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NUMERICAL SOLUTION OF THE INVERSE PROBLEM FOR A SYSTEM OF DIFFERENTIAL EQUATIONS

Abstract

The article considers direct and inverse problems of a system of nonlinear differential equations. Such problems are often found in various fields of science, especially in medicine, chemistry and economics. One of the main methods for solving nonlinear differential equations is the numerical method. The initial direct problem is solved by the Rune-Kutta method with second accuracy and graphs of the numerical solution are shown. The inverse problem of finding the coefficients of a system of nonlinear differential equations with additional information on solving the direct problem is posed. The numerical solution of this inverse problem is reduced to minimizing the objective functional. One of the methods that is applicable to nonsmooth and noisy functionals, unconditional optimization of the functional of several variables, which does not use the gradient of the functional, is the Nelder-Mead method. The article presents the Neller-Mead algorithm. And also a numerical solution of the inverse problem is shown.

Keywords: numerical solution, inverse problem, Runge-Kutta method, Nelder-Mead method, system of differential equations.

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ДИФФЕРЕНЦИАЛДЫҚ ТЕҢДЕУЛЕР ЖҮЙЕСІ ҮШІН КЕРІ ЕСЕПТІ САНДЫҚ ШЕШУ

Мақалада сызықты емес дифференциалдық теңдеулер жүйесінің тура және кері есептері қарастырылады. Мұндай есептер қойылымы ғылымның әртүрлі салаларында, әсіресе медицина, химия, экономика салаларында жиі кездеседі. Сызықты емес дифференциалдық теңдеулерді шешудің негізгі тәсілдерінің бірі сандық тәсіл болып табылады. Бастапқы тура есепті Рунге-Кутта әдісімен екінші дәлдікте шешілуі көрсетіліп, графиктері келтірілген. Тура есеп шешімі туралы қосымша ақпараты арқылы берілген сызықты емес дифференциалдық теңдеулер жүйесінің коэффициенттерін табу кері есебі қойылады. Осы кері есепті сандық шешу мақсатты фунционалды минимималдандыру тиімділеу есебіне келтіріледі. Тегіс емес, қателікпен берілген бірнеше айнымалы функционалды шартсыз, туындыны пайдаланбай минимизациялайтын әдістердің бірі Нелдер-Мид әдісі. Мақалада Нелдер-Мид алгоритмі көрсетілген. Сонымен қатар кері есептің сандық шешімі табылған.

Түйін сөздер: сандық шешім, кері есеп, Рунге-Кутта әдісі, Нелдер-Мид әдісі, дифференциалдық теңдеулер жүйесі.

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ЧИСЛЕННОЕ РЕШЕНИЕ ОБРАТНОЙ ЗАДАЧИ ДЛЯ СИСТЕМЫ ДИФФЕРЕНЦИАЛЬНЫХ УРАВНЕНИЙ

В статье рассматриваются прямые и обратные задачи системы нелинейных дифференциальных уравнений. Такие задачи часто встречаются в различных областях науки, особенно в медицине, химии и экономике. Одним из основных способов решения нелинейных дифференциальных уравнений является численный метод. Исходная прямая задача решена методом Рунге-Кутты со второй точностью и показаны графики численного решения. Поставлена обратная задача о нахождении коэффициентов системы нелинейных дифференциальных уравнений с дополнительной информацией о решении прямой задачи. Численное решения данной обратной задачи сведена к минимизации целевого функционала. Одним из методов, который применим к негладким и зашумлённым функционалам, безусловной оптимизации функционала от нескольких переменных, не использующий градиента функционала является метод Нелдера-Мида. В статье приведен алгоритм Неллера-Мида. А также показаны численное решение обратной задачи.

Ключевые слова: численное решение, обратная задача, метод Рунге-Кутта, метод Нелдера-Мида, система дифференциалных уравнений.

Introduction

One of the most important ways to understand the environment is mathematical modeling. In mathematical modeling, a relationship is derived based on the laws of a subject area and allows you to determine the nature of changes in the system state function depending on its parameters. The intensive development of modern computer technologies will significantly advance the boundaries of mathematical modeling in any field of science and technology.

For the purpose of specifying the given mathematical models the various inverse problems for finding the model parameters are put. Solving the inverse problem can be considered as a complex task. Currently, different gradient, empirical or different combinations of them are used to solve the inverse problem.

