

773/2-77

Z-78



ОБЪЕДИНЕННЫЙ
ИНСТИТУТ
ЯДЕРНЫХ
ИССЛЕДОВАНИЙ

ДУБНА

28/11-77

E10 - 10192

V.B.Zlokazov

THE UNIVERSAL METHOD
OF SPECTRUM ANALYSIS

1976

E10 - 10192

V.B.Zlokazov

**THE UNIVERSAL METHOD
OF SPECTRUM ANALYSIS**

Submitted to "Nuclear Instruments and Methods"



Злоказов В.Б.

E10 - 10192

Универсальный метод анализа спектров

Для решения задачи разложения аппаратного спектра способом, наиболее не зависимым от субъективизма в описании формы полезных компонент спектра, а также формы фона, предложен метод, который использует в качестве моделей реально измеренные гистограммы изолированных компонент спектра, вводя в них некоторых фундаментальные геометрические характеристики функций в качестве параметров. Метод применим к анализу очень широкого класса аппаратных спектров. Подробно описан алгоритмический аспект метода.

Работа выполнена в Лаборатории вычислительной техники и автоматизации ОИЯИ.

Препринт Объединенного института ядерных исследований
Дубна 1976

Zlokazov V.B.

E10 - 10192

The Universal Method of Spectrum Analysis

To solve the problem of the apparatus spectrum decomposition in a way, most independent of the subjectivity in describing the shapes of the spectrum components, both those of the useful ones and that of the background, the method is proposed, which uses as models the really measured histograms of the isolated spectrum components, introducing into them some fundamental geometric characteristics of the functions as parameters. The method is applicable to the analysis of a very large class of apparatus spectra. The algorithmic aspect of the method is described in detail.

The investigation has been performed at the Laboratory of Computing Techniques and Automation, JINR.

Preprint of the Joint Institute for Nuclear Research

Dubna 1976

INTRODUCTION

This paper is the further development and generalization of the method of ref. /1/ to a more large class of problems of spectrum decomposition. In particular, the following problems are considered:

1) the decomposition of a function into peak-like components (the analysis of α -spectra);

2) the decomposition of a function into continuous components (the analysis of β -spectra, of spectra of radioactive decay of several sources, etc.);

3) the mixed problem, i.e., the decomposition of a function into peak-like as well as into continuous components (e.g., the decomposition of γ -spectrum or neutron spectrum into peaks and complicated background; or analysis of neutron diffraction spectrum, when the peak of elastic scattering may be superimposed over the peak of inelastic scattering and both over the background); a specific case is the situation when a continuous component has a fine structure, i.e., consists of peak-like and continuous subcomponents, mutually connected by some constraints (e.g., analysis of X-ray spectra, or decomposition of γ -spectrum into spectra of single isotopes). The background may be regarded as

a valid (although of no interest) component, either continuous or complicated (having peak-like subcomponents).

Contemporarily, the exact analytical form of component functions is unknown for the majority of observed spectra. The use of regression analysis technique for the spectrum processing when the models of components are singled out by occasional means, may be criticized in two relations:

- 1) subjectivity of parametrization;
- 2) inexactitude of models, because the real components have often such a shape, that it is hard to find the appropriate shape function with a little number of parameters.

There is however, an idea arising to take as models the histograms of really measured (sufficiently exactly) isolated components of the spectrum (useful as well as background) and to introduce into these histograms some fundamental geometric characteristics of the functions as parameters.

