A note on the fitting of certain types of experimental data*)

by P. Wynn **)

UDC 311.2

Summary

This paper is concerned with the problem of determining those values of the parameters Z, A_i, α_i $(i = 1, 2, \ldots, h)$ *which provide a best fit of the form*

$$f^*(t) = Z + \sum_{i=1}^{h} A_i e^{-\alpha_i t}$$

to the observed values $f_s = f(t_s)$ $(s = 1, 2, \ldots, n)$ *in the sense that the sum* $\sum_{s=1}^{n} \{f^*(t_s) - f(t_s)\}^2$ *is a minimum.*

Two iterative numerical techniques for the solution of this problem are discussed. The first, a variable gradient method, converges rapidly but involves a relatively large amount of computation; the second involves less computation but converges less rapidly. It is shown that by application of a suitable acceleration technique to the second method, its convergence is made as rapid as that of the first.

Samenvatting

Dit artikel behandelt het probleem der bepaling van die waarden der parameters Z, A_i, α_i $(i = 1, 2, \ldots, h)$, *die de beste benadering geven van de vorm*

$$f^*(t) = Z + \sum_{i=1}^{h} A_i e^{-\alpha_i t}$$

aan de waargenomen waarden $f_s = f(t_s)$ $(s = 1, 2, \ldots, n)$, *in die zin, dat de som* $\sum_{s=1}^{n} \{f^*(t_s) - f(t_s)\}^2$ *een minimum is.*

Twee iteratief numerieke technieken voor de oplossing van dit probleem worden besproken. De eerste, een variabele gradient methode, convergeert snel, doch houdt een relatief groot aantal berekeningen in; de tweede houdt minder berekeningen in, doch convergeert minder snel. Er wordt aangetoond dat, bij toepassing van een geschikte versnellingstechniek bij de tweede methode, de convergentie even snel is als die der eerste.

1. Introduction

A frequently occurring problem in the analysis of experimental data is that of determining parameters Z, A_i, α_i $i = 1, 2, \ldots, h$ such that the sum

*) Communication MR 40 of the Computation Department of the Mathematical Centre, Amsterdam.

**) Mathematical Centre, Amsterdam.

$$Z + \sum_{i=1}^{h} A_i e^{-\alpha_i t} \tag{1}$$

is the best fit to the observations

$$f_s = f(t_s) \qquad s = 1, 2, \ldots, n$$

in the sense that the sum

$$\sum_{s=1}^{n} (f(t_s) - Z - \sum_{i=1}^{h} A_i e^{-\alpha_i t_s})^2 \tag{3}$$

is a minimum.

The normal method of solving this problem is to assume initial values $Z^{(0)}$, $A_i^{(0)}$, $\alpha_i^{(0)}$ $i = 1, 2\ldots, h$ which approximate the required values, and to derive a sequence of increasingly good estimates

$$Z^{(r)}, A_i^{(r)}, \alpha_i^{(r)} \qquad i = 1, 2, \ldots, h; r = 1, 2, \ldots \tag{4}$$

by recourse to a suitable iterative scheme.

We are concerned then to minimise the sum

$$\Theta = \sum_{s=1}^{n} v_s^2 \tag{5}$$

where

$$v_s = f_s - Z - \sum_{i=1}^{h} A_i e^{-\alpha_i t_s} \qquad s = 1, 2, \ldots, n \tag{6}$$

and by partial differentiations derive the $2h + 1$ equations

$$\Phi_u = 0 \qquad u = 0, 1, \ldots, 2h \tag{7}$$

where

$$\Phi_0 = \frac{\partial \Theta}{\partial Z} = -2 \sum_{s=1}^{n} v_s \tag{8}$$

$$\Phi_{2i-1} = \frac{\partial \Theta}{\partial A_i} = -2 \sum_{s=1}^{n} e^{-\alpha_i t_s} v_s \qquad i = 1, 2, \ldots, h \tag{9}$$

$$\Phi_{2i} = \frac{\partial \Theta}{\partial \alpha_i} = 2 A_i \sum_{s=1}^{n} e^{-\alpha_i t_s} v_s t_s \qquad i = 1, 2, \ldots, h \tag{10}$$