Problem statement

Consider the following system of differential equations [1]:

$$\begin{cases} \dot{x}_1 = \left[\frac{a_1}{1+s(t)} - b_1(x_1+x_2)\right] x_1 + a_{12}x_2 - c(t)(x_1)^{\theta} \\ \dot{x}_2 = [a_2 - b_2(x_1+x_2)]x_2 + \frac{a_{21}}{1+s(t)} x_1 \end{cases} \quad (1)$$

where

$$s(t) = \begin{cases} s_*, t \in [t_1, t_2] \\ 0, t \notin [t_1, t_2] \end{cases} \quad (2)$$

Equation (1) is supplemented by the initial conditions

$$x_1(0) = x_{10}, x_2(0) = x_{20}. \quad (3)$$

Numerical solution to the problem

To approximate the equations under consideration, the Runge-Kutta accuracy method is used for the second time.

For this purpose, the time interval $[0, T]$ is divided into a part equal to NN, with a step $h = T/N$. Further, for the k-node of the grids (time step) and for the value of the currently considered functions, the following standard notations are accepted [2]:

$$t_k = kh,\ x_1^k = x_1(t_k),\ x_2^k = x_2(t_k), c^k = c(t_k), k = 0,1,\dots,N$$

The calculations start with the initial conditions:

$$x_1^0 = x_{10},\ x_2^0 = x_{20}$$

In the known values of the functions searched in the k step, the values of the functions that are searched in the intermediate step are calculated over time:

$$x_1^{k+\frac{1}{2}} = x_1^k + \frac{h}{2}\left[a_1\, x_1^k - b_1\left(x_1^k + x_2^k\right) x_1^k + a_{12}\, x_2^k - c^k\left(x_1^k\right)^{\theta}\right],$$
$$x_2^{k+\frac{1}{2}} = x_2^k + \frac{h}{2}\left[a_2\, x_2^k - b_2\left(x_1^k + x_2^k\right) x_2^k + a_{21}\, x_1^k\right],$$

After that, their values are calculated over time for the next step:

$$x_1^{k+1} = x_1^k + \frac{h}{2}\left[a_1\, x_1^{k+\frac{1}{2}} - b_1\left(x_1^{k+\frac{1}{2}} + x_2^{k+\frac{1}{2}}\right) x_1^{k+\frac{1}{2}} + a_{12}\, x_1^{k+\frac{1}{2}} - c^k\left(x_1^k\right)^{\theta}\right],$$
$$x_2^{k+1} = x_2^k + \frac{h}{2}\left[a_2\, x_2^{k+\frac{1}{2}} - b_2\left(x_1^{k+\frac{1}{2}} + x_2^{k+\frac{1}{2}}\right) x_2^{k+\frac{1}{2}} + a_{21}\, x_2^{k+\frac{1}{2}}\right].$$

System parameter values are selected based on the limit values, see the table below:

Table 1. Value of parameters in the problem

a_1	a_2	b_1	b_2	a_{12}	a_{21}	c_*	θ	ε_1	ε_2	N
100	100	0.5	1	1	5	2	2.2	9.5	1	10^4

The calculation results are shown in figure 1 (time change x1, x2) and in figure 2 (time change x1+x2).

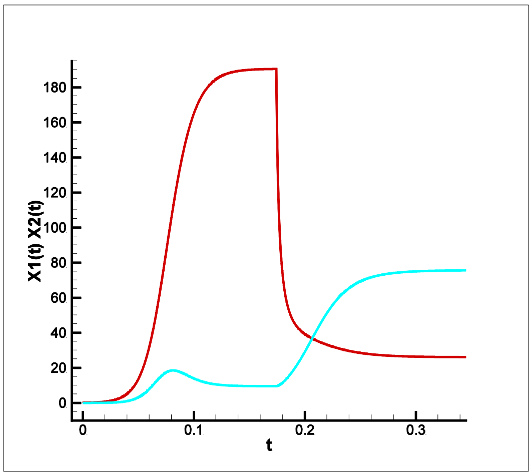

Figure 1 – function graphs $x_1(t), x_2(t)$

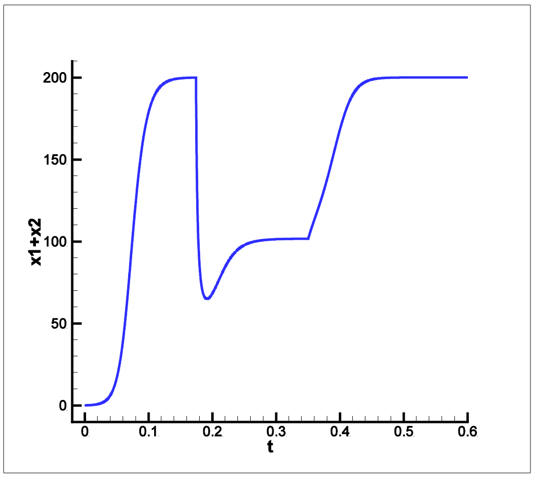

Figure 2 – function graph $x_1(t) + x_2(t)$

Statement of the inverse problem

Consider a system of differential equations

$$\begin{cases} \dot{x}_1 = a_1 x_1 - b_1(x_1 + x_2)x_1 \\ \dot{x}_2 = a_2 x_2 - b_2(x_1 + x_2)x_2 + a_{21}x_1 \end{cases} \tag{4}$$

