Mathematical Modelling and Analysis
Volume 28, Issue 3, 459–468, 2023
https://doi.org/10.3846/mma.2023.16403

Identification of Unknown Parameters of the Dynamic Model of Mass Transfer

Volodymyr Zavialov, Oleksii Lobok, Taras Mysiura, Nataliia Popova, Valentyn Chornyi and Taras Pohorilyi

National University of Food Technologies
Volodymyrska str. 68, UA-01033 Kyiv, Ukraine
E-mail(*corresp.*): val.chor@ukr.net
E-mail: zavialov@nuft.edu.ua

Received January 28, 2022; accepted June 12, 2023

Abstract. An iterative algorithm for identifying unknown parameters of a mathematical model based on the Bayesian approach is proposed, which makes it possible to determine the most probable maximum informative estimates of these parameters. The example of the mathematical model of mass transfer dynamics shows the algorithm for finding the most probable and most informative estimate of the vector of unknown parameters, and also an analysis of the sequence of the corresponding steps is given. The results of computational experiments showed a significant dependence of the results of the calculations on the choice of the initial approximation point and slowing down the rate of convergence of the iterative process (and even its divergence) with an unsuccessful choice of the initial approximation. The validity of the obtained results is provided by analytical conclusions, the results of computational experiments, and statistical modeling. The results of computational experiments make it possible to assert that the proposed algorithm has a sufficiently high convergence for a given degree of accuracy and makes it possible to derive not only estimates of point values of mathematical model parameters based on a posteriori analysis, but also confidence intervals of these estimates. At the same time, it should be noted that the results of calculations depend significantly on the choice of the initial approximation point and the slowing of the convergence rate of the iterative process with an unsuccessful choice of the initial approximation. Analytical studies and results of calculations confirm the effectiveness of the proposed identification algorithm, which makes it possible, with the help of active, purposeful experiments, to build more accurate mathematical models. In accordance with the algorithm, a program was developed in the MatLab mathematics package and computational experiments were performed.

Keywords: iterative algorithm, mass transfer, Bayesian approach, mathematical modeling, variance, experiment.

AMS Subject Classification: 62C12.

1 Introduction

Cause-effect models based on conservation laws are widely used for the mathematical description of various processes and objects of food technology. They reflect the relationship between input (independent) and output (dependent) variables. Along with such variables of a model of this kind include parameters to be determined from experimental data.

Depending on the information available, these parameters can be estimated by the method of least squares, maximum verisimilitude, Bayesian estimation method, etc. [1, 2, 6]. At the same time, the parameters to be evaluated are adopted either by deterministic unknown quantities that, when solving a problem, require the establishment of a confidence probability interval or random variables with an a priori assumed law of distribution. The latter option is related to the Bayesian approach, which represents a more precise and flexible formal apparatus for accounting for a priori information [6] and also gives the possibility of obtaining on the basis of a posteriori analysis, not only point values of estimates of the parameters of a mathematical model, but also the confidence intervals of these estimates.

The novelty of the work is a combined approach to estimating the unknown parameters of mathematical models based on two methods: the Bayesian method of maximizing a posterior probability distribution density and the method of optimal experiment planning based on information theory. An iterative procedure has been developed that makes it possible to obtain the most informative MAP estimates. The results of some computational experiments are presented, based on which conclusions are drawn regarding the effectiveness of this approach.

2 Methodology

In this paper, based on the Bayesian estimation method, an iterative algorithm for identifying unknown parameters of the model is proposed, which makes it possible to determine the most probable maximum informative estimates of these parameters. The method of maximum a posteriori probability density (MAP) or the mode of Bayesian estimation is supplemented by the method of searching for the most informative estimate. Therefore, we can talk about the most informative MAP-estimation.

The optimization problem is difficult since it belongs to the class of conditional multidimensional optimization problems. Even for simple but real models, the objective function of this problem cannot be represented in an analytical form. Therefore, its analytical study for smoothness, multi-extremality, etc. is difficult. Computational experiments in the general case show its multi-extremality (if it starts from different points of the initial approximation, different results may be obtained). Therefore, taking into account its multi-extremality, we solve this problem many times with different initial ap-

proximations and choose the maximum value from local optima. For numerical experiments, the library of optimization methods of the mathematical package MatLab was used.

