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THEORETICAL AND MATHEMATICAL PHYSICS

On the Estimation of the Maximum Possibility for the Parameters of a Measurement Model

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Abstract—The problem of estimating the parameters of the model of a measurement experiment using the results of measurements with an error is considered. The mathematical model of the measurement error is formulated in terms of the theory of possibilities; the distribution of the possibilities on the set of error values determines the order that indicates which error values are preferred (that more probably occur during measurement) and which are less preferred. It is assumed that small error values are preferable to large ones. The mathematical model of the experiment depends on unknown parameters. The problem is to specify the values of these parameters by choosing their estimate for which the difference between the results of experiment and the model prediction is the most possible; this estimate is called the estimate of maximum possibility. An example of estimating the parameters of a Mössbauer spectrometric experiment is given.

Keywords: mathematical measurement model, theory of possibilities, optimal estimates of the model parameters, linear programming, spectrometry.

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INTRODUCTION

In modern experimental investigations the values of studied parameters, g, of objects or phenomena cannot be measured directly; they are estimated from the results of ξ measurements of quantities given by a mathematical model as functions of g.

One example of such an experiment is measurement of the electromagnetic radiation spectrum using a spectrometer [1]. In this case the input signal, g, is the electromagnetic radiation spectrum, $g(\cdot)$; the output signal $q = Ag$ of the spectrometer is formed according to the relationship

$$q(E) = \int_0^\infty a_\vartheta(E, \tilde{E}) g(\tilde{E}) d\tilde{E}, \quad E \in [0, \infty). \tag{1}$$

Here, $a_\vartheta(\cdot,\cdot)$ is the instrument function of the spectrometer; the meaning of this function is that if a monochromatic flux of gamma rays of unit intensity $\tilde{E}$ is supplied to the input of the spectrometer we obtain the following spectrum at the output: $a_\vartheta(E, \tilde{E})$, $E \in [0, \infty)$. The instrument function may depend on the unknown parameter $\vartheta \in \Theta$.

One of the common approaches to solving the problem of measurement interpretation is solving the Fredholm integral equation of the first kind (1) based on the instrument function $a(\cdot, \cdot)$ that is defined with given accuracy and measurements of the function $q(\cdot)$ that is performed with the additive error ν; the error, ν, in this case is assumed to be either bounded with respect to the norm [2] or possess known stochastic properties [3, 4]. It was demonstrated in [2, 5, 6], however, that such a problem may turn out to be ill-posed in the Hadamard sense; in particular, it may turn out to be unsolvable or have a non-unique solution, or its solution (pseudo-solution [5] if the equation $Ag = \xi$ is unsolvable) may be unstable with respect to perturbations of function $q(\cdot)$ or the mathematical measurement models. Regularization methods have been proposed for solving ill-posed problems; the basic idea of these methods is to impose additional constraints on the class of solutions in such a way that as a result the solution to the regularized problem turns out to be unique and tends to the exact solution if the measurement error ν tends to zero [7–10]. In spite of the notable success in creating methods for solving such problems, the interest in them is still strong [11, 12].

In the theory of measurement—numerical systems, unlike, regularization methods, the unknown parameters, g, are estimated from the requirement of maximum accuracy [13]. Formally, it is assumed in these problems that the result, ξ, of the measurement experiment is obtained according to the scheme

$$\xi = Ag + \nu, \tag{2}$$

where ξ is interpreted as the result of the registration of the output signal, Ag, of measurement transformer, A, that is distorted by noise, ν, if the signal, g, from the measured object is supplied to the input of this transformer. The most accurate estimate of either g or the result Ug of the g transform by given operator U is of interest. As a rule, the estimate tends to the exact value of estimated parameters g (or Ug) if the measurement error ν tends to zero. In example (1) the mathematical model of the measurement transformer, A, is given by the integral operator. If the parameters of the mathematical model are known to take any value in some domain, estimates that minimize the maximum error are used [14, 15]. In this case, the estimates are calculated for maximally unfavorable conditions and, as a rule, their errors are unacceptably large. The errors of estimates can be reduced by taking additional information on the measurement model into account.

In this study, a priori data on the measurement model are formulated in the framework of the version of the theory of possibilities that was developed in [16]. In this study, the measure of possibilities, $P(\cdot)$, is constructed on algebra, $\mathcal{F}$, of all subsets of the space of elementary events, Ω, in such a way that for each $A \in \mathcal{F}$ the value of $P(A)$ determines the relative preference, the chance that event A takes place: if $P(A) > P(B)$, event A occurs with higher probability than event B. The following statements are meaningful in the theory of possibilities: "A is more possible (less possible) than B," "A and B are equally possible," therefore, measures of possibilities $P(\cdot)$ and $P'(\cdot)$ are equivalent if a strictly monotonically increasing function $\gamma(\cdot)$ exists: $\mathcal{R}_1 \to \mathcal{R}_1$ such that for any $A \in \mathcal{F}$ the following equality is satisfied: $P(A) = \gamma(P'(A))$. The fundamental idea in this version of the theory of possibilities is the fuzzy element ν of normalized space $\mathcal{R}$ which, by analogy with a random element in probability theory, is given by the distribution of possibilities $\pi^\nu(\cdot)$: $\pi^\nu(x) = p_0$ is the possibility of equality $\nu = x$. If $\pi^\nu(x) = 0$, equality $\nu = x$ is impossible, if $\pi^\nu(x) = 1$, equality $\nu = x$ is quite possible, and if $\pi^\nu(x) > \pi^\nu(y)$, equality $\nu = y$ is less possible than $\nu = x$.

