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MATHEMATICAL PHYSICS

Comparative Analysis of Gradient Methods for Source Identification in a Diffusion-Logistic Model

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Abstract—The paper presents a comparative analysis of the numerical solution of the problem of source identification in the diffusion-logistics model from the data on the diffusion process at fixed points in time and space by gradient methods in continuous and discrete formulations. Expressions are obtained for calculating the gradient of the objective functional for two formulations related to the solution of the corresponding adjoint problems. It is shown that, if the discrete functions of the model are approximated by cubic splines, the accuracy of the solutions of the source identification problem has the same order in the case of continuous and discrete calculation of the gradient. Numerical experiments in solving the source identification problem for a discrete model of information dissemination in online social networks have shown that the use of the discrete approach significantly increases the computational time in comparison with the continuous approach.

Keywords: diffusion-logistic model, source identification problem, inverse problem, gradient methods, adjoint problem, comparative analysis, regularization, optimization, social processes

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INTRODUCTION

Gradient methods for solving source identification problems for differential equations were used in [1–7]. Their main idea is to successively decrease the value of the objective functional $J(q) = \|A(q) - f\|^2$ in the form

$$q^{m+1} = q^m - \alpha_m J'(q^m), \quad q^0 \in Q, \quad \alpha_m > 0, \tag{1}$$

where α_m is the descent parameter, which characterizes one or another gradient method, $J'(q^m)$ is the gradient of the objective functional $J(q^m)$, and $A : Q \to F$ is the operator of the inverse problem.

Depending on the type of space Q (Hilbert, Sobolev, Euclidean, etc.), the domains of the functional $J(q)$ and its gradient $J'(q)$ can be integrable, continuously differentiable, or discrete. In this regard, it is possible to use two approaches: 1) continuous, which consists in formulating the functions used in continuous spaces with subsequent representation of the problem in a finite-difference form, and 2) discrete, in which one first passes to a finite-difference analog, for which discrete functions $J(q)$ and $J'(q)$ are formulated (see [8]).

In this paper, for the source identification problem for the diffusion-logistics model, which arises when describing information dissemination in online social networks and formulated in continuous and discrete forms, both approaches are used. The areas of their applicability are revealed. The gradients of objective functionals are obtained in continuous and discrete formulations related to the solutions of the corresponding adjoint problems. Note that the discrete version of the gradient is not a consequence of discretization of its continuous counterpart, but is obtained by minimizing the Lagrange function (see [9–12]).

The article is organized as follows. The formulations of the direct and inverse problems are given in Section 1. The gradient of the objective functional in discrete form is derived in Section 2.1. The expression for the gradient of the objective functional in continuous form and the corresponding formulation of the adjoint problem are given in Section 2.2. Algorithms of gradient methods for different descent parameters, as well as a comparative analysis of the results of numerical calculations for solving the source identification problem for the diffusion-logistics model, are given in Section 3.

1. FORMULATIONS OF THE DIRECT AND INVERSE PROBLEMS

1.1. Formulation of the Direct Problem

In this work, the direct problem is understood as the problem of simulating the process of information dissemination in online social networks, in which it is required to find the density function of active users, $u(x_j, t_n)$, at each point in space and time. The distance x is an integer quantity that describes the minimum number of friendships between the user and the source of information and is measured in units. Time t is measured in hours, and the density of active users $u(x_j, t_n)$ is measured in the number of people per unit distance.

The data presented in [13] illustrate that interest in information is manifested by users with a distance x ranging from 1 to 6. It is within these boundaries that a significant contribution to the change in the density of active users $u(x_j, t_n)$ occurs. Also, the theory of six handshakes is valid for social networks, according to which most agents are located at a distance of $x \le 6$. Therefore, the model considers Neumann boundary conditions, which describe the absence of information flow across the boundaries at $x = 1, 6$.

The problem of simulating the information dissemination process is based on the law of conservation of information flow:

$$\int_a^b \left(\frac{\partial u}{\partial t} + \frac{\partial H}{\partial x} - g(u,x,t)\right) dx = 0.$$

Namely, for a fixed interval $[a,b]$, the rate of change of the total number of involved users, $\frac{\partial}{\partial t}\int_a^b u(x,t)dx$, in this interval should be equal to the sum of the flow $H(a,t) - H(b,t)$ with which they arrive and the rate $\int_a^b g(u,x,t)dx$ with which new involved users appear within the limits $a < x < b$. Information in a social network is distributed from a high density of involved users to a low one; therefore, the flow can be represented as $H = -d\frac{\partial u}{\partial x}$. In [13], the function $g(u,x,t)$ is chosen in the form $(1 - u/K)r(t)u$ and describes the dynamics of changes in the number of active users. The uncertainty of the constructed model lies in the fact that the distribution of the density of active users at the initial moment of time is unknown and depends on the structure of the social network. Therefore, the task of identifying the initial distribution of users in order to correctly describe the distribution of information in a particular network and its further control/management becomes urgent.

