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MULTILAYER PARAMETRIC MODELS OF PROCESSES IN A POROUS CATALYST PELLET

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Abstract

In this paper, we perform a comparative analysis of new methods for constructing approximate solutions of differential equations. As a test problem, we chose the boundary value problem for a substantially nonlinear second-order differential equation. This problem arose when modeling the processes of heat and mass exchange in a flat granule of a porous catalyst. Previously, we solved this problem with the help of artificial neural networks, using it as a model problem for testing methods developed by us. Our generic neural network approach has been applied to this problem both in the case of constant parameters and parameters varying in some intervals. In the case of constant parameters, the result coincided with the data available in the literature on the subject. Models with variable parameters, which are part of the inputs of neural networks, were first built in our works. One of the significant drawbacks of this approach is the high resource intensity of neural network learning process. In this paper, we consider a new approach, which allows doing without the training procedure. Our approach is based on a modification of known numerical methods – on an application of classical formulas of the numerical solution of ordinary differential equations to an argument change interval with a variable upper limit. The result is an approximate mathematical model in the form of a function, and the parameters of the problem are among the arguments of the function. In this paper, we showed that the new methods have significant advantages. We have considered two such methods. One method is based on a neural network modification of the shooting method. The second method differs in that the shooting is conducted on both sides of the gap. The obtained models are characterized by simplicity and a wide range of parameters for which they are suitable. The models we have built can be easily adapted to observations of real objects. The models we have built can be easily adapted to data observations of real objects.

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Keywords

Catalyst grain; boundary-value problem; approximate solution; neural network modeling; artificial neural network; multilayered modeling; numerical method modification.

МНОГОСЛОЙНЫЕ ПАРАМЕТРИЧЕСКИЕ МОДЕЛИ ПРОЦЕССОВ В ГРАНУЛЕ ПОРИСТОГО КАТАЛИЗАТОРА

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Аннотация

В данной статье мы проводим сравнительный анализ новых методов построения приближённых решений дифференциальных уравнений. В качестве тестовой задачи мы выбрали краевую задачу для существенно нелинейного дифференциального уравнения второго порядка. Данная проблема возникла при моделировании процессов обмена тепла и массы в плоской грануле пористого катализатора. Ранее мы решали эту задачу с помощью искусственных нейронных сетей, используя её как модельную задачу для апробации разработанных нами методов. Наш универсальный нейросетевой подход был применён к данной задаче как в случае постоянных параметров, так и для параметров, изменяющихся в некоторых интервалах. В случае постоянных параметров результат совпал с данными, имеющимися в литературе по данной тематике.

Модели с переменными параметрами, являющимися частью входов нейронных сетей, были впервые построены в наших работах. Одним из существенных недостатков такого подхода является большая ресурсоёмкость процесса обучения нейронных сетей. В данной работе рассматривается разработанный нами новый подход, позволяющий обойтись без процедуры обучения. Наш подход основан на модификации известных численных методов – на применении классических формул численного решения обыкновенных дифференциальных уравнений к интервалу изменения аргумента с переменным верхним пределом. В результате получается приближённая математическая модель в виде функции, причём параметры задачи входят в число аргументов функции. В данной статье мы показали, что новые методы имеют существенные преимущества. Мы рассмотрели два таких метода. Один метод основан на нейросетевой модификации метода пристрелки. Второй метод отличается тем, что пристрелка ведётся с двух сторон промежутка. Для полученных моделей характерны простота и широкая область изменения параметров, для которых они пригодны. Построенные нами модели могут быть легко адаптированы под данные наблюдений за реальными объектами.

Ключевые слова

Гранула катализатора; краевая задача; приближенное решение; нейросетевое моделирование; искусственная нейронная сеть; многослойное моделирование; модификация численного метода.

Introduction

In this paper, we perform a comparative analysis of new methods for constructing approximate solutions of differential equations. As a test problem, we chose a boundary value problem for an essentially nonlinear differential equation of the second order. Some analytical and numerical methods of solutions to similar problems are described in detail in [1-5].

