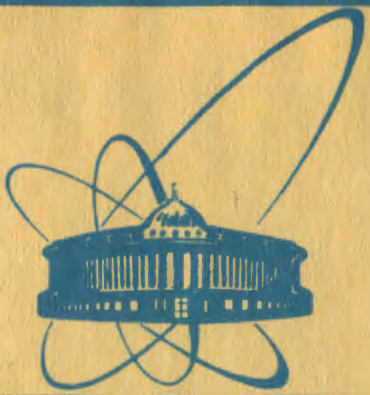

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A FORTRAN-IV COMPUTER CODE FOR THE ANALYSIS OF LATENT EXPONENTS

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1. INTRODUCTION

The analysis of latent exponents is a problem which occurs often in processing of experimental data, e.g., those from measurements of neutron flux in absorbing media, from activity measurements of isotope mixtures, etc. In all such cases a particular problem arises which belongs to the class of latent-regularity analysis [1]. The present paper aims at giving full account on the mathematical and programming means needed for the latent-exponent analysis when using relatively limited hardware: a small computer and without recurring to double-precision computations.

The next section 2 deals with the mathematical formulation of the problem to be solved. In section 3 the iteration scheme applied is described. The extraction of initial guesses from previously marked characteristic points of the input data is the subject of section 4. Section 5 considers the procedure of automatic scaling which ensures an equilibrated iteration-step matrix. The numerical results from processing some test and real experimental data by means of the technique described are presented in section 6.

2. THE PROBLEM TO SOLVE

Let the physical quantity Y be marked at m fixed values of the independent variable q, and let us have at our disposal an evaluation of the measuring accuracy ΔY, i.e., let the sets

$$\{q_i\},\ \{Y_{q_i}\},\quad \{\Delta Y_{q_i}\} \qquad i = 1,2,\ldots,m \tag{2.1}$$

be given. Let a plausible model of the phenomenon studied lead to the representation

$$Y(q) = \sum_{j=1}^{k} A_j \exp(\lambda_j q) + B(q), \tag{2.2}$$

where the amplitudes A_j and the decrements λ_j as well as the background function $B(q)$ are unknown. The latter can be expressed in the form

$$B(q) = \sum_{r=0}^{s} a_r P_r(q), \qquad (2.3)$$

where $P_r(q)$ are polynomials orthonormal over the point set $\{q_i\}$ of (2.1) which are numerically built according to /2/. If we now substitute each pair of Y_{q_i} and q_i from (2.1) in (2.2) taking into account (2.3), the following nonlinear simultaneous equations are obtained:

$$Y_{q_i} = \sum_{j=1}^{k} A_j \exp(\lambda_j q_1) + \sum_{r=0}^{s} a_r P_r(q_i), \quad i = 1,2,\ldots,m. \qquad (2.4)$$

Clearly, the number of unknows is

$$n = 2k + s + 1. \qquad (2.5)$$

As usually m exceeds n, the system (2.4) is overdetermined and, therefore, approximate. Note that in actual measurements it may happen that k itself is also unknown; in the case (2.4) is said to represent a full problem of the analysis of latent exponents /1/. As to the maximum degree of background polynomials s, it may be defined according to statistical criteria /3/.

Each equation of (2.4) is assigned a statistical weight

$$w_i = 1/(\Delta Y_{q_i})^2. \qquad (2.6)$$

If the quantities measured are counts which follow Poisson's distribution, then ΔY are evaluated as $\sqrt{Y}$, and the statistical weights take the form

$$w_i = 1/Y_{q_i}. \qquad (2.7)$$

Let us introduce the notations

$$x = \mathrm{col}(\lambda_1, A_1, \ldots, \lambda_k, A_k, a_0, a_1, \ldots, a_r) \in R^n, \qquad (2.8)$$

$$Y = \mathrm{col}(Y_{q_1}, Y_{q_2}, \ldots, Y_{q_m}) \in R^m, \qquad (2.9)$$

then (2.4) can be written as

$$Y = Fx, \qquad (2.10)$$

where F is the nonlinear operator of the right-hand side of (2.4). Moreover, denoting

$$Fx - Y = fx \qquad (2.11)$$

we compress (2.4) into

$$fx = 0. \tag{2.12}$$

As there is no exact solution of (2.12) it is a usual practice to look for its solution $\tilde{x}$ in the sense of the least squares where $\tilde{x}$ is such as to minimize the weighted Euclidean norm

$$\theta = \sqrt{\frac{\overline{fx}Wfx}{m-n}}, \tag{2.13}$$

which is, in addition, normalized to the number of degrees of freedom m−n. The overscore in (2.13) denotes transposition and

$$W = \mathrm{diag}(w_1, w_2, \ldots, w_m). \tag{2.14}$$

Thus, the problem to be solved when (2.1) are given consists of finding those components of (2.8) which approximately satisfy (2.12) and minimize (2.13). In certain cases the number of terms under the first sum of (2.4) can also be unknown and is to be determined.