In this study, it is assumed that large measurement errors are less possible than small ones. This statement is formalized by defining the distribution $\pi^\nu(\cdot)$ monotonically decreasing with increasing error ν norm. The estimate of the maximum possibility of parameters of measurement model (2) in the simplest case is found from the following considerations. Let $\tilde{g}$ be some estimate of the input signal, g, then $\tilde{\nu} = \xi - A\tilde{g}$ is the measurement error that explains the difference of measurement result ξ from $A\tilde{g}$, its possibility is $\pi^\nu(\xi - A\tilde{g})$. The estimate $\tilde{g}$, which is chosen from the condition $\tilde{g} = \arg\sup_{\tilde{g}} \pi^\nu(\xi - A\tilde{g})$, is called the estimate of the maximum possibility. It is also assumed in this study that model A of the measurement device depends on the unknown parameter $\vartheta \in \Theta$, where Θ is the given bounded set and a priori constraints on the values of input signal g are imposed.

Below, we obtain the estimate $(\hat{\vartheta}, \hat{g})$ of the maximum possibility. We compare the estimate of the maximum possibility and the estimate that minimizes the maximum error under the condition that the error ν in (2) can take any value from a given bounded set. The efficiency of the estimate of the maximum possibility is demonstrated by solving the estimation problem for a Mössbauer spectrum measured with a spectrometer with an instrument function that depends on two scalar parameters from known intervals.

1. A MODEL OF THE MEASUREMENT AND FORMULATION OF THE ESTIMATION PROBLEM FOR MODEL PARAMETERS

1.1. Reducing the Model of the Measurement of an $\mathcal{L}^2(X)$ Element to a Finite-Dimensional Model of Measurement

In practice, the result of measurement is usually a finite set of numbers. Thus, in the example that was considered in the Introduction, the spectrum $q(\cdot)$ in (1) is a continuous function of radiation energy $E \in [0, \infty)$ and its values at points $E_1, \ldots, E_n$ are recorded in the experiment. The result of the spectrum measurement are the numbers $\xi_1, \ldots, \xi_n$, which are interpreted as spectrum values distorted by the noise at the output of the spectrometer for given energy values.

Let us write the result of the measurement ξ_i, $i = 1, \ldots, n$ as

$$\xi_i = q(x_i) + \nu_i = \int_X a_\vartheta(x_i, \tilde{x}) g(\tilde{x}) d\tilde{x} + \nu_i, \quad x \in X, \tag{3}$$

assuming that $g(\cdot) \in \mathcal{L}^2(X)$ is defined by its representative continuous on X, and $a_\vartheta(\cdot, \cdot) \in \mathcal{L}^2(X \times X)$ is defined by its representative continuous on $X \times X$. Then, denoting $\int_X a_\vartheta(x_i, \tilde{x}) g(\tilde{x}) d\tilde{x} = (a_{\vartheta,\, i}, g)$, where $(\cdot, \cdot)$ is the scalar product in $\mathcal{L}^2(X)$, we rewrite (3) as

$$\xi_i = (a_{\vartheta,i}, g) + \nu_i, \quad i = 1, \ldots, n. \tag{4}$$

Here, the following notation is used: $a_{\vartheta,\, i} = a_\vartheta(\cdot) = a_\vartheta(x_i, \cdot) \in \mathcal{L}^2(X)$ and $a_{\vartheta,\, i}$, $i = 1, \ldots, n$, depending on the parameter ϑ, whose value is a priori unknown, while the set Θ of its possible values is given.

Let us denote by $\mathcal{L}_\vartheta] \subset \mathcal{L}^2(X)$ the linear shell of elements $a_{\vartheta,\, i} \in \mathcal{L}^2(X)$, $i = 1, \ldots, n$, and by P_ϑ the orthogonal projector in $\mathcal{L}^2(X)$ onto $\mathcal{L}_\vartheta$. Then, $(I - P_\vartheta)$ is the orthogonal projector onto the orthogonal complement $\mathcal{L}_\vartheta$. Let us also denote by $\mathcal{R}_n$ the arithmetic linear space whose elements are sets of n numbers (coordinates), $\vec{\xi} = (\xi_1, ..., \xi_n)$, $\vec{\nu} = (\nu_1, ..., \nu_n)$, $\vec{f} = (f_1, ..., f_n)$.

Proposition 1. *For any $\vartheta \in \Theta$ the result of measurement* (4) *is independent of the component $(I - P_\vartheta)g$. The value of the component $P_\vartheta g \in \mathcal{L}_\vartheta$ at any point $x \in X$ can be defined as a linear combination $P_\vartheta g(x) = \sum_{i=1}^{n} f_i a_{\vartheta,i}(x)$ of values $a_{\vartheta,i}(x)$ of continuous functions $a_{\vartheta,i}(\cdot)$, $i = 1, ..., n$. Coefficients $f_1, ..., f_n$ are the coordinates of vector $\vec{f} \in \mathcal{R}_n$ that are measured in the experiment according to the linear scheme*

$$\vec{\xi} = B_\vartheta \vec{f} + \vec{n}, \tag{5}$$

where $\vec{\xi} = (\xi_1, ..., \xi_n)$, $\nu = (\nu_1, ..., \nu_n)$, $\{B_\vartheta\}_{ik} = (a_{\vartheta,i}, a_{\vartheta,k})$, $i, k = 1, ..., n$. The vector $\vec{u}$ whose coordinates are the values of $P_\vartheta g(\cdot)$ at points $x_1, ..., x_N \in X$, is connected with the vector $\vec{f}$ by the linear relationship

$$\vec{u} = U_\vartheta \vec{f}, \tag{6}$$

where $U_{\vartheta ji} = a_{\vartheta,i}(x_j)$, $i = 1, ..., n, j = 1, ..., N$.