Let us suppose that the members of the sequence (4) are related by the equations

$$Z^{(r+1)} = Z^{(r)} + \Delta Z^{(r)}, \; A_i^{(r+1)} = A_i^{(r)} + \Delta A_i^{(r)}, \; \alpha_i^{(r+1)} = \alpha_i^{(r)} + \Delta \alpha_i^{(r)}$$
$$i = 1, 2, \ldots, h \tag{11}$$

and let us adopt the column vector notation

$$\Phi_u^{(r)} = \Phi_u(Z^{(r)}, A_1^{(r)}, \alpha_1^{(r)}, A_2^{(r)}, \ldots, \alpha_h^{(r)}) \qquad u = 0, 1, \ldots, 2h \tag{12}$$

then, neglecting second and higher order terms we have

$$(\Phi_0^{(r+1)}, \Phi_1^{(r+1)}, \ldots, \Phi_{2h}^{(r+1)}) = (\Phi_0^{(r)}, \Phi_1^{(r)}, \ldots, \Phi_{2h}^{(r)}) + \\ + J^{(r)} (\Delta Z^{(r)}, \Delta A_1^{(r)}, \Delta\alpha_1^{(r)}, \ldots, \Delta A_h^{(r)}, \Delta\alpha_h^{(r)}) \quad (13)$$

where the vectors in equation (13) (and in (23), (24) below) are of course column vectors, and J is the Jacobian matrix

$$J = \begin{bmatrix} \frac{\partial\Phi_0}{\partial Z} & \frac{\partial\Phi_0}{\partial A_1} & \frac{\partial\Phi_0}{\partial\alpha_1} & \cdots & \frac{\partial\Phi_0}{\partial A_h} & \frac{\partial\Phi_0}{\partial\alpha_h} \\ \frac{\partial\Phi_1}{\partial Z} & \frac{\partial\Phi_1}{\partial A_1} & \frac{\partial\Phi_1}{\partial\alpha_1} & \cdots & \frac{\partial\Phi_1}{\partial\alpha_h} & \frac{\partial\Phi_1}{\partial\alpha_h} \\ \frac{\partial\Phi_2}{\partial Z} & \frac{\partial\Phi_2}{\partial A_1} & \frac{\partial\Phi_2}{\partial\alpha_1} & \cdots & \frac{\partial\Phi_2}{\partial\alpha_h} & \frac{\partial\Phi_2}{\partial\alpha_h} \\ \vdots & \vdots & \vdots & & \vdots & \vdots \\ \frac{\partial\Phi_{2h}}{\partial Z} & \frac{\partial\Phi_{2h}}{\alpha A_1} & \frac{\partial\Phi_{2h}}{\partial\alpha_1} & \cdots & \frac{\partial\Phi_{2h}}{\partial A_h} & \frac{\partial\Phi_{2h}}{\partial\alpha_h} \end{bmatrix} \quad (14)$$

The elements in (14) may be computed from the expressions

$$\frac{\partial\Phi_o}{\partial Z} = 2n \quad (15)$$

$$\frac{\partial\Phi_0}{\partial A_i} = \frac{\partial\Phi_{2i-1}}{\partial Z} = 2\sum_{s=1}^{n} e^{-\alpha_i t_s} \qquad i = 1, 2, \ldots, h \quad (16)$$

$$\frac{\partial\Phi_0}{\partial\alpha_i} = \frac{\partial\Phi_{2i}}{\partial Z} = 2A_i\sum_{s=1}^{n} e^{-\alpha_i t_s} t_s \qquad i = 1, 2, \ldots, h \quad (17)$$

$$\frac{\partial\Phi_{2i-1}}{\partial A_r} = 2\sum_{s=1}^{n} e^{-(\alpha_i+\alpha_r)t_s} \qquad i = 1, 2, \ldots h;\ r = 1, 2, \ldots, h \quad (18)$$

$$A_i^{-1}\frac{\partial\Phi_{2i}}{\partial A_r} = A_r^{-1}\frac{\partial\Phi_{2i-1}}{\partial\alpha_r} = -2\sum_{s=1}^{n} e^{-(\alpha_i+\alpha_r)t_s} t_s \qquad i = 1, 2, \ldots, h \quad (19)$$
$$r = 1, 2, \ldots, i-1, i+1, \ldots, h$$

$$\frac{\partial\Phi_{2i}}{\partial A_i} = \frac{\partial\Phi_{2i-1}}{\partial\alpha_i} = 2\sum_{s=1}^{n} e^{-\alpha_i t_s} v_s t_s - 2A_i\sum_{s=1}^{n} e^{-2\alpha_i t_s} t_s \quad i = 1, 2, \ldots, h \quad (20)$$

