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# Адаптивний метод дистанційного виявлення хімічних та біологічних компонентів, що базується на градієнтному підході

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## Adaptive method for remote detection of chemical and biological components based on the gradient approach

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В роботі описується алгоритм для виявлення хімічних забруднень у рослинності на основі спектральних даних. Для цього ставиться задача апроксимації сигналу, що знадходиться у вигляді лінійної комбінації вектору невідомих параметрів та певних базисних функцій, де в якості базисних функцій беруться ретроспективні спостереження забрудень рослинності різними хімічними компонентами.

Для постановки задачі апроксимації розглядається мінімізація декількох типів нев'язок: середньоквадратичне відхилення сигналу від апроксимації безпосередньо в поточний момент часу та інтегральна нев'язка на всьому проміжку. Для адаптивної корекції вектору параметрів, використовуючи метод градієнтного спуску, будується неперервна ітераційна процедура. Задаючи початкові дані ставиться задача Коші, розвя'зок якої і є шуканим вектором невідомих параметрів.

Досліджено збіжність ітераційної процедури за допомогою використання методів Ляпунова. Ефективність використання даного алгоритму підтверджено експериментально за рахунок визначення хімічних компонентів у рослинах.

Ключові слова: адаптація, сигнали в реальному часі, апроксимація, базисні функції, спектральні дані, диференціальні схеми.

The goal of the task is to define unknown parameters vector in approximation function and to find out chemical and biological components presence in plats by corresponding spectral data. Approximation function is supposed to be a linear combination of basis functions and unknown parameters. Basis functions are taken as retrospective occurrences of plants pollution with different chemical and biological elements.

Adoptive algorithm for signal approximation described. Iterative procedure is built based on gradient descent method for minimizing certain residuals. For this purpose, two types of residuals investigated: directly at the current moment of time and mean square approximation on the continuous time span which is an integral of the mean square deviation between signal and approximation.

System of ordinary differential equations together with initial conditions forms an iterative procedure. Its convergence analysis conducted using Lyapunov methods.

Numerical experiment for chemical components in plants detection conducted to prove experimentally efficiency of the described algorithm. Unknown parameters vector converges to 1 for the corresponding to detected chemical element basis function.

Key Words: adaptation, real-time signal, approximation, basic function, spectral data, differencing schemes.

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#### Introduction

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Despite the fact that there are many works devoted to the problems of approximation both continuous and discrete signals, important practical problems arise, especially in the field of Informatics and applied mathematics [1]. It requires development and testing of new approaches of experimental data approximation. First, it comes from the fact that data processing is mostly conducted in real time. Besides, algorithms should meet strict conditions: they should be constructive, focused on optimal performance and real-time problem solving [3].

These requirements, in our view, meet the below described adaptive algorithms based on gradient approach. Proposed approaches described for the approximation of the continuous processes only, but it is easy to derive discrete counterparts on their basis. As a rule, signals are measured into discrete moments. That is why differencing schemes could prove to be more effective for use.

#### Approximation of continuous signals

Let suppose that we know of uninterrupted, for ease of scalar signal  $x=\varphi(t)$ ,  $t_0 \le t \le T$ , which needs to be approximate with parametrically given assemblage

$$x(t) \approx \psi(t, \alpha) = \psi(t, \alpha_1, \alpha_2, ...\alpha_n).$$
 (1)

If the signal is defined on  $[t_0, t]$ , the task of parameters  $\alpha$  vector adaptive correction is to minimize certain residual [5]. For this purpose, we will consider two types of residuals:

a) directly at the moment t

$$I_1(\alpha) = (\psi(t, \alpha) - \varphi(t))^2; \tag{2}$$

b) mean square approximation of  $[t_0, t]$ 

$$I_2(\alpha) = \int_{t_0}^t (\psi(\tau, \alpha) - \varphi(\tau))^2 d\tau.$$
 (3)

For correction of parameters in order to minimize residual (2) uninterrupted iterative procedure is written down

$$\frac{d\alpha}{dt} = -grad_{\alpha}I_{1}(\alpha) = 
= -2(\psi(t,\alpha) - \varphi(t))grad_{\alpha}\psi(t,\alpha)$$
(4)

with some initial data

$$\alpha(t_0) = \alpha^{(0)}. \tag{5}$$

To find vector parameters  $\alpha$  solution of Cauchy problem is needed (4), (5). If there is a stationary problem solution (4), (5), that is  $\alpha(t) \to \overline{\alpha}$ ,  $t \to \infty$ , you can be taken as a solution of given problem. It is

necessary to notice that for solving some practical tasks such a simple procedure gives good results.