with the initial condition

$$x_1(0) = x_{10}, x_2(0) = 0, \tag{5}$$

By additional information for next (4) system solution

$$x_1(t_m) = y_{1m}, x_2(t_m) = y_{2m}, \quad m = 1, \dots, M \tag{6}$$

a_2, b_2, a_{21} need to determine the coefficients. Let's create the target function

$$I(a_2, b_2, a_{21}) = \sum_{m=1}^{M} (x_1(t_m) - y_{1m})^2 + \sum_{m=1}^{M} (x_2(t_m) - y_{2m})^2$$

The inverse problem consists of minimization of the target functional I. The solution of the problem will be carried out using the Nelder-Mead method.

Nelder-Mead algorithm

The Nelder-Mid method is known as a multifaceted deformation method, it is an unconditional method for optimizing several variable functions that do not use a derivative function, therefore it is easily used for simple functions. The main subject of this method is the gradual displacement and deformation of a simplex around an extremum point. The simplex is a convex polyhedral with the number of ceiling $n + 1$, where n is the number of model parameters.

Let us consider at the k-iteration algorithm and when $k = 0,1,2, \dots$, $\bar{x}_i^k = \left[x_{i1}^k, x_{i2}^k, \dots, x_{in}^k\right]^T$, $i = 1,2, \dots, n + 1$ would be vertex and $f\left(\bar{x}_i^k\right)$ is the value of the given function.

Let's denote the minimum and maximum values. And let's denote them as follows:

$$f(\bar{x}_h^k) = max\{f(\bar{x}_1^k), f(\bar{x}_2^k), \dots, f(\bar{x}_{n+1}^k)\}$$

$$f(\bar{x}_l^k) = min\{f(\bar{x}_1^k), f(\bar{x}_2^k), \dots, f(\bar{x}_{n+1}^k)\}$$

The multifaceted E^n consists of $n+1$ ceilings $\bar{x}_1^k, \bar{x}_2^k, \dots, \bar{x}_{n+1}^k$.

The function has the highest value $\bar{x}_h^k$ without a point $\bar{x}_{n+2}^k$– we set the height by the center of gravity. The coordinates of this meter are calculated by the formula:

$$x_{n+2,j}^k = \frac{1}{n}\left[\sum_{i=1}^{n+1} x_{i,j}^k - x_{h,j}^k\right], j = 1,2,\dots,n.$$

The primary polyhedral is usually chosen as a constant simplex (from the origin to the vertex). Coordinates can be placed in the center of gravity. has the best value E^n the vertex detection procedure consists of the following operations:*1) reflection; 2) stretching; 3) compression; 4) reduction.*

1. Reflection. In accordance with the following relationships, that is, using the center of gravity $\bar{x}_{n+2}^k$ is the design of the point $\bar{x}_h^k$:

$$\bar{x}_{n+3}^k = \bar{x}_{n+2}^k + \alpha(\bar{x}_{n+2}^k - \bar{x}_h^k),$$

where $\alpha > 0 -$ reflection coefficient.

$f(\bar{x}_{n+3}^k)$ calculate the value of the function at the found point. If the value of the function is at this point $f(\bar{x}_{n+3}^k) > f(\bar{x}_h^k)$, then we move on to the fourth part of the algorithm - the reduction operation.

If $f(\bar{x}_{n+3}^k) < f(\bar{x}_h^k) \wedge f(\bar{x}_{n+3}^k) < f(\bar{x}_l^k)$, perform a *stretch* operation.

Otherwise, if $f(\bar{x}_{n+3}^k) < f(\bar{x}_h^k) \wedge f(\bar{x}_{n+3}^k) \geq f(\bar{x}_l^k)$, then the *compression* operation is performed.

2. Stretching. In this operation if $f(\bar{x}_{n+3}^k) < f(\bar{x}_l^k)$ (less than the minimum value in the k-th period), then vectors $(\bar{x}_{n+3}^k - \bar{x}_{n+2}^k)$ lengthens according to the aspect ratio

$$\bar{x}_{n+4}^k = \bar{x}_{n+2}^k + \gamma(\bar{x}_{n+3}^k - \bar{x}_{n+2}^k),$$

where $\gamma > 0 -$ stretching coefficient.

If $f(\bar{x}_{n+4}^k) < f(\bar{x}_l^k)$ then $\bar{x}_l^k$ is replaced by and the procedure continues with the reflection operation at $k = k+1$. Otherwise, $\bar{x}_l^k$ replaced by $\bar{x}_{n+3}^k$ and stretching operation replaced.