$$\frac{\partial\Phi_{2i}}{\partial\alpha_r} = 2A_i A_r\sum_{s=1}^{n} e^{-(\alpha_i+\alpha_r)t_s} t_s^2 \qquad i = 1, 2, \ldots, h;\ r = 1, 2, \ldots$$
$$\ldots, i-1, i+1, \ldots, h \quad (21)$$

$$\frac{\partial\Phi_{2i}}{\partial\alpha_i} = 2A_i^2\sum_{s=1}^{n} e^{-2\alpha_i t_s} t_s^2 - 2A_i\sum_{s=1}^{n} e^{-\alpha_i t_s} v_s t_s^2 \qquad i = 1, 2, \ldots, h \quad (22)$$

and the superscript r in $J^{(r)}$ implies the insertion of the argument set (4) in (14). If we have computed the set $\Phi_u^{(r)}$ $u = 0, 1, \ldots, 2h$ by means of equations (8), (9) and (10), and require those values of $\Delta Z, \Delta A_i^{(r)}, \Delta\alpha_i^{(r)}$ $i = 1, 2, \ldots, h$ which make $\Phi_u^{(r+1)}$ $u = 0, 1, \ldots, 2h$ equal to zero, then from equation (13) we we have approximately

$$(\Delta Z^{(r)}, \Delta A_1^{(r)}, \Delta\alpha_1^{(r)}, \ldots, \Delta A_h^{(r)}, \Delta\alpha_h^{(r)}) = -J^{(r)-1}(\Phi_0^{(r)}, \Phi_1^{(r)}, \ldots, \Phi_{2h}^{(r)}). \quad (23)$$

The vectors in equation (23) (and in (24) below) are of course column vectors.

Improved values of Z, A_i, α_i $i = 1, 2, \ldots, h$ are computed by means of equations (11), and the equation system (8), (9), (10), (15)-(23) used again. (The factor 2 may of course be dropped when using equations (8)-(10), (15)-(22).)

In favorable cases this process, which corresponds to the Newton process for determing the root of an equation, is rapidly convergent. It suffers from the considerable disadvantage however that the evaluation and inversion of the Jacobian matrix at each stage, especially when n is large, involves a considerable amount of computation.

An altermative procedure is as follows. $J^{(0)}$ is computed by means of equations (14)-(22) and inverted.

The iteration then proceeds by means of equations (8)-(11) in conjunction with

$$(\Delta Z^{(r)}, \Delta A_1^{(r)}, \Delta\alpha_1^{(r)}, \ldots, \Delta A_h^{(r)}, \Delta\alpha_h^{(r)}) = -J^{(0)-1}(\Phi_0^{(r)}, \Phi_1^{(r)}, \ldots, \Phi_{2h}^{(r)}) \quad (24)$$

This constant gradient method is considerably less laborious than the previous method, but converges far more slowly.

2. An acceleration technique

The purpose of writing this note is to point out that in favourable cases for the additional cost of a trivial amount of computation, the convergence of the second method may be made as rapid as that of the first. The acceleration technique used consists of the application of the ε-algorithm.

The ε-algorithm is essentially a device for transforming the partial sums of a power series into successive convergents of an associated continued fraction. The continued fraction

$$\sum_{s=0}^{m-1} c_s z^{-s-1} + \frac{c_m z^{-m}}{z - \alpha_0^{(m)} -} \; \frac{\beta_0^{(m)}}{z - \alpha_1^{(m)} -} \; \cdots \; \frac{\beta_{r-1}^{(m)}}{z - \alpha_{r-1}^{(m)} -} \; \cdots \quad (25)$$

is said to be associated with the power series $\sum_{s=0}^{\infty} c_s z^{-s-1}$ if the power series expansion of the n^{th} convergent of (25) agrees with the original power series as far

as the term in $z^{-m-2n-1}$. It is of frequent occurrence that the convergence of the associated continued fraction is far more rapid than that of the original power series. If the r^{th} convergent of (25) is denoted by ${\varepsilon_{2r}}^{(m)}$ the various convergents ${\varepsilon_{2r}}^{(m)}$ $m, r = 0, 1, \ldots$ may be computed by use of the relationships

$$ {\varepsilon_{-1}}^{(m)} = 0, \quad {\varepsilon_0}^{(m)} = \sum_{s=0}^{m-1} c_s z^{-s-1} \qquad m = 0, 1, \ldots \tag{26} $$

$$ {\varepsilon_{s+1}}^{(m)} = {\varepsilon_{s-1}}^{(m+1)} + ({\varepsilon_s}^{(m+1)} - {\varepsilon_s}^{(m)})^{-1} \tag{27} $$

