^T(p)\ Y(p). \qquad (2.10)$$

If the matrix $A^T A$ is nonsingular, this equation determines δp from $Y(p)$.

In the linear theory $p+\delta p$ so determined would be the required solution and the minimum value of S attained there would be

$$S(\bar{p}) = ||Y(p)||^2 - \delta p^T A^T A \delta p \qquad (2.11)$$

In general, $S(p+\delta p)$ will not be the minimal value of S and the whole process is repeated using $p+\delta p$ as an approximation to $\bar{p}$ for the next iteration.

The process we use has the same order of convergence as quasilinearization has (see: Bellman and Kalaba [1965]). The latter process often is called quadratically convergent. In fact, both processes have 2nd order convergence only in the case that the observed values are exact in all decimal places, otherwise they have 1st order convergence (Willems [1972]). So we prefer to speak of first order convergence.

If it appears that $S(p+\delta p) > S(p)$, some other techniques are applied. Firstly the method of steepest descent is used, with p as a point of departure. For this purpose the gradient vector $r = -A^T(p)\, Y(p)$ is calculated and a new trial step is executed with

$$\delta p = r\ ||r||^2/||Ar||^2$$

If even with this δp it appears that $S(p+\delta p) > S(p)$, the direction of the step is not changed, but a relaxation factor is used, the step δp is multiplied by $S(p)/(S(p)+ S(p+\delta p))$ and a new trial step is executed from p.

3. Statistics

Let $\bar{p}$ be the final estimate of p so that $S(p) \geq S(\bar{p})$ for all p: we assume that the linear theory holds in a sufficient large neighbourhoud of $\bar{p}$.

For the perturbations η_i of the observed values y_i we assume an $N(0,\sigma^2)$ distribution and so it follows from equation (2.10) that the estimated value $\bar{p}$ will also be normally distributed. We define $\delta p = \bar{p} - p^*$, hence the expectation of δp will be zero when $p = \bar{p}$. We are also interested in the covariance matrix of δp, i.e. the expected value of $\delta p \delta p^T$.

$$E(\delta p \delta p^T) = E((A^TA)^{-1} A^TY Y^TA (A^TA)^{-1}) =$$

$$= (A^TA)^{-1} A^T E(YY^T) A (A^TA)^{-1} = \sigma^2 (A^TA)^{-1} .$$

From this covariance matrix we derive r_{ij}, the correlations between the estimates δp_i and δp_j.

$$r_{ij} = \frac{q_{ij}}{\sqrt{q_{ii}q_{jj}}} \qquad \text{with } q_{ij} = (A^TA)_{ij} \quad (3.1)$$

By equation (2.10) δp is a linear function of Y. Hence its probability density will be Gaussian and will be given by

$$P(\delta p) = ((2\pi\sigma)^m \det((A^TA)^{-1}))^{-\frac{1}{2}} \exp(-\delta p^T A^T A \delta p/2\sigma^2)$$

From (2.11) follows immediately

$$||Y(\underline{\bar{p}}+\underline{\delta p})||^2 = S(\underline{\bar{p}}) + \underline{\delta p}^T A^TA \underline{\delta p}.$$

Now it is clear that $||\underline{Y}||^2/\sigma^2$, $\delta\underline{p}^TA^TA\underline{\delta p}/\sigma^2$ and $S(\underline{\bar{p}})/\sigma^2$ have a χ^2 distribution with N, m and N-m degrees of freedom, respectively. An estimate of σ^2 is given by

$$s^2 = S(\bar{p})/(N-m) = ||Y(\bar{p})||^2/(N-m) \qquad (3.2)$$

The confidence region at level α is the ellipsoidal region

$$\delta p^T A^TA \delta p \leq \frac{m}{N-m} S(\bar{p}) F_\alpha(m,N-m), \qquad (3.3)$$

where $F_\alpha(n,N-m)$ is the α-point of the F-distribution with m and N-m degrees of freedom.

The principal axes of the ellipsoidal region are given by the eigenvectors of A^TA and the length of the axes is $\lambda_i^{-1/2}$(λ_i is the eigenvalue of the corresponding eigenvector).

The confidence limits for each estimate, supposing that the other estimates are exact, are

$$\bar{p}_i \pm \delta p_i$$

where

$$\delta p_i = \sqrt{\frac{m}{N-m} S(\bar{p})\ F_\alpha/(A^T A)_{ii}} \qquad (3.4)$$

Other confidence limits for the individual estimates (independently) are

$$\bar{p}_i \pm \delta p_i^*$$

where

$$\delta p_i^* = \sqrt{\frac{m}{N-m} S(\bar{p})\ F_\alpha (A^T A)^{-1}_{ii}} \qquad (3.5)$$

The geometrical interpretation is that the tangent planes to the ellipsoïd with normals to the direction i are at a distance δp_i^* from the centre of the ellipsoïd and that the axis i intercepts the ellipsoïd at points δp_i from the centre. Clearly $\delta p_i \leq \delta p_i^*$.

4. Integration of the differential equations

The system of the differential equations which we have to solve in each iteration step of the optimizing process is, in general, a rather large one. In the system we distinguish two parts

1. [see equation (1.1)]

$$\frac{d}{dt} y(t,p) = f(t,y,p) \qquad (4.1)$$

   a coupled system of n differential equations.
2. [see equation (2.8)]

$$\frac{d}{dt} YP = FP + FY.YP\ . \qquad (4.2)$$

This is a set of m systems; each system consists of n differential equations and is coupled with system (4.1).

The structure of the system (4.1-4.2) as a whole can be clarified by writing:

1) the system (4.1 - 4.2) as

$$\begin{aligned} \dot{y} &= f \\ \dot{y}_{p1} &= f_{p1} + f_y\, y_{p1} \\ &\vdots \\ \dot{y}_{pm} &= f_{pm} + f_y\, y_{pm} \end{aligned} \qquad (4.3)$$

where $y_{pi} = \partial y/\partial p_i$, $f_{pi} = \partial f/\partial p_i$ and

$f_y = \partial f/\partial y$ the Jacobian matrix of the system (4.1).

and by writing

2) the Jacobian matrix of the system (4.1-4.2) as

$$J = \begin{pmatrix} f_y & 0 \;\ldots\ldots\; 0 & \\ f_{py1} & f_y & 0 \\ \vdots & 0 & \ddots \quad f_y \\ f_{pym} & & \end{pmatrix}, \qquad (4.4)$$

where $f_{pyi} = \partial(\partial f/\partial p_i)/\partial y$.

In this Jacobian matrix the one way coupling of the system is clearly demonstrated. Besides we notice that the eigenvalues of J are all the same as the eigenvalues of f_y, and so the stability behaviours of system (4.3) and system (4.4) are similar.

In order to solve the system, linear multistep methods are used. Essentially, the integrating procedure used ("multistep"), is the same as the one described in Hemker [1971]. This procedure uses variable steplength and variable order. In the case of stiff differential equations the procedure switches from Adams-Moulton to stiffly stable methods.

In order to solve (4.3) efficiently, we make use of the particular structure mentioned. In each step of the integrating process, equation (4.1) is solved as a independent system. When this part of the integration has been succesfully completed, the m systems of equations (4.2) can be solved with only a little work. We will show this in more detail.

Since we only use implicit linear multistep methods, the solution of one integration step

$$\dot{y} = f(y)$$

corresponds to the solution of the nonlinear equation

$$y_n = h\beta\ f(y_n) + \Phi_n, \qquad (4.4^a)$$

where Φ_n contains the information about a number of completed steps. After the choice of a suitable starting value ${}_{o}y_n$, this equation is solved with a modified Newton-Raphson method

$${}_{r+1}y_n = {}_{r}y_n - (I-h\beta f_y)^{-1}({}_{r}y_m-\Phi_n-h\beta f({}_{r}y_n)). \qquad (4.5)$$

When we solve the system of differential equations

$$\dot{y} = f(y)$$
$$\dot{w} = g(y) + f_y\ w$$

we make use of the one-way coupling of the system. In each step, we have to solve the nonlinear system

$$y_n = h\beta\ f(y_n) + \Phi_n \qquad (4.6)$$

$$w_n = h\beta\ g(y_n) + h\beta\ f_y(y_n).w_n + \Psi_n \qquad (4.7)$$

We do not iterate this system simultaneously, but we solve the nonlinear equation (4.6) by the iteration process (4.5), we substitute the computed value of y_n in (4.7), and we solve the linear equation (4.7) directly. For the solution of this linear equation one needs $(I-h\beta f_y(y_n))^{-1}$: the same factor that will be used in (4.5).

The solution of the system (4.3) is obtained in the same way. In each step of the integration process, the first system of n equations (4.1) is solved by iteration. When this iteration has been completed, each of the m systems of the n equations (4.2) is solved directly. Each one of these m systems needs the L-U-decompsition of one and the same matrix $I-h\beta f_y(y_n)$. Moreover, this L-U-decomposition can be used again in the next modified Newton-Raphson iteration. This implies that each step in the solution of (4.3) only involves:

i) 1 or more (up to 3) evaluations of f.

ii) 1 evaluation of f_{pi}, for i = 1,a,......,m.

iii) 1 evaluation of f_y.

Each evaluation of f_y involves an L-U-decomposition of $I-h\beta f_y$ and each evaluation of f or f_{pi} involves an execution of the second stage of the Gaussian elimination.

When, during an integration step, it appears that the iteration process (4.5) does not converge or that the local error bound is exceeded, the step length is changed and the work mentioned in i) and iii) has to be repeated.

We notice that the possibility of coupling the integration of (4.2) with the integration of (4.1) with this ease, depends cruxially on the form of the linear integration formula (4.4^a). It cannot be done, for instance, with Runge-Kutta methods.

We use another feature of the integration method. On an interval containing some meshpoints, the linear multistep methods approximate the solution of the differential equation to a polynomial of a certain degree. As a consequence, there is no need to take the meshpoints of our integrating procedure together with the points $\{t_i\}$ where the solution is wanted. The solution is obtained by interpolating the approximating polynomial.

5. The procedure odeparest

5.1. General remarks, users manual

Although we know that the iteration process has first order convergence, it is evident that in most practical (nonlinear) problems, we cannot say anything about the a priori fitness of a first estimate. This reason, and others that make parameter estimation an art rather than only a computing technique, lead us to give the output of the procedure in printed form. This prevents the use, without inspectation, of the results as a starting point for further calculations.

INPUT

The input of the procedure can be divided into four parts:

1. The system of differential equations which defines the problem, together with its initial values.
2. The observations to which the parameters will be adjusted.
3. A first estimate of the parameters, together with some upper and lower bounds for them.
4. Some actual parameters of the procedure, by which the optimizing and integration processes will be controlled and one actual parameter which specifies the confidence region desired.

Now we shall treat these four items in detail.

1) The system of differential equations defining the problem has to be supplied by the user as a set of sub-procedures for the procedure odeparest. Four procedures are needed:

a) a procedure which identifies the function f (see equation 1.1).
   This is a procedure with the heading **procedure** call f(r); **value** r; **real** r;.
   By this procedure the values of the left hand part of (1.1), multiplied by the real value r, will be assigned to the array elements of f[1:n].
b) a procedure which identifies the Jacobian matrix of the vector-function f. (I.e. f_y in the equations 4.3 and 4.4).
   This is a procedure with the heading **procedure** call fy(r); **value** r; **real** r;.
   By this procedure the values of the partial derivatives of f_i with respect to y_j multiplied by a real value r, will be assigned to the array element fy[i,j].
c) a procedure which identifies the partial derivatives of f with respect to p.

This is a procedure with the heading procedure call fp(r); value r; real r;.
By this procedure the value of $\partial f_i/\partial p_j * r$ will be assigned to the array element fp[1,j].

d) a procedure by which the initial values of equation (1.1) are supplied.
This is a procedure with the heading procedure call ystart;
By this procedure the initial values of y are assigned to the array elements y[0,i] $(1 \le i \le n)$. However, the procedure has to do another job: some positive values have to be assigned to the array elements ymax[i] $(1 \le i \le n)$. The desired value of ymax[i] corresponds to an estimate of the maximal absolute value of y on the integration interval. If no estimate can be given, the value 1 can be assigned. (For a detailed description of the use of ymax see the manual for the ALGOL 60. procedure MULTISTEP, Hemker [1971]).

N.B. 1. Note that the structure of the system is completely determined by f.f_y and f_p can be derived from f. However, by supplying fy and fp in an analytic form, we are able to solve our problem efficiently.

N.B. 2. f, fy and fp are functions of t, y and p. These values of t, y and p can be obtained from the identifiers (array elements) x, y[0,i] $(1 \le i \le n)$ and par[i] $(1 \le i \le m)$ respectively.

N.B. 3. The initial values may be functions of the parameters p. In that case the initial values of $\partial y/\partial p$ also have to be supplied; thus it is useful to know that $\partial y_i/\partial p_j$ corresponds with y[0,n*j+i].

N.B. 4. Since procedure call ystart is only called once during the integration of an interval, and since "call f", "call fy" and "call fp" are used many times, assignments of the constant value zero to an element of f, fy or fp will be placed in "call ystart".

2) The observations to be fitted to, and
3) the first estimate, upper- and lower-bounds of the parameters, are ashed for by means of a call of the procedure 'data' from the formal parameter list of the procedure 'odeparest'.
The actual declaration of this procedure has the heading

```
procedure data (nobs, tobs, cobs, obs, npar, parlbd,
          par, parubd);
integer nobs, npar; integer array cobs;
array tobs, obs, parlbd, par, par ubd;.
```

nobs and npar are inputparameters, indicating the number of parameters, m, respectively. For each observation a value is assigned to

tobs[i], cobs[i] and obs[i] ($1 \leq i \leq$ nobs)

tobs[i] - the time of observation
cobs[i] - the component of y observed ($1 \leq$ cobs[i] $\leq n$)
obs[i] - the observed value of the component cobs[i] of y at the time tobs[i].

If the time, corresponding to the starting values (given in 'call ystart') does not equal zero, this time has to be provided in tobs[0].
The observations have to be ordered such that tobs[i] $\leq$ tobs[j] if $i \leq j$.
For each parameter in the system (1.1), values are assigned to

parlbd[i], par[i] and parubd[i] ($1 \leq i \leq$ npar)

par[i] - a first estimate of the i-th parameter.
parlbd[i] and parubd[i] - lower- and upper-bounds, respectively, for the parameter value.

N.B. 1. The procedure 'odeparest' only solves the unconstrained optimization problem; parlbd and parubd are provided only to prevent some unwanted effects (e.g. f, fy and fp may be undefined outside the indicated parameter region.

N.B. 2. If the value of 'nobs' is decreased by the procedure 'data', only the first 'nobs' (new value) observations will be used during the calculation.

If the value of 'npar' is decreased by the procedure 'data', only the first 'npar' (new value) parameters will be adjusted.

4) Before we explain the formal procedure parameters of the procedure 'odeparest', by which the process is controled, we give the heading of the procedure:

```
procedure odeparest (n, nobs, npar, data, itmax, converge,
        eps, meshp, stiff, fa);
value n, nobs, npar, itmax, converge, eps, meshp, stiff,
     fa);
integer n, nobs, npar, itmax, meshp; real converge, eps,
       fa;
boolean stiff; procedure data;
```

The actual parameters corresponding to the formal parameters are:

n : < integer expression >;
the number of equations of system (1.1).

nobs : < integer expression >;
the number of observations: N.

npar : < integer expression >;
the number of parameters: m.

data : < procedure >;
this procedure is described in item 2 and 3.

itmax : < integer expression >;
the maximum number of iterations of the optimization process.

converge : < real expression >;
The optimization process is deemed to have converged if the final (estimated) improvement in S(p) (i.e. $|S(p)-S(p+\delta p)|$) is less than

$$\text{converge} * S(p)$$

This test arises from the fact that the difference between $S(\bar{p})$ and $S(p)$, evaluated on the boundary of the confidence region, is

$$\frac{m}{N-m} F_{\alpha}(m, N-m) * S$$

It seems reasonable that some small function fraction of this should be used as convergence criterion.

eps : < real expression >;
a parameter which controls the relative local error bound during the integration process. During the last iteration step of the optimazing process eps is replaced by eps/10.

meshp : < integer expression >;
the maximal number of meshpoints that will be used by the integrating procedure, between two different observation times tobs[i] and tobs[i+1].

stiff : < boolean expression >;
In order to make efficient use of the integrating procedure, 'stiff' can be set <u>true</u>, if the user knows that stiff differential equations will be integrated.

fa : < real expression >;
$F_\alpha(m, N-m)$, fa is the α-point of the F-distribution with npar and nobs-npar degrees of freedom. The confidence regions at level α will be printed.

OUTPUT.

As we mentioned before, a call of procedure 'odeparest' only results in some printed output.
This printout can be of three kinds.

1) Results for each iteration, associated with the fitting of the data.
2) Diagnostic printout.
3) Final results, which include parameter values, confidence regions, correlation- and covariance-matrices.

We describe the printout in more detail.

1) An iteration is called successful, if $S(p_{new}) < S(p_{old})$ holds for the new estimate p_{new} of $\bar{p}$.
   a) Each successful iteration results in the printout 'iteration number' and the number of the iteration performed. The following additional results will be

'computed residue': $||Y(p)||_2^2$ (see equation (1.2))
' computed standard error': $(||Y(p)||^2/(N-m))^{\frac{1}{2}}$
'estimated residue' : $||Y(p+\delta p)||^2$
'estimated standard error': $(||Y(p+\delta p)||^2/(N-m))^{\frac{1}{2}}$
'corrections for parameters': δp_i $(1 \le i \le m)$
'parameter value': $(p+\delta p)_i$ $(1 \le i \le m)$
These additional results will also be printed after the messages:

b) 'boundary constraints jump':
the calculated new parameter value violates the boundary constraints. Linear interpolation gives the maximal permissible jump in the computed direction.

c) 'plus ulta':
even on the boundaries of the permissible region the minimizing vector $\bar{p}$ seems to be beyond these boundaries.

d) 'steepest descent':
the last iteration step was not successful. The old value of p is maintained and a step according to the method of the steepest descent is executed.

e) 'relation par':
even steepest descent was unsatisfactory; the last jump is repeated with a relaxation factor $S(p)/(S(p)+S(p+\delta p))$.

2) Diagnostic printouts are:
'strong nonlinearity'
The differential equation seems to be a very nonlinear one. This may result in a long computing time, since integration is continued with a smaller steplength than specified by 'meshp'. This diagnostic can be avoided by choosing a larger value for 'meshp'. However, this will not avoid the evil. This diagnostic also can appear when fy doesn't represent the Jacobian matrix correctly.
'linear dependence in (dy/dp) [i]'
The matrix A^TA seems to be singular. The initial estimate or the set of sample-times {tobs[i]/1≤i≤N} are not appropriate to solve the problem. This diagnostic

may also occur if fp is not represented correctly.
'the equation was found to be stiff at t='
This message is only given if the formal parameter stiff ≡ <u>false</u>. If the equation appears to be stiff in the greater part of the integration, it will be efficient to set stiff ≡ <u>true</u>.
'some little problems with stiffness < number >'
This message is given if a stiff differential equation is solved. The < number > indicates the number of times that the relative local error bound eps is exeeded. If it is a large number (≈ meshp) it may be better to choose a larger number for meshp.

3) During the last two iterations, information about the confidence region and the linear correlation between the parameters is printed.
This information involves:
   a) the conditional confidence interval:
      the values δp_i (see equation 3.4).
   b) the independent confidence interval:
      the values δp_i^* (see equation 3.5).
   c) the correlation matrix,
   d) the covariance matrix and
   e) the principal axes of the confidence region.
      For detailed information see section 3.

   The last iteration is a special one. It computes $y(t_i,p)$ with an accuracy eps/10 and it computes $p+\delta p$ even in the case $S(p+\delta p) \nless S(p)$.