1. The Approximate Regression Analysis

Let us notice previously some specific properties of the use of regression analysis technique in the experimental physics. Let be given the set of points of measurement $\{x_j, j=1, \dots, M\}$ and the measured quantity $y(x_j)$ such that

$$y(x) = f(x, \vec{p}) + r(x),$$

where $f(x, \vec{p})$ is the superposition of the "true" physical processes (both of interest and those of background), \vec{p} -n-dimensional parameter vector, $r(x)$ -disturbance of measurement-random quantity, independent at dif-

ferent x_j with expectation equal to zero and variance $D_1(x)$. Traditionally we mean by an amount of information of the sample the number M -amount of points of the sample. However, in practice of contemporary experimental physics there is another view on the measurement informativity prevailing, namely: actually the measurement is the sum of regressions of similar nature (events):

$$y(x) = Nf(x, \vec{p}) + \sum_{i=1}^N r_i(x) = Nf(x, \vec{p}) + e(x)$$

and the amount of information (otherwise, statistic) is regarded as the function not of the amount of measurement points but of the amount of events (i.e., N). Such a view is based on profound physical and mathematical foundations:

1) the addition of complementary points x , situated out of a definite interval is either physically or technically senseless; the addition of x , situated in this interval, is limited by the resolution capacity of the apparatus; the improving of the resolution reveals, as a rule, the fine structure of regression $f(x, \vec{p})$; this leads to replacement of $f(x, \vec{p})$ by another function, thus to transition to another problem;

2) the modern experiment theory^{/2/} has instanced many facts, which convince that rather choice of the points than their amount influence the quality of the measurement;

3) the variances of the least squares (L.S.) estimates of parameters \vec{p} of regression $\sum_{i=1}^n p_i \phi_i(x)$ are, as $M \rightarrow \infty$, asymptotically proportional^{/3/} to the quantities $1 / \sum_{j=1}^M \frac{1}{D_1(x_j)} \phi_i^2(x_j)$;

this leads to a paradox: the functions, integrable in square (most suitable in the practice), are unacceptable, for then the L.S.-estimates of the corresponding parameters are inconsistent (their variances do not tend to 0 as $M \rightarrow \infty$).

The fixation of M influences negatively the quality of non-linear L.S.-estimators. Let be, e.g., $f(x, T) = \exp(-\frac{x}{T})$, $e(x) = \alpha(x) - f(x, T)$, where $\alpha(x)$ with probability not equal to 0 assumes the positive values. The probability of registration, e.g., 1 at all points x_j being not equal to zero, and because L.S.-estimate of T is in this case obviously ∞ , we can see, that the unique L.S.-estimate of this simple (but of great importance in experimental physics) problem has no finite expectation and variance.

The rigorous mathematical analysis of properties of L.S.-estimators on condition M being fixed and N (statistic) varied is given in ref.^{/4/}. It has been shown there that, if $f(x, \vec{p})$ is twice continuously differentiable with respect to \vec{p} and $\partial f(x, \vec{p}_0) / \partial p_i$ are linearly independent (\vec{p}_0 - true values of \vec{p}), then the following conditions are sufficient for the existence of strongly consistent (as $N \rightarrow \infty$) L.S.-estimates of parameters \vec{p} of regression $f(x, \vec{p})$:

- 1) sufficiently exact apriori information about \vec{p}_0 is available;
- 2) the disturbance $e(x)$ has been truncated.

The disturbance $\frac{e(x)}{N}$ is truncated for the level $\epsilon > 0$ and statistic N , if

$$\frac{e_{N, \epsilon}(x)}{N} = \begin{cases} \frac{e(x)}{N}, & \text{if } |e(x)| \leq \epsilon \\ \frac{c}{N}, & \text{otherwise; } c \in [0, \epsilon]. \end{cases}$$

The truncation corresponds to such actions of experimenter: before the sample is analysed, all values differing too strongly from the expected ones at these points are corrected.

Now let us consider the approximate models. A physical model $\psi(x)$ may be regarded as the result of a measurement:

$$\psi(x_j) = m(x_j) + \delta(x_j), \quad j = 1, \dots, M_1.$$

where $m(x)$, true model; $\delta(x)$, measurement error - random quantity of the same type as $r(x)$. As a result, we have a histogram $\psi(x_j)$ defined at the points $\{x_j\}$. We can build a smooth function $\phi(x)$ (e.g., by interpolation), coinciding with $\psi(x_j)$ in x_j and consider $\phi(x)$ as a model. We can build such approximate model both for the useful spectrum components and for those of background. Further we can introduce into $\phi(x)$ parameters \vec{q} and apply to $\phi(x, \vec{q})$ the technique of regression analysis. It has been shown in ref.^{/4/} that if the statistic of model measurement increases indefinitely the disturbances $\delta(x)$ being truncated, and the errors of histogram interpolation are negligibly small compared with the variance of $\delta(x)$, then with probability 1 L.S.-estimator, using the approximate model, converges to L.S.-estimator, using the exact model; moreover in the large class of cases it will have asymptotically (as $N \rightarrow \infty$) normal distribution with the covariance matrix of linearized L.S.-estimator (i.e., that of linear regression $f(x, \vec{p}_0) + \sum_{i=1}^n \frac{\partial f(x, \vec{p}_0)}{\partial p_i} (p_i - p_{i0})$). This approach enables to express the biases of estimators in terms of the variances of $\delta_i(x)$.

2. Real Models and Fundamental Parameters

Thus, to avoid the subjectivity of parametrization, it is necessary to take as parameters some fundamental characteristics of functions, possibly similar for all spectra. The measurement gives us the model in the form $\phi_j(x)$, i.e., without implicit dependence on any parameters. Because these parameters are introduced only for the identification of spectrum components, we can consider parametrization problem as a problem of definition of minimal number of geometric function characteristics, which unambiguously determine the component location in the spectrum. Let us define the parameters proceeding from the common properties of relations between the models of isolated components $\phi(x)$ and their images $s(x)$ in the spectrum. These relations are implemented by a set of operators $\{T\}$ such that:

$$s(x) = T\phi(x).$$

The models $\{M_i\}$ and images $\{I_i\}$ have the following properties^{/5/}:

1) reflexivity (each $M_i(I_i)$ is model (image) of itself);

2) symmetry (each $M_i(I_i)$ is image (model) of $I_i(M_i)$);

3) transitivity (if M_1 is model of M_2 , and M_2 -model of M_3 , then M_1 is model of M_3 ; the same case of $\{I_i\}$). These properties mean that $\{T\}$ has a group structure. According to ref. ^{/6/} one can show that $\{T\}$ is a continuous Lie group of plane transformations on itself. The most appropriate from them for our purposes are the linear and projective groups (because the imprimitive groups

require too large a priori information and are too cumbersome for the computation). Let us consider the indicial equation system of linear group in finite form^{/6/}:

$$y_2 = \alpha_{11}y_1 + \alpha_{12}x_1 + \alpha_1; \quad x_2 = \alpha_{21}y_1 + \alpha_{22}x_1 + \alpha_2,$$

where x_1, y_1 are old and x_2, y_2 are new coordinates of plane point. So far as the model and the image in our case are always explicit single-valued functions of one variable, we can neglect the rotation subgroup, whence $\alpha_{12} = \alpha_{21} = 0$. We neglect also the constant shift along Y-axis, that yields $\alpha_1 = 0$. Then

$$y_2 = \alpha_{11}y_1; \quad x_2 = \alpha_{22}x_1 + \alpha_2 \quad \text{or} \quad T\phi(x) = \alpha_{11}\phi(\alpha_{22}x_1 + \alpha_2) \quad (1)$$

The indicial equation system for the projective group is

$$y_2 = \frac{\alpha_{11}y_1 + \alpha_{12}x_1 + \alpha_{13}}{b_{11}y_1 + b_{12}x_1 + 1}; \quad x_2 = \frac{\alpha_{21}y_1 + \alpha_{22}x_1 + \alpha_{23}}{b_{21}y_1 + b_{22}x_1 + b_{23}}.$$

Analogously to considered above, we obtain

$$y_2 = \alpha_{11}y_1; \quad x_2 = \frac{\alpha_{22}x_1 + \alpha_{23}}{b_{22}x_1 + b_{23}}; \quad \text{or} \quad T\phi(x) = \alpha_{11}\phi\left(\frac{\alpha_{22}x_1 + \alpha_{23}}{b_{22}x_1 + b_{23}}\right).$$