Various mathematical methods can be used to describe a wide range of chemical reactions [6,7]. The test problem arose in the simulation of heat and mass exchange processes in a plane porous catalyst granule. The need to obtain solutions to such problems is associated with the widespread use of granular media in the chemical industry, which led to the development of modeling in the field of reactions and processes occurring in the presence of a catalyst [8]. Thus, due to the high degree of use of catalytic chemical reactions, there are a large number of diverse modeling techniques specific boundary value problems by using numerical methods [9-12].

Analysis of the heat-and-mass balance in a porous catalyst pellet at a catalytic chemical reaction leads to the study of boundary value problem with Zaremba's conditions for nonlinear ordinary differential equation [3, 22].

Two methods of numerical solution to the discrete analog of the problem – its difference approximation – are given in the article [21] from the proceedings of the VI International conference NPNJ'2006: Lahae's method [26] and the method of discrete continuation on the best parameter [27]. The results of calculations on these original methods, unfortunately, are not given, but authors argue that they coincide with the results obtained by the method of integral equations, which are given in the famous monograph [22].

Previously, we solved this problem with the help of neural networks. The variety of types [13] and methods of realization of neural networks [14, 15] allows using them for the solution of nonlinear differential equations taking into account certain boundary conditions [16, 17]. In this paper, we showed that our new methods have significant advantages. We considered two methods. One is based on a neural network modification of the shooting method. The second differs in that the shooting is conducted on both sides of the interval using the Euler method [18].

The publication of the authors [28] proposed a variant of the construction of an approximate neural network solution to this problem in the case of fixed system parameters. There was a good agreement of the obtained neural network solution with the results given in the book [22]. Later in the paper [19] the original neural network method of constructing approximate solutions of differential equations [20] was given. This method has been tested on the problem of modeling processes of heat and mass transfer [21, 22, 29]; the generalization of the catalyst problem was considered in the case of interval values of system parameters. The resulting parametric neural network models were also used to describe processes in the non-isothermal chemical reactor.

The complexity of the object modeling, due to the dependence of the process on a set of factors [23, 24], leads to the low accuracy of the corresponding differential models. It is impossible to improve the accuracy of these models without their significant complication, which does not always lead to success due to the impossibility of an accurate description of the features of a particular real object. In this regard, the requirement of adaptability of the model comes to the fore, i.e., the possibility of its refinement according to observations of the object. In works [19, 20] it is shown that our methods of neural network modeling allow building adaptive models, and methods for adjusting models under new data are given.

In this work, we compare these results with the results of our new method for constructing multilayer solutions of differential equations [25]. Method [25] allows building much simpler models while maintaining accuracy. Ttljdfhis fact facilitates their use and adaptation as new data becomes available.

Material and methods

In works [21, 22] processes of heat-and-mass transfer in a flat granule of a porous catalyst are modeled using the boundary value problem for a second-order nonlinear ordinary differential equation

$$\frac{d^2y}{dx^2} = \alpha(1+y)\exp[-\frac{\gamma\beta y}{1-\beta y}] \quad (1)$$

with conditions $y'(0)=0, \quad y(1)=0$. The new approach [25] is a fundamental modification of the known numerical methods such as the Euler method, consisting in the application of these methods to an interval with a variable upper limit.

In this article, we compare two specific methods of this kind.

We obtain the first method by the modification of Störmer's method indicated above [1]. The peculiarity of the problem lies in the fact that classical numerical methods are intended for solving the Cauchy problems, and not for boundary value problems.