Proof. Let P_ϑ be the orthogonal projector in $\mathcal{L}^2(X)$ onto $\mathcal{L}_\vartheta$. Then, coefficients $f_1, ..., f_n$ exist such that

$$P_\vartheta g(x) = \sum_{k=1}^{n} f_k a_{\vartheta,k}(x), \quad x \in X. \tag{7}$$

Since $(a_{\vartheta,i}, g) = (a_{\vartheta,i}, P_\vartheta g + (I - P_\vartheta)g) = (a_{\vartheta,i}, P_\vartheta g)$, substituting the expression $(a_{\vartheta,i}, P_\vartheta g)$ into (4) instead of $(a_{\vartheta,i}, g)$ and taking (7) into account we obtain (5). Substituting the values of $x = x_1, ..., x_N$ into (7)we obtain (6).

The meaning of Proposition 1 is that in the framework of the defined measurement models in the absence of a priori knowledge of $(I - P_\vartheta)$, only the component $P_\vartheta g$ of element g can be estimated from measurements (4), while the values of this component at points $x_1, ..., x_N$ can be estimated from the finite-dimensional measurement scheme (5), (6).

Let us assume that in (4) $a_{\vartheta,i} \in \mathcal{L}^2(X)$, $i = 1, ..., n$ are linearly independent; then the dimensionality of the linear shell $\mathcal{L}_\vartheta$ is equal to n. Let us define a priori constraints on the coordinates $(u_1, ..., u_N)$ of vector $\vec{u}$ in the form of linear inequalities

$$u_{i,\min} \le u_i \equiv \sum_{k=1}^{n} f_k a_{\vartheta,k}(x_i) \le u_{i,\max}, \quad u_{i,\min} \ge -\infty, \quad u_{i,\max} \le \infty; \quad i = 1, \ldots, N. \tag{8}$$

The solution to the system of inequalities (8) determines the set $\mathcal{F}$ that defines a priori constraints on coordinates $f_1, ..., f_n$ of vector $\vec{f}$.

1.2. A Possibilistic Model of the Measurement Error

It was already mentioned in the Introduction that it is natural to assume that in each measurement experiment (3) small values of $|\nu_i|$ are more possible than large ones. To formalize this proposition we assume that $\nu_1, ..., \nu_n$ are fuzzy elements of $\mathcal{R}_1$ with the given possibility distribution $\pi^{\nu_i}(\cdot)$: $\mathcal{R}_1 \to [0, 1]$. The joint possibility distribution of fuzzy elements $\nu_1, ..., \nu_n$ is determined by the formula $\pi^{\nu_1,...,\nu_n}(z_1, ..., z_n) = \min\{\pi^{\nu_1}(z_1), \ldots, \pi^{\nu_n}(z_n)\}$, which formally expresses the independent character of the fuzzy elements $\nu_1, ..., \nu_n$ [16].

If $\pi^{\nu_i}(z) = 0$ for $|z| > \varepsilon_i$, the absolute value of the measurement error ν_i in (4) cannot exceed ε_i, $i = 1, ..., n$. For errors that are bounded with respect to the absolute value, small values of $|\nu_i|$ are more possible than large ones if the possibility distribution $\pi^{\nu_i}(\cdot)$ is given by the relationship

$$\pi^{\nu_i}(z) = \begin{cases} \pi_0\left(\dfrac{|z|}{\varepsilon_i}\right), & |z| \le \varepsilon_i, \\ 0, & |z| > \varepsilon_i, \end{cases} \tag{9}$$

where $\pi_0(\cdot)$ strictly monotonically decreases on the interval [0, 1], $\pi(0) = 1$.

Since the coordinates of the vector $\vec{\nu}$ are independent, their joint possibility distribution with account for (9) is given by the formula $\pi^{\vec{\nu}}(\vec{z}) = \min\{\pi^{\nu_1}(z_1), \ldots, \pi^{\nu_n}(z_n)\} = \pi_0\left(\max_{i=1,\ldots,n} \dfrac{|z_i|}{\varepsilon_i}\right)$.

1.3. The Maximum Possibility Estimate

Let some estimate $\hat{\vartheta}$, $\hat{f}_1$, ..., $\hat{f}_n$ of the values of parameter ϑ and coefficients $f_1, ..., f_n$ in (5) be chosen; then assuming that $\hat{\vartheta}$, $\hat{f}_1$, ..., $\hat{f}_n$ is the true value of these parameters, we obtain that measurement (5) is made with the error $\nu_i = \xi_i - \sum_{k=1}^{n} (a_{\hat{\vartheta},i}, a_{\hat{\vartheta},k}) \hat{f}_k$. The possibility of such error values is determined by the value of function $\pi^{\vec{\nu}}(\cdot)$ at point $\vec{\nu} = \vec{\xi} - B_{\hat{\vartheta}} \hat{\vec{f}}$. According to the possibilistic measurement model error (9), this value is

$$\pi_0\left\{\max_{i=1,\ldots,n}\left\{\frac{1}{\varepsilon_i}\left|\xi_i - \sum_{k=1}^{n} B_{\hat{\vartheta}_{ik}} \hat{f}_k\right|\right\}\right\}. \tag{10}$$

It is natural to choose the values of the estimated parameters $\vartheta \in \Theta$ and $\vec{f} \in \mathcal{F}$ in such a way that possibility (10) of the corresponding measurement error $\tilde{\nu} = \vec{\xi} - B_{\hat{\vartheta}}\hat{\vec{f}}$ is at its maximum.