(The quantities ${\varepsilon_s}^{(m)}$ with odd suffix are auxiliary quantities of no interest in the present application.) The ${\varepsilon_s}^{(m)}$ may be arranged in the following scheme

$$
\begin{array}{ccccccc}
 & & {\varepsilon_0}^{(0)} & & & & \\
 & {\varepsilon_{-1}}^{(1)} & & {\varepsilon_1}^{(0)} & & & \\
 & & {\varepsilon_0}^{(1)} & & {\varepsilon_2}^{(0)} & & \\
 & {\varepsilon_{-1}}^{(2)} & & {\varepsilon_1}^{(1)} & & {\varepsilon_3}^{(0)} & \\
 & & {\varepsilon_0}^{(2)} & & {\varepsilon_2}^{(1)} & \vdots & \\
 & {\varepsilon_{-1}}^{(3)} & & {\varepsilon_1}^{(2)} & \vdots & & \\
 & \vdots & {\varepsilon_0}^{(3)} & \vdots & & & \\
 & & \vdots & & & &
\end{array}
$$

which is built up, column by column, by means of equation (27).

Recently the theory has been extended to consider the case in which the coefficients c_m, ${\alpha_s}^{(m)}$, ${\beta_{s-1}}^{(m)}$ are vectors and matrices. In the present application it is necessary to define the inverse of a vector for use in equation (27). Two possibilities have been exploited:
the primitive inverse

$$ (x_1, x_2, \ldots, x_k)^{-1} \equiv (x_1^{-1}, x_2^{-1}, \ldots, x_k^{-1}) \tag{28} $$

and the Samelson inverse

$$ (x_1, x_2, \ldots, x_k)^{-1} \equiv (\sum_{s=1}^{k} x_s \bar{x}_s)^{-1} (\bar{x}_1, \bar{x}_2, \ldots, \bar{x}_k) \tag{29} $$

The latter is the more efficient in the context of numerical application. The ε-array now becomes an array of vectors, the first two columns of which are given by

$$ {\varepsilon_{-1}}^{(m)} = (0, 0, \ldots, 0), \; {\varepsilon_0}^{(m)} = (Z^{(m)}, {A_1}^{(m)}, {\alpha_1}^{(m)}, \ldots, {A_h}^{(m)}, {\alpha_h}^{(m)}) \qquad m = 0, 1, \ldots \tag{30} $$

(Details of the computation are to be found in [1], and of the theory behind the method are to be found in [2].)

3. The case in which the constant term is zero

In many physical applications it is known a priori that in (1) Z must be zero.

The preceding analysis relates with equal facility to this case. Remove equations (8), (15)—(17), the initial members of the vectors in (23) and (24), and replace the Jacobian (14) by its principal minor.

4. A numerical example

In order to illustrate the methods described an example has been devised in the following way: values of $e^{-0.2\,(s-1)}$ and $e^{-0.5\,(s-1)}$ (both rounded off to four decimal places) for $s = 1(1)10$ have been added together in pairs to provide the required data f_s.

Values of

$$A_1^{(0)} = 1.05,\ \alpha_1^{(0)} = 0.202,\ A_2^{(0)} = 0.95,\ \alpha_2^{(0)} = 0.505 \tag{31}$$

have been used to start off the variable gradient scheme.

The results are displayed in Table I. The bracketed figure accompanying each set of estimates is the corresponding root mean square error

TABLE I

m	$A_1^{(m)}$	$\alpha_1^{(m)}$	$A_2^{(m)}$	$\alpha_2^{(m)}$	
0	1.0500 00	0.2020 00	0.9500 00	0.5050 00	(0.0071 28)
1	1.0177 25	0.2016 93	0.9823 81	0.5044 94	(0.0001 39)
2	1.0005 48	0.2000 51	0.9994 49	0.5001 39	(0.0000 32)
3	1.0008 00	0.2000 67	0.9991 97	0.5002 61	(0.0000 26)
4	1.0008 20	0.2000 69	0.9991 78	0.5002 66	(0.0000 26)
5	1.0008 20	0.2000 69	0.9991 78	0.5002 66	(0.0000 26)

The constant gradient method, in conjuction with an acceleration technique, (the Samelson inverse (28) has been used) has been tested on the same data and initial values (29). The vectors $\varepsilon_{2s}^{(m)}$ with corresponding root mean square error terms are displayed in Table II.