5.2. <u>The procedure text</u>

```
procedure odeparest(n,nobs,npar,data,itmax,converge,eps,meshp,stiff,fa);
value n,nobs,npar,itmax,converge,eps,meshp,stiff,fa;
integer n,nobs,npar,itmax,meshp; real converge,eps,fa; boolean stiff;
begin  comment The procedures: call ystart,call f,call fy,call fp
        define the problem supplied by the user.
        The four procedures inserted here only are examples;
        procedure call ystart;
        begin y[0,1]:= ymax[1]:= ymax[2]:= 1; y[0,2]:= 0 end;

        procedure call f(r); value r; real r;
        begin f[1]:= -r×((1-y[0,2])×y[0,1] - par[2]×y[0,2]);
              f[2]:=  r×par[1]×((1-y[0,2])×y[0,1] -
                                 (par[2]+par[3])×y[0,2])
        end;

        procedure call fy(r); value r; real r;
        begin fy[1,1]:= -r×(1-y[0,2]);
              fy[1,2]:=  r×(par[2]+y[0,1]);
              fy[2,1]:=  r×par[1]×(1-y[0,2]);
              fy[2,2]:= -r×par[1]×(par[2]+par[3]+y[0,1]);
        end;

        procedure call fp(r); value r; real r;
        begin fp[1,1]:= 0; fp[1,2]:= r×y[0,2]; fp[1,3]:= 0;
              fp[2,1]:= r×((1-y[0,2])×y[0,1] - (par[2]+par[3])×y[0,2]);
              fp[2,2]:=-r×par[1]×y[0,2];
              fp[2,3]:=-r×par[1]×y[0,2]
        end last procedure declared by the user;


array y[0:7,1:n×(npar+1)],ymax,f[1:n],fy[1:n,1:n],fp[1:n,1:npar];
proc pr(s); begin nlcr; printtext(s) end;
proc fl(r); flot(5,3,r);
proc pf(s,r); begin pr(s); tab; fl(r) end;

proc out(s,r); string s; real r;
begin int i; if linenumber>50 then new page else nlcr;
        pr(s); print(r);
        pf(⪡computed residue (stand.dev.)⪢,comp error);
        fl(sqrt(comp error/(nobs-npar)));
        pf(⪡estimated residue (stand.dev.)⪢,est error);
        fl(sqrt(est error/(nobs-npar)));
        pr(⪡corrections for parameter⪢); tab;
        for i:=1 step 1 until npar do fl(delta par[i]); nlcr;
        pr(⪡parameter value⪢); tab; tab;
        for i:= 1 step 1 until npar do fl(par[i]);
end;

boolean first,adams; integer k,kold,same,fails;
real x,xold,h,ch,hold,tolconv,tolup,tol,toldwn,a0;
array a[0:7],dd[0:7,0:n],last delta[1:n], jac[1:n,1:n],const[1:45],
     tobs[0:nobs],obs[1:nobs],parl,par,paru[1:npar];
int array cobs[1:nobs],pp[1:n];
```

```
procedure multistep(xend,hmin,hmax,eps);
value xend,hmin,hmax,eps; real xend,hmin,hmax,eps;
begin comment This sub-procedure 'multistep' is essentially the same
      as the procedure 'MULTISTEP' described in Hemker[1971];

      boolean conv; integer i,j,l,knew,np;
      real chnew,c,error,dfi; array delta,df,y0[1:n];

      procedure method;
      begin dd[0,0]:= if adams then -₁₀600 else x; i:= k:= 1;
            if adams then
            begin for const[i]:= 1,1,12,2,1,.5,1,.5,24,12,1,5/12,1,.75,
                  1/6,37.89,24,2,.375,1,11/12,1/3,1/24,53.33,37.89,1,
                  251/720,1,25/24,35/72,5/48,1/120,70.08,53.33,.3158,
                  95/288,1,137/120,.625,17/96,.025,1/720,0,70.08,
                  .07407 do i:= i + 1
            end else
            begin for const[i]:= 1,1,3,2,1,2/3,1,1/3,6,4.5,1,6/11,1,
                  6/11,1/11,9.167,7.333,0.5,.48,1,.7,.2,.02,12.5,
                  10.42,.1667,120/274,1,225/274,85/274,15/274,1/274,
                  15.98,13.7,.04167,180/441,1,58/63,5/12,25/252,
                  3/252,1/1764,0,17.15,.008333 do i:= i + 1
            end
      end method;

      procedure order;
      begin j:= (k-1) × (k+8) / 2 + 1;
            for i:= 0 step 1 until k do a[i]:= const[i+j]; a0:= a[0];
            tolup  := (eps×const[j+k+1])↑2;
            tol    := (eps×const[j+k+2])↑2;
            toldwn:= (eps×const[j+k+3])↑2;
            tolconv:= eps/(2×n×(k+2));
            same:= k+1
      end order;

      procedure evaluate jacobian;
      begin call fy( -a0×h);
            for i:= 1 step 1 until n do
            for j:= 1 step 1 until n do jac[i,j]:= fy[i,j];
            for i:= 1 step 1 until n do jac[i,i]:= jac[i,i] + 1;
            det(jac,n,pp)
      end evaluate jacobian;

      procedure calculate step and order;
      begin real a1,a2,a3; same:= 10;
            a1:= if k<1 then 0 else
                 0.75×(toldwn/sum(i,1,n,(y[k,i]/ymax[i])↑2))↑(0.5/k);
            a2:= 0.80×(tol    /error ) ↑ (0.5/(k+1));
            a3:= if fails≠0 then 0 else
                 0.70×(tolup /sum(i,1,n,((delta[i]-last delta[i])/
                       ymax[i])↑2))↑(0.5/(k+2));
            if a1>a2 ∧ a1>a3 then begin knew:=k-1; chnew:=a1 end else
            if a2>a3         then begin knew:=k  ; chnew:=a2 end else
                                  begin knew:=k+1; chnew:=a3 end
      end calculate step and order;
```

```
procedure reset step;
begin real c;
      if ch < hmin/hold then ch:= hmin/hold else
      if ch > hmax/hold then ch:= hmax/hold;
      x:= xold; h:= hold × ch; c:= 1;
      for j:=0 step 1 until k do
      begin for i:=1 step 1 until n do y[j,i]:= dd[j,i] × c;
            c:= c × ch
      end;
      evaluate jacobian;
      same:= k + 1
end reset step;

procedure begin;
begin hold:= h:= hmin; ch:= 1; call f(h);
      for i:= 1 step 1 until n do
      begin dd[0,i]:= y[0,i]; dd[1,i]:= y[1,i]:= f[i] end;
      fails:= kold:= 0; k:= 1; order; evaluate jacobian
end begin;

if first then
begin first:= false; adams:= ¬stiff; method;
      xold:= x; begin; for i:= 1,2,3 do dd[i,0]:= 0
end;

for l:= 0 while x<xend do
begin x:= x+h;

      comment prediction;
      for i:=0 step 1 until k-1 do
      for j:= k-1 step -1 until i do
      elmrow(1,n,j,j+1,y,y,1);
      for i:= 1 step 1 until n do delta[i]:= 0;


      comment correction and estimation local error;
      for l:=1,2,3 do
      begin call f(h);
            for i:=1 step 1 until n do df[i]:= f[i] - y[1,i];
            sol(jac,n,pp,df);

            conv:= true;
            for i:= 1 step 1 until n do
            begin dfi:= df[i];
                  y[0,i]:= y[0,i] + a0×dfi;
                  y[1,i]:= y[1,i] +    dfi;
                  delta[i]:= delta[i] +dfi;
                  conv:= conv ∧ abs(dfi) < tolconv × ymax[i]
            end;
            if conv then
            begin error:= sum(i,1,n,(delta[i]/ymax[i])↑2);
                  goto convergence
            end
      end;
```

```
comment acceptance or rejection;
if ¬conv then no convergence:
begin if h<hmin×1.0001 then
      begin pr(⩤ strong nonlinearity⩥); hmin:= hmin/4 end;
      ch:= ch/4; reset step
end else convergence:

if error>tol then error test not ok:
begin fails:= fails + 1;
      if h>hmin×1.0001 then
      begin if fails>2 then
            begin k:= 0; reset step; begin end else
            begin calculate step and order;
                  if knew≠k then begin k:= knew; order end;
                  ch:= ch×chnew/fails; reset step
            end
      end else
      if adams then
      begin adams:= false; method;order;reset step end else
      if k≠1 then
      begin k:=1; order; reset step end else
      begin dd[2,0]:= dd[2,0] + 1; goto error test ok end
end else

error test ok:
begin fails:= 0;
      if k>2 then begin for i:=1 step 1 until n do
            elmcolvec(2,k,i,y,a,delta[i]) end;
      for i:= 1 step 1 until n do if abs(y[0,i])>ymax[i]
            then ymax[i]:=abs(y[0,i]);
      same:= same - 1;
      if same=1 then begin for i:=1 step 1 until n do
            last delta[i]:= delta[i] end else
      if same=0 then
      begin calculate step and order;
            if chnew>1.1 then
            begin same:= k + 1;
                  if knew≠k then
                  begin if knew>k then
                        begin for i:=1 step 1 until n do
                              y[knew,i]:= delta[i]×a[k]/knew
                        end;
                        k:= knew; order
                  end;
                  if chnew> hmax/h then chnew:= hmax/h;
                  h:= h × chnew; c:= 1;
                  for j:=1 step 1 until k do
                  begin c:= c × chnew;
                        for i:=1 step 1 until n do
                        y[j,i]:= y[j,i]×c
                  end
            end
      end;
```

```
                for i:= 1 step 1 until n do
                for j:= 0 step 1 until k do dd[j,i]:= y[j,i];

                if h≠ hold then
                begin ch:= h/hold; c:= 1;
                      for j:= 1 step 1 until kold do
                      begin c:= c×ch;
                            for i:= n+1 step 1 until nnp do
                            y[j,i]:= y[j,i]×c;
                      end;  hold:= h;
                end;
                if k>kold then
                for i:= n+1 step 1 until nnp do y[k,i]:= 0;
                kold:= k; xold:= x; ch:= 1;

                evaluate jacobian; call fp(h);

                for i:= 0 step 1 until k-1 do
                for j:=k-1 step -1 until i do
                elmrow(n+1,nnp,j,j+1,y,y,1);

                for j:= 1 step 1 until npar do
                begin np:= j×n;
                      for i:=1 step 1 until n do y0[i]:= y[0,np+i];
                      for i:=1 step 1 until n do df[i]:=
                      fp[i,j] - matvec(1,n,i,fy,y0)/a0 - y[1,np+i];
                      sol(jac,n,pp,df);
                      for i:=1 step 1 until n do
                      elmcolvec(0,k,np+i,y,a,df[i]);
                end;

          end
     end step
end multistep;

integer i,j,l,cobi,iteration,nnp; bool further;
real old comp error,comp error,est error,tobsdif,bound,b,r;
array aux[0:2],em[0:5],delta par,aid,val[1:npar], delta obs[1:nobs],
aa[1:nobs,1:npar],ata,q[1:npar,1:npar]; int array ci,ich[1:npar];

aux[0]:= ₁₀-10; em[0]:= ₁₀-11; em[2]:= ₁₀-8; em[4]:= 5×npar;
old comp error:= ₁₀600; further:= true; tobs[0]:= 0;
data(nobs,tobs,cobs,obs,npar,parl,par,paru);
nnp:= n + n×npar; b:= fa×npar/(nobs-npar);
```

```
for iteration:= 1,iteration+1 while further,iteration do
begin   if ¬further then eps:= eps/10;

        comment integration of the differential equations;
        for i:= n+1 step 1 until nnp do y[0,i]:= 0; x:= tobs[0];
        call ystart; first:= true;
        for i:= 1 step 1 until nobs do
        begin tobsdif:= tobs[i] - tobs[i-1]; if tobsdif>0 then
                multistep(tobs[i],tobsdif/meshp,tobsdif,eps);
                tobsdif:= (tobs[i] - x)/h; cobi:= cobs[i];
                delta obs[i]:= obs[i] - sum(l,0,k,y[l,cobi]×tobsdif↑l);
                for j:= 1 step 1 until npar do
                aa[i,j]:= sum(l,0,k,y[l,n×j+cobi]×tobsdif↑l);
        end;

        comment diagnostic printout;
        if further then else
        for i:= 1 step 1 until nobs do obs[i]:= delta obs[i];
        if ¬stiff ∧ dd[0,0]≠₁₀600 then
        pf(‹the equation was found to be stiff at x =›,dd[0,0]);
        if dd[2,0]≠0 then
        begin pf(‹some little problems with stiffness›,dd[2,0]);nlcrend;

        comment minimization;
        comp error:= sum(i,1,nobs,delta obs[i]↑2);
        old comp error:= old comp error×(1+eps);
        if ¬further ∨ comp error<old comp error then
        begin comment least squares;
                if npar≠ lsqdec(aa,nobs,npar,aux,aid,ci) then
                begin pr(‹linear dependence in (dy/dp)[i]›);
                      further:= false; goto end iteration
                end;
                lsqsol(aa,nobs,npar,aid,ci,delta obs);
                for i:= 1 step 1 until npar do
                begin delta par[i]:= delta obs[i];
                      par[i]:= par[i] + delta par[i]
                end;
                est error:= sum(i,npar+1,nobs,delta obs[i]↑2);
                out(‹iteration number›,iteration);
        end else if est error≠0 then
        begin comment steepest descent;
                for i:= 1 step 1 until npar do
                begin ata[i,i]:= tammat(1,i-1,i,i,aa,aa)+aid[i]↑2;
                      par[i]:= par[i]-deltapar[i];
                      for j:= i+1 step 1 until npar do ata[i,j]:=
                      ata[j,i]:= tammat(1,i-1,i,j,aa,aa)+aa[i,j]×aid[i];
                end;
                for i:= npar step -1 until 1 do if ci[i]≠i then
                begin ichcol(1,npar,i,ci[i],ata);
                      ichrow(1,npar,i,ci[i],ata)
                end;
```

```
        for i:= 1 step 1 until npar do
              val[i]:= matvec(1,npar,i,ata,deltapar);
        for i:= 1 step 1 until npar do
              aid[i]:= matvec(1,npar,i,ata,val);
        r:= vecvec(1,npar,0,val,val)/vecvec(1,npar,0,val,aid);
        for i:= 1 step 1 until npar do
        begin deltapar[i]:= bound:= r × val[i];
              par[i]:= par[i] + bound
        end;  est error:= 0;
        out(⊰steepest descent⊱,r)
end else
begin r:= comp error/(old comp error + comp error);
        if r > .99 then r:= .99;
        for i:= 1 step 1 until npar do
        begin par[i]:= par[i] - r×deltapar[i];
              delta par[i]:= deltapar[i]×(1-r)
        end;  iteration:= iteration + 1;
        eps:= eps/2; further:= iteration < itmax;
        out(⊰relaxation par⊱,1-r);
        goto end iteration
end;

comment constraints; r:= 1;
for i:= 1 step 1 until npar do
begin if par[i]<parl[i] then bound:=parl[i]-par[i] else
      if par[i]>paru[i] then bound:=paru[i]-par[i] else
      goto through; bound:= 1+bound/deltapar[i];
      if bound<r then r:= bound; through:
end;
if 0 < r ∧ r < 1 then
begin for i:= 1 step 1 until npar do
        begin par[i]:= par[i] + (r-1)× delta par[i];
                deltapar[i]:= deltapar[i]×r
        end;
        est error:= est error + r×r×(comp error - est error);
        out(⊰boundary constraints.  jump⊱,r);
end else if r<0 then
begin for i:= 1 step 1 until npar do
        if par[i]<parl[i] then par[i]:= parl[i] else
        if par[i]>paru[i] then par[i]:= paru[i];
        out(⊰plus ultra⊱,r);
end;

further:= further ∧ iteration < itmax-1 ∧
          comp error - est error > converge × est error;
```

```
       comment statistics;
       if ¬ further then
       begin for i:= 1 step 1 until npar do
             begin ata[i,i]:= q[i,i]:=
                   tammat(1,i-1,i,i,aa,aa) + aid[i]×aid[i];
                   for j:= i+1 step 1 until npar do
                   ata[i,j]:= ata[j,i]:= q[i,j]:=
                   tammat(1,i-1,i,j,aa,aa) + aa[i,j]×aid[i];
             end;
             if qrisym(q,npar,val,em)≠0 then
                   pr(⪡qrisym doesnot converge⪢);
             for i:= npar step -1 until 1 do if ci[i]≠i then
             begin ichcol(1,npar,i,ci[i],ata);
                   ichrow(1,npar,i,ci[i],ata);
                   ichrow(1,npar,i,ci[i],q)
             end;

             comment output;
             pr(⪡confidence interval (cond.)⪢); tab;
             for i:= 1 step 1 until npar do
             fl(sqrt(b×est error/ata[i,i]));
             detinv(ata,npar);
             pr(⪡confidence interval (indept.)⪢); tab;
             for i:= 1 step 1 until npar do
             fl(sqrt(b×est error×ata[i,i]));
             if linenumber + 2×npar>53 then new page else nlcr;
             pr(⪡relationships between parameters⪢);
             pr(⪡correlation matrix⪢); space(22);
             printtext(⪡covariance matrix⪢);
             for i:= 1 step 1 until npar do
             begin nlcr; for j:=1 step 1 until npar do
                   begin if i=j then space(40); fl(if i>j then
                         ata[i,j]/sqrt(ata[i,i]×ata[j,j]) else ata[i,j])
                   end;
             end; nlcr;
pr(⪡principal axes (direction cos and conf interval along each axis)⪢);
             for i:= 1 step 1 until npar do
             begin nlcr; for j:= 1 step 1 until npar do fl(q[j,i]);
                   space(5); fl(sqrt(b×est error/val[i]))
             end; new page;
       end;
       old comp error:= comp error; end iteration:
end iteration;
```

```
        tobsdif:= tobs[0];
        pr(⊰residuals, specified for each observation,⊱);
        for i:= 1 step 1 until nobs do
        begin r:= tobs[i]; if r>tobsdif then nlcr else tab;
              tobsdif:= r; absfixt(3,0,i); space(3); fl(obs[i])
        end
end odeparest;
```

```
comment
```

Procedures used

In the body of procedure 'odeparest' a number of procedures are not declared. These procedures (library routines of the EL X8 system of the Mathematical Centre) are:

matvec, tammat, elmrow, elmcolvec, ichrow, ichcol,
det, sol, detinv, lsqdec, lsqsol, qrisym
(see: Dekker [1968] and Dekker and Hoffmann [1968])

and:
nlcr, tab, space, print, printtext, absfixt, flot,
new page, linenumber, sum
(see: Grune[1972]).

;

6 Problems solved

6.1. The ESCEP problem

Our first example originates from biochemistry.
A set of couples chemical reactions

$$E + S \underset{k_{-1}}{\overset{k_1}{\rightleftarrows}} C \overset{k_2}{\rightarrow} E + P$$

is given : a catalyst E combines with a reactant S at one stage and is regenerated in a subsequent stage of the reaction. The problem is to find the rate constants k_1, k_{-1} and k_2 from observations on the overall reaction rate (i.e. velocity of generation of the product P).

Rescaling the problem in some convenient way (see Heineken et al.[1967]), we obtain a description of the system as an initial value problem:

$$ds/dt = -(1-c)s + qc$$
$$dc/dt = M((1-c)s - (p+q)c)$$

$$s(0) = 1 \quad , \; c(0) = 0.$$

Observations on $s(t)$ and $c(t)$ can be made and the unknown (positive) parameters M, p and q have to be determined.

In order to test our algorithm we generated some experimental values $s(t_i)$ and $c(t_i)$ $(i=1,2,\ldots,23)$ using the parameter values

$$M = 1000 \quad ,$$
$$p = 0.99 \quad ,$$
$$q = 0.01 \quad .$$

These parameter values require that we are dealing with a stiff system of diffential equations.

We can distinguish a short initial period in which c(t) increases rapidly and a period in which the steady state hypothesis holds. This represents a common type of enzymatic reaction in biochemistry : after a rapid generation of the complex C there is a period in which the Michaelis - Menten approximation holds.

We made five different tests:

1) we used 23 observations on each of the two components of the system, s(t) and c(t).
   The observations were taken from the initial period as well as from the pseudo-steady state period.
2) Only the 23 observations on the component c(t) were taken.
3) 12 observations were taken on the component c(t) (every $2^{\underline{nd}}$ observation of test (2) was left out).
4) Only the 12 last observations from test (2) were used. All observations are in the pseudo-steady state region.
5) Only the 12 first observations from test (2) were used. Most observations were taken from the initial period.

We note that in tests 1), 2) and 3) our algorithm works highly accurate, since the quality of the observations was perfect : (a) four digits are correct (b) the observations contain information from the initial and from the pseudo-steady state period. In test 4) the parameter M is only approximately correct (1239 in stead of 1000) since this parameter, which is responsible for the initial period, is badly defined by the experimental observations.
In test 5) the parameter M is approximately correct but the other parameters are not determined at all since not enough information is available from the pseudo-steady state region.

NOTE : A component of the correlation matrix which approximately equals one, means that the algorithm cannot fix the parameter vector in some linear subspace of the parameter space.

B13681.138,PHEMKER,T150

```
BEGIN COMMENT THE ESCEP PROBLEM;

        PROC ODEPAREST(N,NOBS,NPAR,DATA,ITMAX,CONVERGE,EPS,MESHP,STIFF,FA);
        VAL N,NOBS,NPAR,ITMAX,CONVERGE,EPS,MESHP,STIFF,FA;
        INT N,NOBS,NPAR,ITMAX,MESHP; REAL CONVERGE,EPS,FA; BOOL STIFF;
        BEGIN COMMENT THE PROCEDURES: CALL YSTART,CALL F,CALL FY,CALL FP
                DEFINE THE PROBLEM SUPPLIED BY THE USER;

                PROC CALL YSTART;
                BEGIN Y[0,1]:= YMAX[1]:= YMAX[2]:= 1; Y[0,2]:= 0; OUTC
                END;
                PROC CALL F(R); VAL R; REAL R;
                BEGIN CF:= CF+1;
                        F[1]:= -R*((1-Y[0,2])*Y[0,1] - PAR[2]*Y[0,2]);
                        F[2]:=  R*PAR[1]*((1-Y[0,2])*Y[0,1] - (PAR[2]+PAR[3])*Y[0,2])
                END;
                PROC CALL FY(R); VAL R; REAL R;
                BEGIN FY[1,1]:= -R*(1-Y[0,2]);            FY[1,2]:= R*(PAR[2]+Y[0,1]);
                      FY[2,1]:=  R*PAR[1]*(1-Y[0,2]);    FY[2,2]:=-R*PAR[1]*(PAR[2]+PAR[3]+Y[0,1]);
                        CFY:= CFY+1;
                END;
                PROC CALL FP(R); VAL R; REAL R;
                BEGIN FP[1,1]:= 0; FP[1,2]:= R*Y[0,2]; FP[1,3]:= 0;
                      FP[2,1]:= R*((1-Y[0,2])*Y[0,1] - (PAR[2]+PAR[3])*Y[0,2]); FP[2,2]:= -R*PAR[1]*Y[0,2];
                      FP[2,3]:=-R*PAR[1]*Y[0,2]; CFP:= CFP+1
                END;

        ARRAY Y[0:7,1:N*(NPAR+1)],YMAX,F[1:N],FY[1:N,1:N],FP[1:N,1:NPAR];
        PROC PR(S); BEGIN NLCR; PRINTTEXT(S) END;
        PROC FL(R); FLOT(5,3,R);
        PROC PF(S,R); BEGIN PR(S); TAB; FL(R) END;

        PROC OUT(S,R); STRING S; REAL R;
        BEGIN INT I; IF LINENUMBER>50 THEN NEW PAGE ELSE NLCR;
                PR(S); PRINT(R);
                PF(<COMPUTED RESIDUE (STAND.DEV.)>,COMP ERROR);
                FL(SQRT(COMP ERROR/(NOBS-NPAR)));
                PF(<ESTIMATED RESIDUE (STAND.DEV.)>,EST ERROR);
                FL(SQRT(EST ERROR/(NOBS-NPAR)));
                PR(<CORRECTIONS FOR PARAMETER>); TAB;
                FOR I:=1 STEP 1 UNTIL NPAR DO FL(DELTA PAR[I]); NLCR;
                PR(<PARAMETER VALUE>); TAB; TAB;
                FOR I:= 1 STEP 1 UNTIL NPAR DO FL(PAR[I]);
        END;

        BOOL FIRST,ADAMS; INTEGER K,KOLD,SAME,FAILS;
        REAL X,XOLD,H,CH,HOLD,TOLCONV,TOLUP,TOL,TOLDWN,A0;
        ARRAY A[0:7],DD[0:7,0:N],LAST DELTA[1:N], JAC[1:N,1:N],CONST[1:45],
                TOBS[0:NOBS],OBS[1:NOBS],PARL,PAR,PARU[1:NPAR];
        INT ARRAY COBS[1:NOBS],PP[1:N];

        PROC MULTISTEP(XEND,HMIN,HMAX,EPS);
        VALUE XEND,HMIN,HMAX,EPS; REAL XEND,HMIN,HMAX,EPS;

        BEGIN BOOLEAN CONV; INTEGER I,J,L,KNEW,NP;
              REAL CHNEW,C,ERROR,DF; ARRAY DELTA,DF,Y0[1:N];
```

```
                    TAMMAT(1,I-1,I,I,AA,AA) + AID[I]*AID[I];
                    FOR J:= I+1 STEP 1 UNTIL NPAR DO
                    ATA[I,J]:= ATA[J,I]:= Q[I,J]:=
                    TAMMAT(1,I-1,I,J,AA,AA) + AA[I,J]*AID[I];
                END;
                IF QRISYM(Q,NPAR,VAL,EM)≠0 THEN
                    PR(‡QRISYM DOESNOT CONVERGE‡);
                FOR I:= NPAR STEP -1 UNTIL 1 DO IF CI[I]≠I THEN
                BEGIN ICHCOL(1,NPAR,I,CI[I],ATA); ICHROW(1,NPAR,I,CI[I],ATA);
                    ICHROW(1,NPAR,I,CI[I],Q)
                END;

                COMMENT OUTPUT;
                PR(‡CONFIDENCE INTERVAL (COND.)‡); TAB;
                FOR I:= 1 STEP 1 UNTIL NPAR DO FL(SQRT(B*EST ERROR/ATA[I,I]));
                DETINV(ATA,NPAR); PR(‡CONFIDENCE INTERVAL (INDEPT.)‡); TAB;
                FOR I:= 1 STEP 1 UNTIL NPAR DO FL(SQRT(B*EST ERROR*ATA[I,I]));
                IF LINENUMBER + 2*NPAR>53 THEN NEW PAGE ELSE NLCR;
                PR(‡RELATIONSHIPS BETWEEN PARAMETERS‡);
            PR(‡CORRELATION MATRIX‡);SPACE(22);PRINTTEXT(‡COVARIANCE MATRIX‡);
                FOR I:= 1 STEP 1 UNTIL NPAR DO
                BEGIN NLCR; FOR J:=1 STEP 1 UNTIL NPAR DO
                    BEGIN IF I=J THEN SPACE(40); FL(IF I>J THEN
                        ATA[I,J]/SQRT(ATA[I,I]*ATA[J,J]) ELSE ATA[I,J])
                    END;
                END; NLCR;
     PR(‡PRINCIPAL AXES (DIRECTION COSINES AND CONFIDENCE INTERVAL ALONG EACH AXIS)‡);
                FOR I:= 1 STEP 1 UNTIL NPAR DO
                BEGIN NLCR; FOR J:= 1 STEP 1 UNTIL NPAR DO FL(Q[J,I]);
                    SPACE(5); FL(SQRT(B*EST ERROR/VAL[I]))
                END; NEW PAGE;
            END;
            OLD COMP ERROR:= COMP ERROR; END ITERATION:
    END ITERATION;

    TOBSDIF:= TOBS[0]; PR(‡RESIDUALS, SPECIFIED FOR EACH OBSERVATION,↓);
    FOR I:= 1 STEP 1 UNTIL NOBS DO
    BEGIN R:= TOBS[I]; IF R>TOBSDIF THEN NLCR ELSE TAB; TOBSDIF:= R;
            ABSFIXT(3,0,I); SPACE(3); FL(OBS[I])
    END
    END ODEPAREST;

    PROC READ OBS AND PAR(NOBS,TOBS,COBS,OBS,NPAR,PARL,PAR,PARU);
    BEGIN INT I; REAL R,S; NLCR; PR(‡THE OBSERVATIONS WERE:‡); PR(‡   I    TOBS[I]    COBS[I]    OBS[I]‡);
            TOBS[0]:= S:= READ; NLCR; ABSFIXT(3,0,0); SPACE(3); FL(TOBS[0]);
            FOR I:= 1 STEP 1 UNTIL NOBS DO
            BEGIN TOBS[I]:= R:= READ; COBS[I]:= READ; OBS[I]:= READ; IF R>S THEN NLCR ELSE TAB; S:= R;
                    ABSFIXT(3,0,I); SPACE(3); FL(R); FIXT(3,0,COBS[I]); SPACE(2); FL(OBS[I]);
            END; NLCR; NLCR; PR(‡THE PARAMETER ESTIMATES WERE:‡);
            PR(‡   I    PARLWB[I]      PAR[I]         PARUPB[I]‡);
            FOR I:= 1 STEP 1 UNTIL NPAR DO
            BEGIN PARL[I]:= READ; PAR[I]:= READ; PARU[I]:= READ; NLCR;
                    ABSFIXT(3,0,I); FOR R:= PARL[I],PAR[I],PARU[I] DO BEGIN  FL(R); SPACE(2) END;
            END;    NEW PAGE;
    END;

    PROC PR(S); BEGIN NLCR; PRINTTEXT(S) END;
    PROC P(S,R); BEGIN PR(S); TAB; PRINT(R) END;
    PROC FL(R); FLOT(5,3,R);
    PROC PF(S,R); BEGIN PR(S); TAB; FL(R) END;
```

```
        INT CF,CFY,CFP;
        PROC OUTC;
        BEGIN INT R; NLCR; SPACE(100); IF CF=0 THEN
                BEGIN SPACE(6); PRINTTEXT(‡EVALUATIONS OF‡); NLCR; SPACE(106);PRINTTEXT(‡F       FY       FP‡) END ELSE
                FOR R:= CF,CFY,CFP DO ABSFIXT(6,0,R);
                CF:= CFY:= CFP:= 0;
        END;

        PROC JOB(N,NOBS,NPAR,ITMAX,CONVERGE,EPS,MESHP,STIFF,FA);
        VAL N,NOBS,NPAR,ITMAX,CONVERGE,MESHP,STIFF,FA;
        INT N,NOBS,NPAR,ITMAX,MESHP; REAL CONVERGE,EPS,FA; BOOL STIFF;
        BEGIN REAL TIM;
                PR(‡PROCEDURE ODEPAREST WAS CALLED WITH THE PARAMETERS:‡);
                P(‡N     =‡,N); P(‡NPAR =‡,NPAR); P(‡NOBS =‡,NOBS); P(‡ITMAX=‡,ITMAX);
                P(‡CONVERGE =‡,CONVERGE); P(‡EPS       =‡,EPS); P(‡MESHP=‡,MESHP);
                PR(‡STIFF= ‡); TAB; IF STIFF THEN PRINTTEXT(‡  TRUE‡) ELSE PRINTTEXT(‡  FALSE‡);
                P(‡FA    =    ‡,FA); PR(‡THE CONFIDENCE REGION AT LEVEL A IS PRINTED‡);
                PR(‡FA IS THE A-POINT OF THE F-DISTIBUTION WITH NPAR AND NOBS-NPAR DEGREES OF FREEDOM‡);
                NLCR; CF:= CFY:= CFP:= 0; TIM:= TIME;
                ODEPAREST(N,NOBS,NPAR,READ OBS AND PAR,ITMAX,CONVERGE,EPS,MESHP,STIFF,FA);
                TIM:= TIME-TIM; OUTC; NLCR;NLCR; NLCR;
                PR(‡THE ENTIRE CALCULATION CONSUMED‡); ABSFIXT(3,2,TIM); PRINTTEXT(‡SEC. ON THE EL X8.‡);
        END JOB;

              JOB(2,READ,3,16,0.01,₁₀-4,100,FALSE,4.28);
              COMMENT 4.28=F[0.01](3,43);
    END
```