To overcome the emerging difficulty, we use the Störmer method formula to write down an approximate multilayer solution of the Cauchy problem

$$y_{k+1}(x,p)=2y_k(x,p)-y_{k-1}(x,p)+\frac{x^2}{n^2}f(y_k(x,p)), \quad (2)$$

where

$$f(y)=\alpha(1+y)\exp[-\frac{\gamma\beta y}{1-\beta y}]. \quad (3)$$

In formula (2), the parameter is the unknown condition for the solution at the left end: $y_0(x,p)\equiv p$. We are looking for this parameter in the form of a neural network function of the task parameters $p=p(\alpha,\beta,\gamma)$; we choose the weights based on the condition on the right end $y(1,p)=0$.

In the second method of constructing the solution, we constructed an approximate solution $y(x,p)$ from two sides of the gap, with a smooth docking in the middle. При этом уравнение (1) переписывается в виде системы

$$\begin{cases}\frac{dy}{dx}=z\\ \frac{dz}{dx}=f(y)\end{cases} \quad (2)$$

The initial conditions have the form $z(0)=0$, $y(0)=p$.

Next follows the implementation of 4 variants of the algorithm.

1) The first step is done by Euler's method

$$y_1=p+hz_0=p,$$

$$z_1=z(0)+hf(p)=hf(p). \quad (4)$$

The second step by Euler's method leads to the equalities

$$y_2=y_1+hz_1=p+h^2f(p),$$

$$z_2=z_1+hf(y_1)=2hf(p). \quad (5)$$

In this case $h=x/2$, whence $y_2(x)=p+\frac{x^2}{4}f(p)$.

2) The first step is done according to Euler's method. The second step is done according to the refined Euler method [1,18]

$$y_2=p+2hz_1=p+2h^2f(p),$$

$$z_2=z_0+2hf(y_1)=2hf(p), \quad (6)$$

whence $y_2(x)=p+xz_1(x)=p+\frac{x^2}{2}f(p)$.

3) We make two steps according to the Euler method with $h=x/4$, whence $z_2(x)=\frac{x}{2}f(p)$.

Next, we make the step of the refined Euler method

$$y_3(x)=p+4hz_2(x)=p+8h^2f(p)=p+\frac{x^2}{2}f(p).$$

4) We are implementing the second option with $h=x/4$, whence $z_2(x)=\frac{x}{2}f(p)$.

Next, we make the step of the refined Euler method

$$y_3(x)=p+4hz_2(x)=p+8h^2f(p)=p+\frac{x^2}{2}f(p).$$

We can see that the formulas for the second, third and fourth variants coincide.

On the right, we make a replacement $x=1-t$, the form of equation (1) does not change, wherein we reduce it to the system again $\begin{cases}\frac{dy}{dt}=z,\\ \frac{dz}{dt}=f(y).\end{cases}$

The boundary conditions have the form $z(0)=q$, $y(0)=0$.

We implement the same four options.

1) The first step is done by Euler's method

$$y_5=y_4+hq=hq,$$

$$z_5=z_4+hf(q)=q+hf(0). \quad (7)$$

The second step by Euler's method leads to the equalities

$$y_6=y_5+hz_5(t)=2hq+h^2f(0),$$

$$z_6=z_5+hf(y_5)=q+hf(0)+hf(hq). \quad (8)$$

In this case $h=t/2$, whence

$$y_6(x)=tq+\frac{t^2}{4}f(0)=(1-x)q+\frac{(1-x)^2}{4}f(0).$$

2) The second step is done according to the refined Euler method

$$y_6=y_4+2hq=2hq+2h^2f(0),$$

$$z_6=q+2hf(y_5)=q+2hf(hq), \quad (9)$$

whence

$$y_6(t)=tq+\frac{t^2}{2}f(0)=(1-x)q+\frac{(1-x)^2}{2}f(0).$$

3) We make two steps according to the Euler method with $h=t/4$, whence

$$z_6=q+\frac{t}{4}f(0)+\frac{t}{4}f\left(\frac{tq}{4}\right).$$

Next, we make the step of the refined Euler method

$$y_7=y_4+4hz_6=tq+\frac{t^2}{4}f(0)+\frac{t^2}{4}f\left(\frac{tq}{4}\right)=(1-x)q+\frac{(1-x)^2}{4}\left(f(0)+f\left(\frac{(1-x)q}{4}\right)\right).$$

4) We are implementing the second option with $h=x/4$, whence $z_6=q+\frac{t}{2}f\left(\frac{tq}{4}\right)$.