Denote the initial values of the density of involved users by $u(x_{i+1}, 1) = q_i$, $i = 0, \dots, 5$. Interpolating the vector of values $q = (q_0, \dots, q_5)$ by cubic splines, we pass to a continuous formulation of the initial-boundary value problem for the diffusion logistic model described by a parabolic partial differential equation (see [13]):

$$\begin{cases} u_t = du_{xx} + \left(1 - \dfrac{u}{K}\right) r(t)u, \quad l \le x \le L, \quad t \ge 1, \\ u(x,1) = Q(x), \quad l \le x \le L, \\ u_x(l,t) = u_x(L,t) = 0, \quad t \ge 1. \end{cases} \tag{2}$$

Here, $Q(x) \ge 0$ is the initial density function corresponding to the vector q. Specifically, $Q(x_i) = q_{i-1}$, $i = 1,\dots,6$, and, on each interval $[x_i, x_{i+1}]$, $i = 1,\dots,5$, the function Q is a third-degree polynomial $Q_i(x)$ satisfying the smoothness conditions

$$Q_i(x_{i+1}) = Q_{i+1}(x_{i+1}), \quad Q_i'(x_{i+1}) = Q_{i+1}'(x_{i+1}), \quad Q_i''(x_{i+1}) = Q_{i+1}''(x_{i+1}), \quad i = \overline{1,4}.$$

Table 1. Parameters of model (2) describing information dissemination in an online social network

Parameter	Description	Average value	Units of measure
d	popularity of information that favors information dissemination through non-structural activities such as the purposeful search by the user for the information under consideration	0.01	dist^2/h
K	throughput: maximum possible number of active users	25	people/ dist
$r(t)$	$=\dfrac{\beta_2}{\beta_1}-e^{-\beta_1(t-1)}\left(\dfrac{\beta_2}{\beta_1}-\beta_3\right)$ growth rate of the number of involved users	—	1/h
β_1	rate of decline in interest in information over time	1.5	—
β_2	residual speed	0.375	—
β_3	initial active user growth rate	1.65	—

The class of initial distribution densities of active users is defined as

$$\tilde{Q} := \left\{Q(x)\in C^2(l,L),\ Q'(l)=Q'(L)=0,\ dQ''+\left(1-\frac{Q}{K}\right)rQ \geq 0,\ Q(i)=q_{i-1},\ i=\overline{1,6}\right\}.$$

According to [13], if $Q(x)\in\tilde{Q}$, then, by the maximum principle, there exists a unique positive solution $u(x,t)\in C^{2,1}((l,L)\times(1,+\infty))\cap C^{1,0}([l,L]\times[1,+\infty))$ of direct problem (2).

The average values and descriptions of the model parameters are presented in Table 1. Parameters β_1, β_2, and β_3 in the considered model correspond to those presented in [13].

1.2. Formulation of the Inverse Problem

Assume that there is additional information of the following form:

$$u(x_i,t_k;q) = f_{ik},\quad i=1,\ldots,N_1,\quad k=1,\ldots,N_2, \tag{3}$$

where $u(x,t;q)$ is the solution of the direct problem for the initial density function $Q(x)$, determined from the set of parameters q, $N_1\leq 6$. The inverse problem (2)–(3) consists in determining the set of parameters q from data f_{ik} of the form (3). The inverse problem can be written as $Aq=f$, where $f=(f_{11},\ldots,f_{1N_2},f_{21},\ldots,f_{2N_2},f_{N_11},\ldots,f_{N_1N_2})\in\mathbb{R}^{N_1N_2}$ and A is the operator of the inverse problem.

Note that, in the linear approximation for $N_1N_2=6$ and $\det A\neq 0$, there is a unique solution of the system $Aq=f$. In the case of $N_1N_2>6$, the solution is understood as a normal pseudosolution, i.e., a solution realizing the minimum of the residual norm

$$J(q)=\|Aq-f\|^2.$$

In [14], in a linear approximation, the stability of the solution of the inverse problem (2)–(3) was studied and it was shown that the condition number of the matrix A has the order of 10^{16}, which indicates the instability of the solution of the inverse problem.

In this paper, the residual has the form

$$J(q)=w\sum_{i=1}^{N_1}\sum_{k=1}^{N_2}\int_l^L\int_1^T|u(x,t;q)-f(x,t)|^2\,\delta(x-x_i)\delta(t-t_k)\,dt\,dx, \tag{4}$$

where $w=(L-l)(T-1)/(N_1N_2)$.