Definition. Estimates ϑ^*, f_1^*, ..., f_n^* of the maximum possibility are the values of the variables ϑ, f_1, ..., f_n that provide the maximum of functional (10) for $\vartheta \in \Theta$ and f_1, ..., f_n satisfying (8).

Note that if ϑ^*, $\vec{f}^*$ are the estimates of the maximum reliability of parameters ϑ, $\vec{f}$, then

$$\vec{u} = U_\vartheta \vec{f}^* \tag{11}$$

have the same possibility as ϑ^*, $\vec{f}^*$ and thus are estimates of the maximum possibility of the values of the sought vector $\vec{u}$.

Proposition 2. *Let* $a_{\vartheta,\, i}(\cdot)$: $X \to \mathcal{R}_1$, $i = 1$, ..., n *be continuous functions in measurement scheme* (4) *whose square is integrable on* X *and* ν_i, $i = 1$, ..., n be *independent fuzzy elements with possibility distribution* (9). *Then, the estimates of the maximum possibility of the values of parameter* ϑ *and orthogonal projection* $P_\vartheta g(\cdot)$ *of function* $g(\cdot)$ *on linear shell* $\mathcal{L}_\vartheta$ *of functions* $a_{\vartheta,\, i}(\cdot)$: $X \to \mathcal{R}_1$, $i = 1$, ..., n *at points* $\{x_1, ..., x_N\} \in X$ *under condition* (8) *are* $\hat{\vartheta} = \vartheta^*$, $P_\vartheta \hat{g}(x_j) = P_{\vartheta^*} g(x_j) = \sum_{k=1}^{n} f_k^* a_{\vartheta^*,k}(x_j)$, $j = 1$, ..., N, *where* ϑ^*, f_i^*, $i = 1$, ..., n *is the solution to the problem*

$$(\vartheta^*, f_1^*, \ldots, f_n^*) = \arg \min_{\vartheta, f_1, \ldots, f_n} \left\{ \max_{i=1,\ldots,n} \left\{ \frac{1}{\varepsilon_i} \left| \xi_i - \sum_{k=1}^{n} B_{\vartheta ik} f_k \right| \right\} \middle| \vartheta \in \Theta, \quad u_{j,\min} \le \sum_{k=1}^{n} U_{\vartheta ik} f_k \le u_{j,\max} \right\}, \quad j = 1, \ldots, N. \tag{12}$$

If the minimum of the functional in (12) *is larger* than *unity, the mathematical measurement model* (4) *does not conform with its result.*

Proof. The problem of the maximization of the possibility (10) under conditions (8) is equivalent to problem (12) due to the monotonous character of function $\pi_0(\cdot)$. If the value of the minimum in (12) is larger than unity, the possibility of such an estimate is equal to zero, which means that the model and the result of measurement (4) are inconsistent.

If problem (12) has more than one unique solution, each of them is the estimate of maximum possibility of parameters $(\vartheta, \vec{f})$ and each of the values $\vec{u}^* = U_{\vartheta^*}\vec{f}^*$ is the sought estimate of the maximum possibility of vector $\vec{u}$. In order to limit the set of estimates of the vector $\vec{u}$, additional concepts are required.

For a fixed ϑ finding the minimum in problem (12) with respect to f_1, ..., f_n is reduced to a linear programming problem [13, 18]. Minimization with respect to $\vartheta \in \Theta$ is performed numerically. Note that if the minimum of the functional in (12) is larger than unity, the possibility of such an estimate is equal to zero, which indicates that the applied mathematical model is inadequate.

1.4. Minimax Estimates of the Coordinates of the Vector $\vec{u}$

The disadvantage of the estimates that are proposed above is that the error of estimating $u_i = P_\vartheta g(x_i)$, $i = 1$, ..., N, is not minimal, since these estimates are obtained from the principle of the maximum possibility, rather than the principle of minimization of the maximum error. In this regard, the problem is of interest in which the estimate $\hat{\vartheta} = \vartheta^*$ of parameter ϑ of the measurement transformer model is chosen from the principle of the minimization of the maximum error of the estimate. In this case it is assumed that errors ν_i, $i = 1$, ..., n in (4) satisfy the constraints

$$|\nu_i| \le \varepsilon_i, \quad i = 1, \ldots, n, \tag{13}$$

and there is no preference of small errors over large errors.

For formulating and solving the problem of minimax estimation we note that for fixed $\vartheta = \vartheta^*$ the sought value $u_j = P_\vartheta g(x_j)$ can be written as the scalar product

$$u_j = \sum_{k=1}^{n} U_{\vartheta^* jk} f_k = (\vec{f}, \vec{d}_j), \tag{14}$$

where $(\vec{d}_j)_k = a_{\vartheta^*,k}(x_j)$. Finding the minimum and maximum values of this scalar product under linear constraints (8), (13) written in the form

$$u_{i,\min} \le (\vec{f}, \vec{d}_i) \le u_{i,\max}, \quad i = 1, \ldots, N; \qquad \left| \xi_i - \sum_{k=1}^{n} B_{\vartheta^* ik} f_k \right| \le \varepsilon_i, \quad i = 1, \ldots, n, \tag{15}$$

as the solutions to the corresponding linear programming problems, we obtain the interval in which the sought value u_j lies; then the minimax estimate of u_j is the middle of this interval, and its error is one half of its length. The minimum and maximum values are the solutions to the minimum and maximum problems for linear functional (14) under linear constraints (15).

Let us formulate these results in the form of the following proposition.