3 Results

Consider the process of mass transfer of matter [5], the dynamics of which is described by the mathematical model:

$$\begin{cases} \frac{ds(t)}{dt} = k_L \left(s^* - s(t)\right), \\ s\left(t_0\right) = s_0, \end{cases} \tag{3.1}$$

where $s\left(t\right)$ is the actual concentration of the substance in the flow at the time t, s_0 is a given initial concentration of the substance at the initial time t_0, k_L defines the mass transfer coefficient, s^* is the equilibrium concentration of this substance (concentration of the substance saturation), the parameters k and s^* are unknown and they to be determined.

Suppose that the concentrations $s\left(t\right)$ are measured at time moments t_j. These measurements are described by a model:

$$y\left(t_j\right) = s\left(t_j\right) + \xi\left(t_j\right), \quad j = 1, 2, ..., m, \tag{3.2}$$

where $y\left(t_j\right)$ is the result of the j-th measurement, $\xi\left(t_j\right)$ are random measurement errors at time t_j, these errors are distributed according the normal (Gaussian) distribution law with zero mathematical expectation and variance σ^2, i.e.,

$$M\left\{\xi\left(t_j\right)\right\} = 0, \quad D\left\{\xi\left(t_j\right)\right\} = M\left\{\xi^2\left(t_j\right)\right\} = \sigma^2, \quad j = 1, 2, ..., m.$$

We will also assume that measurement errors $\xi\left(t_j\right)$ at different time moments are uncorrelated, i.e.,

$$Cov\left(\xi\left(t_i\right), \xi\left(t_j\right)\right) = 0.$$

Further, we consider various random variables ξ (scalar or vector) defined by normally distributed random variables with mathematical expectation a and variance σ^2 (or covariance matrix V). They will be denotes as $\xi \sim N\left(a, \sigma^2\right)$ (or $\xi \sim N\left(a, V\right)$).

Based on measurements of (3.2) it is necessary to find the most reliable (probable) estimates of unknown parameters k_L and s^* of the mathematical model (3.1), such that they would have the greatest informativeness. These estimates will be found using the Bayesian estimation method, which assumes maximizing a posteriori probability density of parameter distribution and methods of active experiment planning given in the theory of information [3, 4].

By assuming the constancy of parameters k_L and s^*, the solution of the Equation (3.1) at $t_0 = 0$ can be represented as:

$$s\left(t; k_L, s^*\right) = e^{-k_L t}\left(s_0 - s^*\right) + s^*, \tag{3.3}$$

where notations $s\left(t\right) = s\left(t; k_L, s^*\right)$ are introduced. They emphasize the dependence of the concentration of the substance $s\left(t\right)$ on parameters k_L, s^*.

For convenience, we also introduce the following notation $\varphi_2 = s^*$, $\varphi = (\varphi_1, \varphi_2)^T$. Then relation (3.3) can be written as:

$$s(t;\varphi) = e^{-\varphi_1 t}(s_0 - \varphi_2) + \varphi_2, \tag{3.4}$$

and measurement equation (3.2) in the form

$$y(t_j) = s(t_j;\varphi) + \xi(t_j), \quad j = 1, 2, ..., m. \tag{3.5}$$

To find the estimate of vector of unknown parameters φ we use procedure of linearization of function $s(t_j;\varphi)$. Let $\hat{\varphi}_k$ be some the estimate of parameter vector φ computed at k-th iteration. Then $s(t_j;\varphi)$ in the neighborhood of point $\hat{\varphi}_k$ can be represented in a linearized form:

$$s(t_j;\varphi) \approx s(t_j;\hat{\varphi}_k) + H(t_j;\hat{\varphi}_k)(\varphi - \hat{\varphi}_k), \tag{3.6}$$

where $H(t_j;\hat{\varphi}_k)$ is the gradient of $s(t_j;\varphi)$ at point $\hat{\varphi}_k$:

$$H(t_j;\hat{\varphi}_k) = \left(\frac{\partial s(t_j;\varphi)}{\partial\varphi_1}, \frac{\partial s(t_j;\varphi)}{\partial\varphi_2}\right)\Bigg|_{\varphi=\hat{\varphi}_k} \tag{3.7}$$

where

$$\frac{\partial s(t_j;\varphi)}{\partial\varphi_1} = t_j e^{-\varphi_1 t_j}(\varphi_2 - s_0), \quad \frac{\partial s(t_j;\varphi)}{\partial\varphi_2} = 1 - e^{-\varphi_1 t_j}. \tag{3.8}$$