PROCEDURE ODEPAREST WAS CALLED WITH THE PARAMETERS:

```
N        =        +2
NPAR =            +3
NOBS =            +46
ITMAX=            +16
CONVERGE =     +.1000000000001⏨-  1
EPS      =     +.9999999999999⏨-  4
MESHP=            +100
STIFF=            FALSE
FA   =         +.4279999999999⏨+  1
```

THE CONFIDENCE REGION AT LEVEL A IS PRINTED
FA IS THE A-POINT OF THE F-DISTIBUTION WITH NPAR AND NOBS-NPAR DEGREES OF FREEDOM

THE OBSERVATIONS WERE:

I	TOBS[I]	COBS[I]	OBS[I]	I	TOBS[I]	COBS[I]	OBS[I]
0	+.00000⏨- 0						
1	+.20000⏨- 3	+1	+.99980⏨- 0	2	+.20000⏨- 3	+2	+.16480⏨- 0
3	+.40000⏨- 3	+1	+.99970⏨- 0	4	+.40000⏨- 3	+2	+.27530⏨- 0
5	+.60000⏨- 3	+1	+.99960⏨- 0	6	+.60000⏨- 3	+2	+.34930⏨- 0
7	+.80000⏨- 3	+1	+.99960⏨- 0	8	+.80000⏨- 3	+2	+.39900⏨- 0
9	+.10000⏨- 2	+1	+.99960⏨- 0	10	+.10000⏨- 2	+2	+.43220⏨- 0
11	+.12000⏨- 2	+1	+.99950⏨- 0	12	+.12000⏨- 2	+2	+.45450⏨- 0
13	+.14000⏨- 2	+1	+.99950⏨- 0	14	+.14000⏨- 2	+2	+.46950⏨- 0
15	+.16000⏨- 2	+1	+.99950⏨- 0	16	+.16000⏨- 2	+2	+.47950⏨- 0
17	+.18000⏨- 2	+1	+.99950⏨- 0	18	+.18000⏨- 2	+2	+.48620⏨- 0
19	+.20000⏨- 2	+1	+.99950⏨- 0	20	+.20000⏨- 2	+2	+.49070⏨- 0
21	+.20000⏨- 1	+1	+.99940⏨- 0	22	+.20000⏨- 1	+2	+.49990⏨- 0
23	+.40000⏨- 1	+1	+.99930⏨- 0	24	+.40000⏨- 1	+2	+.49980⏨- 0
25	+.60000⏨- 1	+1	+.99920⏨- 0	26	+.60000⏨- 1	+2	+.49980⏨- 0
27	+.80000⏨- 1	+1	+.99910⏨- 0	28	+.80000⏨- 1	+2	+.49980⏨- 0
29	+.10000⏨- 0	+1	+.99900⏨- 0	30	+.10000⏨- 0	+2	+.49980⏨- 0
31	+.10000⏨+ 1	+1	+.99450⏨- 0	32	+.10000⏨+ 1	+2	+.49860⏨- 0
33	+.20000⏨+ 1	+1	+.98950⏨- 0	34	+.20000⏨+ 1	+2	+.49730⏨- 0
35	+.50000⏨+ 1	+1	+.97470⏨- 0	36	+.50000⏨+ 1	+2	+.49360⏨- 0
37	+.10000⏨+ 2	+1	+.95020⏨- 0	38	+.10000⏨+ 2	+2	+.48720⏨- 0
39	+.15000⏨+ 2	+1	+.92600⏨- 0	40	+.15000⏨+ 2	+2	+.48080⏨- 0
41	+.20000⏨+ 2	+1	+.90210⏨- 0	42	+.20000⏨+ 2	+2	+.47430⏨- 0
43	+.25000⏨+ 2	+1	+.87860⏨- 0	44	+.25000⏨+ 2	+2	+.46770⏨- 0
45	+.30000⏨+ 2	+1	+.85530⏨- 0	46	+.30000⏨+ 2	+2	+.46100⏨- 0

THE PARAMETER ESTIMATES WERE:

I	PARLWB[I]	PAR[I]	PARUPB[I]
1	+.00000⏨- 0	+.16000⏨+ 4	+.25000⏨+ 4
2	+.00000⏨- 0	+.80000⏨- 0	+.20000⏨+ 1
3	+.00000⏨- 0	+.12000⏨+ 1	+.20000⏨+ 1

```
                                                                                          EVALUATIONS OF
                                                                                          F      FY     FP
THE EQUATION WAS FOUND TO BE STIFF AT X =      +.11572⏨- 0
SOME LITTLE PROBLEMS WITH STIFFNESS      +.10000⏨+ 1

ITERATION NUMBER               +1
COMPUTED RESIDUE (STAND.DEV.)    +.71050⏨+  1 +.40649⏨-  0
ESTIMATED RESIDUE (STAND.DEV.)   +.56079⏨+  1 +.36113⏨-  0
CORRECTIONS FOR PARAMETER        -.13012⏨+  4 +.11222⏨+  1 -.23527⏨+  1

PARAMETER VALUE                  +.29883⏨+  3 +.19222⏨+  1 -.11527⏨+  1

BOUNDARY CONSTRAINTS, JUMP+.5100630429897⏨-  0
COMPUTED RESIDUE (STAND.DEV.)    +.71050⏨+  1 +.40649⏨-  0
ESTIMATED RESIDUE (STAND.DEV.)   +.59974⏨+  1 +.37346⏨-  0
CORRECTIONS FOR PARAMETER        -.66368⏨+  3 +.57238⏨-  0 -.12000⏨+  1

PARAMETER VALUE                  +.93632⏨+  3 +.13724⏨+  1 -.00000⏨-  0
                                                                                          328    162    149
THE EQUATION WAS FOUND TO BE STIFF AT X =      +.16794⏨- 0
SOME LITTLE PROBLEMS WITH STIFFNESS      +.10000⏨+ 1

ITERATION NUMBER               +2
COMPUTED RESIDUE (STAND.DEV.)    +.14767⏨-  0 +.58602⏨-  1
ESTIMATED RESIDUE (STAND.DEV.)   +.27718⏨-  3 +.25389⏨-  2
CORRECTIONS FOR PARAMETER        +.38729⏨+  2 -.44803⏨-  0 +.93545⏨-  2

PARAMETER VALUE                  +.97505⏨+  3 +.92434⏨-  0 +.93545⏨-  2
                                                                                          189    102     94
THE EQUATION WAS FOUND TO BE STIFF AT X =      +.18076⏨- 0
SOME LITTLE PROBLEMS WITH STIFFNESS      +.10000⏨+ 1

ITERATION NUMBER               +3
COMPUTED RESIDUE (STAND.DEV.)    +.48038⏨-  2 +.10570⏨-  1
ESTIMATED RESIDUE (STAND.DEV.)   +.10903⏨-  5 +.15924⏨-  3
CORRECTIONS FOR PARAMETER        +.23473⏨+  2 +.63419⏨-  1 +.56504⏨-  3

PARAMETER VALUE                  +.99852⏨+  3 +.98776⏨-  0 +.99196⏨-  2
                                                                                          189     99     92
THE EQUATION WAS FOUND TO BE STIFF AT X =      +.13005⏨- 0
SOME LITTLE PROBLEMS WITH STIFFNESS      +.10000⏨+ 1

ITERATION NUMBER               +4
COMPUTED RESIDUE (STAND.DEV.)    +.87965⏨-  5 +.45229⏨-  3
ESTIMATED RESIDUE (STAND.DEV.)   +.97692⏨-  7 +.47664⏨-  4
CORRECTIONS FOR PARAMETER        +.16552⏨+  1 +.21989⏨-  2 +.67811⏨-  4

PARAMETER VALUE                  +.10002⏨+  4 +.98996⏨-  0 +.99874⏨-  2
                                                                                          162     85     78
THE EQUATION WAS FOUND TO BE STIFF AT X =      +.12673⏨- 0
SOME LITTLE PROBLEMS WITH STIFFNESS      +.10000⏨+ 1
```

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ITERATION NUMBER              +5
COMPUTED RESIDUE (STAND.DEV.)     +.17284⏨-  6 +.63399⏨-  4
ESTIMATED RESIDUE (STAND.DEV.)    +.78876⏨-  7 +.42829⏨-  4
CORRECTIONS FOR PARAMETER         +.71049⏨-  1 +.59385⏨-  5 +.10685⏨-  4

PARAMETER VALUE                   +.10002⏨+  4 +.98997⏨-  0 +.99981⏨-  2                 160     84     77

THE EQUATION WAS FOUND TO BE STIFF AT X =      +.12673⏨-  0
SOME LITTLE PROBLEMS WITH STIFFNESS     +.10000⏨+  1


ITERATION NUMBER              +6
COMPUTED RESIDUE (STAND.DEV.)     +.80423⏨-  7 +.43247⏨-  4
ESTIMATED RESIDUE (STAND.DEV.)    +.77181⏨-  7 +.42366⏨-  4
CORRECTIONS FOR PARAMETER         +.68692⏨-  2 -.42558⏨-  6 +.19919⏨-  5

PARAMETER VALUE                   +.10003⏨+  4 +.98997⏨-  0 +.10000⏨-  1                 160     84     77

THE EQUATION WAS FOUND TO BE STIFF AT X =      +.12672⏨-  0
SOME LITTLE PROBLEMS WITH STIFFNESS     +.10000⏨+  1


ITERATION NUMBER              +7
COMPUTED RESIDUE (STAND.DEV.)     +.77027⏨-  7 +.42324⏨-  4
ESTIMATED RESIDUE (STAND.DEV.)    +.76914⏨-  7 +.42293⏨-  4
CORRECTIONS FOR PARAMETER         +.74688⏨-  3 -.11067⏨-  6 +.37276⏨-  6

PARAMETER VALUE                   +.10003⏨+  4 +.98997⏨-  0 +.10000⏨-  1
CONFIDENCE INTERVAL (COND.)       +.35182⏨-  0 +.14758⏨-  3 +.53040⏨-  5
CONFIDENCE INTERVAL (INDEPT.)     +.37275⏨-  0 +.15651⏨-  3 +.53096⏨-  5

RELATIONSHIPS BETWEEN PARAMETERS
CORRELATION MATRIX                          COVARIANCE MATRIX
                                            +.60497⏨+  7 +.83833⏨+  3 -.26443⏨-  1
+.33004⏨-  0                                             +.10665⏨+  1 -.15708⏨-  2
-.30686⏨-  3 -.43414⏨-  1                                             +.12275⏨-  2

PRINCIPAL AXES (DIRECTION COSINES AND CONFIDENCE INTERVAL ALONG EACH AXIS)
-.22444⏨-  6 +.16512⏨-  2 +.10000⏨+  1      +.53040⏨-  5
+.13857⏨-  3 -.10000⏨+  1 +.16512⏨-  2      +.14774⏨-  3
+.10000⏨+  1 +.13857⏨-  3 -.43711⏨-  8      +.37275⏨-  0
```

```
THE EQUATION WAS FOUND TO BE STIFF AT X =        +.11394⏨-  0
SOME LITTLE PROBLEMS WITH STIFFNESS      +.10000⏨+  1

ITERATION NUMBER               +8
COMPUTED RESIDUE (STAND.DEV.)      +.57579⏨-  7 +.36593⏨-  4
ESTIMATED RESIDUE (STAND.DEV.)     +.39239⏨-  7 +.30208⏨-  4
CORRECTIONS FOR PARAMETER          -.28749⏨-  0 +.30690⏨-  4 -.38921⏨-  6

PARAMETER VALUE                    +.99997⏨+  3 +.99000⏨-  0 +.10000⏨-  1
CONFIDENCE INTERVAL (COND.)        +.25607⏨-  0 +.10540⏨-  3 +.37908⏨-  5
CONFIDENCE INTERVAL (INDEPT.)      +.27126⏨-  0 +.11175⏨-  3 +.37948⏨-  5

RELATIONSHIPS BETWEEN PARAMETERS
CORRELATION MATRIX                            COVARIANCE MATRIX
                                              +.62801⏨+  7 +.85279⏨+  3 -.28560⏨-  1
+.32962⏨-  0                                               +.10659⏨+  1 -.15691⏨-  2
-.32508⏨-  3 -.43352⏨-  1                                               +.12290⏨-  2

PRINCIPAL AXES (DIRECTION COSINES AND CONFIDENCE INTERVAL ALONG EACH AXIS)
-.21946⏨-  6 +.16496⏨-  2 +.10000⏨+  1     +.37908⏨-  5
+.13579⏨-  3 -.10000⏨+  1 +.16496⏨-  2     +.10551⏨-  3
+.10000⏨+  1 +.13579⏨-  3 -.45477⏨-  8     +.27126⏨-  0
```

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RESIDUALS, SPECIFIED FOR EACH OBSERVATION,

1	-.35018$_{10}$-4	2	-.48515$_{10}$-4
3	-.24118$_{10}$-4	4	-.28407$_{10}$-4
5	-.49451$_{10}$-4	6	-.84650$_{10}$-4
7	+.91730$_{10}$-6	8	-.14189$_{10}$-4
9	+.35006$_{10}$-4	10	-.77490$_{10}$-4
11	-.41823$_{10}$-4	12	-.66609$_{10}$-4
13	-.25959$_{10}$-4	14	-.85430$_{10}$-5
15	-.14997$_{10}$-4	16	-.23427$_{10}$-4
17	-.73200$_{10}$-5	18	-.36063$_{10}$-4
19	-.18458$_{10}$-5	20	-.34154$_{10}$-4
21	-.27884$_{10}$-5	22	+.40917$_{10}$-4
23	-.28382$_{10}$-5	24	-.35671$_{10}$-4
25	-.28931$_{10}$-5	26	-.12226$_{10}$-4
27	-.29617$_{10}$-5	28	+.20054$_{10}$-4
29	-.30339$_{10}$-5	30	+.50819$_{10}$-4
31	-.19363$_{10}$-4	32	-.32695$_{10}$-4
33	-.40349$_{10}$-4	34	-.80809$_{10}$-4
35	+.21362$_{10}$-4	36	+.32362$_{10}$-5
37	+.37013$_{10}$-4	38	-.30868$_{10}$-4
39	+.30840$_{10}$-4	40	+.10424$_{10}$-4
41	+.33316$_{10}$-7	42	+.26133$_{10}$-4
43	+.41227$_{10}$-4	44	+.14388$_{10}$-4
45	-.49611$_{10}$-4	46	-.26659$_{10}$-4

155 79 74

THE ENTIRE CALCULATION CONSUMED 131.72 SEC. ON THE EL X8.

```
PROCEDURE ODEPAREST WAS CALLED WITH THE PARAMETERS:
N     =              +2
NPAR  =              +3
NOBS  =              +23
ITMAX=               +16
CONVERGE =        +.1000000000001⏨-  1
EPS      =        +.9999999999999⏨-  4
MESHP=             +100
STIFF=             FALSE
FA    =           +.4940000000002⏨+  1
THE CONFIDENCE REGION AT LEVEL A IS PRINTED
FA IS THE A-POINT OF THE F-DISTIBUTION WITH NPAR AND NOBS-NPAR DEGREES OF FREEDOM


THE OBSERVATIONS WERE:
   I       TOBS(I)    COBS(I)    OBS(I)
   0     +.00000⏨-  0
   1     +.20000⏨-  3    +2    +.16480⏨-  0
   2     +.40000⏨-  3    +2    +.27530⏨-  0
   3     +.60000⏨-  3    +2    +.34930⏨-  0
   4     +.80000⏨-  3    +2    +.39900⏨-  0
   5     +.10000⏨-  2    +2    +.43220⏨-  0
   6     +.12000⏨-  2    +2    +.45450⏨-  0
   7     +.14000⏨-  2    +2    +.46950⏨-  0
   8     +.16000⏨-  2    +2    +.47950⏨-  0
   9     +.18000⏨-  2    +2    +.48620⏨-  0
  10     +.20000⏨-  2    +2    +.49070⏨-  0
  11     +.20000⏨-  1    +2    +.49990⏨-  0
  12     +.40000⏨-  1    +2    +.49980⏨-  0
  13     +.60000⏨-  1    +2    +.49980⏨-  0
  14     +.80000⏨-  1    +2    +.49980⏨-  0
  15     +.10000⏨-  0    +2    +.49980⏨-  0
  16     +.10000⏨+  1    +2    +.49860⏨-  0
  17     +.20000⏨+  1    +2    +.49730⏨-  0
  18     +.50000⏨+  1    +2    +.49360⏨-  0
  19     +.10000⏨+  2    +2    +.48720⏨-  0
  20     +.15000⏨+  2    +2    +.48080⏨-  0
  21     +.20000⏨+  2    +2    +.47430⏨-  0
  22     +.25000⏨+  2    +2    +.46770⏨-  0
  23     +.30000⏨+  2    +2    +.46100⏨-  0


THE PARAMETER ESTIMATES WERE:
   I    PARLWB(I)          PAR(I)           PARUPB(I)
   1 +.00000⏨-  0     +.16000⏨+  4     +.25000⏨+  4
   2 +.00000⏨-  0     +.80000⏨-  0     +.20000⏨+  1
   3 +.00000⏨-  0     +.12000⏨+  1     +.20000⏨+  1
```

```
                                                                              EVALUATIONS OF
                                                                              F      FY     FP

THE EQUATION WAS FOUND TO BE STIFF AT X =        +.11572⏨- 0
SOME LITTLE PROBLEMS WITH STIFFNESS     +.10000⏨+ 1


ITERATION NUMBER              +1
COMPUTED RESIDUE (STAND.DEV.)    +.17718⏨+ 1 +.29764⏨- 0
ESTIMATED RESIDUE (STAND.DEV.)   +.11735⏨+ 1 +.24223⏨- 0
CORRECTIONS FOR PARAMETER        -.12620⏨+ 4 +.18566⏨+ 1 -.30514⏨+ 1

PARAMETER VALUE                  +.33798⏨+ 3 +.26566⏨+ 1 -.18514⏨+ 1

BOUNDARY CONSTRAINTS,  JUMP+.3932632438264⏨- 0
COMPUTED RESIDUE (STAND.DEV.)    +.17718⏨+ 1 +.29764⏨- 0
ESTIMATED RESIDUE (STAND.DEV.)   +.12660⏨+ 1 +.25160⏨- 0
CORRECTIONS FOR PARAMETER        -.49631⏨+ 3 +.73015⏨- 0 -.12000⏨+ 1