Proposition 3. *The quantity* $(z_{i,\max} + z_{i,\min})/2$ *minimizes the maximum error of the value of orthogonal projection* $P_\vartheta g(\cdot)$ *of function* $g(\cdot)$ *on* $\mathcal{L}(\vartheta)$ *at point* $x_i \in X$ *with error* $(z_{i,\max} + z_{i,\min})/2$, *where* $z_{i,\max}$ *and* $z_{i,\max}$ *are the maximum and minimum values of the linear functional* $(\vec{f}, \vec{a}_i)$ *defined in* (14) *with constraints* (15), $i = 1, \ldots, N$. *If the system of inequalities* (15) *is inconsistent, the mathematical measurement models in* (4) *are inadequate.*

2. AN ESTIMATE OF THE MAXIMUM POSSIBILITY OF THE PARAMETERS OF A MÖSSBAUER SPECTROMETRIC EXPERIMENT

The method that was proposed above was applied for interpreting the results of a Mössbauer spectrometric experiment in which the absorption spectrum $g(\cdot)$ is measured according to scheme [1]

$$\xi_i = C - \int_{-\infty}^{+\infty} w(v - v_i)\, g(v) dv + \nu_i, \quad i = 1, \ldots, n. \quad (16)$$

Here, $w(v) = (1 - \alpha) w_L(v, \Gamma) + \alpha_{wG}(v, \Gamma)$ is the instrument function of a Mössbauer spectrometer with the signal $g(v)$ supplied to the input, $v \in \mathcal{R}_1$ is the Doppler velocity, functions $w_L(\cdot, \Gamma)$ and $w_G(\cdot, \Gamma)$ are defined by the following relationships: $w_L(v, \Gamma) = \dfrac{1}{\pi\Gamma} \dfrac{1}{1 + (v/\Gamma)^2}$, $w_G(v, \Gamma) = \dfrac{1}{\sqrt{2\pi\Gamma^2}} e^{-v^2/(2\Gamma^2)}$, $v \in (-\infty, \infty)$, parameters α and Γ are unknown, while the intervals of their variation are known: $\alpha \in [0, 1]$, $\Gamma \in [\Gamma_{\min}, \Gamma_{\max}]$. Measurements are performed for $n = 400$ values of the Doppler velocity near zero, from -1.879 mm/s to 2.109 mm/s with a uniform step. The constant C in (16) is the intensity of the incident radiation; its value belongs to the given interval $[C_{\min}, C_{\max}]$.

The input spectrum is nonnegative for all $v \in \mathcal{R}_1$ and $g(v) \to 0$ for $|v| \to \infty$. The latter relationship makes it possible to replace the infinite integration limits in (16) by finite ones with an error that is comparable with the measurement error,

$$\xi_i = C - \int_{v_1}^{v_n} w(v - v_i)\, g(v) dv + \nu_i, \quad i = 1, \ldots, n. \quad (17)$$

Let us seek the estimate of the projection of the input spectrum at the same points, $v_1, \ldots, v_n$, in which measurements (16) were performed. Then, assuming that in (5) $\vartheta = (\alpha, \Gamma) \in R_2$, $a_{\vartheta, i}(v) = w(v - v_i)$, $v \in (-\infty, \infty)$, $i = 1, \ldots, n$, we rewrite (5) with account for (17) in the explicit form,

$$\xi_i = C - \sum_{j=1}^{n} (a_{\vartheta,i}, a_{\vartheta,j}) f_j + \nu_i, \quad i = 1, \ldots, n, \quad (18)$$

approximating the scalar product in $\mathcal{L}^2(-\infty, \infty)$ with an accuracy that is comparable with the measurement error by the sum

$$(a_{\vartheta,i}, a_{\vartheta,j}) = \sum_{k=1}^{n} w(v_k - v_i) w(v_k - v_j)$$

and taking the fact into account that for such a replacement, (5) is written as

$$u_i = P_\vartheta g(v_i) = \sum_{k=1}^{n} w(v_k - v_i) f_k,$$

we obtain instead of (16)

$$\xi_i = C - \sum_{j=1}^{n} w(v_j - v_i) u_j + \nu_i, \quad i = 1, \ldots, n. \quad (19)$$

or, in a shorter notation, $\vec{\xi} = C\vec{e} - U\vec{u} + \vec{\nu}$, where $\vec{e} = (1, 1, \ldots, 1) \in \mathcal{R}_n$, u_j is the sought value of the input spectrum estimate at point v_j, $j = 1, \ldots, n$, $U \in \mathcal{R}_n \to \mathcal{R}_n$ is the finite-dimensional operator defined by the symmetric matrix $U_{ij} = w(v_j - v_i)$, $i, j = 1, \ldots, n$. Now, relationship (17) can be rewritten as

$$\xi_i = (\vec{e}\,(-U)) \begin{pmatrix} C \\ \vec{u} \end{pmatrix} + \vec{\nu}, \quad (20)$$

Here, $\vec{e}\,(-U)$ is a block matrix with the size $(n + 1) \times n$, its first block $\vec{e}$ is a column that consists of n unities, and the second block is the matrix U with the opposite sign.

Thus, the scheme of measurements is reduced to the finite-dimensional scheme

$$\vec{\xi}_0 = A\vec{g}_0 + \vec{\nu}, \quad (21)$$

in which operator A is given by the matrix $A = (\vec{e}\,(-U))$, and vector $\vec{g}_0 = \begin{pmatrix} C \\ \vec{u} \end{pmatrix} \in \mathcal{R}_{n+1}$; the matrix elements of operator A depend on the two-dimensional parameter $\vartheta = (\alpha, \Gamma)$, $\alpha \in [0, 1]$, $\Gamma \in [\Gamma_{\min}, \Gamma_{\max}]$. The following constraints are imposed on the coordinates of the vector $\vec{g}_0$: $g_{0_1} \equiv C \in [C_{\min}, C_{\max}]$, $g_{0_k} \equiv u_{k-1} \geqslant 0$, $k = 2, \ldots, n + 1$.