Substituting correlation (3.6) into the measurement model (3.5), we obtain the linearized equation of obsevations

$$y_j^k = H_j^k \Delta\varphi_k + \xi_j, \qquad j = 1, 2, ..., m; \qquad \xi_j \sim N(0, \sigma^2), \tag{3.9}$$

where the following notation is introduced

$$y_j^k = y(t_j) - s(t_j;\hat{\varphi}_k),\ H_j^k = H(t_j;\hat{\varphi}_k),\ \Delta\varphi_k = \varphi - \hat{\varphi}_k,\ \xi_j = \xi(t_j). \tag{3.10}$$

Using the results of work [6] and correlations (3.9), (3.10), it can be shown that the most informative Bayesian estimate of vector of unknown parameters φ, which maximizes the posterior probability density can be represented by $\{\hat{\varphi}_k\}$. The elements of it are calculated by the following iterative procedure

$$\hat{\varphi}_{k+1} = \hat{\varphi}_k + \Delta\hat{\varphi}_k, \quad k = 0, 1, 2, ..., \tag{3.11}$$

where

$$\Delta\hat{\varphi}_k = \left(\sum_{j=1}^{m} \left(H^k\left(t_j^k\right)\right)^T H^k\left(t_j^k\right) + \sigma^2 \hat{V}_k^{-1}\right)^{-1} \times \left(\sum_{j=1}^{m} \left(H^k\left(t_j^k\right)\right)^T \left(y\left(t_j^k\right) - s\left(t_j^k;\hat{\varphi}_k\right)\right)\right). \tag{3.12}$$

Here, $H^k\left(t_j^k\right) = H\left(t_j^k;\hat{\varphi}_k\right)$ is the gradient, defined by formulas (3.7), (3.8), $\left(t_1^k, t_2^k, ..., t_m^k\right) = \arg\max\limits_{t_1,t_2,...,t_m} Q_k\left(t_1, t_2, ..., t_m\right)$, i.e., $\left(t_1^k, t_2^k, ..., t_m^k\right)$ are moments that maximize objective function $Q_k\left(t_1, t_2, ..., t_m\right)$ of form:

$$Q_k\left(t_1, t_2, ..., t_m\right) = \det\left(\sum_{j=1}^{m}\left(H^k\left(t_j^k\right)\right)^T H^k\left(t_j^k\right) + \sigma^2\hat{V}_k^{-1}\right).$$

Remark 1. If variance of measurement errors σ^2 is unknown, then can find its estimate $\hat{\sigma}_k^2$ as solution of next nonlinear equation [4] relative to σ^2:

$$\sigma^2 = \frac{1}{m}\sum_{j=1}^{m}\left(y_j^k - H_j^k\Delta\hat{\varphi}_k\right)^2,$$

where $\Delta\hat{\varphi}_k$ defined by formula (3.12).

A posteriori covariance evaluation matrix $\hat{\varphi}_{k+1}$ herewith is determined by recurrence formula:

$$\begin{cases} \hat{V}_{k+1} = \sigma^2\left(\sum\limits_{j=1}^{m}\left(H^k\left(t_j^k\right)\right)^T H^k\left(t_j^k\right) + \sigma^2\hat{V}_k^{-1}\right)^{-1}, \quad k = 0, 1, 2, ..., \\ \hat{V}_0 = V_a, \end{cases}$$

where V_a – a priori estimation of covariance matrix of selective vector $\hat{\varphi}_0$.

The Bayesian approach uses a priori information about the normal distribution law of the estimated parameters. We note that a priori knowledge of the parameter estimates and the covariance matrix is necessary only at the initial step of the iterative procedure, later they are recalculated according to the above formulas.

Remark 2. If a priori information about estimated parameters $\varphi = (\varphi_1, \varphi_2) = (k_L, s^*)$ is absent or insufficient, then we can assume $V_a = \rho E$, where $\rho > 0$ is a sufficiently large value (constant), E is a unit matrix.