By analogy, we formulate a discrete formulation of the objective functional:

$$I(q)=w\sum_{i=1}^{N_1}\sum_{k=1}^{N_2}\left|v_i^k-f_{ik}\right|^2, \tag{5}$$

where $v_i^k := u(x_i,t_k;q)$.

2. CONTINUOUS AND DISCRETE FORMULATIONS OF THE GRADIENTS OF THE FUNCTIONAL

The study of continuous and discrete solutions of direct and inverse problems for the diffusion-logistic model was inspired by Karchevskii [8], in which a similar analysis was done to solve the inverse problem for the hyperbolic equation.

There are two approaches to the numerical solution of the formulated inverse problem (2)–(3). The first consists of the following steps:

- pass from a continuous formulation of the direct problem $L_q u = 0$ (L_q is the operator of the direct problem) to a discrete one $\Lambda_p v = 0$ (Λ_p is a finite-difference analogue of the operator of the direct problem; the function p is some approximation of the function Q and $p_j = q_{s-1}$ for $x_j = s$, $s = 1, \dots, 6$);
- write out the objective functional in a discrete formulation, $I(q)$;
- obtain the formulation of the adjoint problem $\Lambda_p^* \phi = 0$ and the gradient of the objective functional in discrete form, $I'(q)$;
- solve the problem of minimizing the functional $I(q)$.

The second approach implies the following scheme of actions:

- write out the objective functional in a continuous formulation, $J(q)$;
- obtain the formulation of the adjoint problem $L_q^* \psi = 0$ and the expression for the gradient of the objective functional in continuous form, $J'(q)$;
- pass to the problem $\Lambda_p v = 0$;
- write out the objective functional $I(q)$ approximating $J(q)$;
- from the statement of the adjoint problem $L_q^* \psi = 0$, pass to the problem $\Lambda_p^* \phi = 0$;
- get the relation for $I'(q)$, approximating the gradient of the objective functional $J'(q)$;
- solve the problem of minimizing the functional $J(q)$.

The specificity of the formulation of the inverse problem (2)–(3) is the discrete character of additional measurements, as well as the determination of the set of parameters $q = (q_0, \dots, q_5)$ instead of the function $Q(x)$.

2.1. Gradient of the Functional in the Discrete Formulation

The discrete gradient obtained using the approach of Yu.G. Evtushenko and F.L. Chernous'ko [9–12] is formulated for the discrete formulation of the considered model, i.e., for the problem

$$\begin{cases} \dfrac{v_j^{n+1} - v_j^n}{\tau} = d\,\dfrac{v_{j+1}^n - 2v_j^n + v_{j-1}^n}{h^2} + \left(1 - \dfrac{v_j^n}{K}\right) r^n v_j^n, \quad j = 1, \dots, N_x - 1, \quad n = 0, \dots, N_t - 1, \\ v_j^0 = p_j, \quad j = 0, \dots, N_x, \\ v_0^{n+1} = \dfrac{4v_1^{n+1} - v_2^{n+1}}{3}, \quad n = 0, \dots, N_t - 1, \\ v_{N_x}^{n+1} = \dfrac{4v_{N_x-1}^{n+1} - v_{N_x-2}^{n+1}}{3}, \quad n = 0, \dots, N_t - 1. \end{cases} \tag{6}$$

We transform it to the constraint

$$\Phi(n, v^n; q) = 0, \quad n = 0, \dots, N_t, \tag{7}$$

where v^n is the set of vectors v_j, $j = 0, \dots, N_x$.

To each condition in (7), we put into correspondence a vector $\phi^n \in \mathbf{R}^{N_x+1}$; their union is the vector $\phi^{\mathrm{T}} = (\phi_0^{\mathrm{T}}, \dots, \phi_{N_t}^{\mathrm{T}})$, $\phi \in \mathbf{R}^{(N_t+1)\times(N_x+1)}$. We consider an analogue of the Lagrange function for a multistep process (7):

$$E(v, \phi; q) = I(q) - \sum_{n=0}^{N_t} \Phi^{\mathrm{T}}(n, v^n; q)\phi^n. \tag{8}$$

Then (see [9]),

$$\phi^{i_n} = E_{v^{i_n}}(v,\phi;q) = I_{v^{i_n}}(q) - \sum_{n=0}^{N_t}\Phi^{\mathrm{T}}_{v^{i_n}}(n,v^n;q)\phi^n, \quad i_n = 0, \dots, N_t, \tag{9}$$

$$\frac{\partial I(q)}{\partial q_{i_s}} = E_{q_{i_s}}(v,\phi;q) = I_{q_{i_s}}(q) - \sum_{n=0}^{N_t}\Phi^{\mathrm{T}}_{q_{i_s}}(n,v^n;q)\phi^n, \quad i_s = 0,\dots,5. \tag{10}$$

We have the following lemma.