3. Compression. If $f(\bar{x}_{n+3}^k) > f(\bar{x}_i^k)$ $f(\bar{x}_{n+3}^k) > f(\bar{x}_i^k)$ where $\forall i, i \neq h$, then the vectors $(\bar{x}_h^k - \bar{x}_{n+2}^k)$ compressed according to the formula

$$\bar{x}_{n+5}^k = \bar{x}_{n+2}^k + \beta(\bar{x}_h^k - \bar{x}_{n+2}^k),$$

where $0 < \beta < 1 -$ compression coefficient. After that, point $\bar{x}_h^k$ replaces by $\bar{x}_{n+5}^k$, and with $k = k + 1$. *Reflection* operation is performed. Search again $\bar{x}_h^{k+1}$.

4. Reduction. If $(\bar{x}_{n+3}^k) \geq f(\bar{x}_h^k)$, then all vectors $(\bar{x}_i^k - \bar{x}_l^k)$ when $i = 1,2,\dots(n+1)$ from point $\bar{x}_l^k$ it doubles according to the formula below

$$\bar{x}_i^k = \bar{x}_l^k + 0.5 \cdot (\bar{x}_i^k - \bar{x}_l^k), i = 1,2,\dots(n+1)$$

and the transition to the reflection operation is performed (at the beginning of the algorithm $k = k+1$).

Rules such as other algorithms can be obtained as a stop criterion.

The following ratio is used to cancel the algorithm

$$\left\{\frac{1}{n+1}\sum_{i=1}^{n+1}\left[f\left(x_i^k\right)-f\left(x_{n+2}^k\right)\right]^2\right\}^{1/2} < \varepsilon$$

The selection of coefficients is usually empirical. After multifaceted massaging, its dimensions should remain unchanged until changes in the topology require multifacetedness in another form [3].

Numerical solution of the problem of restoring report parameters

To check the performance of the algorithms, we give a clear solution $a_{2ex} = 0.1, b_{2ex} = 0.01, a_{21ex} = 0.0001$ determine the value of the experimental results $y_{1m} = x_1(t_m), y_{2m} = x_2(t_m),\quad m = 1,\dots,M.$ $M = 30$. With these values, we reduce the given function. The following parameter values are selected: $T = 1.0, N_t = 10^3, a_1 = 0.5, b_1 = 0.01, x_{10} = 0.1.$

The results of the iteration count in accordance with the specified algorithm are shown in table 2.

Table 2. Results of iteration calculations

Iteration	a_2	b_2	a_{21}	$I(a_2, b_2, a_{21})$
1	1.07466	1.01741	1.08589	3.26474e-013
2	1.07466	1.01741	1.08589	3.26474e-013
3	1.07466	1.01741	1.08589	3.26474e-013
4	1.07466	1.01741	1.08589	3.26474e-013
5	1.07466	1.01741	1.08589	3.26474e-013
6	1.07466	1.01741	1.08589	3.26474e-013
7	1.07466	1.01741	1.08589	3.26474e-013
8	1.07466	1.01741	1.08589	3.26474e-013
9	1.07466	1.01741	1.08589	3.26474e-013
10	1.07466	1.01741	1.08589	3.26474e-013
11	1.07466	1.01741	1.08589	3.26474e-013
12	1.07466	1.01741	1.08589	3.26474e-013
13	1.07466	1.01741	1.08589	3.26474e-013
14	1.07466	1.01741	1.08589	3.26474e-013
15	1.07466	1.01741	1.08589	3.26474e-013
16	1.07466	1.01741	1.08589	3.26474e-013
17	1.07466	1.01741	1.08589	3.26474e-013
18	0.0995178	0.00457442	9.98016e-005	1.95726e-014
19	0.0995178	0.00457442	9.98016e-005	1.95726e-014
20	0.0995178	0.00457442	9.98016e-005	1.95726e-014
exact	0.1	0.01	0.0001	0

As you can see from the result, search parameters are restored quickly and with high accuracy.

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References:

1 Serovajsky S., Nurseitov D., Kabanikhin S., et al. (2017). Identification of mathematical model of bacteria population under the antibiotic influence. Journal of Inverse and Ill-posed Problems, 26(5), pp. 565-576. doi:10.1515/jiip-2017-0102

2 Samarsky, A.A., Gulin, A.V.: Numerical Methods. Nauka, Moscow (1989)

3 Attetkov A.V., Galkin S. V., Zarubin B. S.. Optimization methods: Studies. for universities. 2nd ed. Moscow: MGTU publishing House. N. E. Bauman, 2003. – 440p.