Denoting $\alpha_{23}/\alpha_{22} = -P$, $b_{23}/\alpha_{22} = W$, $b_{22}/\alpha_{22} = K$, $\alpha_{11} = A$, we have

$$s(x) = T\phi(x) = A\phi\left(\frac{x-P}{Kx+W}\right). \quad (2)$$

Let us put $T\phi(x) = Ay(x, P, W, K)$ and normalize $\phi(x)$:

$$T_1\phi(x) = \frac{1}{|\phi(x_0)|} \phi\left(\frac{x-x_0}{x_2-x_1}\right),$$

where x_0 is a maximum point of $\phi(x)$, x_1 and x_2 are the nearest to x_0 left and right points such that $\phi(x_1) = \phi(x_2) = \frac{1}{2}\phi(x_0)$. Then $T_1\phi(x) = 1 \cdot y(x, 0, 1, 0)$. On the one hand, the parameters A, P, W, K as parameters of common transformation groups

are the desired fundamental characteristics of the functions, on the other hand, they have a clear physical sense: A - amplitude, P - position, W - fwhm, K - coefficient of linear dependence of width on x.

The relation (2) enables a calculation of the partial derivatives of regression function with respect to the parameters A, P, W, K, which are required by L.S.-estimator:

$$\frac{\partial s}{\partial A} = \phi(z), \frac{\partial s}{\partial P} = -\frac{A}{Kx+W} \phi'_x(z), \frac{\partial s}{\partial W} = -\frac{Az}{Kx+W} \phi'_x(z), \frac{\partial s}{\partial K} = -\frac{Azx}{Kx+W} \phi'_x(z), \quad (3)$$

where $z = (x-P)/(Kx+W)$. Similarly, the derivatives of higher orders are calculated. The relation (3) enables also the determination of component area:

$$S = \int A \phi \left(\frac{x-P}{Kx+W} \right) dx = A(W+KP) \int \phi(z) \frac{1}{(1-Kz)^2} dz.$$

The integration is carried out in the domain of values of normalized model not equal to zero. For the linear group $K=0$ and

$$S = AW \int \phi(z) dz = AWc.$$

In the practice all four parameters are required only in the complicated cases (background description, decomposition into groups, etc.). For the decomposition into peak-like functions A, P, W are sufficient (if necessary, the model should be corrected for different spectrum intervals). For the description of exponentials and exponential-like functions A and W are sufficient. The combined evaluation of background and useful components gives the more exact results. The use of the background subtraction technique achieves the most success, if the absolutely exact theoretical background is known. If only its estimate is

available then after its subtraction the residual background (sometimes more regularly shaped, e.g., more close to a polynomial) remains in the spectrum and still requires the estimating parameters in the regression function in order to avoid the biasedness of the estimates of useful parameters.

3. The Sensitivity and the Resolution of the Method

We obtain the L.S.-estimates of parameters by minimizing

$$F(x, \vec{p}, e(x)) = \sum_{j=1}^M \frac{1}{D(x_j)} \left\{ s(x_j) - \sum_{i=1}^n A_i y_i(x_j, P_i, W_i, K_i) \right\}^2 \quad (4)$$

provided that n-number of components - is known. Let us now explore the uniqueness of decomposition. This is very important because minimization of (4) optimally fits the summary regression line to spectrum values, but the distribution of the components inside this regression may be arbitrary, if, e.g., the parameters are correlated or the initial values fail to be sufficiently good. Furthermore, the minimum of (4) is found from: $\text{grad } F(x, \vec{p}, e(x)) = 0$. However, $\text{grad } F$ may be equal to zero not only at minimum points. Let us consider the cases:

1) the alteration of component numbers; physically the problem does not change, but formally it means a transformation of coordinates of the space of parameter values. Hence, $F(x, \vec{p}, e(x))$ always has at least n! minimum points, between which the local maxima, the saddle points, etc., interpose.