Lemma. *The gradient of functional* (5) *has the form*

$$\begin{cases} I'(q)[0] = -\dfrac{d}{h^2}\phi_1^0, \\ I'(q)[s] = -\dfrac{\phi_{j_s}^0}{\tau} - d\dfrac{\phi^0_{j_{(s-1)}} - 2\phi^0_{j_s} + \phi^0_{j_{(s+1)}}}{h^2} - r^0\phi^0_{j_s} + \dfrac{2r^0 q_s}{K}\phi^0_{j_s}, \quad s = 1, 2, 3, 4, \\ I'(q)[5] = -\dfrac{d}{h^2}\phi^0_{N_x-1}, \end{cases} \tag{11}$$

where $\phi^0_{j_s}$ *corresponds to the value of* ϕ *at a point* $(x_j = s+1, t_0)$ *and the function* ϕ_j^n *satisfies the adjoint problem*

$$\begin{cases} \dfrac{\phi_j^{n-1} - \phi_j^n}{\tau} = d\dfrac{\phi^n_{j-1} - 2\phi^n_j + \phi^n_{j+1}}{h^2} + r^n\phi^n_j - \dfrac{2r^n v^n_j}{K}\phi^n_j - \dfrac{[\phi]}{\tau h}, \quad j = 1, \dots, N_x - 1, \quad n = 1, \dots, N_t, \\ \phi_j^{N_t} = 0, \quad j = 0 \dots, N_x, \\ \phi_0^n = \dfrac{d}{h^2}\phi_1^n, \quad n = 0 \dots, N_t - 1, \\ \phi^n_{N_x} = \dfrac{d}{h^2}\phi^n_{N_x-1}, \quad n = 0 \dots, N_t - 1, \end{cases} \tag{12}$$

where $[\phi] = 2w(v_i^k - f_{ik})$ *at* $(x_j, t_n) = (x_i, t_k)$ *and* $[\phi] = 0$ *at* $(x_j, t_n) \neq (x_i, t_k)$.

Proof. The function E defined by formula (8) has the form

$$\frac{E(v,q,\phi)}{\tau h} = \frac{I(q)}{\tau h} + \sum_{j=1}^{N_x-1}\sum_{n=1}^{N_t-1}\left[\frac{v_j^{n+1} - v_j^n}{\tau} - d\frac{v^n_{j+1} - 2v^n_j + v^n_{j-1}}{h^2} - r^n v^n_j + \frac{r^n(v^n_j)^2}{K}\right]\phi^n_j$$
$$+ \sum_{j=1}^{N_x-1}\left[\frac{v_j^1 - p_j}{\tau} - d\frac{p_{j+1} - 2p_j + p_{j-1}}{h^2} - r^0 p_j + \frac{r^0(p_j)^2}{K}\right]\phi^0_j$$
$$+ \sum_{n=0}^{N_t-1}\left[v_0^{n+1} - \frac{1}{3}(4v_1^{n+1} - v_2^{n+1})\right]\phi_0^n + \sum_{n=0}^{N_t-1}\left[v^{n+1}_{N_x} - \frac{1}{3}(4v^{n+1}_{N_x-1} - v^{n+1}_{N_x-2})\right]\phi^n_{N_x} = 0.$$

We find the derivative of the function E with respect to v_j^n, which, according to (9), is a formula for determining the function ϕ_j^n:

$$\frac{[\phi]}{\tau h} + \frac{\phi_j^{n-1} - \phi_j^n}{\tau} - d\frac{\phi^n_{j-1} - 2\phi^n_j + \phi^n_{j+1}}{h^2} - r^n\phi^n_j + \frac{2r^n v^n_j}{K}\phi^n_j = 0,$$

for $j = 1, \dots, N_x - 1$, $n = 1, \dots, N_t$. In the case of $j = 0$ and $j = N_x$, for all $0 \le n \le N_t$,

$$\phi_0^{n-1} = \frac{d}{h^2}\phi_1^n, \quad \phi^{n-1}_{N_x} = \frac{d}{h^2}\phi^n_{N_x-1}.$$

Table 2. Discretized initial density function $Q(x)$ used as an exact solution q_{ex} of the inverse problem

Parameter	q_0	q_1	q_2	q_3	q_4	q_5
Value	5.8	1.7	1.9	1	0.95	0.7

For all $0 \le j \le N_x$, the component v_j^0 does not enter into the expression for the function E; therefore, we can set

$$\phi_j^{N_t} = 0, \quad j = 0, \ldots, N_x.$$

Thus, we have obtained the formulation of the adjoint problem (12).