For the integral residual we write down the same system of ordinary differential equations

$$\frac{d\alpha}{dt} = -\operatorname{grad}_{\alpha} I_{2}(\alpha) = 
= -2 \int_{t_{0}}^{t} (\psi(\tau, \alpha) - \varphi(\tau)) \operatorname{grad}_{\alpha} \psi(\tau, \alpha) d\tau.$$
(6)

As (6) is a system of ordinary differential equations of order n, recorded in normal form, initial conditions for it must be selected similarly to the previous case

$$\alpha(t_0) = \alpha^{(0)}. (7)$$

That means, in another case is needed to solve the problem numerically with one of the methods, such as Runge-Kutta, a Cauchy (6), (7).

Comment 1. The original data is to be chosen from the convergence of the proposed iterative procedures, e.g. using Lyapunov second method.

Consider a more specific problem of formulated type. Suppose we have a system of basic functions  $\varphi_1(t), \varphi_2(t), ..., \varphi_n(t), \quad t \ge t_0$ , (8)

and function  $\psi(t,\alpha)$  will choose as a linear combination of

$$\psi(t,\alpha) = \sum_{j=1}^{n} \alpha_{j} \varphi_{j}(t). \tag{9}$$

In this case, the system of ordinary differential equations (4) we write in this form

$$\frac{d\alpha_i}{dt} = -2\varphi_i(t)\sum_{j=1}^n \varphi_j(t)\alpha_j + 2\varphi(t)\varphi_i(t), \tag{10}$$

i = 1, 2, ..., n

System (10) is a linear nonparallel sentence system of ordinary differential equations which can be re rewritten in a vector-matric form

$$\frac{d\alpha}{dt} = A(t)\alpha + f(t), \quad t \ge t_0. \tag{11}$$

According to Cauchy's formula solution of problem (5), (11) can be written as follows

$$\alpha(t) = W(t, t_0)\alpha^{(0)} + \int_{t_0}^t W(t, \tau)f(t)d\tau, \qquad (12)$$

where  $W(t,\tau)$  – scaled under the moment  $\tau$  fundamental matrix of a homogeneous system, which corresponds to (11), i.e.

$$\frac{dW}{dt} = A(t)W, \quad W(\tau, \tau) = E_n. \tag{13}$$

By analogy, you can extract systems of differential equations for the integral residual (3)

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provided (9). In this case, the system (6) could be written in this form

$$\frac{d\alpha_i}{dt} = -2 \int_{t_0}^t \left( \sum_{j=1}^n \alpha_j \varphi_j(\tau) - \varphi(\tau) \right) \varphi_i(\tau) d\tau,$$

$$i = 1.2 \qquad n \tag{14}$$

A linear system (14) could be written in a vectormatrix form

$$\frac{d\overline{\alpha}}{dt} = \overline{A}(t)\alpha + 2\overline{f},\tag{15}$$

where 
$$\bar{f}^T(t) = \int_{t_0}^t f^T(\tau) d\tau$$
,  $\overline{A}(t) = \int_{t_0}^t A(\tau) d\tau$ .

However, a diverse linear system of ordinary differential equations (14), in effect (7), you need to consider under partially fixed initial conditions. In order to find an overall system solution (14) under any  $\alpha^{(0)}$ , will use the Cauchy formula

$$\alpha(t) = \overline{W}(t, t_0)\alpha^{(0)} + \int_{t_0}^{t} \overline{W}(t, \tau)\overline{f}(\tau)d\tau , \qquad (16)$$

where  $\overline{W}(t,\tau)$  – converging for a moment  $\tau$  fundamental matrix for homogeneous system

$$\frac{d\alpha}{dt} = \overline{A}(t)\alpha . {17}$$

This matrix satisfies the system with a single initial conditions

$$\frac{dW}{dt} = \overline{A}(t)\overline{W}, \quad \overline{W}(t_0, t_0) = E_n. \tag{18}$$

#### Analysis of iterative procedures convergence

Let us conduct analysis of the convergence of iterative procedures using Lyapunov methods of practical stability [4].

Consider two types of residuals (2) and (3).

