DOI https://doi.org/10.15407/csc.2022.02.033
UDC 6:004.8

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PROBLEM OF CONSTRUCTING THE GMDH NEURAL NETWORKS WITH ACTIVE NEURONS

Characteristics of the existing neural networks of GMDH with active neurons are given and their main advantages and disadvantages are analyzed. Two approaches of increasing efficiency of inductive construction of complex system models from statistical data based on a new hybrid GMDH neural networks with active neurons using methods of computational intelligence are proposed. Effectiveness of these networks are compared with classical approaches on artificial inductive modelling tasks (noisy linear and nonlinear models).

Keywords: *inductive modeling, GMDH neural network, active neurons, computational intelligence, genetic algorithms.*

Introduction

The Group Method of Data Handling (GMDH) [1–4] is one of the most successful methods of inductive modeling methods which extract knowledge directly from the data based on experimental or statistical measurements. It is used in various tasks of data analysis and knowledge discovery, forecasting and systems modeling, classification and pattern recognition.

Main GMDH advantages are as follows [5]:

- the model structure and its parameters are found automatically; optimal complexity of the model structure is found adequately to the noise level in data sample.
- the method uses information directly from a data sample and minimizes the impact of a priori assumptions on the modeling results;
- relationships in data are found and informative input variables are selected;
- the model structure and its parameters are found automatically;
- optimal complexity of the model structure is found adequately to the noise level in the data sample;
- any non-linear functions or factors that could affect the output variable are used as input variables (arguments).

As of today, a great variety of GMDH algorithms of the sorting-out and iteration types was developed and explored [6–8 2, 3]. The sorting-out algorithms are effective as the tool for structural identification but only for limited number of arguments. Iterative GMDH such us the MIA GMDH is effective data mining tool developed by O. Ivakhnenko in 1965 as multilayer deep feed

forward neural network (NN) with unlimited number of layers which settings during learning process [9, 10]. These algorithms are capable of working with a lot of arguments but often need too much time to achieve desired accuracy. Currently the most effective GMDH neural network is GIA with "active neurons" [11–15] with optimization of every partial model structure by combinatorial algorithm [6–8] to avoid inclusion of spurious arguments in the final model and overfitting the model complexity. However, such optimization needs to sort-out all models structure, which would require a lot of computational time.

It is known [17] that hybridization of neural network and genetic algorithm (GA) [18–21] is a good way to combine their strengths, speed up training process of neural networks and obtain better modelling results.

To enhance GIA GMDH algorithm two novel versions of this algorithm "with active neurons" are proposed in this paper. The first one performs optimization of every partial model structure by genetic algorithm, whilst the second one optimizes all partial model structures simultaneously using GA. To verify the effectiveness of proposed algorithms they are compared to multilayered perceptron and GIA GMDH on artificially generated data of different complexity.

General characteristics of the GMDH as an inductive method of model building

The main goal of GMDH network is to fit the given data using a feed-forward network of the special type, where each neuron has a second-degree transfer activation function. The method uses information directly from a data sample and minimizes the *a*-priori assumptions impact an author on the modeling results; finds regularity in data and selects informative input arguments; automatically finds the model structure and its parameters.

Any GMDH algorithm solves a discrete optimization task to construct the optimal complexity model by the given external criterion minimum based on the data sample separation:

$$f^* = \arg\min_{f\in\Phi} CR(f),$$

where CR is a selection criterion as a measure of the quality of the model $f \in \Phi$ quality.

A model selection criterion is called "external" if it is based on additional information that is not contained in the data used for calculation of model parameters. The models set Φ being explored can be formed using iterative and sorting-out model structures generators of diverse complexities which differ by variants generation techniques and organization of a given external criterion minimum search based on additional information that is not contained in the data used for calculation of model parameters.