Since $p_j = q_{s-1}$ for $x_j = s$, we find the derivatives of the function E with respect to q_{s-1}:

$$-\frac{\phi_{j_s}^0}{\tau} - d\frac{\phi_{j(s-1)}^0 - 2\phi_{j_s}^0 + \phi_{j(s+1)}^0}{h^2} - r^0\phi_{j_s}^0 + \frac{2r^0 q_{s-1}}{K}\phi_{j_s}^0,$$

for $s = 2, 3, 4, 5$, where $\phi_{j_s}^0$ corresponds to the value of ϕ at the point $(x_j = s, t_0)$. For $s = 1$ and $s = 6$, the derivatives are, respectively,

$$E_{q_0} = -\frac{d}{h^2}\phi_1^0, \quad E_{q_5} = -\frac{d}{h^2}\phi_{N_x-1}^0.$$

Then (10) implies (11), which completes the proof of the lemma.

2.2. Gradient of the Functional in the Continuous Formulation

The gradient of functional (4) has the form

$$J'(q) = -\psi(x,1), \tag{13}$$

where the function $\psi(x,t)$ satisfies the solution of the adjoint problem

$$\begin{cases} \psi_t = -d\psi_{xx} - r(t)\psi + \dfrac{2r(t)u}{K}\psi + \xi, \quad 1 \le t \le T, \quad l \le x \le L, \\ \psi(x,T) = 0, \quad l \le x \le L, \\ \psi_x(l,t) = \psi_x(L,t) = 0, \quad 1 \le t \le T, \end{cases}$$

where $\xi = 2w\sum_{i=1}^{N_1}\sum_{k=1}^{N_2}\int_l^L\int_1^T |u(x,t;q) - f(x,t)|^2\,\delta(x - x_i)\delta(t - t_k)dtdx.$

In [15], formula (13) was derived for a more general formulation of problem (2) with an arbitrary right-hand side.

Note that, due to the properties of the delta function, the adjoint problem can be written as (see [16])

$$\begin{cases} \psi_t = -d\psi_{xx} - r(t)\psi + \dfrac{2r(t)u}{K}\psi, \quad 1 \le t \le T, \quad l \le x \le L, \\ \psi(x,T) = 0, \quad l \le x \le L, \\ \psi_x(l,t) = \psi_x(L,t) = 0, \quad 1 \le t \le T, \\ [\psi]_{\substack{x=x_i \\ t=t_k}} = 2w\left(u(x_i,t_k;q) - f_{ik}\right), \quad i = 1, \ldots, N_1, \quad k = 1, \ldots, N_2 \end{cases}$$

3. NUMERICAL EXPERIMENTS

To solve the inverse problem (2)–(3), as synthetic data f_{ik}, we took the values of the solution of the direct problem for the parameter values presented in Tables 1 and 2, at every tenth point in $x < N_x$ and at every twenty-fifth point in $t \ge 50$, i.e., $N_1 = 5$ and $N_2 = 22$. The parameter values in Table 2 imitate real data from the news site Digg.com, obtained in [13].

In addition to the value of the functional, we measured the relative error

$$\delta = \frac{\|q_{\text{ex}} - \tilde{q}\|^2}{\|q_{\text{ex}}\|^2}.$$

Here, q_{ex} are the exact values of the discretized function $Q(x)$ and $\tilde{q}$ is the found solution of the inverse problem, which corresponds to the minimum of the functional $J(q)$ (4).

3.1. Gradient Methods

The solution to the problem of minimizing the objective functionals $J(q)$ and $I(q)$ was obtained using two gradient methods:

1. The gradient descent method (GDM) (see [17, 18]) is a classical one-step gradient method (1) with a constant descent parameter $\alpha_m = \alpha$. The rate of convergence in the functional (see [18]) is

$$J(q^m) \le \frac{\left\|q^0 - q_{\text{ex}}\right\|^2}{m\alpha\left(1 - \alpha\|A\|^2\right)}.$$

2. The multilevel gradient method (MGM) (see [19, 20]) is a method of local optimization of a function of several variables. It is a modification of the gradient descent method, which can significantly increase the convergence rate. The algorithm of the method has the following form:

$$q^{m+1} = \theta_{m+1} z^m + (1 - \theta_{m+1}) y^m, \quad \theta_{m+1} \in \arg\min_{\theta \in [0;1]} J(\theta z^m + (1 - \theta) y^m),$$

$$y^{m+1} = q^{m+1} - \zeta_{m+1} J'(q^{m+1}), \quad \zeta_{m+1} \in \arg\min_{\zeta \ge 0} J(q^{m+1} - \zeta J'(q^{m+1})),$$

$$z^{m+1} = z^m - \eta_{m+1} J'(q^{m+1}), \quad \eta_{m+1} = \frac{1}{2L_{m+1}} + \sqrt{\frac{1}{4L_{m+1}^2} + \eta_m^2}, \quad \eta_0 = 0.$$