2) if some $A_i \rightarrow 0$, hypersurface $F(x, \vec{p}, e(x))$ locally degenerates to a hypercylinder, for then P_i, W_i, K_i cease to influence the values of F ; the degeneration becomes complete as $A_i = 0$;

3) the spectrum components often have the similar shape and equal width (within an interval); then if $P_i \rightarrow P_j$, the hypersurface F locally degenerates to a hypercylinder along the hyperplanes $b_1 A_i + b_2 A_j = \text{const}$; in the case of exponential analysis this occurs as $W_i \rightarrow W_j$; it means that decomposing the multiplets in complex cases we have practically equal chances to obtain any arbitrary combination of amplitudes, in sum equal to some constant. In such a case a menace arises to obtain an inconsistent L.S.-estimate and in order to prevent this menace one should minimize (4) not on all parameter space, but on:

$$A_i \geq s_i; P_{i+1} - P_i \geq r_i; \quad (5) \\ W_{i+1} - W_i \geq r_i$$

on conditions $K_i x_j + W_j \geq c, s_i > 0, r_i > 0$. The quantities s_i and r_i should obviously correspond to the disturbance distribution, namely: for every $e(x)$ (5) must hold with probability 1 (or sufficiently great); these quantities s_i and r_i have a transparent physical sense: they are the sensitivities and the resolutions of our method (analogous to those of instruments). That they are not equal to zero, reflects an obvious fact that the disturbances being present, the sensitivity and the resolution of the method (as well as of the instruments) are not ideal.

Of course, for the arbitrary $e(x)/N$ such quantities s_i and r_i may fail to exist and then the problem of spectrum analysis turns out to be ill-posed, i.e., our method is short of sensitivity and (or) resolution for the analysis of such a spectrum.

If the problem of spectrum analysis is ill-posed, we can (on condition that $F(x, \vec{p}, e(x))$ has no other degeneration points except for the above-mentioned ones) fictitiously select such s_i and r_i , corresponding to distribution of $e(x)$, that the estimator, being a projection of L.S.-estimator onto simplex (5) will be though biased but consistent as $N \rightarrow \infty$.

Formally s_i and r_i may be defined in such a way: let the measurement give only pure disturbances $e(x)$, which are analysed as spectra; then s_i and r_i for every bounded set $\{e(x)\}$ are upper bounds of L.S.-estimates of amplitudes and upper bounds of differences of L.S.-estimates of positions.

We can construct the estimates of these quantities. Let be chosen a level of significance α and d is the upper bound of values of some test for the hypotheses about s_i and r_i such that if $F(x, \vec{p}, e(x)) > d$, the hypothesis is considered as α -nonsignificant. Let denote $\vec{\Delta} = (s_i, r_i)$; then the estimator of $\vec{\Delta}$ is the solution of the problem:

$$\max F(x, \vec{p} + \vec{\Delta}, e(x)) \quad (6)$$

on conditions $F(x, \vec{p} + \vec{\Delta}, e(x)) \leq d, A_i \geq s_i; P_{i+1} > P_i + r_i; Kx_j + W_j \geq c$. The problem (6) is dual to the problem of parameter estimation and s_i and r_i are dual variables to A_i and P_i .

4. The Algorithmic Aspect

Thus, the problem of spectrum analysis is formally posed:

$$\min \sum_{j=1}^M \frac{1}{D(x_j)} \left\{ s(x_j) - \sum_{i=1}^n A_i y(x_j, P_i, W_i, K_i) \right\}^2 \quad (7)$$

on conditions

$$A_i \geq s_i; P_{i+1} \geq P_i + r_i; K_i x_j + W_i \geq c_i. \quad (8)$$

Remarks: 1) for the decomposition into peak-like functions the inequalities (8) have the form:

$$A_i \geq s_i; P_{i+1} \geq P_i + r_i; K_i = 0; W_j = k_j W_i + d_j + \epsilon_j; j > i. \quad (8')$$