To avoid the need to calculate at each iteration inverse matrices $\hat{V}_k^{-1}$, we introduce the change of variables $W_k = \sigma^2\hat{V}_k^{-1}$. Then (3.12) is transformed into

$$\Delta\hat{\varphi}_k = \left(\sum_{j=1}^{m}\left(H^k\left(t_j^k\right)\right)^T H^k\left(t_j^k\right) + W_k\right)^{-1} \times \left(\sum_{j=1}^{m}\left(H^k\left(t_j^k\right)\right)^T\left(y\left(t_j^k\right) - s\left(t_j^k;\hat{\varphi}_k\right)\right)\right), \quad (3.13)$$

where matrices W_k satisfy the recurrence matrix equation

$$\begin{cases} W_{k+1} = W_k + \sum\limits_{j=1}^{m}\left(H^k\left(t_j^k\right)\right)^T H^k\left(t_j^k\right), \quad k = 0, 1, 2, ..., \\ W_0 = \sigma^2 V_a^{-1}, \end{cases} \quad (3.14)$$

and moments of time $\left(t_1^k, t_2^k, \ldots, t_m^k\right)$ are solutions of the optimization problem

$$Q_k\left(t_1, t_2, \ldots, t_m\right) = \det\left(\sum_{j=1}^{m}\left(H^k\left(t_j\right)\right)^T H^k\left(t_j\right) + W_k\right) \to \max_{t_1, t_2, \ldots, t_m}. \quad (3.15)$$

Thus, the search algorithm of the optimal (in the sense of the most probable) and most informative estimate of the vector for unknown parameters of the model (3.1) is defined by the following sequence of steps:

1. Assume that $k = 0$ and set the following quantities: σ^2 is the dispersion of measurement errors (if variance σ^2 is unknown, it should be guided by Remark 2); $\hat{\varphi}_0$ is the initial approximation vector; V_a is a priori estimation of covariance matrix of selective vector $\hat{\varphi}_0$, in particular, we can put $V_a = \rho E$, where $\rho > 1$; ε is the accuracy of calculation.
2. The optimization problem (3.15) is solved, the obtained solution is denoted by $\left(t_1^k, t_2^k, \ldots, t_m^k\right)$.
3. At points $\left(t_1^k, t_2^k, \ldots, t_m^k\right)$ measurements $y\left(t_j^k\right)$ are done of the substance $s\left(t\right)$.
4. Vector $\Delta\hat{\varphi}_k$ is calculated by the formula (3.13).
5. The following approximation is found $\hat{\varphi}_{k+1} = \hat{\varphi}_k + \Delta\hat{\varphi}_k$.
6. Matrix W_{k+1} is calculated by the recurrence equation (3.14).
7. Take $k = k + 1$ and go to the next iteration, i.e., to step 2.

The condition for stopping this iterative algorithm can be taken in form

$$\frac{||\hat{\varphi}_{k+1} - \hat{\varphi}_k||}{1 + ||\hat{\varphi}_{k+1}||} < \varepsilon, \quad (3.16)$$

where $\|\varphi\|$ is the Euclidean norm of vector, ε is the predetermined accuracy of calculations. The degree of reliability of obtained parameter estimates is obtained by using the results of the works [3, 5], the following confidence intervals for the component $\Delta\varphi_{ik}$ vector of parameters $\Delta\varphi_k = (\Delta\varphi_{1,k}, \Delta\varphi_{2,k})$ are defined

$$\Delta\hat{\varphi}_{i,k} - \delta_i^k \le \Delta\varphi_{i,k} \le \Delta\hat{\varphi}_{i,k} + \delta_i^k, \quad \delta_i^k = s_k \cdot \sqrt{c_{ii}^k} \cdot t_{\alpha;m-2}, \quad i = 1, 2, \quad (3.17)$$

where $t_{\alpha;m-2}$ is Student's t-distribution with $m-2$ degrees of freedom and the significance level α (coefficient of trust $\gamma = 1 - \alpha$), s_k^2 is the residual variance estimate:

$$s_k^2 = \frac{1}{m-2}\sum_{j=1}^{m}\left(y_j^k - H_j^k\Delta\hat{\varphi}_k\right)^2, \quad (3.18)$$

c_{ii}^k – i-th diagonal matrix element C_k of form:

$$C_k = \left(\sum_{j=1}^{m}\left(H^k\left(t_j^k\right)\right)^T H^k\left(t_j^k\right) + W_k\right)^{-1}. \quad (3.19)$$

Joint confidence regions play an important role in the analysis of model parameters, which in this case are confidence ellipsoids of the form:

$$(\Delta\varphi_k - \Delta\hat{\varphi}_k)^T C_k^{-1} (\Delta\varphi_k - \Delta\hat{\varphi}_k) \le 2 \cdot s_k^2 \cdot F_{\alpha;2;m-2}. \tag{3.20}$$

Here the value of s_k^2 is determined by the ratio (3.18), $F_{\alpha;2;m-2}$ is the Fisher criterion with degrees of freedom 2 and $m-2$ and level of significance α, C_k is matrix of the form (3.19).