Next, we make the step of the refined Euler method

$$y_7=y_4+4hz_6=tq+\frac{t^2}{2}f\left(\frac{tq}{4}\right)=(1-x)q+\frac{(1-x)^2}{2}f\left(\frac{(1-x)q}{4}\right).$$

In the subsequent calculations, the first two variants were tested.

Version 1. Dock solutions in the middle of the interval

$y_2(0.5)=y_6(0.5)$, $y_2'(0.5)=y_6'(0.5)$, whence

$$p+\frac{1}{16}f(p)=\frac{1}{2}q+\frac{1}{16}f(0),$$

$$\frac{1}{4}f(p)=-q-\frac{1}{4}f(0).$$

From these equalities we obtain an equation for determining p

$$p+\frac{3}{16}f(q)+\frac{1}{16}f(0)=0. \quad (10)$$

We will take into account that $f(0)=\alpha$, then for the first half of the interval we obtain a solution

$$y_2(x)=p-\frac{x^2}{12}(\alpha+16p), \quad (11)$$

and in the second half –

$$y_6(x)=\frac{(x-1)}{12}(3x\alpha-\alpha-16p). \quad (12)$$

Version 2. Dock solutions in the middle of the interval

$y_2(0.5)=y_6(0.5)$, $y_2'(0.5)=y_6'(0.5)$, откуда

$$p+\frac{1}{8}f(p)=\frac{1}{2}q+\frac{1}{8}f(0),\ \frac{1}{2}f(p)=-q-\frac{1}{2}f(0).$$

From these equalities, we obtain an equation for determining p

$$p+\frac{3}{8}f(p)+\frac{1}{8}f(0)=0 \quad (13)$$

We will take into account that $f(0)=\alpha$, then for the first half of the interval we obtain a solution of the form

$$y_2(x)=p-\frac{x^2}{6}(\alpha+8p), \quad (14)$$

and in the second half –

$$y_6(x)=\frac{(1-x)}{3}(\alpha-4p)+\frac{(1-x)^2}{2}\alpha=\frac{(x-1)}{6}(3x\alpha-\alpha-8p) \quad (15)$$

Calculation

The purpose of this work was to qualitatively investigate the relationship between the mean square error values at test points for the equation and in the boundary conditions and various combinations of the number of layers corresponding to the multilayer formula and the neurons in the network approximating the initial condition. In this case, in comparison with [19], the range of variation of the parameters α,β,γ, was sharply expanded, each of which now varied in the interval from 0 to 2.

When implementing the first method to approach a solution $y(x,p,\alpha,\beta,\gamma)$, the number of layers in which is equal to two, we obtain the expression

$$p+0.25x^2\alpha(\mathrm{e}^{-\frac{p\beta\gamma}{1-p\beta}}(1+p)+exp\left[-\frac{\left(p+0.125\mathrm{e}^{-\frac{p\beta\gamma}{1-p\beta}}(1+p)x^2\alpha\right)\beta\gamma}{1-\left(p+0.125\mathrm{e}^{-\frac{p\beta\gamma}{1-p\beta}}(1+p)x^2\alpha\right)\beta}\right](1+p)(1+0.125\mathrm{e}^{-\frac{p\beta\gamma}{1-p\beta}}x^2\alpha)).$$