Thus, the problem of estimating the input spectrum is reduced to the problem that was considered in the previous section by replacing matrix B in (5) by $A = (\vec{e}\,(-U))$ and matrix U in (6) by the identity matrix.

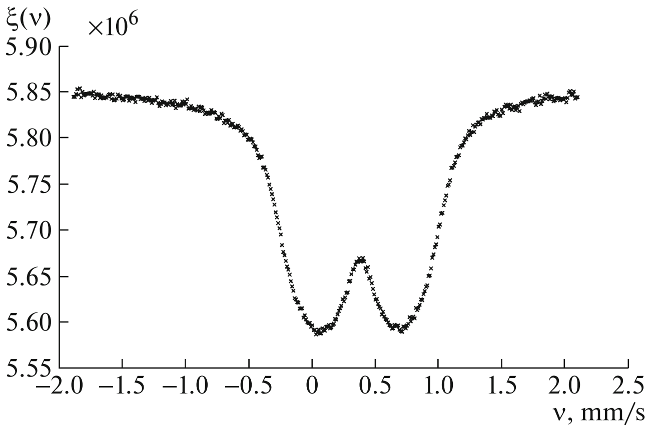

Fig. 1. The result of a Mössbauer spectrum for Doppler velocities from −1.879 mm/s to 2.109 mm/s with a step of 0.001 mm/s. The number of photons is shown along the vertical axis.

The data of Mössbauer spectroscopy that were kindly provided by V. D. Sedykh, a senior researcher of the Institute of Solid State Physics, RAS, were used for spectrum estimation. The plot of the measured spectrum at points $v_1, \ldots, v_n$ is shown in Fig. 1, $n = 400$.

At the first stage, the estimates of the parameters $(\alpha, \Gamma, u_1, \ldots, u_n)$ were obtained. For this purpose, minimax problem (12) was solved. Taking the notation used in this section into account, the problem is rewritten as follows:

$$\Phi(\alpha^*, \Gamma^*, \vec{g}_0^*) = \min_{\alpha, \Gamma, \vec{g}_0} \max_{i=1,\ldots,n}$$
$$\times \left\{ \frac{1}{\varepsilon_i} \left| \xi_i - \sum_{k=1}^{n+1} A_{ik} g_{0_k} \right| \Bigg\| g_{0_{i,\min}} \le g_{0_i} \le g_{0_{i,\max}}, i = 1, \ldots, n \right\}. \tag{22}$$

For fixed α, Γ, minimization problem (22) with respect to $\vec{g}_0$ is reduced to a linear programming problem [13, 18]. Let us denote its solution by $\vec{g}_0^*(\alpha, \Gamma)$; function $\Phi(\alpha, \Gamma, \vec{g}_0^*(\alpha, \Gamma))$ is minimized with respect to α, Γ numerically.

The plot of function $\Phi(\alpha, \Gamma, \vec{g}_0^*(\alpha, \Gamma))$ for $\alpha \in [0, 0.4]$, $\Gamma \in [0.14, 0.19]$ is shown in Fig. 2. It can be seen that for $\Gamma \geqslant 0.14$ $\Phi(\alpha, \Gamma, \vec{g}_0^*(\alpha, \Gamma))$ grows sharply with increasing Γ and is practically independent of (α, Γ) for $\Gamma < 0.14$. For $\alpha \geqslant 0.2$, $\Gamma \geqslant 0.17$ the minimum of the function $\Phi(\alpha, \Gamma, \vec{g}_0^*(\alpha, \Gamma)$ is reached at the boundary of the domain of admissible values, at $\alpha^* = 0.2$, $\Gamma^* = 0.17$. For these values, the estimate of the constant C is 5 867 450. The plot of the instrument function that corresponds to the parameters ($\alpha^* = 0.2$, $\Gamma^* = 0.14$) is

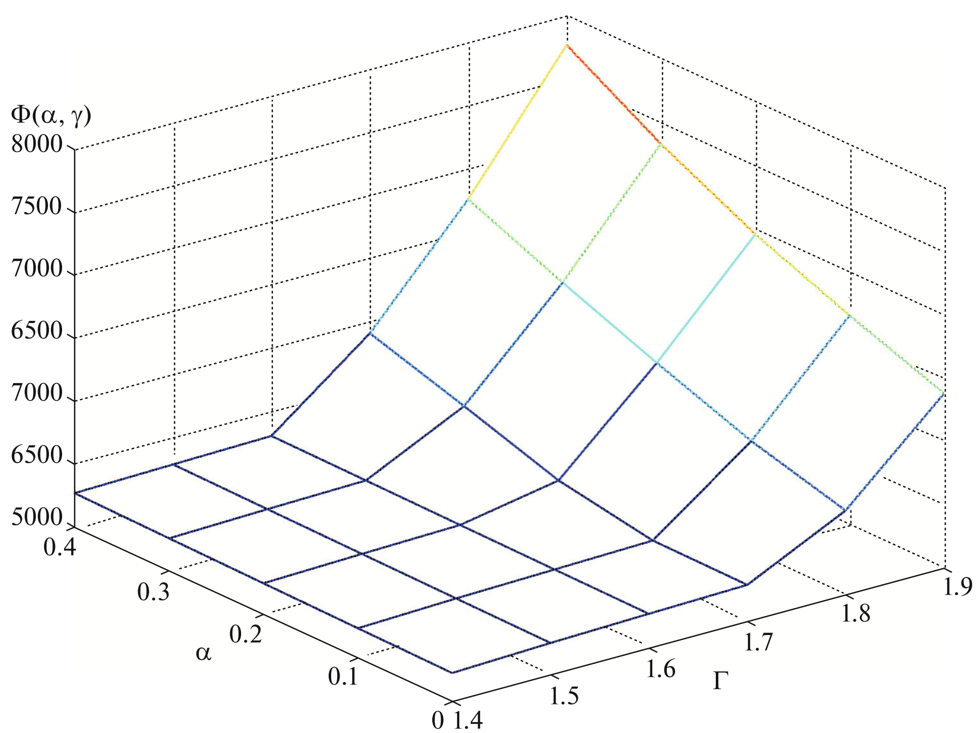

Fig. 2. Functional $\Phi(\alpha, \Gamma, \vec{g}_0^*(\alpha, \Gamma))$ minimized in (22) as a function of (α, Γ).