In the case of MGM, the rate of convergence in the functional is estimated as (see [21])

$$J(q^m) \le \frac{4L\left\|q^0 - q_{\text{ex}}\right\|^2}{(m+1)^2},$$

where L is the Lipschitz constant for the gradient of the functional:

$$\left\|J'(q^{m+1}) - J'(q^m)\right\|_2 \le L\left\|q^{m+1} - q^m\right\|_2.$$

The GDM and MGM with continuous and discrete types of gradients were applied and analyzed. Moreover, in the case of a discrete gradient, the GDM has a descent parameter $\alpha^{(1)} = 10^{-7}$ and the minimum with respect to ζ in the MGM is on the interval $[0, 10^{-6}]$ with a step 10^{-7}. In the case of a continuous gradient, $\alpha^{(2)} = 10^{-3}$, and the minimum in $\zeta \in [0, 10^{-5}]$ is determined with a step of 10^{-6}.

3.2. Finite-Difference Schemes for Solving Direct and Adjoint Problems

To construct difference schemes, we introduce a uniform grid in a closed region $\bar{D} = \{(x,t) | l \le x \le L, 1 \le t \le T\}$:

$$\bar{\omega} = \{(x_j, t_n) | x_j = l + jh, t_n = 1 + n\tau, j = 0, \dots, N_x, n = 0, \dots, N_t\},$$

where $h = (L - l)/N_x$ and $\tau = (T - 1)/N_t$.

To apply the classical continuous approach, the initial approximation function $Q(x)$ is determined from the vector q (see Table 2) by cubic-spline interpolation.

Direct problem (2) is solved using an explicit finite-difference scheme with the order of approximation $O(\tau + h^2)$ in the form (6).

Table 3. Algorithms for solving inverse problem (2)–(3) in the case of continuous and discrete approaches

Discrete approach	Continuous approach
(1) Direct problem (2) is solved by a finite difference method with the order of approximation $O(\tau + h^2)$	
(2) Adjoint problem (12) is solved with the order of approximation $O(\tau + h^2)$	(2) Adjoint problem (14) is solved by a finite difference method with the order of approximation $O(\tau + h^2)$
(3) Objective functional gradient $I'(q)$ is determined by formula (11)	(3) Objective functional gradient $J'(q)$ is determined by formula (13)
(4) Next approximation of the solution to the inverse problem is computed as	
$q^{m+1} = q^m - \alpha_m^{(1)} I'(q^m)$	$q^{m+1} = q^m - \alpha_m^{(2)} J'(q^m)$
$\alpha_m^{(1)} = \alpha^{(1)}$ for GDM	$\alpha_m^{(2)} = \alpha^{(2)}$ for GDM
$\alpha_m^{(1)}$ and $\alpha_m^{(2)}$ for MGM are determined experimentally	

Table 4. Solution of the inverse problem obtained by particle swarm optimization

Parameter	$\hat{q}_0$	$\hat{q}_1$	$\hat{q}_2$	$\hat{q}_3$	$\hat{q}_4$	$\hat{q}_5$
Value	5.809	1.697	1.901	0.999	0.949	0.701

Table 5. Results obtained by gradient descent methods and its modification

Method	q^0	$J(q), \times 10^{-4}$	$\delta, \times 10^{-4}$	N_{iter}	t_{comp}
GDM I	$\hat{q}$	9.604	6.274	5380	3
MGM I	$\hat{q}$	9.544	6.273	397	3
MGM II	0	9.029	6.262	245	2
GDM II	0	9.032	6.262	16374	9
GDM III	$\hat{q}$	9.847	6.276	166862	93
MGM III	$\hat{q}$	9.793	6.276	1372	11
MGM IV	0	9.047	6.261	1630	12
GDM IV	0	9.101	6.266	1005999	569
MGM V	0	11.26	6.254	1586	25

In the column of initial guess q^0, $\hat{q}$ is the vector of the solution of the inverse problem obtained using particle swarm optimization (presented in Table 4), 0 is the zero vector, N_{iter} is the number of iterations, and t_{comp} is the program running time.

In numerical calculations, we set $l = 1$, $L = 6$, $T = 24$, $N_x = 50$, and $N_t = 575$. Such values of l and L were chosen in accordance with the data presented in [13], which illustrate that interest in information is manifested by users with a distance x ranging from 1 to 6. It is within these boundaries that a significant contribution to the change in the density of active users $u(x,t)$ occurs. The grid partition values N_x and N_t are chosen so as to satisfy the Courant–Friedrichs–Lewy condition

$$\tau \leq \frac{2h^2}{4d + r_c h^2}$$

Taking into account that $r_c = \max_t r(t) = 0.44$, we have $h = 0.1$ and $\tau = 0.04$.