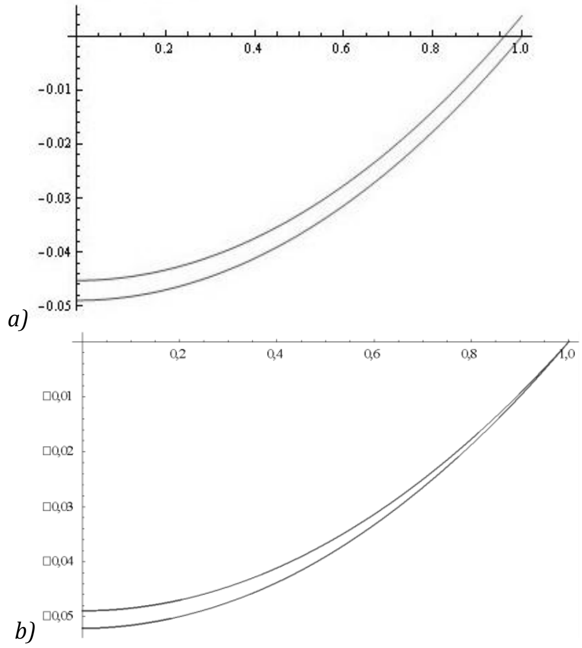

Fig.1. Graphs a) of the solution calculated by the approximate formula of the first method (2) in the case of four layers using a network of 15 neurons for $p(\alpha,\beta,\gamma)$, b) a solution constructed for a network of 100 neurons by the method of [2] for intervals of parameter variation $\alpha\in(0.05;\ 0.15)$, $\beta\in(0.4;\ 0.6)$, $\gamma\in(0.8;\ 1.2)$, and the solution found in package Mathematica. The values of the parameters $\alpha=0.1$, $\beta=0.5$, $\gamma=1$ for which the solution was constructed

The smallest error in the boundary conditions was reached with the maximum number of neurons considered to be 15, it was 0.0012, and for test points for the equation, the smallest mean-square error 0.0025 was obtained for a given number of neurons. When carrying out calculations for the three-layer and four-layer formulas, the time for obtaining an approximate solution and root-mean-square errors has significantly increased. The results of calculations of calculation errors for three-layer formulas showed that the most accurate result is achieved with five neurons in a network that approximates the initial condition.

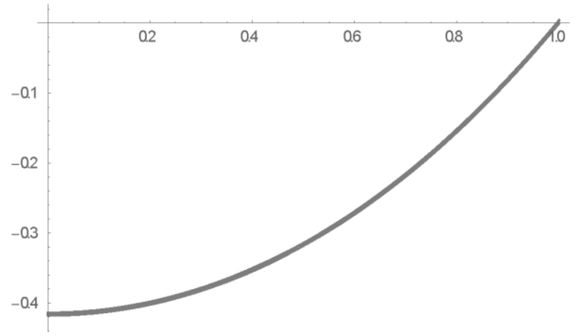

Fig.2. The graphs of the solution, calculated according to the approximate formula of the first method (2) in the case of four layers using a network of 15 neurons for $p(\alpha,\beta,\gamma)$, and the solution found in the Mathematica package. The values of the parameters $\alpha=1$, $\beta=1$, $\gamma=1$ under which the solution was constructed

For trial points for the equation, the smallest mean square error was 0.0025. Subsequent calculations, in which four layers corresponding to the multilayer formula were considered, showed that there is a direct relationship between the increase in the accuracy of the approximate calculation and the number of layers since the smallest error was revealed precisely with the maximum number of layers considered in this paper. Thus, using an approximate network of 5 neurons, the mean square errors were obtained for the trial points of the equation 0.00202 and the boundary conditions 0.00082, respectively. These values showed the minimum error of the approximate solution.

The table below shows the mean square error values for different combinations of the number of layers and neurons of the approximate network. In the upper left corner of each cell are the values for the root-mean-square error for the parameter change area $\alpha,\beta,\gamma\in[0;1]$, and in the lower right corner for the parameter change area $\alpha,\beta,\gamma\in[0;2]$. The selected values are the smallest for the entire series of experiments.