Let us look at the iterative scheme based on minimization of residual (2). Suppose that solution of the Cauchy problem (5), (11) meets the condition  $\alpha^{(1)}(t,t_0,\alpha^{(0)}) \rightarrow \overline{\alpha} = const, \ t \rightarrow \infty$ . Then with the substitute

$$\alpha = \alpha^{(1)}(t, t_0, \alpha^{(0)}) + v(t) \tag{19}$$

we'll come to a homogeneous system of linear differential equations with respect to the new variable v(t)

$$\frac{dv}{dt} = A(t)v , \quad t \ge t_0 . \tag{20}$$

Then, on the assumption that the original data (5) can be perturbed, analysis of convergence of iterative procedure (11) will be equivalent to the research of

stability of solution  $v(t) \equiv 0$ ,  $t \ge t_0$  of linear homogeneous system (20). Fair's the next theorem.

Theorem 1. For the convergence of iterative scheme (13) at perturbed initial data, i.e.

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$$\alpha(t, t_0, \alpha^{(0)} + v^{(0)}) \rightarrow \overline{\alpha}, \ t \rightarrow \infty$$
 (21)

is necessary and sufficient, the converging for a moment fundamental matrix  $W(t,t_0)$ , to meet the conditions

$$W(t,t_0) \to 0$$
, for  $t \to \infty$ . (22)

The proof of the formulated theorem is based on the framework as a replacement (19), recording and analysis of Cauchy problem solution for a homogeneous system (20)

$$v(t) = W(t, t_0) v^{(0)}. (23)$$

Here  $v^{(0)}$  – *n*-dimensional vector of initial data for homogeneous system (20),  $\overline{\alpha}$  –*n*-dimensional stationary vector, which is the solution of the given problem.

### Detection of chemical components in the plants and calculation experiment

Let's show constructiveness and effectiveness of the proposed approach primarily based on spectral data processing of the plants contaminated with chemical elements. We assume that plants pollution is generated by some chemical elements and its spectral data received. They are considered as basic for recognition of them in new experimental data. Let us designate basic spectral functions

$$\varphi_1(t), \varphi_2(t), \dots, \varphi_n(t), \quad t_0 \le t \le T$$
,

which represent the spectral data of plants pollution by known chemical elements.

Let  $\varphi(t), t \in [t_0, T]$  the measured spectral function contaminated by an unknown chemical element. The function  $\psi(t, \alpha)$  will choose as a

linear combination of (9) 
$$\psi(t,\alpha) = \sum_{j=1}^{n} \alpha_{j} \varphi_{j}(t)$$
.

Solution of differential equations system (10) will give us needed parameters vector.

Numerical experiment conducted under the described above adaptive algorithm. Spectral experimental data on a plant specimens were chosen for the basic functions, which were contaminated by the chemical elements CaCl and  $K_2Cr_2O_7$ . Spectral values of basic functions displayed on Figure 1. For the recognition of new experimental data for the contamination with selected chemical elements, an adaptive algorithm is applied and the result are shown on Figure 2.

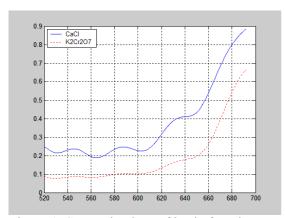


Figure 1. Spectral values of basic functions.

Unknown parameters vector converges to 0 for the experimental data contaminated by CaCl and to 1 for  $K_2Cr_2O_7$  correspondingly. It means that contamination by chemical element  $K_2Cr_2O_7$  is recognized. .

#### Conclusion

Developed concept of adaptive algorithm for approximation of experimental data with discrete dimensions based on gradient approach.

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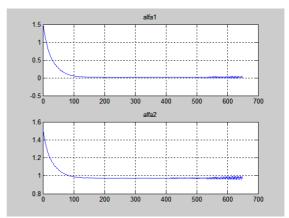


Figure 2. Iterative procedure convergence for experimental data contaminated by the chemical elements CaCl (alfa1) and K<sub>2</sub>Cr<sub>2</sub>O<sub>7</sub> (alfa2).

Adaptive algorithm for approximation of discrete experimental data on the basis of gradient approach created. Convergence of proposed adaptive algorithm for detecting chemical and biological components proven. Particularities of application of adaptive algorithm of forecasting at initial detection of components of different types investigated.

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