To analyze the stability of the solution of the direct problem, the Crank–Nicolson scheme with the order of approximation $O(\tau^2 + h^2)$ was implemented.

3.3. Comparative Analysis of Continuous and Discrete Formulations

We will conduct a comparative analysis of the approaches to solving the inverse problem: with an accurate calculation of the gradient for the discrete problem (6)–(3) and with continuous formulation and dis-

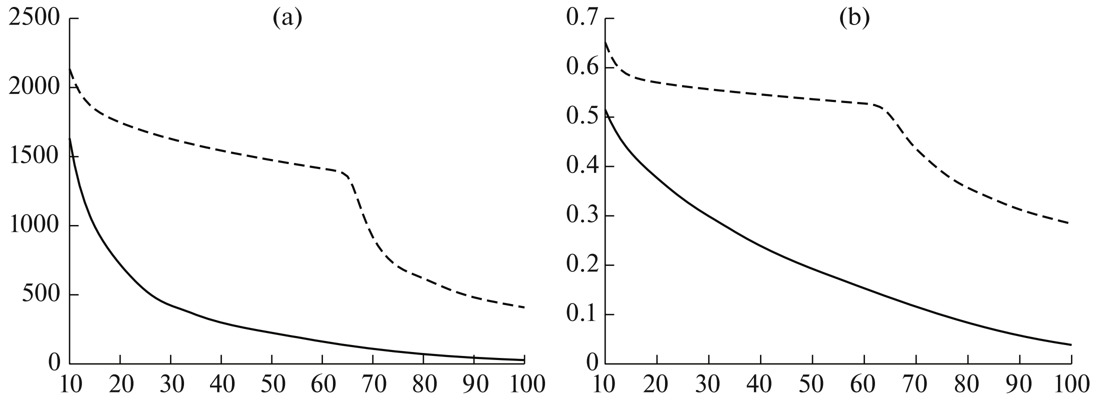

Fig. 1. Graphs of (a) decreasing functionals $J(q)$ and $I(q)$ and (b) relative error δ from 10th to the 100th iterations: the use of (solid line) a continuous gradient and (dotted line) a discrete gradient of the objective functional.

cretization when calculating the gradient (2)–(3). The stages of similarity and differences of algorithms for solving these inverse problems are shown in Table 3. Note that in both cases it is identical the direct problem is solved, and the adjoint problems are solved by one finite-difference scheme, which are included in the corresponding expressions for calculating the gradients of the target functional. The same algorithms are applied to solving the corresponding minimization problems. As a comparison of the two approaches, the value of the target functional and the relative error of the reconstructed solutions are analyzed.

The solution obtained using gradient methods depends on the initial approximation. Two options for choosing the initial approximation were considered (see [19, 22, 23]): the solution of the inverse problem obtained using the method of global particle swarm optimization (PSO), presented in Table 4, and zero initial guess. The zero initial guess was chosen from the physical formulation, since q^0 describes the first reaction of users to the news in the absence of additional information about this reaction. In the above implementation of PSO, the functional $J(\hat{q}) = 1.114\times10^{-3}$ and relative error $\delta = 1.533\times10^{-3}$.

Table 5 presents the results obtained by the following methods:

• GDM I and MGM I: methods with a continuous gradient and an initial approximation in the form of a solution obtained by PSO;

• GDM II and MGM II: methods with continuous gradient and zero initial guess;

• GDM III and MGM III: methods with a discrete gradient and an initial guess in the form of a solution obtained by PSO;

• GDM IV and MGM IV: methods with discrete gradient and zero initial guess;

• MGM V: a method with a zero initial guess and a discrete gradient in the case when the direct and adjoint problems are numerically solved using the Crank–Nicolson finite difference scheme.

Table 6. Results of solving the inverse problem with a noise level $\varepsilon = 1, 5, 10\%$ in the data obtained by the multilevel gradient method with a gradient in discrete and continuous formulations

Initial guess	ε, %	Discrete gradient (11)		Continuous gradient (13)	
		$I(q)$	δ	$J(q)$	δ
Zero	1	1.133×10^{-2}	6.706×10^{-4}	9.628×10^{-2}	7.356×10^{-4}
	5	1.475×10^{-1}	8.447×10^{-4}	3.272×10^{-3}	6.399×10^{-4}
	10	3.461×10^{-2}	7.305×10^{-4}	3.286×10^{-3}	6.407×10^{-4}
Solution by PSO	1	1.242×10^{-3}	6.271×10^{-4}	1.403×10^{-3}	6.262×10^{-4}
	5	3.165×10^{-2}	6.431×10^{-4}	1.865×10^{-3}	6.261×10^{-4}
	10	16.795	1.707×10^{-2}	11.289	1.388×10^{-2}