PARAMETER VALUE                  +.11037⏨+ 4 +.15301⏨+ 1 +.18190⏨- 11      328    162    149

THE EQUATION WAS FOUND TO BE STIFF AT X =        +.46713⏨- 0
SOME LITTLE PROBLEMS WITH STIFFNESS     +.10000⏨+ 1


ITERATION NUMBER              +2
COMPUTED RESIDUE (STAND.DEV.)    +.16227⏨- 0 +.90075⏨- 1
ESTIMATED RESIDUE (STAND.DEV.)   +.48594⏨- 3 +.49292⏨- 2
CORRECTIONS FOR PARAMETER        -.19588⏨+ 3 -.66029⏨- 0 +.96919⏨- 2

PARAMETER VALUE                  +.90782⏨+ 3 +.86986⏨- 0 +.96919⏨- 2       189    101     93

THE EQUATION WAS FOUND TO BE STIFF AT X =        +.69112⏨- 0
SOME LITTLE PROBLEMS WITH STIFFNESS     +.10000⏨+ 1


ITERATION NUMBER              +3
COMPUTED RESIDUE (STAND.DEV.)    +.14980⏨- 1 +.27368⏨- 1
ESTIMATED RESIDUE (STAND.DEV.)   +.44831⏨- 5 +.47345⏨- 3
CORRECTIONS FOR PARAMETER        +.73926⏨+ 2 +.11379⏨- 0 +.25278⏨- 3

PARAMETER VALUE                  +.98174⏨+ 3 +.98365⏨- 0 +.99447⏨- 2       470    239    232

THE EQUATION WAS FOUND TO BE STIFF AT X =        +.14132⏨- 0
SOME LITTLE PROBLEMS WITH STIFFNESS     +.10000⏨+ 1


ITERATION NUMBER              +4
COMPUTED RESIDUE (STAND.DEV.)    +.67976⏨- 4 +.18436⏨- 2
ESTIMATED RESIDUE (STAND.DEV.)   +.21267⏨- 6 +.10312⏨- 3
CORRECTIONS FOR PARAMETER        +.16735⏨+ 2 +.62029⏨- 2 +.58868⏨- 4

PARAMETER VALUE                  +.99848⏨+ 3 +.98985⏨- 0 +.10004⏨- 1       168     88     81

THE EQUATION WAS FOUND TO BE STIFF AT X =        +.12996⏨- 0
SOME LITTLE PROBLEMS WITH STIFFNESS     +.10000⏨+ 1
```

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ITERATION NUMBER             +5
COMPUTED RESIDUE (STAND.DEV.)     +.50229_10-  6 +.15848_10-  3
ESTIMATED RESIDUE (STAND.DEV.)    +.56618_10-  7 +.53206_10-  4
CORRECTIONS FOR PARAMETER         +.16031_10+  1 +.89647_10-  4 +.27540_10-  6

PARAMETER VALUE                   +.10001_10+  4 +.98994_10-  0 +.10004_10-  1          162      85      78

THE EQUATION WAS FOUND TO BE STIFF AT X =     +.12674_10-  0
SOME LITTLE PROBLEMS WITH STIFFNESS     +.10000_10+  1


ITERATION NUMBER             +6
COMPUTED RESIDUE (STAND.DEV.)     +.63747_10-  7 +.56456_10-  4
ESTIMATED RESIDUE (STAND.DEV.)    +.59899_10-  7 +.54726_10-  4
CORRECTIONS FOR PARAMETER         +.15156_10-  0 +.12546_10-  4 -.85614_10-  6

PARAMETER VALUE                   +.10002_10+  4 +.98996_10-  0 +.10003_10-  1          160      84      77

THE EQUATION WAS FOUND TO BE STIFF AT X =     +.12673_10-  0
SOME LITTLE PROBLEMS WITH STIFFNESS     +.10000_10+  1


ITERATION NUMBER             +7
COMPUTED RESIDUE (STAND.DEV.)     +.60422_10-  7 +.54964_10-  4
ESTIMATED RESIDUE (STAND.DEV.)    +.60387_10-  7 +.54949_10-  4
CORRECTIONS FOR PARAMETER         +.13889_10-  1 +.11800_10-  5 -.23603_10-  6

PARAMETER VALUE                   +.10002_10+  4 +.98996_10-  0 +.10003_10-  1
CONFIDENCE INTERVAL (COND.)       +.49107_10-  0 +.20799_10-  3 +.25462_10-  4
CONFIDENCE INTERVAL (INDEPT.)     +.53434_10-  0 +.28756_10-  3 +.33211_10-  4

RELATIONSHIPS BETWEEN PARAMETERS
CORRELATION MATRIX                        COVARIANCE MATRIX
                                          +.63807_10+  7 +.13472_10+  4 -.88117_10+  2
+.39232_10-  J                                           +.18479_10+  1 -.13685_10-  0
-.22219_10-  J -.64123_10-  0                                           +.24649_10-  1

PRINCIPAL AXES (DIRECTION COSINES AND CONFIDENCE INTERVAL ALONG EACH AXIS)
-.23001_10-  5 +.76114_10-  1 +.99710_10-  0       +.25389_10-  4
+.21157_10-  3 -.99710_10-  0 +.76114_10-  1       +.26526_10-  3
+.10000_10+  1 +.21113_10-  3 -.13810_10-  4       +.53434_10-  0
```

THE EQUATION WAS FOUND TO BE STIFF AT X = +.11393$_{10}$- 0
SOME LITTLE PROBLEMS WITH STIFFNESS +.10000$_{10}$+ 1

ITERATION NUMBER	+8		
COMPUTED RESIDUE (STAND.DEV.)	+.40737$_{10}$- 7	+.45131$_{10}$- 4	
ESTIMATED RESIDUE (STAND.DEV.)	+.22182$_{10}$- 7	+.33303$_{10}$- 4	
CORRECTIONS FOR PARAMETER	-.27407$_{10}$- 0	+.49294$_{10}$- 4	-.37172$_{10}$- 5
PARAMETER VALUE	+.99997$_{10}$+ 3	+.99001$_{10}$- 0	+.99990$_{10}$- 2
CONFIDENCE INTERVAL (COND.)	+.30329$_{10}$- 0	+.12604$_{10}$- 3	+.15439$_{10}$- 4
CONFIDENCE INTERVAL (INDEPT.)	+.32990$_{10}$- 0	+.17410$_{10}$- 3	+.20122$_{10}$- 4

RELATIONSHIPS BETWEEN PARAMETERS

CORRELATION MATRIX

+.39160$_{10}$- 0	
-.22146$_{10}$- 0	-.64056$_{10}$- 0

COVARIANCE MATRIX

+.66216$_{10}$+ 7	+.13684$_{10}$+ 4	-.89446$_{10}$+ 2
	+.18440$_{10}$+ 1	-.13653$_{10}$- 0
		+.24635$_{10}$- 1

PRINCIPAL AXES (DIRECTION COSINES AND CONFIDENCE INTERVAL ALONG EACH AXIS)

-.22557$_{10}$- 5	+.76091$_{10}$- 1	+.99710$_{10}$- 0	+.15394$_{10}$- 4
+.20708$_{10}$- 3	-.99710$_{10}$- 0	+.76091$_{10}$- 1	+.16065$_{10}$- 3
+.10000$_{10}$+ 1	+.20665$_{10}$- 3	-.13508$_{10}$- 4	+.32990$_{10}$- 0

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RESIDUALS, SPECIFIED FOR EACH OBSERVATION}

1	-.47636$_{10}$-	4
2	-.27446$_{10}$-	4
3	-.83974$_{10}$-	4
4	-.13932$_{10}$-	4
5	-.77666$_{10}$-	4
6	-.67177$_{10}$-	4
7	-.94434$_{10}$-	5
8	-.24595$_{10}$-	4
9	-.37443$_{10}$-	4
10	-.33695$_{10}$-	4
11	+.30925$_{10}$-	4
12	-.37656$_{10}$-	4
13	-.14209$_{10}$-	4
14	+.10067$_{10}$-	4
15	+.40861$_{10}$-	4
16	-.34399$_{10}$-	4
17	-.82217$_{10}$-	4
18	+.27244$_{10}$-	5
19	-.29857$_{10}$-	4
20	+.12995$_{10}$-	4
21	+.30298$_{10}$-	4
22	+.20180$_{10}$-	4
23	-.19205$_{10}$-	4

155 79 74

THE ENTIRE CALCULATION CONSUMED 151,97 SEC. ON THE EL X8.

```
PROCEDURE ODEPAREST WAS CALLED WITH THE PARAMETERS:
N     =            +2
NPAR  =            +3
NOBS  =            +12
ITMAX=             +16
CONVERGE =      +.1000000000001⏨-  1
EPS      =      +.9999999999999⏨-  4
MESHP=             +100
STIFF=             FALSE
FA    =         +.3860000000001⏨+  1
THE CONFIDENCE REGION AT LEVEL A IS PRINTED
FA IS THE A-POINT OF THE F-DISTIBUTION WITH NPAR AND NOBS-NPAR DEGREES OF FREEDOM

THE OBSERVATIONS WERE:
   I      TOBS(I)     COBS(I)    OBS(I)
   0    +.00000⏨-  0
   1    +.20000⏨-  3    +2    +.16480⏨-  0
   2    +.60000⏨-  3    +2    +.34930⏨-  0
   3    +.10000⏨-  2    +2    +.43220⏨-  0
   4    +.14000⏨-  2    +2    +.46950⏨-  0
   5    +.18000⏨-  2    +2    +.48620⏨-  0
   6    +.20000⏨-  1    +2    +.49990⏨-  0
   7    +.60000⏨-  1    +2    +.49980⏨-  0
   8    +.10000⏨-  0    +2    +.49980⏨-  0
   9    +.20000⏨+  1    +2    +.49730⏨-  0
  10    +.10000⏨+  2    +2    +.48720⏨-  0
  11    +.20000⏨+  2    +2    +.47430⏨-  0
  12    +.30000⏨+  2    +2    +.46100⏨-  0

THE PARAMETER ESTIMATES WERE:
   I   PARLWB(I)          PAR(I)            PARUPB(I)
   1 +.00000⏨-  0    +.16000⏨+  4    +.25000⏨+  4
   2 +.00000⏨-  0    +.80000⏨-  0    +.20000⏨+  1
   3 +.00000⏨-  0    +.12000⏨+  1    +.20000⏨+  1
```

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                                                                                         EVALUATIONS OF
                                                                                         F       FY       FP

THE EQUATION WAS FOUND TO BE STIFF AT X =        +.10969⏨-  0
SOME LITTLE PROBLEMS WITH STIFFNESS     +.10000⏨+  1


ITERATION NUMBER               +1
COMPUTED RESIDUE (STAND,DEV.)    +.92495⏨-  0 +.32058⏨-  0
ESTIMATED RESIDUE (STAND,DEV.)   +.65942⏨-  0 +.27068⏨-  0
CORRECTIONS FOR PARAMETER        -.11607⏨+  4 +.14314⏨+  1 -.27008⏨+  1

PARAMETER VALUE                  +.43934⏨+  3 +.22314⏨+  1 -.15008⏨+  1

BOUNDARY CONSTRAINTS,  JUMP+.4443101165480⏨-  0
COMPUTED RESIDUE (STAND,DEV.)    +.92495⏨-  0 +.32058⏨-  0
ESTIMATED RESIDUE (STAND,DEV.)   +.71184⏨-  0 +.28124⏨-  0
CORRECTIONS FOR PARAMETER        -.51569⏨+  3 +.63597⏨-  0 -.12000⏨+  1

PARAMETER VALUE                  +.10843⏨+  4 +.14360⏨+  1 -.18190⏨- 11       316     157     144

THE EQUATION WAS FOUND TO BE STIFF AT X =        +.10620⏨-  0
SOME LITTLE PROBLEMS WITH STIFFNESS     +.10000⏨+  1


ITERATION NUMBER               +2
COMPUTED RESIDUE (STAND,DEV.)    +.58275⏨-  1 +.80467⏨-  1
ESTIMATED RESIDUE (STAND,DEV.)   +.18511⏨-  3 +.45352⏨-  2
CORRECTIONS FOR PARAMETER        -.14259⏨+  3 -.52644⏨-  0 +.83665⏨-  2

PARAMETER VALUE                  +.94172⏨+  3 +.90953⏨-  0 +.83665⏨-  2       127      68      60

THE EQUATION WAS FOUND TO BE STIFF AT X =        +.11552⏨-  0
SOME LITTLE PROBLEMS WITH STIFFNESS     +.10000⏨+  1


ITERATION NUMBER               +3
COMPUTED RESIDUE (STAND,DEV.)    +.40825⏨-  2 +.21298⏨-  1
ESTIMATED RESIDUE (STAND,DEV.)   +.21711⏨-  5 +.49115⏨-  3
CORRECTIONS FOR PARAMETER        +.48692⏨+  2 +.76334⏨-  1 +.12889⏨-  2

PARAMETER VALUE                  +.99041⏨+  3 +.98587⏨-  0 +.96554⏨-  2       115      60      57

THE EQUATION WAS FOUND TO BE STIFF AT X =        +.10938⏨-  0
SOME LITTLE PROBLEMS WITH STIFFNESS     +.10000⏨+  1


ITERATION NUMBER               +4
COMPUTED RESIDUE (STAND,DEV.)    +.21798⏨-  4 +.15563⏨-  2
ESTIMATED RESIDUE (STAND,DEV.)   +.47063⏨-  7 +.72313⏨-  4
CORRECTIONS FOR PARAMETER        +.87943⏨+  1 +.40871⏨-  2 +.26612⏨-  3

PARAMETER VALUE                  +.99921⏨+  3 +.98995⏨-  0 +.99215⏨-  2       131      68      61

THE EQUATION WAS FOUND TO BE STIFF AT X =        +.10926⏨-  0
SOME LITTLE PROBLEMS WITH STIFFNESS     +.10000⏨+  1
```

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ITERATION NUMBER                  +5
COMPUTED RESIDUE (STAND.DEV.)     +.30026⏨-  6 +.18265⏨-  3
ESTIMATED RESIDUE (STAND.DEV.)    +.12146⏨-  7 +.36737⏨-  4
CORRECTIONS FOR PARAMETER         +.93699⏨-  0 +.10383⏨-  3 +.58812⏨-  4

PARAMETER VALUE                   +.10001⏨+  4 +.99006⏨-  0 +.99803⏨-  2                  131     68     61

THE EQUATION WAS FOUND TO BE STIFF AT X =       +.10920⏨-  0
SOME LITTLE PROBLEMS WITH STIFFNESS     +.10000⏨+  1


ITERATION NUMBER                  +6
COMPUTED RESIDUE (STAND.DEV.)     +.24964⏨-  7 +.52667⏨-  4
ESTIMATED RESIDUE (STAND.DEV.)    +.12413⏨-  7 +.37139⏨-  4
CORRECTIONS FOR PARAMETER         +.10410⏨-  0 +.63844⏨-  5 +.14649⏨-  4

PARAMETER VALUE                   +.10002⏨+  4 +.99006⏨-  0 +.99949⏨-  2                  131     68     61

THE EQUATION WAS FOUND TO BE STIFF AT X =       +.10920⏨-  0
SOME LITTLE PROBLEMS WITH STIFFNESS     +.10000⏨+  1


ITERATION NUMBER                  +7
COMPUTED RESIDUE (STAND.DEV.)     +.13175⏨-  7 +.38260⏨-  4
ESTIMATED RESIDUE (STAND.DEV.)    +.12430⏨-  7 +.37163⏨-  4
CORRECTIONS FOR PARAMETER         +.12096⏨-  1 -.49038⏨-  6 +.37842⏨-  5

PARAMETER VALUE                   +.10003⏨+  4 +.99006⏨-  0 +.99987⏨-  2                  131     68     61

THE EQUATION WAS FOUND TO BE STIFF AT X =       +.10919⏨-  0
SOME LITTLE PROBLEMS WITH STIFFNESS     +.10000⏨+  1


ITERATION NUMBER                  +8
COMPUTED RESIDUE (STAND.DEV.)     +.12465⏨-  7 +.37216⏨-  4
ESTIMATED RESIDUE (STAND.DEV.)    +.12416⏨-  7 +.37142⏨-  4
CORRECTIONS FOR PARAMETER         +.15564⏨-  2 -.36539⏨-  6 +.99306⏨-  6

PARAMETER VALUE                   +.10003⏨+  4 +.99006⏨-  0 +.99997⏨-  2
CONFIDENCE INTERVAL (COND.)       +.40706⏨-  0 +.17383⏨-  3 +.17489⏨-  4
CONFIDENCE INTERVAL (INDEPT.)     +.43723⏨-  0 +.23291⏨-  3 +.22285⏨-  4

RELATIONSHIPS BETWEEN PARAMETERS
CORRELATION MATRIX                                COVARIANCE MATRIX
                                                  +.11967⏨+  8 +.23191⏨+  4 -.12316⏨+  3
+.36381⏨-  0                                                   +.33957⏨+  1 -.20121⏨-  0
-.20192⏨-  0 -.61929⏨-  0                                                   +.31088⏨-  1

PRINCIPAL AXES (DIRECTION COSINES AND CONFIDENCE INTERVAL ALONG EACH AXIS)
-.14473⏨-  5 +.60476⏨-  1 +.99817⏨-  0      +.17457⏨-  4
+.19407⏨-  5 -.99817⏨-  0 +.60476⏨-  1      +.21734⏨-  3
+.10000⏨+  1 +.19380⏨-  3 -.10292⏨-  4      +.43723⏨-  0
```

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170772- 10     8 13681.138 PHEMKER                12                                    00
                                                                           131    68    61

THE EQUATION WAS FOUND TO BE STIFF AT X =      +.11763⏨-  0
SOME LITTLE PROBLEMS WITH STIFFNESS      +.10000⏨+  1


ITERATION NUMBER                +9
COMPUTED RESIDUE (STAND.DEV.)    +.27909⏨-  7 +.55687⏨-  4
ESTIMATED RESIDUE (STAND.DEV.)   +.14187⏨-  7 +.39703⏨-  4
CORRECTIONS FOR PARAMETER        -.40836⏨-  0 -.92822⏨-  4 +.36651⏨-  5

PARAMETER VALUE                  +.99985⏨+  3 +.98997⏨-  0 +.10003⏨-  1
CONFIDENCE INTERVAL (COND.)      +.44179⏨-  0 +.18544⏨-  3 +.20321⏨-  4
CONFIDENCE INTERVAL (INDEPT.)    +.47480⏨-  0 +.25066⏨-  3 +.26121⏨-  4

RELATIONSHIPS BETWEEN PARAMETERS
CORRELATION MATRIX                          COVARIANCE MATRIX
                                            +.12350⏨+  8 +.23794⏨+  4 -.13852⏨+  3
+.30495⏨-  0                                             +.34419⏨+  1 -.22516⏨-  0
-.20387⏨-  0 -.62774⏨-  0                                             +.37379⏨-  1