3. THE ITERATION SCHEME

There exist well-known difficulties encountered when one attempts a numerical solution of the problem just posed [4,5]. Since it is a nonlinear one, the application of an iteration procedure is indispensable whose steps are, as a rule, ill-conditioned. To improve the situation and to achieve convergence regularization is applied - either is a specific two-step linearizing approach [5,6] or, more generally, when using authoregularization [7]. We renounced the former while hardware limitations did not allow for the latter; therefore, another way ought to be sought for. Our choice fell on the regularized Gauss-Newton method with an exponentially-decreasing regularizer [1,7]. There are at least two reasons to justify it: (i) the method performs quite well when applied to the analysis of latent Gaussians and (ii) it may be implemented on a small computer without double-precision options [8-11]. Since in a previous paper [9] we described this method in detail, only the basic iteration formulae are repeated here.

$$x^0;\ x^{t+1} = x^t - [V(x^t) + \alpha^t I]^{-1}\,\overline{f'(x^t)}Wfx^t, \tag{3.1}$$

$$V(x^t) = \overline{f'(x^t)}Wf'(x^t), \tag{3.2}$$

$$[f'(x^t)]_{ij} = \partial f_i(x^t)/\partial x_j^t \,, \tag{3.3}$$

$$\alpha^t = \alpha_0 e^{-rt} + \alpha_\infty \,, \tag{3.4}$$

$$\alpha_0 = \begin{cases} e^{r_0\theta(x^0)} & \text{if } \theta(x^0) < \theta_{max} \\ e^{r_0\theta_{max}} & \text{if } \theta(x^0) \geq \theta_{max} \end{cases} \,, \tag{3.5}$$

where x^0 is the vector of initial guesses; I is a unit matrix of rank n; r, α_∞, r_0 and θ_{max} are experimentally-chosen constants.

4. THE INITIAL-GUESS VECTOR

Both the convergence itself and the number of iterations $\tilde{t}$ required to reach the solution $\tilde{x}$ depend on the suitable choice of the initial-guess vector x^0. We suppose that the raw experimental data have been pre-processed in a man-machine dialogue carried out by means of a graphical display [12,13]. Apart from formatting and sectioning, the main purpose of the dialogue is to point out three characteristic points for each exponent present or suspected in the input data. Let the characteristic points for the i^{th} exponent be (q_1, Y_1), (q_2, Y_2) and (q_3, Y_3) respectively, the i-subscript being omitted for the sake of brevity. Then the initial values of λ_i^0 and A_i^0 can be computed according to the second-difference formulae reported in [12]. If, in addition, we request that the abscisses q_1, q_2 and q_3 be equidistant, a more precise evaluation is easily obtained:

$$\lambda_i^0 = [\ln \frac{Y_1 - Y_2}{Y_2 - Y_3}] / (q_1 - q_2) \tag{4.1}$$

and

$$A_i^0 = (Y_1 - Y_2)/(e^{\lambda_i^0 q_1} - e^{\lambda_i^0 q_2}) \,. \tag{4.2}$$

Each couple of values λ_i^0 and A_i^0 yields also an evaluation of the background

$$B_i = Y_1 - A_i^0 e^{\lambda_i^0 q_1} \tag{4.3}$$

and these, in turn, lead to

$$a_0^0 = \frac{1}{P_0 k} \sum_{j=1}^{k} B_j , \qquad (4.4)$$

where at given values of (2.1) P_0 is calculated according to[2]. All the remaining initial guesses $a_2^0, \ldots, a_s^0$ are taken to be zeroes.

Note that when the input data contain one exponent on a constant background (4.1)-(4.4) are as accurate as are the measurements, i.e., the formulae are not based on simplifying assumptions. Hence, in such cases the solution $\bar{x}$ can be reached in a very limited number (1 to 3) of iterations. Our practice of processing data from measurements of non-stationary neutron transport confirms largely this conclusion.