(in particular, for γ -spectrum analysis often $k_j = 1, d_j = \epsilon_j = 0$). 2) for the decomposition into exponential-like functions (in particular, into peaks with the same positions, but with different widths) the inequalities (8) have the form:

$$A_i \geq s_i; W_{i+s} \geq W_i + r_i; K_i = 0; P_j = k_j P_i + d_j + \epsilon_j; j > i; \quad (8'')$$

(for pure exponentials $k_j = d_j = \epsilon_j = 0$;) 3) in all cases s_i and r_i should be previously determined. Further, for improving the properties of estimates one can add the following constraints:

$$A_j = \alpha_j A_i + \gamma_j; P_j = P_i + b_j + \delta_j; j > i; \quad (9)$$

$$P_{i\ell} \leq P_i \leq P_{i\ell}; P_i = \{ A_i, P_i, W_i, K_i \} \quad (10)$$

provided that the region, bounded by (9), (10) contains \vec{p}_0 .

To solve this problem the following computation procedure has been used:

1) First, the damped iterations of Gauss-Newton process^{/7/} on condition that all intermediate estimates are projected onto region (8), (9), (10) are used;

2) Last, the iterations of Newton process are used, on condition that their matrices are positive definite.

This procedure has the following advantages:

1) The constraints do not allow the estimates exceed the region of their consistency and iteration convergency;

2) The Newton process does not require the length of the step of parameter corrections (always 1);

3) The break-up of the process is more safe (strictly speaking, the Newton process is practically the unique process, which has the property: the littleness of corrections indicates the nearness of the minimum point);

4) It is possible, having tested the positive definiteness of the matrix to be convinced of the correspondence of the solution to minimum of F , but not to other zeroes of gradient of F . The last is very important because one can instance many complicated spectra, the decomposition of which with the aid of only Gauss-Newton process (even applying the damping technique) gives the results disagreeing with the true values to an inadmissibly great extent, although all outward indicators testify that the minimization has been carried out well (the accuracy of fit is achieved, $F(x, \vec{p}, e(x))$ significantly agree with χ^2 -distribution,

the graphs of components in the spectrum look very likely). The matrices were tested in the following way: all diagonal minors of 1st and 2nd order of direct and inverse matrix were calculated and their positiveness was considered as the indicator of the positive definiteness of the matrix.

Let us adduce the analytical form of the projection operators of vector \vec{p} on the inequality simplex (8), (9), (10). The projection \vec{q} of the vector \vec{p} onto (10) is performed:

$$q_i = \begin{cases} p_i, & \text{if } p_{i\ell} \leq p_i \leq p_{iu} \\ p_{i\ell}, & \text{if } p_i < p_{i\ell} \\ p_{iu}, & \text{if } p_i > p_{iu} \end{cases}$$

The projection \vec{q} of vector \vec{p} onto simplex: $p_{i+1} - p_i \geq r_i$ is performed with the aid of the procedure:

a) the indices $i\ell$ and iu are found such that for every j ($i\ell \leq j \leq iu$) the inequalities do hold: $p_{j+1} - p_j < r_j$;

b) the components of the vector q are calculated:

$$q_{iu} = \frac{1}{m} \left(\sum_{k=i\ell}^{iu} p_k + \sum_{k=i\ell}^{iu-1} (k - i\ell + 1) r_k \right), \quad m = iu - i\ell + 1;$$

$$q_j = p_j, \quad j > iu, \quad j < i\ell;$$

$$q_j = q_j - \sum_{k=j}^{iu-1} r_k, \quad i\ell \leq j < iu;$$

c) the inequalities $q_{i\ell} - q_{i\ell-1} \geq r_{i\ell-1}$; $q_{iu+1} - q_{iu} \geq r_{iu}$; are verified; if the 1st does not hold, assume $i\ell = i\ell - 1$; if the 2nd does not hold, assume $iu = iu + 1$ and repeat the actions of the points a) and b), until the

the inequalities of point c) hold; d) the next group of indices $i\ell$ and iu is found, for which b) and c) are performed; if it occurs that for the groups $\{i\ell, iu\} \{k\ell, ku\}$ $k\ell = iu + 1$ and $q_{k\ell} - q_{iu} < r_{iu}$ take place, then both the groups are united and q_i are recalculated according to formulas b); and so on until for all q_i $q_{i+1} - q_i \geq r_i$ hold.