PRINCIPAL AXES (DIRECTION COSINES AND CONFIDENCE INTERVAL ALONG EACH AXIS)
-.16944⏨-  5 +.66880⏨-  1 +.99776⏨-  0      +.20276⏨-  4
+.19298⏨-  3 -.99776⏨-  0 +.66880⏨-  1      +.23389⏨-  3
+.10000⏨+  1 +.19266⏨-  3 -.11216⏨-  4      +.47480⏨-  0
```

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RESIDUALS, SPECIFIED FOR EACH OBSERVATION,

1	-.48093$_{10}$- 4
2	-.78147$_{10}$- 4
3	-.64658$_{10}$- 4
4	+.87488$_{10}$- 5
5	-.16034$_{10}$- 4
6	+.63975$_{10}$- 4
7	+.16068$_{10}$- 4
8	+.71642$_{10}$- 4
9	-.57228$_{10}$- 4
10	-.10386$_{10}$- 4
11	+.45301$_{10}$- 4
12	-.74947$_{10}$- 5

147 75 72

THE ENTIRE CALCULATION CONSUMED 115.92 SEC. ON THE EL X8.

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170772-  8      B 13681.138 PHEMKER                                    9                                          00

PROCEDURE ODEPAREST WAS CALLED WITH THE PARAMETERS:
N      =            +2
NPAR  =             +3
NOBS  =            +12
ITMAX=             +16
CONVERGE =     +.1000000000001⏨-  1
EPS      =     +.9999999999999⏨-  4
MESHP=           +100
STIFF=           FALSE
FA    =        +.3860000000001⏨+  1
THE CONFIDENCE REGION AT LEVEL A IS PRINTED
FA IS THE A-POINT OF THE F-DISTIBUTION WITH NPAR AND NOBS-NPAR DEGREES OF FREEDOM


THE OBSERVATIONS WERE:
  I        TOBS(I)    COBS(I)     OBS(I)
  0     +.00000⏨-  0
  1     +.40000⏨-  1    +2    +.49980⏨-  0
  2     +.60000⏨-  1    +2    +.49980⏨-  0
  3     +.80000⏨-  1    +2    +.49980⏨-  0
  4     +.10000⏨-  0    +2    +.49980⏨-  0
  5     +.10000⏨+  1    +2    +.49860⏨-  0
  6     +.20000⏨+  1    +2    +.49730⏨-  0
  7     +.50000⏨+  1    +2    +.49360⏨-  0
  8     +.10000⏨+  2    +2    +.48720⏨-  0
  9     +.15000⏨+  2    +2    +.48080⏨-  0
 10     +.20000⏨+  2    +2    +.47430⏨-  0
 11     +.25000⏨+  2    +2    +.46770⏨-  0
 12     +.30000⏨+  2    +2    +.46100⏨-  0

THE PARAMETER ESTIMATES WERE:
  I    PARLWB(I)          PAR(I)            PARUPB(I)
  1 +.00000⏨-  0     +.10000⏨+  2     +.20000⏨+  4
  2 +.00000⏨-  0     +.50000⏨-  0     +.20000⏨+  1
  3 +.00000⏨-  0     +.50000⏨-  0     +.20000⏨+  1
```

```
                                                                                       EVALUATIONS OF
                                                                                       F       FY      FP

ITERATION NUMBER              +1
COMPUTED RESIDUE (STAND.DEV.)    +.13332⏨+  1 +.38488⏨-  0
ESTIMATED RESIDUE (STAND.DEV.)   +.93934⏨-  0 +.32307⏨-  0
CORRECTIONS FOR PARAMETER        +.10240⏨+  2 +.10058⏨+  1 -.63001⏨-  0

PARAMETER VALUE                  +.20240⏨+  2 +.15058⏨+  1 -.13001⏨-  0

BOUNDARY CONSTRAINTS,  JUMP+.7936380460351⏨-  0
COMPUTED RESIDUE (STAND.DEV.)    +.13332⏨+  1 +.38488⏨-  0
ESTIMATED RESIDUE (STAND.DEV.)   +.11874⏨+  1 +.36323⏨-  0
CORRECTIONS FOR PARAMETER        +.81267⏨+  1 +.79823⏨-  0 -.50000⏨-  0

PARAMETER VALUE                  +.18127⏨+  2 +.12982⏨+  1 -.22737⏨- 12             185     89      84

ITERATION NUMBER              +2
COMPUTED RESIDUE (STAND.DEV.)    +.71146⏨-  1 +.88911⏨-  1
ESTIMATED RESIDUE (STAND.DEV.)   +.36949⏨-  3 +.64074⏨-  2
CORRECTIONS FOR PARAMETER        +.13619⏨+  2 -.34389⏨-  0 +.10731⏨-  1

PARAMETER VALUE                  +.31746⏨+  2 +.95434⏨-  0 +.10731⏨-  1             477     239     234

THE EQUATION WAS FOUND TO BE STIFF AT X =        +.40000⏨-  3
SOME LITTLE PROBLEMS WITH STIFFNESS     +.20000⏨+  1

ITERATION NUMBER              +3
COMPUTED RESIDUE (STAND.DEV.)    +.14864⏨-  2 +.12851⏨-  1
ESTIMATED RESIDUE (STAND.DEV.)   +.20890⏨-  4 +.15235⏨-  2
CORRECTIONS FOR PARAMETER        +.11780⏨+  2 +.31567⏨-  1 -.92586⏨-  3

PARAMETER VALUE                  +.43526⏨+  2 +.98590⏨-  0 +.98050⏨-  2             154     79      76

THE EQUATION WAS FOUND TO BE STIFF AT X =        +.40000⏨-  3
SOME LITTLE PROBLEMS WITH STIFFNESS     +.20000⏨+  1

ITERATION NUMBER              +4
COMPUTED RESIDUE (STAND.DEV.)    +.32891⏨-  3 +.60453⏨-  2
ESTIMATED RESIDUE (STAND.DEV.)   +.70040⏨-  6 +.27897⏨-  3
CORRECTIONS FOR PARAMETER        +.13151⏨+  2 +.19592⏨-  2 +.62856⏨-  4

PARAMETER VALUE                  +.56677⏨+  2 +.98394⏨-  0 +.98678⏨-  2             144     75      73

THE EQUATION WAS FOUND TO BE STIFF AT X =        +.40000⏨-  3
SOME LITTLE PROBLEMS WITH STIFFNESS     +.20000⏨+  1
```

```
ITERATION NUMBER                    +5
COMPUTED RESIDUE (STAND.DEV.)    +.37965⏨-  4 +.20539⏨-  2
ESTIMATED RESIDUE (STAND.DEV.)   +.45848⏨-  7 +.71374⏨-  4
CORRECTIONS FOR PARAMETER        +.13034⏨+  2 +.26511⏨-  3 +.68927⏨-  4

PARAMETER VALUE                  +.69711⏨+  2 +.98421⏨-  0 +.99368⏨-  2          148    77    73

THE EQUATION WAS FOUND TO BE STIFF AT X =        +.40000⏨-  3
SOME LITTLE PROBLEMS WITH STIFFNESS      +.12000⏨+  2


ITERATION NUMBER                    +6
COMPUTED RESIDUE (STAND.DEV.)    +.47230⏨-  5 +.72442⏨-  3
ESTIMATED RESIDUE (STAND.DEV.)   +.15631⏨-  7 +.41674⏨-  4
CORRECTIONS FOR PARAMETER        +.15652⏨+  2 +.91192⏨-  3 +.28762⏨-  4

PARAMETER VALUE                  +.85363⏨+  2 +.98512⏨-  0 +.99655⏨-  2          140    72    70

THE EQUATION WAS FOUND TO BE STIFF AT X =        +.40000⏨-  3
SOME LITTLE PROBLEMS WITH STIFFNESS      +.12000⏨+  2


ITERATION NUMBER                    +7
COMPUTED RESIDUE (STAND.DEV.)    +.48319⏨-  6 +.23171⏨-  3
ESTIMATED RESIDUE (STAND.DEV.)   +.10383⏨-  7 +.33966⏨-  4
CORRECTIONS FOR PARAMETER        +.15148⏨+  2 +.68799⏨-  3 +.75665⏨-  5

PARAMETER VALUE                  +.10051⏨+  3 +.98581⏨-  0 +.99731⏨-  2          169    87    79

THE EQUATION WAS FOUND TO BE STIFF AT X =        +.40000⏨-  3
SOME LITTLE PROBLEMS WITH STIFFNESS      +.22000⏨+  2


ITERATION NUMBER                    +8
COMPUTED RESIDUE (STAND.DEV.)    +.64722⏨-  7 +.84801⏨-  4
ESTIMATED RESIDUE (STAND.DEV.)   +.15466⏨-  7 +.41454⏨-  4
CORRECTIONS FOR PARAMETER        +.10587⏨+  2 +.32942⏨-  3 +.39064⏨-  5

PARAMETER VALUE                  +.11110⏨+  3 +.98614⏨-  0 +.99770⏨-  2          158    81    76

THE EQUATION WAS FOUND TO BE STIFF AT X =        +.40000⏨-  3
SOME LITTLE PROBLEMS WITH STIFFNESS      +.22000⏨+  2


ITERATION NUMBER                    +9
COMPUTED RESIDUE (STAND.DEV.)    +.18350⏨-  7 +.45155⏨-  4
ESTIMATED RESIDUE (STAND.DEV.)   +.14919⏨-  7 +.40715⏨-  4
CORRECTIONS FOR PARAMETER        +.55563⏨+  1 +.16825⏨-  3 +.10748⏨-  5

PARAMETER VALUE                  +.11665⏨+  3 +.98631⏨-  0 +.99781⏨-  2          155    80    76

THE EQUATION WAS FOUND TO BE STIFF AT X =        +.40000⏨-  3
SOME LITTLE PROBLEMS WITH STIFFNESS      +.22000⏨+  2
```

```
ITERATION NUMBER              +10
COMPUTED RESIDUE (STAND,DEV.)    +.14573⏨-  7 +.40240⏨-  4
ESTIMATED RESIDUE (STAND,DEV.)   +.14462⏨-  7 +.40086⏨-  4
CORRECTIONS FOR PARAMETER        -.11656⏨-  0 -.18476⏨-  4 +.22602⏨-  6

PARAMETER VALUE                  +.11654⏨+  3 +.98629⏨-  0 +.99783⏨-  2
CONFIDENCE INTERVAL (COND.)      +.42130⏨+  1 +.16229⏨-  3 +.16557⏨-  4
CONFIDENCE INTERVAL (INDEPT.)    +.54661⏨+  2 +.21016⏨-  2 +.23138⏨-  4

RELATIONSHIPS BETWEEN PARAMETERS
CORRELATION MATRIX                          COVARIANCE MATRIX
                                            +.16057⏨+ 12 +.61377⏨+  7 +.42263⏨+  4
+.99418⏨-  0                                             +.23737⏨+  3 -.34272⏨-  1
+.62182⏨-  1 -.13115⏨-  1                                             +.28770⏨-  1

PRINCIPAL AXES (DIRECTION COSINES AND CONFIDENCE INTERVAL ALONG EACH AXIS)
-.27524⏨-  5 +.71319⏨-  1 +.99745⏨-  0      +.16515⏨-  4
+.38126⏨-  4 -.99745⏨-  0 +.71319⏨-  1      +.22693⏨-  3
+.10000⏨+  1 +.38225⏨-  4 +.26321⏨-  7      +.54661⏨+  2
```

```
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                                                                                              156     80     76

THE EQUATION WAS FOUND TO BE STIFF AT X =        +.40000⏨-  3
SOME LITTLE PROBLEMS WITH STIFFNESS      +.52000⏨+  2

ITERATION NUMBER              +11
COMPUTED RESIDUE (STAND.DEV.)    +.12301⏨-  7 +.36970⏨-  4
ESTIMATED RESIDUE (STAND.DEV.)   +.11350⏨-  7 +.35513⏨-  4
CORRECTIONS FOR PARAMETER        +.73885⏨+  1 +.25030⏨-  3 +.22481⏨-  5

PARAMETER VALUE                  +.12393⏨+  3 +.98654⏨-  0 +.99806⏨-  2
CONFIDENCE INTERVAL (COND.)      +.37436⏨+  1 +.14387⏨-  3 +.14446⏨-  4
CONFIDENCE INTERVAL (INDEPT.)    +.38757⏨+  2 +.15053⏨-  2 +.20256⏨-  4

RELATIONSHIPS BETWEEN PARAMETERS
CORRELATION MATRIX                           COVARIANCE MATRIX
                                             +.10285⏨+ 12 +.39590⏨+  7 -.35743⏨+  4
+.99102⏨-  0                                              +.15516⏨+  3 -.33241⏨-  0
-.66491⏨-  1 -.15921⏨-  0                                              +.28096⏨-  1

PRINCIPAL AXES (DIRECTION COSINES AND CONFIDENCE INTERVAL ALONG EACH AXIS)
-.26757⏨-  5 +.70414⏨-  1 +.99752⏨-  0       +.14410⏨-  4
+.38399⏨-  4 -.99752⏨-  0 +.70414⏨-  1       +.20178⏨-  3
+.10000⏨+  1 +.38492⏨-  4 -.34752⏨-  7       +.38757⏨+  2
```

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```
RESIDUALS, SPECIFIED FOR EACH OBSERVATION;
   1    +.29508⏨- 4
   2    +.38775⏨- 5
   3    +.28449⏨- 4
   4    +.53371⏨- 4
   5    -.20235⏨- 4
   6    -.66102⏨- 4
   7    +.15118⏨- 4
   8    -.21777⏨- 4
   9    +.16383⏨- 4
  10    +.28219⏨- 4
  11    +.12223⏨- 4
  12    -.32582⏨- 4
```

211 110 105

THE ENTIRE CALCULATION CONSUMED 171.93 SEC. ON THE EL X8.

```
PROCEDURE ODEPAREST WAS CALLED WITH THE PARAMETERS:
N     =             +2
NPAR  =             +3
NOBS  =            +12
ITMAX=              +9
CONVERGE =      +.1000000000001⏨-  1
EPS      =      +.9999999999999⏨-  4
MESHP=            +100
STIFF=            FALSE
FA    =         +.3860000000001⏨+  1
THE CONFIDENCE REGION AT LEVEL A IS PRINTED
FA IS THE A-POINT OF THE F-DISTIBUTION WITH NPAR AND NOBS-NPAR DEGREES OF FREEDOM

THE OBSERVATIONS WERE:
   I       TOBS(I)    COBS(I)     OBS(I)
   0    +.00000⏨-  0
   1    +.20000⏨-  3    +2    +.16480⏨-  0
   2    +.40000⏨-  3    +2    +.27530⏨-  0
   3    +.60000⏨-  3    +2    +.34930⏨-  0
   4    +.80000⏨-  3    +2    +.39900⏨-  0
   5    +.10000⏨-  2    +2    +.43220⏨-  0
   6    +.12000⏨-  2    +2    +.45450⏨-  0
   7    +.14000⏨-  2    +2    +.46950⏨-  0
   8    +.16000⏨-  2    +2    +.47950⏨-  0
   9    +.18000⏨-  2    +2    +.48620⏨-  0
  10    +.20000⏨-  2    +2    +.49070⏨-  0
  11    +.20000⏨-  1    +2    +.49990⏨-  0
  12    +.40000⏨-  1    +2    +.49980⏨-  0

THE PARAMETER ESTIMATES WERE:
   I    PARLWB(I)          PAR(I)            PARUPB(I)
   1 +.00000⏨-  0    +.10000⏨+  2    +.20000⏨+  4
   2 +.00000⏨-  0    +.50000⏨-  0    +.20000⏨+  1
   3 +.00000⏨-  0    +.50000⏨-  0    +.20000⏨+  1
```

```
                                                                                             EVALUATIONS OF
                                                                                             F      FY     FP

ITERATION NUMBER          +1
COMPUTED RESIDUE (STAND.DEV.)   +.17749⏨+ 1 +.44409⏨- 0
ESTIMATED RESIDUE (STAND.DEV.)  +.55124⏨- 1 +.78261⏨- 1
CORRECTIONS FOR PARAMETER       +.31497⏨+ 3 +.20610⏨+ 5 -.20182⏨+ 5

PARAMETER VALUE                 +.32497⏨+ 3 +.20611⏨+ 5 -.20181⏨+ 5

BOUNDARY CONSTRAINTS,  JUMP+.2477474026819⏨- 4
COMPUTED RESIDUE (STAND.DEV.)   +.17749⏨+ 1 +.44409⏨- 0
ESTIMATED RESIDUE (STAND.DEV.)  +.55124⏨- 1 +.78261⏨- 1
CORRECTIONS FOR PARAMETER       +.78033⏨- 2 +.51061⏨- 0 -.50000⏨- 0

PARAMETER VALUE                 +.10008⏨+ 2 +.10106⏨+ 1 -.00000⏨- 0          33     24     23

ITERATION NUMBER          +2
COMPUTED RESIDUE (STAND.DEV.)   +.17749⏨+ 1 +.44409⏨- 0
ESTIMATED RESIDUE (STAND.DEV.)  +.55107⏨- 1 +.78250⏨- 1
CORRECTIONS FOR PARAMETER       +.31500⏨+ 3 +.20596⏨+ 5 -.20168⏨+ 5

PARAMETER VALUE                 +.32501⏨+ 3 +.20597⏨+ 5 -.20168⏨+ 5

PLUS ULTRA                -0
COMPUTED RESIDUE (STAND.DEV.)   +.17749⏨+ 1 +.44409⏨- 0
ESTIMATED RESIDUE (STAND.DEV.)  +.55107⏨- 1 +.78250⏨- 1
CORRECTIONS FOR PARAMETER       +.31500⏨+ 3 +.20596⏨+ 5 -.20168⏨+ 5

PARAMETER VALUE                 +.32501⏨+ 3 +.20000⏨+ 1 +.00000⏨- 0          33     24     23

ITERATION NUMBER          +3
COMPUTED RESIDUE (STAND.DEV.)   +.46667⏨- 0 +.22771⏨- 0
ESTIMATED RESIDUE (STAND.DEV.)  +.67799⏨- 3 +.86794⏨- 2
CORRECTIONS FOR PARAMETER       +.43920⏨+ 3 +.81988⏨+ 1 -.93965⏨+ 1

PARAMETER VALUE                 +.76421⏨+ 3 +.10199⏨+ 2 -.93965⏨+ 1

PLUS ULTRA                -0
COMPUTED RESIDUE (STAND.DEV.)   +.46667⏨- 0 +.22771⏨- 0
ESTIMATED RESIDUE (STAND.DEV.)  +.67799⏨- 3 +.86794⏨- 2
CORRECTIONS FOR PARAMETER       +.43920⏨+ 3 +.81988⏨+ 1 -.93965⏨+ 1

PARAMETER VALUE                 +.76421⏨+ 3 +.20000⏨+ 1 +.00000⏨- 0          70     37     36

ITERATION NUMBER          +4
COMPUTED RESIDUE (STAND.DEV.)   +.22241⏨- 0 +.15720⏨- 0
ESTIMATED RESIDUE (STAND.DEV.)  +.12114⏨- 4 +.11602⏨- 2
CORRECTIONS FOR PARAMETER       +.17156⏨+ 3 -.12622⏨+ 1 -.23002⏨- 0

PARAMETER VALUE                 +.93577⏨+ 3 +.73783⏨- 0 -.23002⏨- 0
```

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PLUS ULTRA                   -0
COMPUTED RESIDUE (STAND,DEV,)    +,22241⏨-  0 +,15720⏨-  0
ESTIMATED RESIDUE (STAND,DEV,)   +,12114⏨-  4 +,11602⏨-  2
CORRECTIONS FOR PARAMETER        +,17156⏨+  3 -,12622⏨+  1 -,23002⏨-  0

PARAMETER VALUE                  +,93577⏨+  3 +,73783⏨-  0 +,00000⏨-  0            71    37    36


ITERATION NUMBER                +5
COMPUTED RESIDUE (STAND,DEV,)    +,26571⏨-  1 +,54336⏨-  1
ESTIMATED RESIDUE (STAND,DEV,)   +,83682⏨-  5 +,96426⏨-  3
CORRECTIONS FOR PARAMETER        +,52095⏨+  2 +,81563⏨-  0 -,57725⏨-  0

PARAMETER VALUE                  +,98786⏨+  3 +,15535⏨+  1 -,57725⏨-  0

PLUS ULTRA                   -0
COMPUTED RESIDUE (STAND,DEV,)    +,26571⏨-  1 +,54336⏨-  1
ESTIMATED RESIDUE (STAND,DEV,)   +,83682⏨-  5 +,96426⏨-  3
CORRECTIONS FOR PARAMETER        +,52095⏨+  2 +,81563⏨-  0 -,57725⏨-  0

PARAMETER VALUE                  +,98786⏨+  3 +,15535⏨+  1 +,00000⏨-  0            83    43    42


STEEPEST DESCENT+,1724278651036⏨+  1
COMPUTED RESIDUE (STAND,DEV,)    +,78790⏨-  1 +,93565⏨-  1
ESTIMATED RESIDUE (STAND,DEV,)   +,00000⏨-  0 +,00000⏨-  0
CORRECTIONS FOR PARAMETER        +,22507⏨-  0 +,32972⏨-  2 -,15959⏨+  1

PARAMETER VALUE                  +,93599⏨+  3 +,74113⏨-  0 -,10187⏨+  1

BOUNDARY CONSTRAINTS,   JUMP+,3617034401022⏨-  0
COMPUTED RESIDUE (STAND,DEV,)    +,78790⏨-  1 +,93565⏨-  1
ESTIMATED RESIDUE (STAND,DEV,)   +,10308⏨-  1 +,33843⏨-  1
CORRECTIONS FOR PARAMETER        +,81409⏨-  1 +,11926⏨-  2 -,57725⏨-  0

PARAMETER VALUE                  +,93585⏨+  3 +,73902⏨-  0 -,00000⏨-  0           107    54    51


ITERATION NUMBER                +7
COMPUTED RESIDUE (STAND,DEV,)    +,26290⏨-  1 +,54048⏨-  1
ESTIMATED RESIDUE (STAND,DEV,)   +,82542⏨-  5 +,95767⏨-  3
CORRECTIONS FOR PARAMETER        +,52066⏨+  2 +,80885⏨-  0 -,57145⏨-  0

PARAMETER VALUE                  +,98791⏨+  3 +,15479⏨+  1 -,57145⏨-  0

PLUS ULTRA                   -0
COMPUTED RESIDUE (STAND,DEV,)    +,26290⏨-  1 +,54048⏨-  1
ESTIMATED RESIDUE (STAND,DEV,)   +,82542⏨-  5 +,95767⏨-  3
CORRECTIONS FOR PARAMETER        +,52066⏨+  2 +,80885⏨-  0 -,57145⏨-  0

PARAMETER VALUE                  +,98791⏨+  3 +,15479⏨+  1 +,00000⏨-  0            83    43    42
```

```
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STEEPEST DESCENT+.1728280197774⏨+  1
COMPUTED RESIDUE (STAND.DEV.)     +.77513⏨-  1 +.92804⏨-  1
ESTIMATED RESIDUE (STAND.DEV.)    +.00000⏨-  0 +.00000⏨-  0
CORRECTIONS FOR PARAMETER         +.22614⏨-  0 +.31859⏨-  2 -.15917⏨+  1

PARAMETER VALUE                   +.93607⏨+  3 +.74221⏨-  0 -.10202⏨+  1

BOUNDARY CONSTRAINTS,  JUMP+.3590277575213⏨-  0
COMPUTED RESIDUE (STAND.DEV.)     +.77513⏨-  1 +.92804⏨-  1
ESTIMATED RESIDUE (STAND.DEV.)    +.99915⏨-  2 +.33319⏨-  1
CORRECTIONS FOR PARAMETER         +.81189⏨-  1 +.11438⏨-  2 -.57145⏨-  0

PARAMETER VALUE                   +.93593⏨+  3 +.74017⏨-  0 -.00000⏨-  0
CONFIDENCE INTERVAL (COND.)       +.20830⏨-  0 +.64131⏨+  1 +.10787⏨+  2
CONFIDENCE INTERVAL (INDEPT.)     +.20915⏨-  0 +.11173⏨+  2 +.18793⏨+  2

RELATIONSHIPS BETWEEN PARAMETERS
CORRELATION MATRIX                           COVARIANCE MATRIX
                                             +.34026⏨+  1 +.15611⏨+  2 +.26143⏨+  2
+.85885⏨-  1                                              +.97104⏨+  4 +.13372⏨+  5
+.85504⏨-  1 +.81871⏨-  0                                              +.27473⏨+  5

PRINCIPAL AXES (DIRECTION COSINES AND CONFIDENCE INTERVAL ALONG EACH AXIS)
+.55306⏨-  3 +.88127⏨-  0 -.47262⏨-  0       +.57131⏨+  1
+.87805⏨-  3 +.47262⏨-  0 +.88127⏨-  0       +.21104⏨+  2
+.10000⏨+  1 -.90237⏨-  3 -.51241⏨-  3       +.20830⏨-  0
```

```
ITERATION NUMBER              +9
COMPUTED RESIDUE (STAND.DEV.)    +.26038⏨- 1 +.53788⏨- 1
ESTIMATED RESIDUE (STAND.DEV.)   +.50102⏨- 5 +.74612⏨- 3
CORRECTIONS FOR PARAMETER        +.50012⏨+ 2 +.73464⏨- 0 -.50023⏨- 0

PARAMETER VALUE                  +.98594⏨+ 3 +.14748⏨+ 1 -.50023⏨- 0

PLUS ULTRA              -0
COMPUTED RESIDUE (STAND.DEV.)    +.26038⏨- 1 +.53788⏨- 1
ESTIMATED RESIDUE (STAND.DEV.)   +.50102⏨- 5 +.74612⏨- 3
CORRECTIONS FOR PARAMETER        +.50012⏨+ 2 +.73464⏨- 0 -.50023⏨- 0

PARAMETER VALUE                  +.98594⏨+ 3 +.14748⏨+ 1 +.00000⏨- 0
CONFIDENCE INTERVAL (COND.)      +.44407⏨+ 1 +.33383⏨- 2 +.33192⏨- 2
CONFIDENCE INTERVAL (INDEPT.)    +.62234⏨+ 1 +.51518⏨- 0 +.51090⏨- 0

RELATIONSHIPS BETWEEN PARAMETERS
CORRELATION MATRIX                         COVARIANCE MATRIX
                                           +.60081⏨+ 7 +.24877⏨+ 6 -.24479⏨+ 6
+.50019⏨- 0                                            +.41171⏨+ 5 -.40828⏨+ 5
-.49631⏨- 0 -.99997⏨- 0                                            +.40490⏨+ 5

PRINCIPAL AXES (DIRECTION COSINES AND CONFIDENCE INTERVAL ALONG EACH AXIS)
-.30110⏨- 3 +.70507⏨- 0 +.70914⏨- 0     +.23538⏨- 2
+.58788⏨- 1 -.70790⏨- 0 +.70386⏨- 0     +.62800⏨- 0
+.99827⏨- 0 +.41901⏨- 1 -.41236⏨- 1     +.62340⏨+ 1
```

```
170772-  5      B 13681.138 PHEMKER.                    14                                                          00

RESIDUALS, SPECIFIED FOR EACH OBSERVATION;
   1      +.50671⏨-  2
   2      +.22413⏨-  3
   3      -.90022⏨-  2
   4      -.19413⏨-  1
   5      -.29608⏨-  1
   6      -.38639⏨-  1
   7      -.46255⏨-  1
   8      -.52587⏨-  1
   9      -.57679⏨-  1
  10      -.61692⏨-  1
  11      -.74608⏨-  1
  12      -.74706⏨-  1
                                                                                               107      54      53

THE ENTIRE CALCULATION CONSUMED  63.87 SEC. ON THE EL X8.
```

6.2. Bellman's problem

This test problem is taken from an example given in an article by Bellman c.s. [1967]. It originates from a chemical experiment on the reaction

$$2\ NO + O_2 \rightleftarrows 2NO_2$$

reported by Bodonstein [1922].
The differential equation reads

$$dy/dt = p(126.2-y)\ (91.9-y)^2 - q\ y^2\ .$$

The parameters p and q have to be determined from 14 given observations.