5. THE AUTOMATIC SCALING PROCEDURE

As in[9], we shall take advantage of scaling in R^n to achieve an equilibrated iteration-step matrix V with a possibly lower condition number cond V. Let $z \in R^n$ and

$$x = Cz, \qquad (5.1)$$

where

$$C = \mathrm{diag}(c_1, c_2, \ldots, c_n). \qquad (5.2)$$

The iteration process (3.1)-(3.5) can now easily be re-written with respect to the new variable z; obviously the step matrix $V' = V(z^t)$ will take the form

$$V' = CVC, \qquad (5.3)$$

and the elements of C should be suitably selected. Note that both V and V′ are symmetric and positively-defined. Furthermore, from the non-negative weights w_i and from the Cauchy-Schwarz inequality it follows that for any couple of subscripts i and j

$$v_{ii} \cdot v_{jj} \geq (v_{ij})^2 . \qquad (5.4)$$

This inequality holds for both V and V′. Therefore, if we are able to make the V′ diagonal elements equal to unity, equlibration of V′ would be accomplished.

Now, combining (3.2), (3.3) and (5.3), we obtain

$$v'_{ii} = \sum_{j=1}^{m} c_i^2 w_j (f'_{ji})^2 \qquad (5.5)$$

or, taking also into account (2.7),

$$v'_{ii} = c_i^2 \sum_{j=1}^{m} (f'_{ji})^2 / Y_{q_j} . \qquad (5.6)$$

The values of the diagonal elements v'_{ii} are supposed to be made as close to unity as possible by means of suitably chosen c_i.

The direct calculation of the sum in (5.6) for each iteration is a time-consuming procedure which should - and can - be simplified; moreover, we request that $v'_{ii} \sim 1$ rather than the precise equality $v'_{ii} = 1$. Hence, in case our initial guesses are of the same order of magnitude as the components of the solution vector $\tilde{x}$, we can scale once only, at iteration number $t=0$; then

$$c_i = (S_i^0)^{-1/2} , \qquad (5.7)$$

where S_i^0 stands for the sum in (5.6) at the initial values of the unknown parameters. To compute approximately S_i^0 the following steps are carried out:

- summation is replaced by integration over dq from q_1 to q_m;
- derivatives are obtained according to (2.4);
- instead of the precise denominator Y_{q_j} the i-th exponential term of (2.4) is substituted while the background is neglected.

With these assumptions one obtains analytically:

5.1. For the decrement scaling coefficients -

$$c_{2i-1} = [(\lambda_i^0)^3 / A_i^0 \xi_i]^{1/2} ; \quad i = 1,2,\ldots,k , \qquad (5.8)$$

where

$$\xi_i = e^{u_m} (u_m^2 - 2u_m + 2) - e^{u_1} (u_1^2 - 2u_1 + 2) \qquad (5.9)$$

with

$$u_m = \lambda_i^0 q_m \qquad (5.10)$$

and

$$u_1 = \lambda_i^0 q_1 . \qquad (5.11)$$

5.2. For the amplitude scaling coefficients -

$$c_{2i} = [\lambda_i^0 A_i^0/(e^{u_m} - e^{u_1})]^{1/2} \; ; \quad i = 1,2,\ldots,k. \qquad (5.12)$$

5.3. Note that when $i > 2k$ the corresponding matrix elements of V are equal to unity by their very construction /2/. Therefore, no scaling of the background coefficients is needed.

5.4. And, last but not least, to avoid additional round-off errors in the scaling-descaling transforms we use not the values computed according to (5.8) and (5.12) but the nearest to them integer degrees of the base 2, i.e., these transforms affect the binary exponents rather than the respective mantissas.

6. IMPLEMENTATION AND NUMERICAL RESULTS

6.1. The method described was implemented in a FORTRAN-IV computer code EXPØN which is being run on IZØT-0310, a machine compatible with PDP-8 at instruction level. The computer uses 23-bit mantissa and does not possess double-precision options. Implementation is based on the KATØK-F modules /10,11/ and on the subroutine package /2/ which builds numerically a polynomial family orthogonal over a point set. EXPØN consists of the total of 19 modules:

(i)	KUBØK (main)
(ii)	KATØK
(iii)	FLSTK
(iv)	THETL
(v)	ALPHA
(vi)	ALFO
(vii)	GRAPH
(viii)	EXPØN
(ix)	PORTHN
(x)	INVKA
(xi)	INØUT
(xii)	INØU1
(xiii)	INØU2
(xiv)	INØU3
(xv)	INØU5
(xvi)	INØU6
(xvii)	INØU7
(xviii)	ØRTHØN
(xix)	ERØRTH

whose role is exactly as described in refs. [2,10,11]. Modules ii - vii, ix - x, xii, xv and xvii - xix have been borrowed without modifications; module xiii contains insignificant FØRMAT changes concerning the output headers; the text of modules i, viii, xi, xiv and xvi is available from the author.