Given the ratio (3.11), (3.17), (3.20), we can obtain interval estimates for unknown parameters $\varphi_{i,k+1} = \hat{\varphi}_{i,k} + \Delta\varphi_{i,k}$ at each iteration

$$\hat{\varphi}_{i,k+1} - \delta_i^k \le \varphi_{i,k+1} \le \hat{\varphi}_{i,k+1} + \delta_i^k, \quad i = 1, 2,$$

and their joint confidence ellipsoid

$$(\varphi_{k+1} - \hat{\varphi}_{k+1})^T C_k^{-1} (\varphi_{k+1} - \hat{\varphi}_{k+1}) \le 2 \cdot s_k^2 \cdot F_{\alpha;2;m-2}.$$

We now consider special case of estimating one parameter $k_L(\varphi_1 = k_L)$ of model (3.1) under the assumption that equilibrium concentration $s^*(\varphi_1 = s^*)$ is known. Then $H(t_j; \hat{\varphi}_k)$ becomes a scalar function of the form

$$H(t_j; \hat{\varphi}_k) = \left.\frac{\partial s(t_j; \varphi)}{\partial \varphi_1}\right|_{\varphi=\hat{\varphi}_k} = t_j e^{-\hat{\varphi}_{1,k} t_j} (\varphi_2 - s_0) = t_j e^{-\hat{\varphi}_{1,k} t_j} (s^* - s_0)$$

and the optimal moments of measurement $\left(t_1^k, t_2^k, \ldots, t_m^k\right)$ are solutions to the problem of maximizing the objective function

$$q_k(t_1, t_2, \ldots, t_m) = \sum_{j=1}^{m} \left(H(t_j; \hat{\varphi}_k)\right)^2 = \sum_{j=1}^{m} \left(t_j e^{-\hat{\varphi}_{1,k} t_j} (s^* - s_0)\right)^2$$
$$= (s^* - s_0)^2 \sum_{j=1}^{m} \left(t_j^2 e^{-2\hat{\varphi}_{1,k} t_j}\right). \tag{3.21}$$

Analysis of this function shows that its maximum is reached at points $t_j^k \equiv$ $\equiv t^k = 1/\hat{\varphi}_{1,k}$, $j = 1, 2, \ldots, m$, i.e., to obtain the most informative estimate of the mass transfer coefficient $\varphi_1 = k_L$ it is necessary to perform m parallel measurements of the concentration of the substance $s(t)$ at moment $t^k = 1/\hat{\varphi}_{1,k}$.

If parallel measurements are impossible and all measurements should be carried out in dynamics, then all m measurements must be concentrated in the vicinity of time moment $t^k = 1/\hat{\varphi}_{1,k}$.

Note that if measurements can be performed only on a given time interval $[0, T]$, then

$$t^k = \begin{cases} 1/\hat{\varphi}_{1,k}, & 1/\hat{\varphi}_{1,k} < T, \\ T, & 1/\hat{\varphi}_{1,k} \ge T. \end{cases}$$

Moreover, from the ratio (3.21) it follows that if in active experiment we can change initial concentration of the substance s_0 and/or the equilibrium concentration s^*, then to obtain the most informative estimate of the coefficient k_L it is necessary that a difference in these concentrations $s^* - s_0$ be as big as possible.

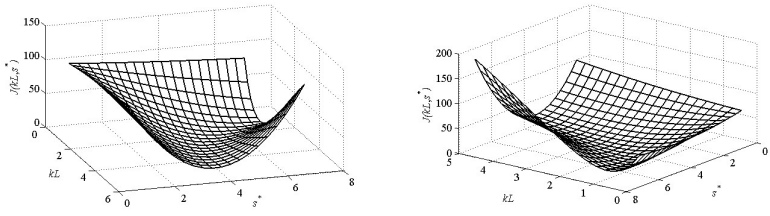
Based on the above algorithm, a Matlab solver was developed and computational experiments were performed, the results of which are shown below.