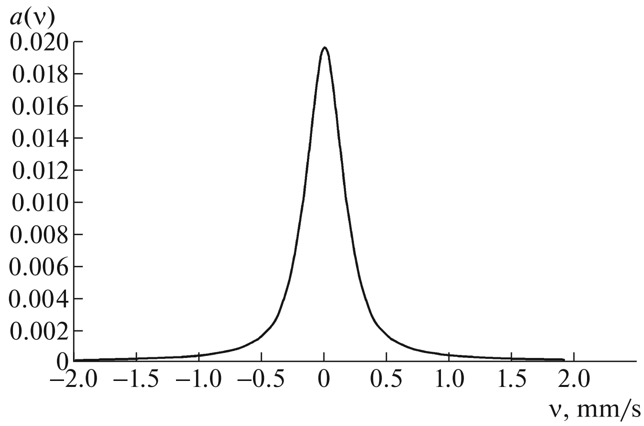

Fig. 3. The instrument function of a Mössbauer spectrometer, step 0.01 mm/s.

shown in Fig. 3 and the plot of the estimate of the input spectrum, the vector $\bar{u}^*$ is shown in Fig. 4.

To study the information value of the experiment we obtained the minimax estimate of the values of the spectrum projection for the same wavelengths. The constraints on the noise ε_i in (15) were chosen proportional to $\sqrt{\xi_i}$, $I = 1, ..., n$. The intervals $[z_{i,\min}, z_{i,\max}]$, $i = 1, ..., n$, of the variation of the spectrum coordinates (arb. u.) are shown in Fig. 5. It follows from Section 1.4 that in order to construct these estimates it is necessary to calculate the minimum and maximum values of each coordinate u_i of vector $\vec{u}$, $i = 1, ..., n$. Their arithmetic average yields the minimax estimate of the corresponding coordinate, while their half-difference yields the estimate error. The minimum values of each coordinate u_i in the analyzed experiment turned out to be practically zero for each $i = 1, ..., n$; they are shown by the points on the abscissa axis. The maximum values of the coordinates u_i, $i = 1, ..., n$, are shown in Fig. 5 as the upper base of a curvilinear trapezoid. The minimax estimate is given by the "median" of this trapezoid. It can be seen from Fig. 5 that the measurement contains insufficient information for the reliable detection of six absorption lines. Taking the additional information that large measurement errors are less possible than small ones into account yields the much better result that is shown in Fig. 4.

Such a strong difference between the results of minimax estimation and estimation of the maximum possibility in the general formulation was discussed in [14]; it was demonstrated there that minimax estimates can correspond to a situation in which realization of the measurement error has the maximum admissible norm. This situation is a low-probability case for a researcher, since experiments, as a rule, are formulated in such a way that measurement errors are as small as possible. It can be seen from comparison of Figs. 4 and 5 that taking this circumstance into account substantially improves the result of solving the problem of interpretation of measurements. Moreover, the constraint of the nonnegativeness of the coordinates of the input spectrum plays an important role in the considered problem; it can be seen from the result (Fig. 4) that a large number of coordinates of the estimate are zero, i.e., they lie at the boundary of the admissible domain, which testifies to the efficiency of these constraints.

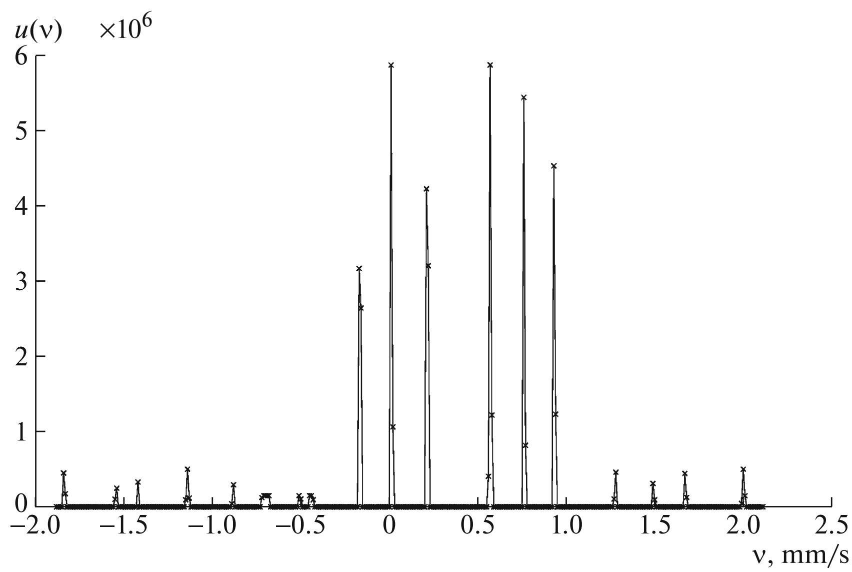

Fig. 4. The estimate of the input spectrum using the method of maximum possibility, arb. u.