The projection onto $Kx + W \geq c$ under assumption that $Kx + W$ has the form of Chebyshev polynomial is carried out in such a way ($x \in [-1, +1]$):

$$1) \quad q_1 = K, \quad q_2 = W, \quad \text{if } W - K \geq c, \quad W + K \geq c;$$

$$2) \quad q_1 = 0, \quad q_2 = c, \quad \text{if } W - K < c, \quad W + K < c;$$

$$3) \quad q_1 = (c - W + K)/2, \quad q_2 = (c + W - K)/2, \quad \text{if } W - K \geq c, \quad W + K < c;$$

$$4) \quad q_1 = (K + W - c)/2, \quad q_2 = (c + W + K)/2, \quad \text{if } W - K < c, \quad W + K \geq c;$$

The projection \vec{q} of the vector \vec{p} onto simplex, bounded by the inequalities:

$$p_j = k_j p_i + h_j \pm \epsilon_j, \quad j > i \quad (11)$$

is carried out with the aid of following procedure:

a) all j for which $|p_j - k_j p_i - h_j| > \epsilon_j, j > i$, are found;

b) $\delta_j = \epsilon_j \text{ sign}\{p_j - k_j p_i - h_j\} + h_j$ are calculated;

c) the components q_i are calculated:

$$q_t = p_t \quad \text{if } t \notin \{j\}$$

$$q_i = \left(\sum_{\ell=2}^m k_\ell (p_\ell - \delta_\ell) + p_i \right) / \left(1 + \sum_{\ell=2}^m k_\ell^2 \right),$$

m - number of indices j ; $q_s = k_s q_i + \delta_s, s \in \{j\}$.

d) then the inequalities of point a) are verified, and if new indices, for which these

inequalities hold, are found, they are added to $\{j\}$, and the actions of the points $b)$, $c)$, $d)$ are repeated, until (11) hold.

R e m a r k: if some $\epsilon_i = 0$, it is more preferable to construct the projections on such equalities, transforming the matrix of the iterational processes (it makes the matrix better conditioned); a possible algorithm is given in ref.^{8/}

The method, described in this paper, has been implemented in the subroutine UPEAK, written in FORTRAN-4 language and oriented to be used on the computers with the memory capacity about 32K. The UPEAK can interact with any arbitrary subroutine (e.g., display-oriented software, etc.). The experimentally measured components (background and useful components, simultaneously not more than two for each spectrum interval) may be used as models. The UPEAK was successfully used for the analysis of γ - and X-ray spectra neutron diffraction spectra, fragment spectra, spectra of radioactive decay and so on.

ACKNOWLEDGEMENTS

The author is deeply grateful to Prof. N.N.Govorun for his stimulating support in this work. He would like also to thank Prof. E.P.Zhidkov for useful discussions.

REFERENCES

1. V.B.Zlokazov. Nucl.Instr.and Meth., 130, 543 (1975).
2. V.V.Nalimov. The Theory of an Experiment (in Russian) (Moscow, Nauka, 1971).

3. E.Malinvaud. Ann.Math.Statist., 41 (3), 856 (1970).
4. V.B.Zlokazov. JINR, P11-10186, Dubna, 1976 (in Russian).
5. Chao Young Cheng. Mathematical Logic and Its Applications (Moscow, Nauka, 1965) (in Russian).
6. V.S.Fain. Pattern recognition (Moscow, Nauka, 1970) (in Russian).
7. A.R.Gallant. Amer.Statist., 29(2), 73 (1975).
8. E.V.Meerwall. Comp.Phys.Commun., 9(2), 117 (1975).

Received by Publishing Department
on October 28, 1976.