Calculations were performed with the following model initial data: $t_0 = 0$, $T = 5$, $s_0 = 1$, $\sigma = 0.5$, $\rho = 10^4$, $\alpha = 0.05$, $\varepsilon = 10^{-6}$, $m = 5$. The array of initial time points of measurements was chosen in the form $\left(t_1^{(0)}, t_2^{(0)}, t_3^{(0)}, t_4^{(0)}, t_5^{(0)}\right) = = (0.1; 0.2; 0.3; 0.4; 0.5)$, and initial approximations of the unknown parameters $k_L (k_L = \varphi_1)$ and $s^* (s^* = \varphi_2)$ were taken as $\hat{\varphi}_{1,0} = 3$, $\hat{\varphi}_{2,0} = 4$. The value of the Student's test for $m - 2 = 3$ degrees of freedom and significance level $\alpha = 0.05$ (confidence coefficient $\gamma = 1 - \alpha = 0.95$) is equal to $t_{\alpha;m-2} = t_{0.05;3} = 2.53$ [5].

Because measurement errors $\xi(t_j)$ and a priori distribution function of vector of unknown parameters φ obey the normal distribution law, then, as can be easily shown, maximization of the posterior distribution function of these parameters is equivalent to minimizing a function of form

$$J\left(k_L, s^*\right) = J\left(\varphi\right) = \sigma^{-2} \sum_{j=1}^{m} \left(y\left(t_j\right) - s\left(t_j; \varphi\right)\right)^2 + \rho^{-1} (\varphi - \varphi_0)^T \left(\varphi - \varphi_0\right),$$

where the functions $s\left(t_j; \varphi\right)$ and $y\left(t_j\right)$ are determined by ratio (3.4) and (3.5), φ_0 is the given initial a priori value of vector of estimated parameters φ. The function $J\left(k_L, s^*\right)$, whose minimum determines the estimate of the unknown parameters is called a generalized discrepancy function.



a) b)

Figure 1. Graph of generalized discrepancy function $J\left(k_L, s^*\right)$.

In Figure 1 the graph of the function $J\left(k_L, s^*\right)$ is presented, from which it can be concluded that the search for a minimum point of this function with a high degree of accuracy is quite a complex computational problem, since in the neighborhood of the minimum point the surface of the function is fairly shallow, and, consequently, the numerical solution of this optimization problem depends essentially on a good choice of an initial approximation.

In computational experiments to simulate some measurement results as test values of the required parameters k_L (mass transfer coefficient) and s^* (equilibrium concentration of the substance) we selected $k_L = 2$, $s^* = 5$. Below are the results of some numerical experiments. Table 1 shows dynamics of changes in estimates of the parameters $(\hat{\varphi}_{1,k}, \hat{\varphi}_{2,k})$ and the most informative moments of measurement time (t_i^k) for different numbers of iterations (k). It can be seen that the most significant change in estimates occurs at the beginning of the given iterative procedure, after that the covergence to the point of optimum

is slowed. The most informative is the final time moment $T = 5$, at which it is necessary to perform all five measurements of the substance concentration $s(t)$, performing so-called repeated measurements.

Table 1. The dynamics of change of parameter estimates.

k	$\hat{\varphi}_{1,k}$	$\hat{\varphi}_{2,k}$	t_1^k	t_2^k	t_3^k	t_4^k	t_5^k
0	3.0	4.0	0.1	0.2	0.3	0.4	0.5
1	3.2131	4.3133	0.33328	0.33335	0.33335	0.33338	5.0
2	2.1786	4.7323	0.30588	0.30588	0.30588	0.30588	5.0
10	1.9133	5.1130	0.49715	0.49715	0.49715	0.49715	5.0
15	1.9594	5.0634	0.51179	0.51179	0.51179	0.51179	5.0
35	2.0301	4.9953	5.0	5.0	5.0	5.0	5.0
154	2.0009	4.9992	5.0	5.0	5.0	5.0	5.0

Herewith are the values δ_1^k and δ_2^k, which determine the confidence intervals for the mass transfer coefficient $k_L = \varphi_1$ and equilibrium concentration of the substance $s^* = \varphi_2$, equally $\delta_1^k = 0.68239$, $\delta_2^k = 0.05826$.