It can be seen from Table 5 that the MGM finds a solution with a given accuracy, making 10 times fewer iterations than the GDM under the same initial conditions and forms of finding the gradient of the objective functional. In the case of an initial approximation $\hat{q}$ and a continuous gradient (i.e., GDM I and MGM I), the running times of the programs do not differ, but, in implementations of gradient methods, the MGM finds a solution with a given accuracy several times faster than the GDM. With a zero initial guess, the methods work several times longer but achieve greater accuracy only at the sixth decimal place. In the case of a discrete gradient, the MGM reaches a solution of the same order several times longer, and the GDM is more than 30 times longer in time. At the same time, MGM V has the smallest error among all the considered methods, but works several times longer than other implementations of the MGM. In Fig. 1, the continuous lines represent the curves obtained by MGM II in the case of continuous calculation of the gradient of the functional, and the dotted lines represent the curves obtained by MGM IV in the case of a discrete implementation of the gradient. It follows from Fig. 1 that the value of the functional and the error in the case of MGM II decrease faster.

We also analyzed the case of noisy data:

$$f_{ik}^{\varepsilon} = f_{ik} + \varepsilon\gamma \max|f_{ik}|, \quad i = 1, \ldots, N_1, \quad k = 1, \ldots, N_2,$$

where $\varepsilon \in (0, 1)$ is the noise level and γ is a random variable with a standard normal distribution.

For noisy data of the inverse problem, the MGM was implemented with different initial approximations and the direct problem was solved by the finite difference method using the Crank–Nicolson scheme. The results of numerical experiments for this formulation of the inverse problem in the case of discrete and continuous gradients are given in Table 6. It can be seen that, in the case of a zero initial guess, the discrete gradient method has the smallest relative error for noise of 1%, while the continuous gradient method has the smallest value for noise of 5 and 10%. In the case of the initial approximation in the form of a solution obtained using PSO, the accuracy of the recovered solutions of the inverse problem differ insignificantly.

This paper investigates two approaches to solving the problem of source recovery, in which two finite-difference schemes were implemented, in which the order of approximation in the spatial variable coincides and equals 2, and in the temporal have the 1st and 2nd (Krank–Nicholson) orders. Tables 5 and 6 show experimentally that the convergence result is not sensitive to the order of approximation by the time variable. Based on convergence estimates and iterative expressions for determining the solution of the inverse problem, the order of approximation by a spatial variable when solving direct and adjoint problems has a great influence on the accuracy of the obtained solution and, most likely, on the convergence rate of gradient methods. In the case of determining the density of the initial distribution of users relative to popular news in online social networks with high bandwidth (Twitter, Facebook, Reddit, etc.), it is necessary to qualitatively determine the type of user engagement and the distribution structure. Separate studies are needed to obtain more accurate estimates of the relationship between the convergence rate of gradient methods and approximation accuracy.

CONCLUSIONS

This paper presents a comparative analysis of the numerical solution of the source identification problem for the diffusion-logistics model based on the data on the diffusion process at fixed points in time and space by gradient methods for the cases of continuous (classical) and discrete formulations. Expressions for calculating the gradient of the objective functional in the case of two formulations related to the solution of the corresponding adjoint problems have been obtained.

The direct and adjoint problems were solved using an explicit scheme with an order of approximation $O(\tau + h^2)$ and the Courant–Friedrichs–Lewy condition and a semi-implicit Crank–Nicolson scheme with an order of approximation $O(\tau^2 + h^2)$. The problem minimizing an objective functional was solved by gradient descent methods with a constant descent parameter and by a multilevel gradient method. Two variants of the initial approximation of the solution of the inverse problem were analyzed: zero guess and an approximation obtained by particle swarm optimization. It has been shown that, in the case of a nonzero initial guess, using the expression for the gradient of the objective functional in a continuous formulation, the running times of the programs do not differ; however, in other implementations of the gradient methods, the multilevel gradient method finds a solution with a given accuracy several times faster than the gradient descent method. With a zero initial guess, the methods work several times longer but achieve higher accuracy. In the case of a discrete gradient, the multilevel gradient method is several times longer in reaching a solution of the same order, and the gradient descent method is more than 30 times longer.

It has been shown that, in the case of cubic-spline approximation of discrete functions in the direct problem, differences in the accuracy of the obtained solutions of the inverse problems for continuous and discrete formulations are observed only in the sixth decimal place in the case of noise-free synthetic data describing the dynamics of involved users in an online social network. However, the computer time for solving the inverse problem in discrete form is greater than its continuous counterpart.

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CONFLICT OF INTEREST

The authors declare that they have no conflicts of interest.

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