Table 1

The number of layers corresponding to the multilayered formula / The number of neurons in approaching network	2	3	4
2	0.00337 / 0.0363	0.00349 / 0.0299	0.00377 / 0.0250
5	0.00274 / 0.00837	0.00246 / 0.0124	0.00201 / 0.00852
15	0.00246 / 0.00802	0.00251 / 0.00832	0.00230252 / 0.0107

Thus, the solution constructed in this way, in comparison with the previous approach [19], preserves the accuracy of an essentially wider set of task parameters with a smaller number of selectable network weights.

For the second method, the result of applying two variants of the application of the algorithm differs significantly. For the first variant (formulas (10-12)), the error is too big.

An increase in the number of neurons does not lead to a significant decrease in the error. The second variant of the second method (formulas (13-15)) leads to qualitatively better results.

An even more striking result was obtained when trying to predict the result for a parameter $\alpha = \beta = \gamma = 1.5$ value using a network that was trained for parameter $\alpha, \beta, \gamma \in [0;1]$ change intervals.

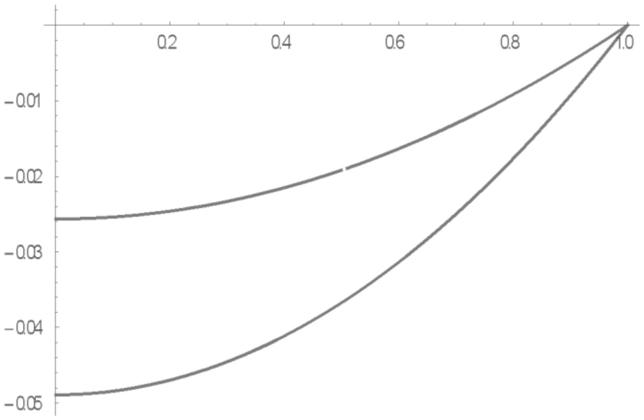

Fig.3. The graphs of the solution, calculated according to the approximate formula of the first variant of the second method (formulas (10-12)) using a network of 5 neurons for the solution $p(\alpha, \beta, \gamma)$ found in the package Mathematica. The neural network was trained for intervals of parameter changes $\alpha, \beta, \gamma \in [0;1]$. The values of the parameters $\alpha = 0.1,\ \beta = 0.5,\ \gamma = 1$ for which the solution was constructed

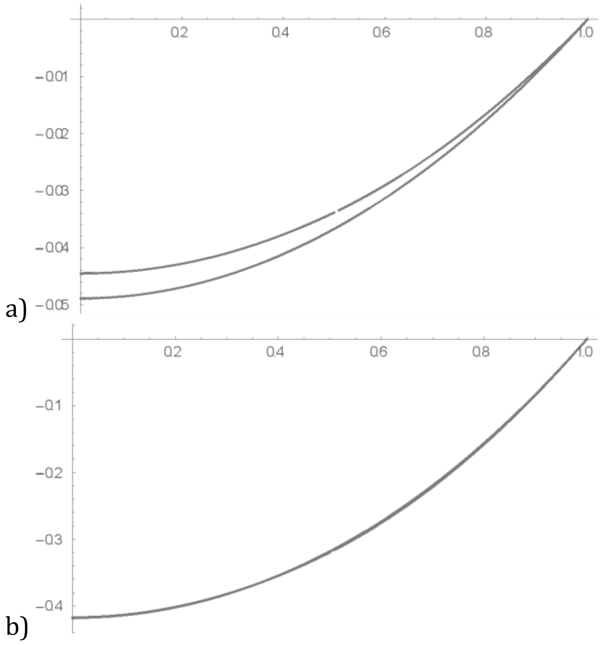

Fig.4. The graphs of the solution calculated by formulas (13-15) of the second variant of the second method using a network of 15 neurons for $p(\alpha,\beta,\gamma)$ and the solution found in the Mathematica package. The neural network was trained for intervals of parameter $\alpha,\beta,\gamma\in[0;1]$ changes. a) The values of the parameters $\alpha=0.1$, $\beta=0.5$, $\gamma=1$ under which the solution was constructed. b) The values of the parameters $\alpha=\beta=\gamma=1$ at which the solution was constructed