There are two points which emerge from a study of Table II. The first is that an indication of the accuracy of the estimated values of the parameters is provided by observing the change in the root mean square error which is produced by small changes in the parameter.

Secondly it will be observed that the parameter set

$$A_1 = A_2 = 1.0 \quad \alpha_1 = 0.2, \quad \alpha_2 = 0.5$$

does not provide the best approximation to the given data (this may be verified by substitution and comparing the resulting root mean square error term with others occuring in Table II). This appears to be one of the cases in which a statistical estimate of the solution provides a better result than the correct answer.

TABLE II

m\s	0	2	4	6	
0	1.0500 00 0.2020 00 0.9500 00 0.5050 00 (0.0071 28)	$(A_1^{(0)})$ $(\alpha_1^{(0)})$ $(A_2^{(0)})$ $(\alpha_2^{(0)})$			
1	1.0177 25 0.2016 93 0.9823 81 0.5044 94 (0.0001 39)	1.0164 93 0.2015 64 0.9836 02 0.5041 70 (0.0001 28)			
2	1.0165 37 0.2015 73 0.9835 59 0.5041 92 (0.0001 29)	0.9954 17 0.2014 46 1.0059 55 0.5012 43 (0.0035 68)	1.0052 86 0.2006 00 0.9946 26 0.5009 46 (0.0001 03)		
3	1.0154 12 0.2014 64 0.9846 79 0.5039 13 (0.0001 20)	1.0052 96 0.2006 01 0.9946 14 0.5009 48 (0.0001 03)	1.0029 06 0.2004 56 0.9970 97 0.5005 98 (0.0002 23)	1.0006 39 0.2000 55 0.9993 50 0.5002 26 (0.0000 28)	
4	1.0143 99 0.2013 67 0.9856 85 0.5036 57 (0.0001 12)	1.0008 06 0.2001 11 0.9991 97 0.5002 63 (0.0000 71)	1.0006 48 0.2000 57 0.9993 40 0.5002 28 (0.0000 28)		
5	1.0134 56 0.2012 78 0.9866 22 0.5034 19 (0.0001 05)	1.0006 51 0.2000 59 0.9993 38 0.5002 29 (0.0000 29)			
6	1.0125 78 0.2011 94 0.9874 94 0.5031 98 (0.0000 98)				

The data in this numerical example is given at equidistant intervals; this means that the parameters A_i, α_i $i = 1,2$ may be estimated by the method of Prony [3]. Briefly this proceeds in the given example as follows: constants X, Y are estimated by the method of least squares from the n—2 equations

$$f_{s+2} + Xf_{s+1} + Yf_s = 0 \qquad s = 1, 2, \ldots, n\text{—}2 \quad (32)$$

If the roots of the equation

$$x^2 + Xx + Y = 0 \quad (33)$$

are given by x_1, x_2 then approximations to α_1, α_2 are given by

$$\alpha_i^* = -\log(x_i) \qquad i = 1, 2 \quad (34)$$

Estimates of A_1, A_2 are provided by applying the method of least squares to the n equations

$$A_1 e^{-\alpha_1^* s} + A_2 e^{-\alpha_2^* s} = f_s \qquad s = 1, 2, \ldots, n \quad (35)$$

Applying this method to the example in hand we derive the approximations

$$A_1 = 1.0025\,26 \quad \alpha_1 = 0.2002\,35 \quad A_2 = 0.9974\,81 \quad \alpha_2 = 0.5006\,78 \quad (36)$$

and the corresponding root mean square error (0.0000 30). The set (36) may of course be used as initial values for the iteration procedures described, but it transpires that in both cases convergence to the solution is so rapid as to render the initial values (36) unsuitable for the purposes of display, and therefore slightly worse estimates have been chosen to illustrate the theory.

Acknowledgement

The numerical results in Tables I and II were computed upon the X1 in Amsterdam, using the ALGOL compiler constructed by J. A. Zonneveld and E. W. Dijkstra.

References

[1] Wynn P., Acceleration Techniques for Iterated Vector and Matrix Problems, Maths. of Comp., to appear.

[2] Wynn P., Continued Fractions whose Coefficients obey a Non-Commutative Law of Multiplication, to appear.

[3] Whittaker E. T. and Robinson G., The Calculus of Observations, 4*th* Ed., London 1944, p. 369.