The actual values of constants used in (3.4) and (3.5) have been experimentally set to

$$r = 0.5,$$

$$\alpha_{\infty} = 0.00001,$$

$$r_0 = 0.0125,$$

$$\theta_{max} = 24.0.$$

Note that by inverting the order of cycles in computing the V-matrix it became possible to drop the largest array FIXT (100,40) in all CØMMØNs which leads to core economy and allows for loading the whole code into 28K 12-bit memory without recurring to overlay.

6.2. To test the entire package we composed an artificial problem with three exponents where the background is constant

$$Y_q = 40000\,e^{-.2q} + 20000\,e^{-.1q} + 10000\,e^{-.05q} + 5000$$

are calculated Y_q for $q = 0,1,2,\ldots,99$ up to the tenth decimal digit. These values rounded to the nearest integer (to simulate pulse counts as in real measurements) represent the input and are shown in Table 1. The last four rows in the table are the co-ordinates of the same number of characteristic-point groups, i.e., we suppose the number of exponents to be unknown and presume them not to exceed four.

These characteristic points yield according to (4.1)-(4.4)

λ_1^0 = -.169008	A_1^0 = 61935.2	B_1 = 13064.8	
λ_2^0 = -.084993	A_2^0 = 35061.5	B_2 = 5587.75	
			$\bar{B}$=7169.25
λ_3^0 = -.056181	A_3^0 = 15438.1	B_3 = 5017.55	
λ_4^0 = -.053949	A_4^0 = 13671.0	B_4 = 5006.86	

After the third iteration the program drops the forth exponent as insignificant and starts the process anew with three exponents only. The significance test is continuously carried out but no other superfluous component is detected. Solution is

Table 1

Input data of artificial test Problem with three exponents and constant background

(q -values from 0 to 99 follow in groups of ten along each row)

75000	65358	57236	50376	44567	39634	35432	31842	28766	26120
23836	21859	20141	18642	17330	16178	15162	14263	13465	12754
12118	11548	11036	10574	10155	9776	9431	9117	8830	8567
8326	8105	7901	7713	7539	7378	7229	7091	6963	6844
6733	6630	6533	6444	6360	6281	6208	6139	6074	6014
5957	5904	5854	5807	5763	5722	5683	5646	5611	5578
5548	5519	5491	5465	5441	5418	5396	5376	5356	5338
5320	5304	5288	5273	5259	5246	5234	5222	5211	5200
5190	5180	5171	5163	5154	5147	5139	5132	5126	5120
5114	5108	5103	5097	5093	5088	5084	5080	5076	5072

0	75000	2	57236	4	44567
25	9776	30	8326	35	7378
60	5548	70	5320	80	5190
70	5320	84	5154	98	5076

reached at the 35th iteration with θ^{35}=.0037 which cannot be further lowered because of the round-off errors present in the input. The solution vector restores the input counts within less than ±.5 units at each point which corresponds to the accuracy of data processed. At point q=93 only the approximation differs by .6 units which can be attributed to disadvantageous rounding before input and/or to piling of round-off errors during the last iteration. The output values of parameters are

$\lambda_1 = -.2001 \pm 0.001$ $A_1 = 39901 \pm 68$

$\lambda_2 = -.1004 \pm .0003$ $A_2 = 19989 \pm 25$ $B = 5000.36 \pm .25$

$\lambda_3 = -.0502 \pm .0001$ $A_3 = 10109 \pm 61$,

i.e., the agreement is very good - both as absolute figures and as accuracy estimation.

6.3. The EXPØN program is currently being used for processing data from measurements of non-stationary neutron transport in various media [14]. So far some ten series of measurements have been carried out and over 100 time-spectra processed. Divergence of the iteration process described was never observed; moreover, since a typical spectrum contains one exponent on a constant background, the display-assisted preliminary processing [13] ensures good initial guesses and a very limited number of iterations (1-3) is usually needed to reach the solution.

7. CONCLUSIONS

Latent-exponent analysis leads to ill-conditioned iteration-step matrices which can be numerically inverted if - and only if - special care is taken for improving their condition. Such care includes both process regularization and suitable scaling. None of these two measures taken separately is able to ensure convergence in single-precision computations. When combined, however, they allow for performing the analysis aimed at on small computers with limited memory and relatively slow floating point operations, i.e., on mini-machines which are usually at hand in any physical laboratory.

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