For realizing the external supplement principle, the parameter estimations by the least squares method *LSM* (usually) and criteria values are calculated on various sample $W = [X, y]$ parts, where X, y are matrix and n measurements vector of m arguments and one output respectively. The input sample W splits into training (A) and checking (B) subsets. The regularity criterion calculated for a model $f \in \Phi$ is most commonly used among GMDH criteria:

$$AR_{B|A}(f) = \left\| y_B - \hat{y}_{B|A}(f) \right\|^2 = \left\| y_B - X_{Bf}\hat{\theta}_{Af} \right\|^2,$$

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and means "the error of the model $f(\cdot)$ on dataset B with parameters obtained on A", and X_{Af}, X_{Bf} are the submatrices of the matrix X that contain columns that correspond to a partial model $f \in \Phi$ being considered.

Building bricks of the iterative GMDH algorithm are simple initial models with the polynomial partial description. Such models can be considered as the GMDH neural network elementary neurons. The network originality with such neurons consists in high speed of the process of local adjustment of neuron weights and automatic global optimization of the network structure (number of units and iterations or hidden layers).The GMDH NN solves discrete optimization problem by successive approaching to the criterion minimum using a network-type procedure based on the analogy with the biological selection of living organisms: the models complication on a layer arise due to the pairwise "crossing" F best models from the previous layer.

The complication process stops after the value of criterion starts to increase.

Previous researches of the GMDH neural networks with active neurons

Presently, the classical multilayered iterative algorithm MIA GMDH [1–4] is the most widely known. However it has some substantial drawbacks:

1) possibility of loss of informative arguments if they were eliminated at the beginning of the selection procedure;

2) inclusion of spurious arguments to the final model if they were included at the beginning of the selection procedure;

3) exponential growth of the polynomial degree (1, 2, 4, 8, ...) due to using the non-linear (quadratic) partial description, and others.

To enhance the efficiency of the iterative GMDH algorithm, various modifications of MIA have been proposed in different periods of its evolution. Main variants of them are presented below.

To enhance the efficiency of the iterative GMDH algorithm, various modifications of MIA have been proposed in different periods of its evolution [15, 16].

In all kinds of standard (passive) neurons, any mechanisms of optimization of the set of input variables are not used, only parametric optimization is performed. The mechanisms are realized in the complex process of self-organization of the whole system of many neurons in general.

A combined method was proposed by prof. Ivakhnenko in [23] extending the theory of self-organization from fixed passive structures to active neural networks. An algorithm known as "neural network with active neurons" [23–28] is used in the GMDH architecture. Both multilayered and combinatorial GMDH algorithm can be used as active neurons; that leads to increasing the accuracy and reducing the calculation time.

The advantage of GMDH neural networks with active neurons as compared to the conventional neural network with uniform neurons consists in that self-organizing of the network is simplified: each neuron finds necessary connections and its own structure in the process of self-organization. The idea of active neurons served also as the basis for generalization of the previous modifications in order to significantly improve the efficiency of iterative GMDH algorithms such as GMDH-type neural network with feedback [29], Group of Adaptive Models Evolution [30–31], Hybrid of Differential Evolution and GMDH for Inductive Modeling [32]. These algorithms eliminate only some of the shortcomings of MIA GMDH. An Generalized Iterative Algorithm GIA GMDH [10–16] algorithm was developed to removing all three previously mentioned shortcomings. For this purpose, the algorithm uses:

- enabling the use of the initial arguments in each layer to prevent losing the relevant ones in the multilayer self-organizing process;
- using the idea of active neurons by performing the optimization of every partial model structure by combinatorial algorithm to avoid inclusion of spurious arguments in the final model and over fitting the model complexity;
- using various partial descriptions in the form of linear, bilinear or nonlinear functions on different layers;
- enabling to a user applying different modes of the modeling process.

This algorithm makes it possible to get the following basic variants of the GMDH algorithms of iterative type:

1) classical MIA GMDH algorithm with the use of pairwise combinations of only intermediate arguments;

2) an algorithm with adding to intermediate arguments only initial ones;

3) an algorithm with equal usage of both the intermediate and initial arguments in the partial descriptions;

4) in any of the three variants, the optimization of every partial model structure by combinatorial algorithm may or may not be used;

5) in the case of using the optimization, this architecture becomes a typical hybrid algorithm with active neurons.