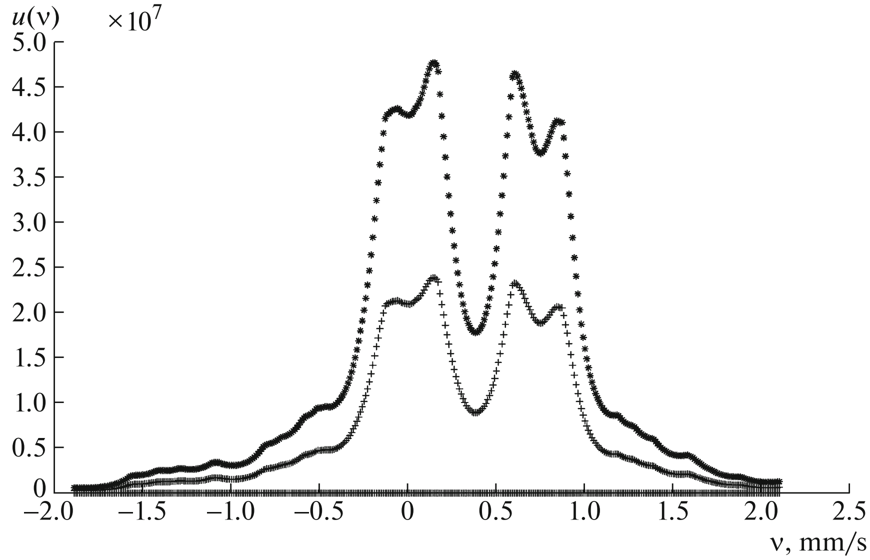

Fig. 5. The minimum, maximum, and average values of the estimated input spectrum. The minimum values for each v_i, $i = 1, ..., 400$ are practically zero; their plot coincides with the abscissa axis. The plot of the maximum spectrum values for different v_i is marked by "*"; it forms the upper base of a curvilinear trapezoid. The minimax spectrum estimate is given by the "median" of this trapezoid marked by "+."

CONCLUSIONS

The estimates of the maximum possibility of parameter values of measurement models with a finite number of linear functionals of a studied function were constructed and methods for their calculation were given. The estimate possibility was determined by the fuzzy model of the measurement error of functionals, in which it was assumed that large errors were less possible than small ones. The efficiency of the method was illustrated by estimating the parameters of a Mössbauer spectrometer and the measured spectrum for the given set of wavelengths. The obtained estimates of the spectrum values were compared with minimax estimates that were constructed under the assumption that the error of the measurement of linear functionals was bounded and arbitrary within a given interval. It was demonstrated that the assumption of high possibility of small measurement error values made it possible to obtain adequate idea of the measured spectrum, while the minimax estimates indicate that without this assumption the information that is contained in measurements was insufficient to obtain adequate spectrum estimates.

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REFERENCES

1. V. S. Rusakov, *Fundamentals of Mossbauer Spectroscopy* (Moscow, 2011) [in Russian].
2. A. N. Tikhonov and V. Ya. Arsenin, *Methods for Solving Non-Correct Problems* (Moscow, 1979) [in Russian].
3. A. M. Fedotov, *Non-Correct Problems with Accidental Errors in Data* (Novosibirsk, 1990) [in Russian].
4. V. F. Turchin, V. P. Kozlov, and M. S. Malkevich, Sov. Phys. Usp. **13**, 681 (1971).
5. V. K. Ivanov, V. V. Vasin, and V. P. Tanana, *Theory of Linear Non-Correct Problems and Its Applications* (Moscow, 1978) [in Russian].
6. M. M. Lavrent'ev, *Some Non-Correct Problems of Mathematical Physics* (Novosibirsk, 1962) [in Russian].
7. A. N. Tikhonov, A. V. Goncharskii, V. V. Stepanov, and A. G. Yagola, *Numerical Methods for Solving Non-Correct Problems* (Moscow, 1990) [in Russian].
8. A. G. Yagola, Van Yanfei, I. E. Stepanova, and V. N. Titarenko, *Inverse Problems and Methods for Solving Them. Applications to Geophysics* (Moscow, 2014) [in Russian].
9. A. A. Samarskii and P. N. Vabishchevich, *Numerical Methods for Solving Inverse Problems of Mathematical Physics* (Moscow, 2009) [in Russian].
10. V. N. Vapnik, *Reconstruction of Dependences Based on Experimental Data* (Moscow, 1979) [in Russian].

11. S. Eichstadt, F. Schmahling, G. Wubbeler, et al., in *Proc. 16th Int. Congress on Metrology, 2013*, p. 14005.

12. A. J. Silva Neto and N. Cella, Comput. Appl. Math. **25** (2, 3), 139 (2006).

13. Yu. P. Pytiev, *Methods of Mathematical Simulation of Measurement-Computational Systems* (Moscow, 2004) [in Russian].

14. A. I. Chulichkov and B. Yuan, Mash. Obuchenie Anal. Dannykh **1** (9), 1246 (2014).

15. A. I. Chulichkov and T. A. Kopit, in *Proc. 9th Int. Conf.: Intellectualization of Data Treatment, 2012,* pp. 648–651.

16. Yu. P. Pytiev, *Possibility as Alternative to Probability. Mathematical and Empirical Foundations, Application* (Moscow, 2007) [in Russian].

17. A. I. Chulichkov and B. Yuan, Moscow Univ. Phys. Bull. **69** (3), 218 (2014).

18. K. V. Kirillov and A. I. Chulichkov, Moscow Univ. Phys. Bull. **54** (2), 83 (1999). http://vmu.phys.msu.ru/abstract/1999/2/99-2-62.