The left-hand side of inequality (3.16), which is condition for end of the iterative process, is $||\hat{\varphi}_{k+1} - \hat{\varphi}_k||/(1 + ||\hat{\varphi}_{k+1}||)^{-1} = 1.3543 \cdot 10^{-7}$, which indicates achievement of a specified degree of acuracy $\varepsilon = 10^{-6}$.

Thus, the required (estimated) parameters are equal $k_L = \varphi_1 = \hat{\varphi}_{1,k} \pm \delta_1^k = = 2.0009 \pm 0.68239$, $s^* = \varphi_2 = \hat{\varphi}_{2,k} \pm \delta_2^k = 4.9992 \pm 0.05826$, which agrees well with the test values $k_L = 2$, $s^* = 5$.

Figure 2 shows the course of computational process when searching for the most informative optimal estimates of unknown parameters in accordance with the algorithm proposed above.

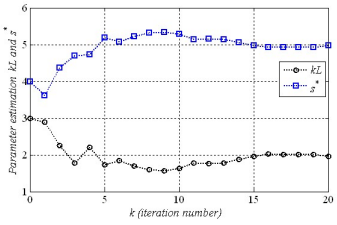


Figure 2. Dynamics of changes in the estimation of parameters at test values $k_L = 2$ and $s^* = 5$.

Computational experiments show a significant dependence of results of calculations on choice of point of initial approximation and slowing of speed of convergence of the iterative process (and even its divergence) with an unsuccessful choice of the initial approximation.

Figure 3 shows the result of another computational experiment. Here the initial starting point did not change. However, in connection with the presence of random errors in the measurement of the concentration of the substance, trajectory of motion of estimates to true values of parameters is somewhat

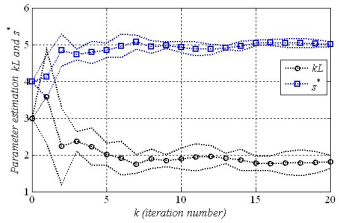


Figure 3. Trajectory of motion of parameter estimates with confidence limits.

different. The same graph shows the dynamics of confidence intervals for the estimated parameters.

4 Conclusions

In the paper, the algorithm for the identification of unknown parameters of the mathematical model, which makes it possible to determine the most probable maximum informative estimates of these parameters, is proposed. The algorithm is based on an information identification criterion and Bayesian estimation method, which represents a more precise and flexible formal apparatus for accounting for a priori information. The results of computational experiments make it possible to assert that the proposed algorithm has a sufficiently high convergence for a given degree of accuracy and makes it possible to derive based on a posteriori analysis not only point values of estimates of the parameters of the mathematical model but also the confidence intervals of these estimates.

References

[1] A.M. Andronov, E.A. Kopytov and L.Ya. Gringlaz. *Teoriya veroyatnostey i matematicheskaya statistika*. Piter, Saint Petersburg, 2004. (in Russian)

[2] S.A. Ayvazyan and S.A. Mkhitaryan. *Prikladnaya Statistika i Osnovy Ekonometriki*. UNITY, Moscow, 1998. (in Russian)

[3] G.I. Ivchenko and Yu.I. Medvedev. *Vvedeniye v matematicheskuyu statistiku*. Publishing house LCI, Moscow, 2010. (in Russian)

[4] V. Zavialov, V. Bodrov, T. Misyura, N. Popova, Y. Zaporozhets and V. Dekanskiy. Development of mathematical models of external mass exchange under conditions of vibroextraction from vegetable raw materials. *Chemistry & Chemical Technology*, **9**(3):367–374, 2015. https://doi.org/10.23939/chcht09.03.367.

[5] V. Zavialov, V. Dekanskiy, O. Lobok and T. Misyura. Matematychne modelyuvannya masoobminu pry vibroekstrahuvanni iz roslynnoyi syrovyny v umovakh kombi-novanoyi diyi mekhanichnykh kolyvan riznoyi chastoty. *Scientific works of NUFT*, **21**(3):161–168, 2015. (in Ukrainian)

[6] A. Zelner. *Bayyesovskiye metody v ekonometrii*. Statistika, Moscow, 1980. (in Russian)