Bellman reports as parameter values and computed residue (apart from a printing error in his article)

$$p = .4577_{10} - 5$$

$$q = .2793_{10} - 5$$

$$s = 22.7$$

We note that the 1% confidence regions are

$$\delta p = .31_{10} - 6 \quad \text{and} \quad \delta q = .48_{10} - 3\ .$$

Our algorithm finds respectively

$$p = .44_{10} - 5 \qquad \delta p = .30_{10} - 6$$

$$q = .23_{10} - 3 \qquad \delta p = .43_{10} - 3$$

$$s = 25.12$$

The computed residue is slightly greater but the difference is by no means important.

B13681.138,PHEMKER,T150

```
BEGIN COMMENT BELLMAN'S PROBLEM, SEE: MATH.BIOSC. 1(67)71 ;

        PROC ODEPAREST(N,NOBS,NPAR,DATA,ITMAX,CONVERGE,EPS,MESHP,STIFF,FA);
        VAL N,NOBS,NPAR,ITMAX,CONVERGE,EPS,MESHP,STIFF,FA;
        INT N,NOBS,NPAR,ITMAX,MESHP; REAL CONVERGE,EPS,FA; BOOL STIFF;
        BEGIN COMMENT THE PROCEDURES: CALL YSTART,CALL F,CALL FY,CALL FP
                DEFINE THE PROBLEM SUPPLIED BY THE USER;

                PROC CALL YSTART;
                BEGIN Y[0,1]:= 0; YMAX[1]:= 50; OUTC
                END;
                PROC CALL F(R); VAL R; REAL R;
                BEGIN CF:= CF+1; F[1]:= R*(PAR[1]*(126.2-Y[0,1]) * (91.9-Y[0,1])↑2
                                -PAR[2]*Y[0,1]↑2    )
                END;
                PROC CALL FY(R); VAL R; REAL R;
                BEGIN FY[1,1]:= R*(
                        -PAR[1]*(-91.9*344.3 + 620.0*Y[0,1] -3*Y[0,1]↑2)
                        -PAR[2]*Y[0,1]↑2        ));
                        CFY:= CFY+1;
                END;
                PROC CALL FP(R); VAL R; REAL R;
                BEGIN FP[1,1]:= R*(126.2-Y[0,1])*(91.1-Y[0,1])↑2 ;
                      FP[1,2]:=-R*Y[0,1]↑2; CFP:= CFP+1
                END;

        ARRAY Y[0:7,1:N*(NPAR+1)],YMAX,F[1:N],FY[1:N,1:N],FP[1:N,1:NPAR];
        PROC PR(S); BEGIN NLCR; PRINTTEXT(S) END;
        PROC FL(R); FLOT(5,3,R);
        PROC PF(S,R); BEGIN PR(S); TAB; FL(R) END;

        PROC OUT(S,R); STRING S; REAL R;
        BEGIN INT I; IF LINENUMBER>50 THEN NEW PAGE ELSE NLCR;
                PR(S); PRINT(R);
                PF(≮COMPUTED RESIDUE (STAND.DEV.)≯,COMP ERROR);
                FL(SQRT(COMP ERROR/(NOBS-NPAR)));
                PF(≮ESTIMATED RESIDUE (STAND.DEV.)≯,EST ERROR);
                FL(SQRT(EST ERROR/(NOBS-NPAR)));
                PR(≮CORRECTIONS FOR PARAMETER≯): TAB;
                FOR I:=1 STEP 1 UNTIL NPAR DO FL(DELTA PAR[I]); NLCR;
                PR(≮PARAMETER VALUE≯); TAB; TAB;
                FOR I:= 1 STEP 1 UNTIL NPAR DO FL(PAR[I]);
        END;

        BOOL FIRST,ADAMS; INTEGER K,KOLD,SAME,FAILS;
        REAL X,XOLD,H,CH,HOLD,TOLCONV,TOLUP,TOL,TOLDWN,A0;
        ARRAY A[0:7],DD[0:7,0:N],LAST DELTA[1:N], JAC[1:N,1:N],CONST[1:45],
                TOBS[0:NOBS],OBS[1:NOBS],PARL,PAR,PARU[1:NPAR];
        INT ARRAY COBS[1:NOBS],PP[1:N];

        PROC MULTISTEP(XEND,HMIN,HMAX,EPS);
        VALUE XEND,HMIN,HMAX,EPS; REAL XEND,HMIN,HMAX,EPS;

        BEGIN BOOLEAN CONV; INTEGER I,J,L,KNEW,NP;
              REAL CHNEW,C,ERROR,DFI; ARRAY DELTA,DF,Y0[1:N];
```

```
280772-171      B 13681.138 PHEMKER                    9                                  00

PROCEDURE ODEPAREST WAS CALLED WITH THE PARAMETERS:
N     =               +1
NPAR  =               +2
NOBS  =              +14
ITMAX=               +14
CONVERGE =      +.1999999999999⏨-  2
EPS      =      +.9999999999996⏨-  5
MESHP=             +100
STIFF=             FALSE
FA   =          +.6930000000000⏨+  1
THE CONFIDENCE REGION AT LEVEL A IS PRINTED
FA IS THE A-POINT OF THE F-DISTIBUTION WITH NPAR AND NOBS-NPAR DEGREES OF FREEDOM


THE OBSERVATIONS WERE:
   I      TOBS(I)    COBS(I)   OBS(I)
   0   +.10000⏨+  1
   1   +.20000⏨+  1    +1   +.14000⏨+  1
   2   +.30000⏨+  1    +1   +.63000⏨+  1
   3   +.40000⏨+  1    +1   +.10400⏨+  2
   4   +.50000⏨+  1    +1   +.14200⏨+  2
   5   +.60000⏨+  1    +1   +.17600⏨+  2
   6   +.70000⏨+  1    +1   +.21400⏨+  2
   7   +.80000⏨+  1    +1   +.23000⏨+  2
   8   +.10000⏨+  2    +1   +.27000⏨+  2
   9   +.12000⏨+  2    +1   +.30400⏨+  2
  10   +.15000⏨+  2    +1   +.34400⏨+  2
  11   +.20000⏨+  2    +1   +.38800⏨+  2
  12   +.25000⏨+  2    +1   +.41600⏨+  2
  13   +.30000⏨+  2    +1   +.43500⏨+  2
  14   +.40000⏨+  2    +1   +.45300⏨+  2

THE PARAMETER ESTIMATES WERE:
   I   PARLWB(I)         PAR(I)          PARUPB(I)
   1 +.00000⏨-  0    +.10000⏨-  5    +.10000⏨-  2
   2 +.00000⏨-  0    +.10000⏨-  3    +.10000⏨-  1
```

```
                                                                        EVALUATIONS OF
                                                                        F      FY     FP

ITERATION NUMBER                  +1
COMPUTED RESIDUE (STAND.DEV.)    +.40843⏨+ 4 +.18449⏨+ 2
ESTIMATED RESIDUE (STAND.DEV.)   +.13275⏨+ 3 +.33261⏨+ 1
CORRECTIONS FOR PARAMETER        +.14831⏨- 5 +.18734⏨- 2

PARAMETER VALUE                  +.24831⏨- 5 +.19734⏨- 2
                                                                        43     24     23

ITERATION NUMBER                  +2
COMPUTED RESIDUE (STAND.DEV.)    +.21964⏨+ 4 +.13529⏨+ 2
ESTIMATED RESIDUE (STAND.DEV.)   +.10301⏨+ 3 +.29299⏨+ 1
CORRECTIONS FOR PARAMETER        -.69354⏨- 7 -.30568⏨- 1

PARAMETER VALUE                  +.24138⏨- 5 -.28595⏨- 1

BOUNDARY CONSTRAINTS,  JUMP+.6455684411230⏨-  1
COMPUTED RESIDUE (STAND.DEV.)    +.21964⏨+ 4 +.13529⏨+ 2
ESTIMATED RESIDUE (STAND.DEV.)   +.11174⏨+ 3 +.30515⏨+ 1
CORRECTIONS FOR PARAMETER        -.44773⏨- 8 -.19734⏨- 2

PARAMETER VALUE                  +.24786⏨- 5 -.00000⏨- 0
                                                                        133    78     64

ITERATION NUMBER                  +3
COMPUTED RESIDUE (STAND.DEV.)    +.70601⏨+ 3 +.76704⏨+ 1
ESTIMATED RESIDUE (STAND.DEV.)   +.60001⏨+ 2 +.22361⏨+ 1
CORRECTIONS FOR PARAMETER        +.70689⏨- 6 +.70937⏨- 3

PARAMETER VALUE                  +.31855⏨- 5 +.70937⏨- 3
                                                                        68     30     29

ITERATION NUMBER                  +4
COMPUTED RESIDUE (STAND.DEV.)    +.65954⏨+ 3 +.74136⏨+ 1
ESTIMATED RESIDUE (STAND.DEV.)   +.17928⏨+ 2 +.12223⏨+ 1
CORRECTIONS FOR PARAMETER        +.21550⏨- 6 -.60068⏨- 2

PARAMETER VALUE                  +.34010⏨- 5 -.52974⏨- 2

BOUNDARY CONSTRAINTS,  JUMP+.1180947078510⏨-  0
COMPUTED RESIDUE (STAND.DEV.)    +.65954⏨+ 3 +.74136⏨+ 1
ESTIMATED RESIDUE (STAND.DEV.)   +.26876⏨+ 2 +.14966⏨+ 1
CORRECTIONS FOR PARAMETER        +.25450⏨- 7 -.70937⏨- 3

PARAMETER VALUE                  +.32110⏨- 5 -.00000⏨- 0
                                                                        100    53     48

ITERATION NUMBER                  +5
COMPUTED RESIDUE (STAND.DEV.)    +.22422⏨+ 3 +.43226⏨+ 1
ESTIMATED RESIDUE (STAND.DEV.)   +.32133⏨+ 2 +.16364⏨+ 1
CORRECTIONS FOR PARAMETER        +.41967⏨- 6 +.37065⏨- 3

PARAMETER VALUE                  +.36307⏨- 5 +.37065⏨- 3
                                                                        76     31     30
```

```
280772-171     B 13681.138 PHEMKER                      11                                                      00

ITERATION NUMBER              +6
COMPUTED RESIDUE (STAND.DEV.)     +.20569⏨+  3 +.41401⏨+  1
ESTIMATED RESIDUE (STAND.DEV.)    +.12692⏨+  2 +.10284⏨+  1
CORRECTIONS FOR PARAMETER         +.25951⏨-  6 -.15412⏨-  2

PARAMETER VALUE                   +.38902⏨-  5 -.11705⏨-  2

BOUNDARY CONSTRAINTS,  JUMP+.2404997579242⏨-  0
COMPUTED RESIDUE (STAND.DEV.)     +.20569⏨+  3 +.41401⏨+  1
ESTIMATED RESIDUE (STAND.DEV.)    +.23855⏨+  2 +.14099⏨+  1
CORRECTIONS FOR PARAMETER         +.62412⏨-  7 -.37065⏨-  3

PARAMETER VALUE                   +.36931⏨-  5 -.00000⏨-  0                                    105     57     50

ITERATION NUMBER              +7
COMPUTED RESIDUE (STAND.DEV.)     +.10666⏨+  3 +.29813⏨+  1
ESTIMATED RESIDUE (STAND.DEV.)    +.21888⏨+  2 +.13506⏨+  1
CORRECTIONS FOR PARAMETER         +.25365⏨-  6 +.23346⏨-  3

PARAMETER VALUE                   +.39467⏨-  5 +.23346⏨-  3                                     82     32     31

ITERATION NUMBER              +8
COMPUTED RESIDUE (STAND.DEV.)     +.67884⏨+  2 +.23785⏨+  1
ESTIMATED RESIDUE (STAND.DEV.)    +.18095⏨+  2 +.12280⏨+  1
CORRECTIONS FOR PARAMETER         +.23093⏨-  6 -.33316⏨-  3

PARAMETER VALUE                   +.41776⏨-  5 -.99699⏨-  4

BOUNDARY CONSTRAINTS,  JUMP+.7007490319338⏨-  0
COMPUTED RESIDUE (STAND.DEV.)     +.67884⏨+  2 +.23785⏨+  1
ESTIMATED RESIDUE (STAND.DEV.)    +.42544⏨+  2 +.18829⏨+  1
CORRECTIONS FOR PARAMETER         +.16183⏨-  6 -.23346⏨-  3

PARAMETER VALUE                   +.41085⏨-  5 +.11102⏨- 15                                     98     48     44

STEEPEST DESCENT+.2868668658626⏨- 14
COMPUTED RESIDUE (STAND.DEV.)     +.93932⏨+  2 +.27978⏨+  1
ESTIMATED RESIDUE (STAND.DEV.)    +.00000⏨-  0 +.00000⏨-  0
CORRECTIONS FOR PARAMETER         +.16175⏨-  6 -.64924⏨- 10

PARAMETER VALUE                   +.41085⏨-  5 +.23346⏨-  3                                     84     33     32

ITERATION NUMBER             +10
COMPUTED RESIDUE (STAND.DEV.)     +.44502⏨+  2 +.19257⏨+  1
ESTIMATED RESIDUE (STAND.DEV.)    +.19447⏨+  2 +.12730⏨+  1
CORRECTIONS FOR PARAMETER         +.16612⏨-  6 -.23518⏨-  3

PARAMETER VALUE                   +.42746⏨-  5 -.17164⏨-  5
```

```
280772-171     B 1368!.138 PHEMKER                    12                                                00

BOUNDARY CONSTRAINTS,  JUMP+.9927016284564⏨-  0
COMPUTED RESIDUE (STAND.DEV.)    +.44502⏨+  2 +.19257⏨+  1
ESTIMATED RESIDUE (STAND.DEV.)   +.44138⏨+  2 +.19178⏨+  1
CORRECTIONS FOR PARAMETER        +.16491⏨-  6 -.23346⏨-  3

PARAMETER VALUE                  +.42734⏨-  5 +.71124⏨- 16                      93      41      38

STEEPEST DESCENT+.3050702941380⏨- 14
COMPUTED RESIDUE (STAND.DEV.)    +.10711⏨+  3 +.29876⏨+  1
ESTIMATED RESIDUE (STAND.DEV.)   +.00000⏨-  0 +.00000⏨-  0
CORRECTIONS FOR PARAMETER        +.16482⏨-  6 -.71060⏨- 10

PARAMETER VALUE                  +.42733⏨-  5 +.23346⏨-  3                      84      33      32

ITERATION NUMBER            +12
COMPUTED RESIDUE (STAND.DEV.)    +.29872⏨+  2 +.15778⏨+  1
ESTIMATED RESIDUE (STAND.DEV.)   +.21001⏨+  2 +.13229⏨+  1
CORRECTIONS FOR PARAMETER        +.10159⏨-  6 -.13714⏨-  3

PARAMETER VALUE                  +.43749⏨-  5 +.96321⏨-  4                      94      42      39

STEEPEST DESCENT+.3166938513554⏨- 14
COMPUTED RESIDUE (STAND.DEV.)    +.53079⏨+  2 +.21032⏨+  1
ESTIMATED RESIDUE (STAND.DEV.)   +.00000⏨-  0 +.00000⏨-  0
CORRECTIONS FOR PARAMETER        +.10154⏨-  6 -.44067⏨- 10

PARAMETER VALUE                  +.43748⏨-  5 +.23346⏨-  3
CONFIDENCE INTERVAL (COND.)      +.00000⏨-  0 +.00000⏨-  0
CONFIDENCE INTERVAL (INDEPT.)    +.00000⏨-  0 +.00000⏨-  0

RELATIONSHIPS BETWEEN PARAMETERS
CORRELATION MATRIX                       COVARIANCE MATRIX
                                         +.97565⏨- 44 +.42403⏨- 52
+. 7558⏨- 14                                          +.59778⏨- 31

PRINCIPAL AXES (DIRECTION COSINES AND CONFIDENCE INTERVAL ALONG EACH AXIS)
+.10000⏨+  1 +.00000⏨-  0       +.00000⏨-  0
+.00000⏨-  1 +.10000⏨+  1       +.00000⏨-  0
```

ITERATION NUMBER +14
COMPUTED RESIDUE (STAND.DEV.) +.25124$_{10}$+ 2 +.14469$_{10}$+ 1
ESTIMATED RESIDUE (STAND.DEV.) +.21983$_{10}$+ 2 +.13535$_{10}$+ 1
CORRECTIONS FOR PARAMETER +.68717$_{10}$- 7 -.72843$_{10}$- 4

PARAMETER VALUE +.44435$_{10}$- 5 +.16062$_{10}$- 3
CONFIDENCE INTERVAL (COND.) +.29635$_{10}$- 6 +.43013$_{10}$- 3
CONFIDENCE INTERVAL (INDEPT.) +.34822$_{10}$- 6 +.50541$_{10}$- 3

RELATIONSHIPS BETWEEN PARAMETERS
CORRELATION MATRIX COVARIANCE MATRIX
+.47757$_{10}$- 14 +.36396$_{10}$- 11
+.52508$_{10}$-) +.10060$_{10}$- 7

PRINCIPAL AXES (DIRECTION COSINES AND CONFIDENCE INTERVAL ALONG EACH AXIS)
+. 0000$_{10}$+ 1 -.36177$_{10}$- 3 +.29635$_{10}$- 6
+.36177$_{10}$- 3 +.10000$_{10}$+ 1 +.50541$_{10}$- 3

RESIDUALS, SPECIFIED FOR EACH OBSERVATION,

```
  1    -.29614⏨+ 1
  2    -.18947⏨+ 1
  3    -.11908⏨+ 1
  4    -.42015⏨- 0
  5    +.26207⏨- 0
  6    +.16116⏨+ 1
  7    +.99253⏨- 0
  8    +.11359⏨+ 1
  9    +.13101⏨+ 1
 10    +.13794⏨+ 1
 11    +.96308⏨- 0
 12    +.41278⏨- 0
 13    -.67007⏨- 1
 14    -.12272⏨+ 1                                   138    64    58
```

THE ENTIRE CALCULATION CONSUMED 65.05 SEC. ON THE EL X8.

6.3. Gear's problem

This test originates from a problem in Gear [1971, p.229-230]. The system of differential equations is

$$dy/dt = - k_1 \, y + k_2 \, z \, (b-z-2y)$$

$$dz/dt = - k_3 \, z + k_4 \, (b-z-2y) \, (a-z-y) - dy/dt$$

$$y(0) = 0.25 \quad , \quad z(0) = 0.5 \; .$$

Apparently this system originates from the chemical reactions

$$A + B \underset{k_3}{\overset{k_4}{\rightleftarrows}} AB$$

$$AB + B \underset{k_1}{\overset{k_2}{\rightleftarrows}} ABB$$

with z = [AB] and y = [ABB].

No solution was given for this problem.
At any rate, the solution found by our algorithm is a sufficient one since the residuals for each observation are less than the experimental error (3 digit accuracy) .