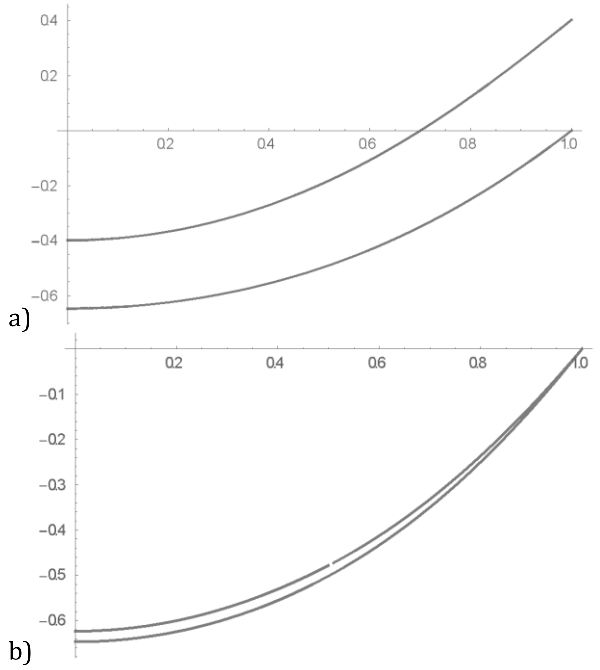

Fig.5. Solution graphics, using a network of 5 neurons for $p(\alpha,\beta,\gamma)$ and the solution found in the Mathematica package. The neural network was trained for intervals of parameter $\alpha,\beta,\gamma\in[0;1]$ changes. The values of the parameters $\alpha=\beta=\gamma=1.5$ under which the solution was constructed. a) The approximate formula of the first method (2) is used in the case of four layers. b) The formulas (13-15) of the second variant of the second method are used

Table 2. The root-mean-square errors for the second variant of the second method are formulas (13-15)

The number of neurons in approaching network	Intervals for changing parameters about network training $\alpha,\beta,\gamma\in[0,1]$	Intervals for changing parameters about network training $\alpha,\beta,\gamma\in[0,2]$
2	0.00317	0.0156
5	0.00232	0.00648
15	0.00141	0.00389

Results and Discussion

Comparison of the new approach [25] with the old one [19, 20] shows its superiority in several aspects.

First, the application of a new campaign allows us to drastically expand the range of parameters for which the model is built. Moreover, the second variant of the second method allows extrapolating the model to a wider range of parameter changes than the one used in the construction of the model.

Secondly, the new approach allows you to build much less complex models while maintaining accuracy. The model constructed with the help of the second variant of the second method with two neurons is a convenient approximate analytical model that can be used not only for computer calculations.

$$\begin{cases} 0.169+x^2(-0.224-0.167\alpha)+(0.374-0.499x^2)\tanh\begin{bmatrix}0.391-0.44\alpha\\ -0.0839\beta-0.101\gamma\end{bmatrix}+ \\ +(-0.564+0.752x^2)\tanh[0.618+0.799\alpha-0.071\beta-0.0904\gamma] \end{cases}, x<0.5;$$

$$\frac{x-1}{6}\left(-\alpha+3x\alpha-8\begin{pmatrix}0.168+0.374\tanh[0.391-0.44\alpha-0.0839\beta-0.101\gamma]- \\ 0.564\tanh[0.618+0.798\alpha-0.071\beta-0.0904\gamma]\end{pmatrix}\right), x\ge 0.5$$

Third, the new approach allows us to create a wider palette of approximate formulas, which is especially relevant in the situation where equation (1) poorly describes the real object. In such a situation, it is required to choose the model most accurately reflecting the observations of the object, so a wider set of models makes it possible to find among them more adequate.

The second method allowed building more accurate models, but it requires more accuracy, which is shown by the first version of this method, based on the formulas (10-12).

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