813681.138,PHEMKER,T150

```
BEGIN COMMENT GEAR'S PROBLEM , SEE: GEAR[1971]P.230 ;

        PROC ODEPAREST(N,NOBS,NPAR,DATA,ITMAX,CONVERGE,EPS,MESHP,STIFF,FA);
        VAL N,NOBS,NPAR,ITMAX,CONVERGE,EPS,MESHP,STIFF,FA;
        INT N,NOBS,NPAR,ITMAX,MESHP; REAL CONVERGE,EPS,FA; BOOL STIFF;
        BEGIN COMMENT THE PROCEDURES: CALL YSTART,CALL F,CALL FY,CALL FP
                DEFINE THE PROBLEM SUPPLIED BY THE USER;

                PROC CALL YSTART;
                BEGIN
                        Y[0,2]:= YMAX[1]:= YMAX[2]:= 0.5; Y[0,1]:= 0.25;
                        FP[1,3]:= FP[1,4]:= U; OUTC
                END;
                PROC CALL F(R); VAL R; REAL R;
                BEGIN REAL Q,Z,W; COMMENT ; CF:= CF+1;
                        COMMENT A=1, B= 2;
                        Q:= Y[0,1]; Z:= Y[0,2]; W:= 2-Q-Q-Z;
                        F[1]:= R*(-PAR[1]*Q + PAR[2]*W*Z);
                        F[2]:= R*(-PAR[3]*Z + PAR[4]*W*(1-Q-Z)) - F[1];
                END;
                PROC CALL FY(R); VAL R; REAL R;
                BEGIN REAL Q,Z,W,V,F1,F2;
                        Q:= Y[0,1]; Z:= Y[0,2]; W:= 2-Q-Q-Z; V:= 1-Q-Z;
                        FY[1,1]:= F1:= R*(-PAR[1] - 2*PAR[2]*Z);
                        FY[1,2]:= F2:= R*( PAR[2]*(W-Z));
                        FY[2,1]:=       R*(-PAR[4]*(V+V+W)) - F1;
                        FY[2,2]:=       R*(-PAR[3] - PAR[4]*(V+W)) - F2;
                        CFY:= CFY+1;
                END;
                PROC CALL FP(R); VAL R; REAL R;
                BEGIN REAL Q,Z,W,F1,F2;
                        Q:= Y[0,1]; Z:= Y[0,2]; W:= 2-Q-Q-Z;
                        F1:= FP[1,1]:= -Q*R;     F2:= FP[1,2]:= W*Z*R;
                        FP[2,1]:= -F1;           FP[2,2]:= -F2;
                        FP[2,3]:= -Z*R;          FP[2,4]:= W*(1-Q-Z)*R;
                        CFP:= CFP + 1;
                END;

        ARRAY Y[0:7,1:N*(NPAR+1)],YMAX,F[1:N],FY[1:N,1:N],FP[1:N,1:NPAR];
        PROC PR(S); BEGIN NLCR; PRINTTEXT(S) END;
        PROC FL(R); FLOT(5,3,R);
        PROC PF(S,R); BEGIN PR(S); TAB; FL(R) END;

        PROC OUT(S,R); STRING S; REAL R;
        BEGIN INT I; IF LINENUMBER>50 THEN NEW PAGE ELSE NLCR;
                PR(S); PRINT(R);
                PF({COMPUTED RESIDUE (STAND.DEV.)},COMP ERROR);
                FL(SQRT(COMP ERROR/(NOBS-NPAR)));
                PF({ESTIMATED RESIDUE (STAND.DEV.)},EST ERROR);
                FL(SQRT(EST ERROR/(NOBS-NPAR)));
                PR({CORRECTIONS FOR PARAMETER}); TAB;
                FOR I:=1 STEP 1 UNTIL NPAR DO FL(DELTA PAR[I]); NLCR;
                PR({PARAMETER VALUE}); TAB; TAB;
                FOR I:= 1 STEP 1 UNTIL NPAR DO FL(PAR[I]);
        END;
```

```
PROCEDURE ODEPAREST WAS CALLED WITH THE PARAMETERS:
N      =              +2
NPAR   =              +4
NOBS   =              +8
ITMAX=               +24
CONVERGE  =       +.1000000000001⏨-  1
EPS       =       +.9999999999999⏨-  4
MESHP=               +100
STIFF=               FALSE
FA     =          +.6680000000000⏨+  1
THE CONFIDENCE REGION AT LEVEL A IS PRINTED
FA IS THE A-POINT OF THE F-DISTIBUTION WITH NPAR AND NOBS-NPAR DEGREES OF FREEDOM


THE OBSERVATIONS WERE:
   I      TOBS(I)    COBS(I)   OBS(I)
   0    +.01000⏨-  0
   1    +.33300⏨-  0   +1   +.30100⏨-  0         2    +.33300⏨-  0   +2   +.40300⏨-  0
   3    +.67200⏨-  0   +1   +.32400⏨-  0         4    +.67200⏨-  0   +2   +.36200⏨-  0
   5    +.11120⏨+  1   +1   +.33500⏨-  0         6    +.10120⏨+  1   +2   +.34500⏨-  0
   7    +.11000⏨+  3   +1   +.34500⏨-  0         8    +.10000⏨+  3   +2   +.33200⏨-  0

THE PARAMETER ESTIMATES WERE:
   I   PARLWB(I)         PAR(I)          PARUPB(I)
   1 +.00000⏨-  0   +.10000⏨+  1   +.10000⏨+  2
   2 +.00000⏨-  0   +.10000⏨+  1   +.10000⏨+  2
   3 +.00000⏨-  0   +.10000⏨+  1   +.10000⏨+  2
   4 +.00000⏨-  0   +.10000⏨+  1   +.10000⏨+  2
```

```
                                                                                              EVALUATIONS OF
                                                                                              F      FY     FP

ITERATION NUMBER              +1
COMPUTED RESIDUE (STAND.DEV.)   +.29886⏨-  3 +.86438⏨-  2
ESTIMATED RESIDUE (STAND.DEV.)  +.29652⏨-  5 +.86098⏨-  3
CORRECTIONS FOR PARAMETER       -.24647⏨-  0 -.18866⏨-  0 -.76952⏨-  1 -.23282⏨-  1

PARAMETER VALUE                 +.75353⏨-  0 +.81134⏨-  0 +.92305⏨-  0 +.97672⏨-  0    145     73     65

ITERATION NUMBER              +2
COMPUTED RESIDUE (STAND.DEV.)   +.74640⏨-  5 +.13660⏨-  2
ESTIMATED RESIDUE (STAND.DEV.)  +.24398⏨-  6 +.24697⏨-  3
CORRECTIONS FOR PARAMETER       +.38606⏨-  1 +.30865⏨-  1 -.27768⏨-  1 -.33981⏨-  1

PARAMETER VALUE                 +.79213⏨-  0 +.84220⏨-  0 +.89528⏨-  0 +.94274⏨-  0     90     45     42

ITERATION NUMBER              +3
COMPUTED RESIDUE (STAND.DEV.)   +.25409⏨-  6 +.25204⏨-  3
ESTIMATED RESIDUE (STAND.DEV.)  +.21613⏨-  6 +.23245⏨-  3
CORRECTIONS FOR PARAMETER       +.33519⏨-  2 +.29445⏨-  2 -.16623⏨-  2 -.17801⏨-  2

PARAMETER VALUE                 +.79549⏨-  0 +.84515⏨-  0 +.89362⏨-  0 +.94096⏨-  0    117     59     52

ITERATION NUMBER              +4
COMPUTED RESIDUE (STAND.DEV.)   +.23171⏨-  6 +.24068⏨-  3
ESTIMATED RESIDUE (STAND.DEV.)  +.23049⏨-  6 +.24005⏨-  3
CORRECTIONS FOR PARAMETER       -.14616⏨-  3 -.66320⏨-  4 -.50710⏨-  3 -.64300⏨-  3

PARAMETER VALUE                 +.79534⏨-  0 +.84508⏨-  0 +.89311⏨-  0 +.94031⏨-  0
CONFIDENCE INTERVAL (COND.)     +.33666⏨-  2 +.29626⏨-  2 +.48223⏨-  2 +.59231⏨-  2
CONFIDENCE INTERVAL (INDEPT.)   +.21905⏨-  1 +.19434⏨-  1 +.39016⏨-  1 +.47636⏨-  1

RELATIONSHIPS BETWEEN PARAMETERS
CORRELATION MATRIX                              COVARIANCE MATRIX
                                                +.31163⏨+  3 +.27263⏨+  3 -.20151⏨+  3 -.23865⏨+  3
+.98606⏨-  0                                                 +.24530⏨+  3 -.18052⏨+  3 -.20853⏨+  3
-.36304⏨-  0 -.36657⏨-  0                                                 +.98869⏨+  3 +.11959⏨+  4
-.35215⏨-  0 -.34682⏨-  0 +.99074⏨-  0                                                 +.14738⏨+  4

PRINCIPAL AXES (DIRECTION COSINES AND CONFIDENCE INTERVAL ALONG EACH AXIS)
+.62649⏨-  0 -.71559⏨-  0 -.23960⏨-  0 +.19502⏨-  0    +.21513⏨-  2
+.21834⏨-  0 -.21937⏨-  0 +.73818⏨-  0 -.59941⏨-  0    +.42281⏨-  2
+.73223⏨-  0 +.64910⏨-  0 +.11517⏨-  0 +.17101⏨-  0    +.26782⏨-  1
+.15387⏨-  0 +.13594⏨-  0 -.62001⏨-  0 -.75725⏨-  0    +.62523⏨-  1
```

```
THE EQUATION WAS FOUND TO BE STIFF AT X =        +.33300_10-  2
SOME LITTLE PROBLEMS WITH STIFFNESS      +.20000_10+  1


ITERATION NUMBER                  +5
COMPUTED RESIDUE (STAND.DEV.)     +.22630_10- 6 +.23785_10- 3
ESTIMATED RESIDUE (STAND.DEV.)    +.22372_10- 6 +.23649_10- 3
CORRECTIONS FOR PARAMETER         -.26061_10- 3 -.30077_10- 3 -.27050_10- 3 -.20842_10- 3

PARAMETER VALUE                   +.79508_10- 0 +.84478_10- 0 +.89284_10- 0 +.94011_10- 0
CONFIDENCE INTERVAL (COND.)       +.33630_10- 2 +.29853_10- 2 +.48538_10- 2 +.59251_10- 2
CONFIDENCE INTERVAL (INDEPT.)     +.22231_10- 1 +.19927_10- 1 +.39679_10- 1 +.48069_10- 1

RELATIONSHIPS BETWEEN PARAMETERS
CORRELATION MATRIX                              COVARIANCE MATRIX
                                                +.33071_10+ 3 +.29242_10+ 3 -.22553_10+ 3 -.26467_10+ 3
+.98649_10- J                                                 +.26570_10+ 3 -.20503_10+ 3 -.23516_10+ 3
-.38209_10- J -.38753_10- 0                                                 +.10535_10+ 4 +.12646_10+ 4
-.37013_10- J -.36690_10- 0 +.99088_10- 0                                                 +.15461_10+ 4

PRINCIPAL AXES (DIRECTION COSINES AND CONFIDENCE INTERVAL ALONG EACH AXIS)
+.62932_10- J -.71268_10- 0 -.24003_10- 0 +.19606_10- 0     +.21588_10- 2
+.22108_10- J -.21815_10- 0 +.73575_10- 0 -.60184_10- 0     +.42503_10- 2
+.72729_10- J +.65077_10- 0 +.12218_10- 0 +.18064_10- 0     +.27026_10- 1
+. 6167_10- J +.14495_10- 0 -.62139_10- 0 -.75281_10- 0     +.63429_10- 1
```

RESIDUALS, SPECIFIED FOR EACH OBSERVATION;

1	+.28751₁₀- 4	2	-.13850₁₀- 3
3	-.17981₁₀- 3	4	+.89109₁₀- 4
5	+.19571₁₀- 3	6	+.29093₁₀- 3
7	-.79138₁₀- 4	8	-.19186₁₀- 3

135 70 67

THE ENTIRE CALCULATION CONSUMED 57.28 SEC. ON THE EL X8.

6.4. Barnes' problem

This problem was suggested during the FEBS summerschool on computing techniques in biochemistry (Edinburgh 1968). The system of differential equations

$$dx/dt = k_1x - k_2xy$$
$$dy/dt = k_2xy - k_3y$$

originates from the chemical reactions

$$A \xrightarrow{k_1} A + A$$
$$A + B \xrightarrow{k_2} B + B$$
$$B \xrightarrow{k_3} C$$

This is an oscillating system of the Lotka-Volterra type (see Lotka [1956], Volterra [1931]), which also has many applications in theoretical biology.

As approximate results for a set of given observations, it is known that

$$k_1 = 0.861 \pm 0.14$$
$$k_2 = 2.080 \pm 0.39$$
$$k_3 = 1.816 \pm 0.42$$

confidence interval 1%.
These values agree fairly well with our results.

B1368'.138,PHEMKER,T150

```
BEGIN COMMENT BARNES' PROBLEM;

        PROC ODEPAREST(N,NOBS,NPAR,DATA,ITMAX,CONVERGE,EPS,MESHP,STIFF,FA);
        VAL N,NOBS,NPAR,ITMAX,CONVERGE,EPS,MESHP,STIFF,FA;
        INT N,NOBS,NPAR,ITMAX,MESHP; REAL CONVERGE,EPS,FA; BOOL STIFF;
        BEGIN COMMENT THE PROCEDURES: CALL YSTART,CALL F,CALL FY,CALL FP
                DEFINE THE PROBLEM SUPPLIED BY THE USER;

                PROC CALL YSTART;
                BEGIN Y[0,1]:= YMAX[1]:= 1; Y[0,2]:= 0.3; YMAX[2]:= 0.5;
                        FP[1,3]:= FP[2,1]:= 0; OUTC
                END;
                PROC CALL F(R); VAL R; REAL R;
                BEGIN CF:= CF+1;
                        F[1]:= R*Y[0,1]*(PAR[1]-PAR[2]*Y[0,2]);
                        F[2]:= -R*Y[0,2]*(PAR[3]-PAR[2]*Y[0,1]);
                END;
                PROC CALL FY(R); VAL R; REAL R;
                BEGIN REAL F12; CFY:= CFY+1;
                        FY[1,1]:= R*(PAR[1]-PAR[2]*Y[0,2]);
                        FY[1,2]:= F12:= -R*PAR[2]*Y[0,2];  FY[2,1]:= -F12;
                        FY[2,2]:= R*(PAR[2]*Y[0.1]-PAR[3]);
                END;
                PROC CALL FP(R); VAL R; REAL R;
                BEGIN REAL F12; CFP:= CFP+1;
                        FP[1,1]:= Y[0,1]*R;
                        F12:= FP[1,2]:= -Y[0,1]*Y[0,2]*R;
                        FP[2,2]:= -F12;
                        FP[2,3]:= -Y[0,2]*R;
                END;

        ARRAY Y[0:7,1:N*(NPAR+1)],YMAX,F[1:N],FY[1:N,1:N],FP[1:N,1:NPAR];
        PROC PR(S); BEGIN NLCR; PRINTTEXT(S) END;
        PROC FL(R); FLOT(5,3,R);
        PROC PF(S,R); BEGIN PR(S); TAB; FL(R) END;

        PROC OUT(S,R); STRING S; REAL R;
        BEGIN INT I; IF LINENUMBER>50 THEN NEW PAGE ELSE NLCR;
                PR(S); PRINT(R);
                PF({COMPUTED RESIDUE (STAND.DEV.)},COMP ERROR);
                FL(SQRT(COMP ERROR/(NOBS-NPAR)));
                PF({ESTIMATED RESIDUE (STAND.DEV.)},EST ERROR);
                FL(SQRT(EST ERROR/(NOBS-NPAR)));
                PR({CORRECTIONS FOR PARAMETER}); TAB;
                FOR I:=1 STEP 1 UNTIL NPAR DO FL(DELTA PAR[I]); NLCR;
                PR({PARAMETER VALUE}); TAB; TAB;
                FOR I:= 1 STEP 1 UNTIL NPAR DO FL(PAR[I]);
        END;

        BOOL FIRST,ADAMS; INTEGER K,KOLD,SAME,FAILS;
        REAL X,XOLD,H,CH,HOLD,TOLCONV,TOLUP,TOL.TOLDWN,A0;
        ARRAY A[0:7],DD[0:7,0:N],LAST DELTA[1:N], JAC[1:N,1:N],CONST[1:45],
                TOBS[0:NOBS],OBS[1:NOBS],PARL,PAR,PARU[1:NPAR];
        INT ARRAY COBS[1:NOBS],PP[1:N];

        PROC MULTISTEP(XEND,HMIN,HMAX,EPS);
```

```
PROCEDURE ODEPAREST WAS CALLED WITH THE PARAMETERS:
N     =              +2
NPAR  =              +3
NOBS  =              +20
ITMAX=               +24
CONVERGE =      +.1000000000001⏨-  1
EPS      =      +.9999999999999⏨-  4
MESHP=               +100
STIFF=               FALSE
FA    =         +.5180000000000⏨+  1
THE CONFIDENCE REGION AT LEVEL A IS PRINTED
FA IS THE A-POINT OF THE F-DISTIBUTION WITH NPAR AND NOBS-NPAR DEGREES OF FREEDOM


THE OBSERVATIONS WERE:
  I     TOBS(I)    COBS(I)    OBS(I)
  0   +.00000⏨-  0
  1   +.50000⏨-  0   +1   +.11000⏨+  1        2   +.50000⏨-  0   +2   +.35000⏨-  0
  3   +.10000⏨+  1   +1   +.13000⏨+  1        4   +.10000⏨+  1   +2   +.40000⏨-  0
  5   +.15000⏨+  1   +1   +.11000⏨+  1        6   +.15000⏨+  1   +2   +.50000⏨-  0
  7   +.20000⏨+  1   +1   +.90000⏨-  0        8   +.20000⏨+  1   +2   +.50000⏨-  0
  9   +.25000⏨+  1   +1   +.70000⏨-  0       10   +.25000⏨+  1   +2   +.40000⏨-  0
 11   +.30000⏨+  1   +1   +.50000⏨-  0       12   +.30000⏨+  1   +2   +.30000⏨-  0
 13   +.35000⏨+  1   +1   +.60000⏨-  0       14   +.35000⏨+  1   +2   +.25000⏨-  0
 15   +.40000⏨+  1   +1   +.70000⏨-  0       16   +.40000⏨+  1   +2   +.25000⏨-  0
 17   +.45000⏨+  1   +1   +.80000⏨-  0       18   +.45000⏨+  1   +2   +.30000⏨-  0
 19   +.50000⏨+  1   +1   +.10000⏨+  1       20   +.50000⏨+  1   +2   +.35000⏨-  0

THE PARAMETER ESTIMATES WERE:
  I   PARLWB(I)        PAR(I)         PARUPB(I)
  1 +.00000⏨-  0   +.10000⏨+  1   +.30000⏨+  1
  2 +.00000⏨-  0   +.10000⏨+  1   +.30000⏨+  1
  3 +.00000⏨-  0   +.13000⏨+  1   +.30000⏨+  1
```

```
                                                                                    EVALUATIONS OF
                                                                                    F       FY      FP

ITERATION NUMBER              +1
COMPUTED RESIDUE (STAND.DEV.)    +.20345⏨+  2 +.10940⏨+  1
ESTIMATED RESIDUE (STAND.DEV.)   +.50795⏨+  1 +.54662⏨-  0
CORRECTIONS FOR PARAMETER        -.63413⏨-  1 +.45862⏨-  0 +.29026⏨-  0

PARAMETER VALUE                  +.93659⏨-  0 +.14586⏨+  1 +.15903⏨+  1             117      45      43

ITERATION NUMBER              +2
COMPUTED RESIDUE (STAND.DEV.)    +.31463⏨+  1 +.43020⏨-  0
ESTIMATED RESIDUE (STAND.DEV.)   +.37049⏨-  0 +.14763⏨-  0
CORRECTIONS FOR PARAMETER        -.26418⏨-  1 +.38646⏨-  0 +.13818⏨-  0

PARAMETER VALUE                  +.91017⏨-  0 +.18451⏨+  1 +.17284⏨+  1             127      49      43

ITERATION NUMBER              +3
COMPUTED RESIDUE (STAND.DEV.)    +.43549⏨-  0 +.16005⏨-  0
ESTIMATED RESIDUE (STAND.DEV.)   +.13641⏨-  0 +.89579⏨-  1
CORRECTIONS FOR PARAMETER        -.60317⏨-  2 +.22838⏨-  0 +.12969⏨-  0

PARAMETER VALUE                  +.90414⏨-  0 +.20735⏨+  1 +.18581⏨+  1             111      41      37

ITERATION NUMBER              +4
COMPUTED RESIDUE (STAND.DEV.)    +.18044⏨-  0 +.10303⏨-  0
ESTIMATED RESIDUE (STAND.DEV.)   +.15356⏨-  0 +.95042⏨-  1
CORRECTIONS FOR PARAMETER        -.14002⏨-  1 +.57202⏨-  1 +.87401⏨-  2

PARAMETER VALUE                  +.89014⏨-  0 +.21307⏨+  1 +.18669⏨+  1              97      38      35

ITERATION NUMBER              +5
COMPUTED RESIDUE (STAND.DEV.)    +.16852⏨-  0 +.99565⏨-  1
ESTIMATED RESIDUE (STAND.DEV.)   +.16509⏨-  0 +.98545⏨-  1
CORRECTIONS FOR PARAMETER        -.12529⏨-  1 -.23028⏨-  3 -.20624⏨-  1

PARAMETER VALUE                  +.87761⏨-  0 +.21304⏨+  1 +.18463⏨+  1              91      36      33

STEEPEST DESCENT+.6783314817062⏨-  1
COMPUTED RESIDUE (STAND.DEV.)    +.16865⏨-  0 +.99602⏨-  1
ESTIMATED RESIDUE (STAND.DEV.)   +.00000⏨-  0 +.00000⏨-  0
CORRECTIONS FOR PARAMETER        -.12279⏨-  1 -.17576⏨-  2 -.10166⏨-  2

PARAMETER VALUE                  +.87786⏨-  0 +.21289⏨+  1 +.18659⏨+  1              93      37      33
```

```
ITERATION NUMBER                +7
COMPUTED RESIDUE (STAND.DEV.)    +.16779⏨-  0 +.99349⏨-  1
ESTIMATED RESIDUE (STAND.DEV.)   +.16507⏨-  0 +.98539⏨-  1
CORRECTIONS FOR PARAMETER        -.80093⏨-  3 +.14125⏨-  1 -.55416⏨-  2

PARAMETER VALUE                  +.87705⏨-  0 +.21430⏨+  1 +.18603⏨+  1                    93     37     33

STEEPEST DESCENT+.1364513087151⏨-  0
COMPUTED RESIDUE (STAND.DEV.)    +.17039⏨-  0 +.10012⏨-  0
ESTIMATED RESIDUE (STAND.DEV.)   +.00000⏨-  0 +.00000⏨-  0
CORRECTIONS FOR PARAMETER        +.44054⏨-  3 +.13373⏨-  1 +.51776⏨-  3

PARAMETER VALUE                  +.87830⏨-  0 +.21423⏨+  1 +.18664⏨+  1                    94     37     34

ITERATION NUMBER                +9
COMPUTED RESIDUE (STAND.DEV.)    +.16984⏨-  0 +.99954⏨-  1
ESTIMATED RESIDUE (STAND.DEV.)   +.16845⏨-  0 +.99542⏨-  1
CORRECTIONS FOR PARAMETER        -.68080⏨-  2 -.89510⏨-  2 -.22265⏨-  1

PARAMETER VALUE                  +.87149⏨-  0 +.21333⏨+  1 +.18441⏨+  1
CONFIDENCE INTERVAL (COND.)      +.10461⏨-  0 +.14431⏨-  0 +.13694⏨-  0
CONFIDENCE INTERVAL (INDEPT.)    +.23298⏨-  0 +.47408⏨-  0 +.47495⏨-  0

RELATIONSHIPS BETWEEN PARAMETERS
CORRELATION MATRIX                                 COVARIANCE MATRIX
                                                   +.35250⏨-  0 +.62722⏨-  0 +.63825⏨-  0
+.87443⏨-  )                                                    +.14596⏨+  1 +.13895⏨+  1
+.88817⏨-  ) +.95023⏨-  0                                                    +.14650⏨+  1

PRINCIPAL AXES (DIRECTION COSINES AND CONFIDENCE INTERVAL ALONG EACH AXIS)
-.30574⏨-  ) -.67210⏨-  0 -.67439⏨-  0       +.69525⏨-  0
-.47602⏨-  ) +.72133⏨-  0 -.50308⏨-  0       +.10859⏨-  0
-.82458⏨-  ) -.16722⏨-  0 +.54047⏨-  0       +.97191⏨-  1
```

```
ITERATION NUMBER            +10
COMPUTED RESIDUE (STAND.DEV.)    +.16984⏨- 0 +.99953⏨- 1
ESTIMATED RESIDUE (STAND.DEV.)   +.16967⏨- 0 +.99903⏨- 1
CORRECTIONS FOR PARAMETER        +.74720⏨- 3 +.29422⏨- 2 -.19381⏨- 2

PARAMETER VALUE                  +.87224⏨- 0 +.21363⏨+ 1 +.18422⏨+ 1
CONFIDENCE INTERVAL (COND.)      +.10956⏨- 0 +.14536⏨- 0 +.13861⏨- 0
CONFIDENCE INTERVAL (INDEPT.)    +.24304⏨- 0 +.48772⏨- 0 +.47880⏨- 0

RELATIONSHIPS BETWEEN PARAMETERS
CORRELATION MATRIX                        COVARIANCE MATRIX
                                          +.38085⏨- 0 +.67084⏨- 0 +.66409⏨- 0
+.87775⏨- )                                           +.15337⏨+ 1 +.14326⏨+ 1
+.88512⏨- ) +.95148⏨- 0                                           +.14781⏨+ 1

PRINCIPAL AXES (DIRECTION COSINES AND CONFIDENCE INTERVAL ALONG EACH AXIS)
-.31258⏨- ) -.67786⏨- 0 -.66544⏨- 0     +.70991⏨- 0
+.77151⏨- ) +.22750⏨- 0 -.59416⏨- 0     +.10212⏨- 0
+.55414⏨- ) -.69911⏨- 0 +.45186⏨- 0     +.10859⏨- 0
```

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RESIDUALS, SPECIFIED FOR EACH OBSERVATION,

1	+.11570$_{10}$-	1	2	-.15551$_{10}$-	1
3	+.21867$_{10}$-	0	4	-.67389$_{10}$-	1
5	+.13641$_{10}$-	0	6	-.57497$_{10}$-	1
7	+.91303$_{10}$-	1	8	-.70121$_{10}$-	1
9	-.22814$_{10}$-	2	10	-.10476$_{10}$-	0
11	-.16528$_{10}$-	0	12	-.11376$_{10}$-	0
13	-.91623$_{10}$-	1	14	-.87445$_{10}$-	1
15	-.65997$_{10}$-	1	16	-.40703$_{10}$-	1
17	-.77560$_{10}$-	1	18	+.22896$_{10}$-	1
19	-.73487$_{10}$-	3	20	+.49724$_{10}$-	1

132   51   47

THE ENTIRE CALCULATION CONSUMED 78.20 SEC. ON THE EL X8.

6.5. Analyzing a sum of exponentials

As another example of parameter estimation we report some experiences with linear differential equations. Analysing a sum of exponentials can be considered as the estimation of parameters in a linear initial value problem. Here the parameters appear as well in the differential equations as in the initial values. Since the parameters appear in a nonlinear way, our estimation problem is a nonlinear one. However, the linearity of the differential equation causes a rather efficient use of the integration method.

We consider the sum of exponentials

$$y(t) = a + be^{\lambda t} + ce^{\mu t} \quad .$$

To this function $y(t)$ we associate a system of linear differential equations

$$\dot{y}(t) = z$$

$$\dot{z}(t) = -\lambda\mu y + (\lambda+\mu)z + \lambda\mu a \; .$$

This system has the general solution

$$\begin{pmatrix} y \\ z \end{pmatrix} = c_1 \begin{pmatrix} 1 \\ \lambda \end{pmatrix} e^{\lambda t} + c_2 \begin{pmatrix} 1 \\ \mu \end{pmatrix} e^{\mu t} + \begin{pmatrix} a \\ 0 \end{pmatrix} .$$

With initial conditions

$$y(0) = a + b + c$$
$$z(0) = \lambda b + \mu c$$

this system has the particular solution

$$y(t) = a + be^{\lambda t} + ce^{\mu t}$$
$$z(t) = be^{\lambda t} + ce^{\mu t}$$

It appears from the general solution that it will be difficult to determine the parameters in the case that $\lambda \approx \mu$. In order to be able to determine the complete set of parameters, it is evident that the observations should contain information about both exponentials: some observations have to represent $e^{\lambda t}$ (sample times t, with the order of magnitude $1/\lambda$) and some observations have to represent $e^{\mu t}$. The example shown below satisfies these conditions.

In order to make intelligible the details of the example we give the initial values and functions as they are used in the program.

Notation $y1 = y(t)$; $y2 = z(t)$; $f1 = \dot{y}(t)$; $f2 = \dot{z}(t)$.
Initial values (t=0):

$y1$	$= a + b + c$	$y2$	$= \lambda b + \mu c$
$\partial f1/\partial a =$	1	$\partial f2/\partial a =$	0
$\partial f1/\partial b =$	1	$\partial f2/\partial b =$	λ
$\partial f1/\partial c =$	1	$\partial f2/\partial c =$	μ
$\partial f1/\partial \lambda =$	0	$\partial f2/\partial \lambda =$	b
$\partial f1/\partial \mu =$	0	$\partial f2/\partial \mu =$	c

Functions :

$f1 = y2$
$f2 = (\lambda+\mu)\, y2 + \lambda\mu(a-y1)$

$\partial f1/\partial y1 = 0$ $\qquad$ $\partial f1/\partial y2 = 1$
$\partial f2/\partial y1 = -\lambda\mu$ $\qquad$ $\partial f2/\partial y2 \quad \lambda + \mu$

$\partial f1/\partial a = \partial f1/\partial b = \partial f1/\partial c = \partial f1/\partial \lambda = \partial f1/\partial \mu = 0$
$\partial f2/\partial b = \partial f2/\partial c = 0$
$\partial f2/\partial a = \lambda\mu$
$\partial f2/\partial \lambda = y2 + \mu(a-y1)$
$\partial f2/\partial \mu = y2 + \lambda(a-y1)$

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```
BEGIN COMMENT ANALIZING A SUM OF EXPONENTIALS;

        PROC ODEPAREST(N,NOBS,NPAR,DATA,ITMAX,CONVERGE,EPS,MESHP,STIFF,FA);
        VAL N,NOBS,NPAR,ITMAX,CONVERGE,EPS,MESHP,STIFF,FA;
        INT N,NOBS,NPAR,ITMAX,MESHP; REAL CONVERGE,EPS,FA; BOOL STIFF; PROC DATA;
        BEGIN COMMENT     Y[0,    1    2
                 PAR[1]= C        3    4
                 PAR[2]= MU       5    6
                 PAR[3]= B        7    8
                 PAR[4]= LAMBDA   9   10
                 PAR[5]= A       11   12  ];

                 PROC CALL YSTART;
                 BEGIN YMAX[1]:= SUM(I,0,2,ABS(PAR[1+I+I]));
                        YMAX[2]:= ABS(PAR[1]*PAR[2]) + ABS(PAR[3]*PAR[4]);
                          Y[0,1]:= SUM(I,0,2,PAR[1+I+I]);
                          Y[0,2]:= PAR[1]*PAR[2] + PAR[3]*PAR[4];
                          Y[0,3]:= Y[0,7]:= Y[0,11]:= 1;
                          Y[0,4]:= PAR[2]; Y[0,6]:= PAR[1];
                          Y[0,8]:= PAR[4]; Y[0,10]:= PAR[3];
                          FOR I:= 1,2,3,4,5 DO FP[1,I]:= 0;
                          FP[2,1]:= FP[2,3]:= FY[1,1]:= 0; OUTC
                 END;

                 PROC CALL F(R); VAL R; REAL R;
                 BEGIN    F[1]:= R*Y[0,2];          CF:= CF + 1;
                          F[2]:= R*((PAR[2]+PAR[4])*Y[0,2]
                                   + PAR[2]*PAR[4]*(PAR[5]-Y[0,1]));
                 END;

                 PROC CALL FY(R); VAL R; REAL R;
                 BEGIN    FY[1,2]:= R;              CFY:= CFY + 1;
                          FY[2,1]:= -R*PAR[2]*PAR[4];
                          FY[2,2]:= R*(PAR[2]+PAR[4]);
                 END;

                 PROC CALL FP(R); VAL R; REAL R;
                 BEGIN    FP[2,5]:= R*PAR[2]*PAR[4];     CFP:= CFP + 1;
                          FP[2,2]:= R*(Y[0,2] + PAR[4]*(PAR[5]-Y[0,1]));
                          FP[2,4]:= R*(Y[0,2] + PAR[2]*(PAR[5]-Y[0,1]));
                 END;

        ARRAY Y[0:7,1:N*(NPAR+1)],YMAX,F[1:N],FY[1:N,1:N],FP[1:N,1:NPAR];
        PROC PR(S); BEGIN NLCR; PRINTTEXT(S) END;
        PROC FL(R); FLOT(5,3,R);
        PROC PF(S,R); BEGIN PR(S); TAB; FL(R) END;

        PROC OUT(S,R); STRING S; REAL R;
        BEGIN INT I; IF LINENUMBER>50 THEN NEW PAGE ELSE NLCR;
                 PR(S); PRINT(R);
                 PF({COMPUTED RESIDUE (STAND.DEV.)},COMP ERROR);
                 FL(SQRT(COMP ERROR/(NOBS-NPAR)));
                 PF({ESTIMATED RESIDUE (STAND.DEV.)},EST ERROR);
                 FL(SQRT(EST ERROR/(NOBS-NPAR)));
                 PR({CORRECTIONS FOR PARAMETER}); TAB;
                 FOR I:=1 STEP 1 UNTIL NPAR DO FL(DELTA PAR[I]); NLCR;
```

```
PROC PF(S,R); BEGIN PR(S); TAB; FL(R) END;

INT CF,CFY,CFP;
PROC OUTC;
BEGIN INT R; NLCR; SPACE(100); IF CF=0 THEN
        BEGIN SPACE(6); PRINTTEXT(‡EVALUATIONS OF‡); NLCR; SPACE(106);PRINTTEXT(‡F       FY       FP‡) END ELSE
        FOR R:= CF,CFY,CFP DO ABSFIXT(6,0,R);
        CF:= CFY:= CFP:= 0;
END;

PROC EXP DATA(N,T,CT,O,NP,PL,P,PU);
BEGIN REAL A,B,C,L,M,TOBS,TT; INT I,NOBS,NPAR;
        TT:= TIME;
        A:= P[5]:= READ; B:= P[3]:= READ; C:= P[1]:= READ; L:= P[4]:= READ; M:= P[2]:= READ;
        NLCR; NLCR; PRINTTEXT(‡THE PROGRAM TRIES TO FIT THE SUM OF EXPONENTIALS‡);
        NLCR;FIXT(3,2,C); PRINTTEXT(‡ * EXP( ‡); FIXT(3,2,M); PRINTTEXT(‡ * T) ‡);
        FIXT(3,2,B); PRINTTEXT(‡ * EXP( ‡); FIXT(3,2,L); PRINTTEXT(‡ * T) ‡); FIXT(3,2,A); NLCR; NLCR;
        NLCR; NLCR;TOBS:= T[0]:= 0; N:= NOBS:= READ;
        PRINTTEXT(‡THE FUNCTION WAS SAMPLED AT T=‡); NLCR;
        FOR I:= 1 STEP 1 UNTIL NOBS DO
        BEGIN TOBS:= T[I]:= READ; CT[I]:= 1; FL(TOBS);
              O[I]:= A + B*EXP(L*TOBS) + C*EXP(TOBS*M);
              IF PRINTPOS>70 THEN NLCR ELSE TAB;
        END;  NLCR;
        NP:= NPAR:= READ; NLCR; PRINTTEXT(‡THE PARAMETER ESTIMATES WERE:‡);
        PR(‡    I    PARLWB[I]      PAR[I]        PARUPB[I]‡);
        FOR I:= 1 STEP 1 UNTIL NPAR DO
        BEGIN NLCR; ABSFIXT(3,0,I); A:=PL[I]:= READ; FL(A); A:= P[I]:= READ; FL(A); A:= PU[I]:= READ; FL(A) END;
        NEW PAGE; TIM:= TIM + TT - TIME
END;
REAL TIM;

PROC EXP JOB(N,NOBS,NPAR,ITMAX,CONVERGE,EPS,MESHP,STIFF,FA);
VAL N,NOBS,NPAR,ITMAX,CONVERGE,MESHP,STIFF,FA;
INT N,NOBS,NPAR,ITMAX,MESHP; REAL CONVERGE,EPS,FA; BOOL STIFF;
BEGIN   PR(‡PROCEDURE ODEPAREST WAS CALLED WITH THE PARAMETERS:‡);
        P(‡N      =‡,N); P(‡NPAR =‡,NPAR); P(‡NOBS =‡,NOBS); P(‡ITMAX=‡,ITMAX);
        P(‡CONVERGE =‡,CONVERGE); P(‡EPS        =‡,EPS); P(‡MESHP=‡,MESHP);
        PR(‡STIFF= ‡); TAB; IF STIFF THEN PRINTTEXT(‡  TRUE‡) ELSE PRINTTEXT(‡  FALSE‡);
        P(‡FA    =    ‡,FA); PR(‡THE CONFIDENCE REGION AT LEVEL A IS PRINTED‡);
        PR(‡FA IS THE A-POINT OF THE F-DISTIBUTION WITH NPAR AND NOBS-NPAR DEGREES OF FREEDOM‡);
        NLCR; CF:= CFY:= CFP:= 0; TIM:= TIME;
        ODEPAREST(N,NOBS,NPAR,EXP DATA,ITMAX,CONVERGE,EPS,MESHP,STIFF,FA);
        TIM:= TIME-TIM; OUTC; NLCR;NLCR; NLCR;
        PR(‡THE ENTIRE CALCULATION CONSUMED‡); ABSFIXT(3,2,TIM); PRINTTEXT(‡SEC, ON THE EL X8,‡);
END JOB;

EXP JOB(2,READ,5,16,0.01,-4.100,TRUE,5.06);
COMMENT 5.06= F[0.01](5,12);
END
```

```
PROCEDURE ODEPAREST WAS CALLED WITH THE PARAMETERS:
N      =              +2
NPAR =                +5
NOBS =               +17
ITMAX=               +16
CONVERGE  =      +.1000000000001⏨-  1
EPS       =      +.9999999999999⏨-  4
MESHP=                +100
STIFF=               TRUE
FA    =          +.5059999999998⏨+  1
THE CONFIDENCE REGION AT LEVEL A IS PRINTED
FA IS THE A-POINT OF THE F-DISTIBUTION WITH NPAR AND NOBS-NPAR DEGREES OF FREEDOM


THE PROGRAM TRIES TO FIT THE SUM OF EXPONENTIALS
  -3.00   * EXP(  -20.00  * T)   +2.00   * EXP(   -1.00   * T)   +1.00



THE FUNCTION WAS SAMPLED AT T=
+.20000⏨-  1     +.40000⏨-  1     +.60000⏨-  1     +.80000⏨-  1     +.10000⏨-  0
+.20000⏨-  )     +.40000⏨-  0     +.60000⏨-  0     +.80000⏨-  0     +.10000⏨+  1
+.20000⏨+  1     +.30000⏨+  1     +.40000⏨+  1     +.50000⏨+  1     +.10000⏨+  2
+.15000⏨+  2     +.20000⏨+  2

THE PARAMETER ESTIMATES WERE:
   I    PARLWB(I)         PAR(I)          PARUPB(I)
   1 -.1000)⏨+  2 -.50000⏨+  1 +.10000⏨+  2
   2 -.4000)⏨+  2 -.10000⏨+  2 -.10000⏨-  1
   3 -.5000)⏨+  1 +.50000⏨+  1 +.50000⏨+  1
   4 -.5000)⏨+  1 -.50000⏨-  0 -.10000⏨-  0
   5 -.5000)⏨+  1 +.50000⏨-  0 +.50000⏨+  1
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						EVALUATIONS OF P	PY	FP
ITERATION NUMBER +1								
COMPUTED RESIDUE (STAND.DEV.)	+.23845$_{10}$+ 2	+.14097$_{10}$+ 1						
ESTIMATED RESIDUE (STAND.DEV.)	+.16545$_{10}$- 1	+.37132$_{10}$- 1						
CORRECTIONS FOR PARAMETER	+.22491$_{10}$+ 1	-.42683$_{10}$+ 1	-.30728$_{10}$+ 1	-.10424$_{10}$- 0	+.51105$_{10}$- 0			
PARAMETER VALUE	-.27509$_{10}$+ 1	-.14268$_{10}$+ 2	+.19272$_{10}$+ 1	-.60424$_{10}$- 0	+.10111$_{10}$+ 1	165	84	82
ITERATION NUMBER +2								
COMPUTED RESIDUE (STAND.DEV.)	+.75052$_{10}$- 0	+.25009$_{10}$- 0						
ESTIMATED RESIDUE (STAND.DEV.)	+.23014$_{10}$- 2	+.13849$_{10}$- 1						
CORRECTIONS FOR PARAMETER	-.25946$_{10}$- 0	-.50296$_{10}$+ 1	+.63934$_{10}$- 1	-.24332$_{10}$- 0	+.10982$_{10}$- 2			
PARAMETER VALUE	-.30104$_{10}$+ 1	-.19298$_{10}$+ 2	+.19911$_{10}$+ 1	-.84756$_{10}$- 0	+.10122$_{10}$+ 1	152	78	76
ITERATION NUMBER +3								
COMPUTED RESIDUE (STAND.DEV.)	+.76284$_{10}$- 1	+.79731$_{10}$- 1						
ESTIMATED RESIDUE (STAND.DEV.)	+.22978$_{10}$- 4	+.13838$_{10}$- 2						
CORRECTIONS FOR PARAMETER	-.59071$_{10}$- 2	-.69262$_{10}$- 0	+.15834$_{10}$- 1	-.13000$_{10}$- 0	-.10842$_{10}$- 1			
PARAMETER VALUE	-.30163$_{10}$+ 1	-.19991$_{10}$+ 2	+.20070$_{10}$+ 1	-.97756$_{10}$- 0	+.10013$_{10}$+ 1	159	81	79
ITERATION NUMBER +4								
COMPUTED RESIDUE (STAND.DEV.)	+.22891$_{10}$- 2	+.13812$_{10}$- 1						
ESTIMATED RESIDUE (STAND.DEV.)	+.12321$_{10}$- 5	+.32042$_{10}$- 3						
CORRECTIONS FOR PARAMETER	+.16256$_{10}$- 1	-.59411$_{10}$- 2	-.57463$_{10}$- 2	-.22140$_{10}$- 1	-.13863$_{10}$- 2			
PARAMETER VALUE	-.30001$_{10}$+ 1	-.19996$_{10}$+ 2	+.20012$_{10}$+ 1	-.99970$_{10}$- 0	+.99992$_{10}$- 0	162	82	80
ITERATION NUMBER +5								
COMPUTED RESIDUE (STAND.DEV.)	+.80985$_{10}$- 5	+.82151$_{10}$- 3						
ESTIMATED RESIDUE (STAND.DEV.)	+.23709$_{10}$- 6	+.14056$_{10}$- 3						
CORRECTIONS FOR PARAMETER	+.12845$_{10}$- 3	+.27472$_{10}$- 2	-.97612$_{10}$- 3	-.66138$_{10}$- 3	+.12205$_{10}$- 3			
PARAMETER VALUE	-.29999$_{10}$+ 1	-.19994$_{10}$+ 2	+.20002$_{10}$+ 1	-.10004$_{10}$+ 1	+.10000$_{10}$+ 1	162	82	80
ITERATION NUMBER +6								
COMPUTED RESIDUE (STAND.DEV.)	+.23464$_{10}$- 6	+.13983$_{10}$- 3						
ESTIMATED RESIDUE (STAND.DEV.)	+.22232$_{10}$- 6	+.13611$_{10}$- 3						
CORRECTIONS FOR PARAMETER	-.67500$_{10}$- 4	-.58372$_{10}$- 4	+.15898$_{10}$- 4	+.51143$_{10}$- 4	+.32551$_{10}$- 5			
PARAMETER VALUE	-.30000$_{10}$+ 1	-.19994$_{10}$+ 2	+.20003$_{10}$+ 1	-.10003$_{10}$+ 1	+.10000$_{10}$+ 1	162	82	80

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ITERATION NUMBER                 +7
COMPUTED RESIDUE (STAND.DEV.)     +.22367 10- 6 +.13653 10- 3
ESTIMATED RESIDUE (STAND.DEV.)    +.22362 10- 6 +.13651 10- 3
CORRECTIONS FOR PARAMETER         +.19926 10- 5 -.28885 10- 4 +.16144 10- 5 +.46270 10- 6 -.39176 10- 6

PARAMETER VALUE                   -.30000 10+ 1 -.19994 10+ 2 +.20003 10+ 1 -.10003 10+ 1 +.10000 10+ 1
CONFIDENCE INTERVAL (COND.)       +.84794 10- 3 +.68985 10- 2 +.28098 10- 3 +.42610 10- 3 +.16653 10- 3
CONFIDENCE INTERVAL (INDEPT.)     +.18685 10- 2 +.18846 10- 1 +.78593 10- 3 +.93961 10- 3 +.30832 10- 3

RELATIONSHIPS BETWEEN PARAMETERS
CORRELATION MATRIX                          COVARIANCE MATRIX
                                            +.74056 10+ 1 +.39859 10+ 2 -.68451 10- 0 +.12606 10- 0 -.30724 10- 1
                                                          +.75334 10+ 3 +.17964 10+ 2 -.23259 10+ 2 +.22636 10+ 1
+.53365 10- 0                                                           +.13102 10+ 1 -.99803 10- 0 -.59142 10- 1
-.21975 10- 0 +.57179 10- 0                                                           +.18726 10+ 1 -.32541 10- 0
+.33852 10- 1 -.61924 10- 0 -.63718 10- 0                                                           +.20162 10- 0
-.25144 10- 1 +.18367 10- 0 -.11507 10- 0 -.52958 10- 0

PRINCIPAL AXES (DIRECTION COSINES AND CONFIDENCE INTERVAL ALONG EACH AXIS)
+.93584 10- 1 -.99677 10- 2 +.43473 10- 0 +.25681 10- 0 +.85802 10- 0      +.14504 10- 3
+.33243 10- 0 -.43710 10- 1 +.82575 10- 0 -.24470 10- 0 -.38190 10- 0      +.43795 10- 3
-.21247 10- 1 +.35278 10- 1 +.19399 10- 0 +.89379 10- 0 -.34222 10- 0      +.62653 10- 3
-.91256 10- 1 +.32859 10- 1 +.30160 10- 0 -.27269 10- 0 +.28725 10- 1      +.17145 10- 2
+.53060 10- 2 +.99783 10- 0 +.23724 10- 1 -.30773 10- 1 +.29953 10- 2      +.18887 10- 1
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                                                                                       162      82      80

ITERATION NUMBER               +8
COMPUTED RESIDUE (STAND.DEV.)    +.65081⏨- 7 +.73644⏨- 4
ESTIMATED RESIDUE (STAND.DEV.)   +.34802⏨- 8 +.17030⏨- 4
CORRECTIONS FOR PARAMETER        -.70770⏨- 4 -.52746⏨- 2 -.15823⏨- 3 +.30427⏨- 3 -.43664⏨- 4

PARAMETER VALUE                  -.30001⏨+ 1 -.19999⏨+ 2 +.20001⏨+ 1 -.10000⏨+ 1 +.10000⏨+ 1
CONFIDENCE INTERVAL (COND.)      +.10607⏨- 3 +.85182⏨- 3 +.34906⏨- 4 +.53470⏨- 4 +.20775⏨- 4
CONFIDENCE INTERVAL (INDEPT.)    +.23551⏨- 3 +.23471⏨- 2 +.99371⏨- 4 +.12023⏨- 3 +.38646⏨- 4

RELATIONSHIPS BETWEEN PARAMETERS
CORRELATION MATRIX                          COVARIANCE MATRIX
                                            +.75589⏨+ 1 +.39869⏨+ 2 -.71520⏨- 0 +.16214⏨- 0 -.33804⏨- 1
+.52925⏨- )                                             +.75076⏨+ 3 +.18270⏨+ 2 -.24004⏨+ 2 +.23198⏨+ 1
-.22424⏨- ) +.57479⏨- 0                                             +.13458⏨+ 1 -.10593⏨+ 1 -.55403⏨- 1
+.42615⏨- ( -.62415⏨- 0 -.65057⏨- 0                                             +.19702⏨+ 1 -.33403⏨- 0
-.27253⏨- ( +.18766⏨- 0 -.10586⏨- 0 -.52747⏨- 0                                             +.20355⏨- 0

PRINCIPAL AXES (DIRECTION COSINES AND CONFIDENCE INTERVAL ALONG EACH AXIS)
+.93553⏨- 1 -.10092⏨- 1 +.43782⏨- 0 +.25578⏨- 0 +.85676⏨- 0      +.18069⏨- 4
+.33183⏨- ) -.44053⏨- 1 +.82569⏨- 0 -.23500⏨- 0 -.38854⏨- 0      +.54925⏨- 4
-.22276⏨- ) +.36959⏨- 1 +.18706⏨- 0 +.89436⏨- 0 -.33784⏨- 0      +.78621⏨- 4
-.91032⏨- ) +.32233⏨- 1 +.30162⏨- 0 -.28009⏨- 0 +.29269⏨- 1      +.21730⏨- 3
+.53256⏨- 1 +.99777⏨- 0 +.24211⏨- 1 -.31868⏨- 1 +.30802⏨- 2      +.23523⏨- 2
```

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RESIDUALS, SPECIFIED FOR EACH OBSERVATION,

1	$-.44339_{10}-5$
2	$+.10727_{10}-3$
3	$+.80554_{10}-4$
4	$+.51513_{10}-4$
5	$+.14461_{10}-4$
6	$-.66740_{10}-4$
7	$-.48047_{10}-4$
8	$+.16470_{10}-4$
9	$+.61385_{10}-4$
10	$+.96188_{10}-4$
11	$+.94246_{10}-4$
12	$+.69905_{10}-4$
13	$+.97097_{10}-5$
14	$-.29693_{10}-4$
15	$-.56893_{10}-4$
16	$-.43462_{10}-4$
17	$-.65404_{10}-4$

225   114   109

THE ENTIRE CALCULATION CONSUMED 153.13 SEC, ON THE EL X8.

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