Due to these features the GIA algorithm with quadratic partial description can build linear, bilinear and nonlinear models of complex systems and

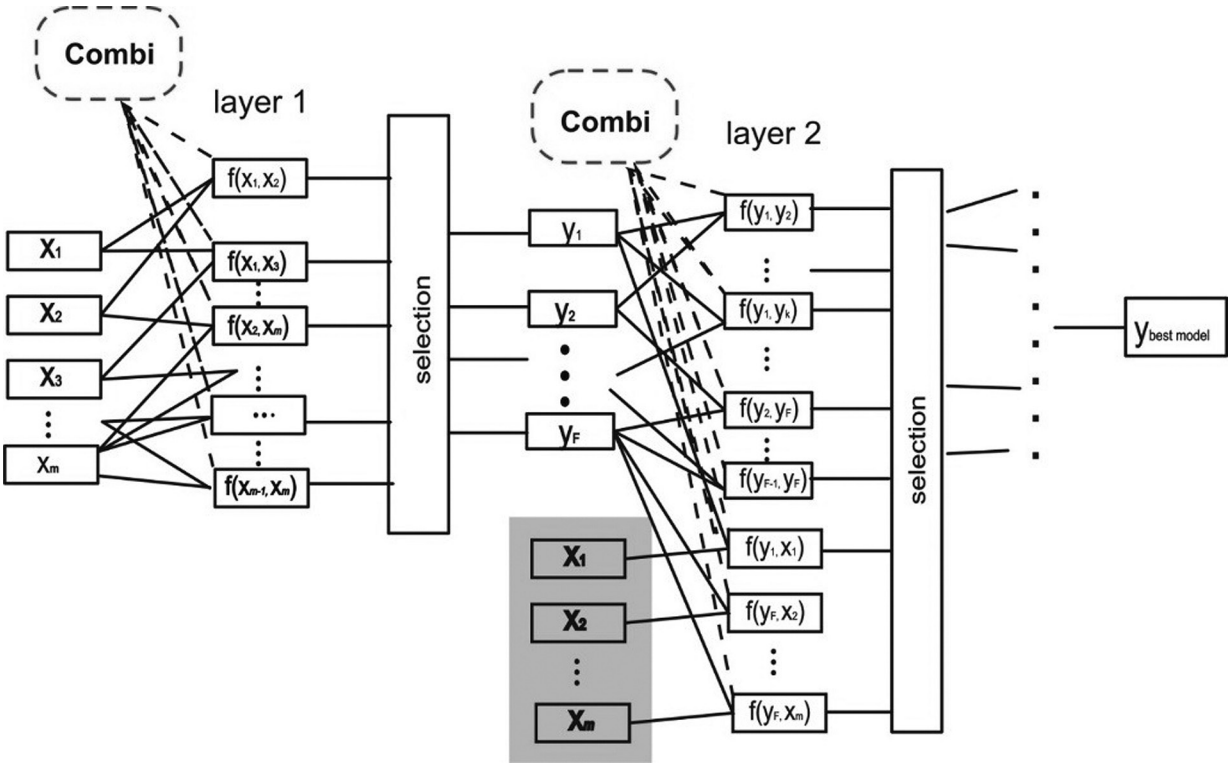

Fig. 1. The generalized architecture of GIA GMDH

processes. Let's consider its description in more detail.

GIA GMDH algorithm description

Formally, in general case, a layer of the GIA GMDH may be defined as follows [16]:

1) the input matrix is $X_{r+1} = (y_1^r, ..., y_F^r, x_1, ..., x_m)$ for a layer $r+1$, where $x_1, \ldots, x_m$, $x_1, \ldots, x_m$ are the initial arguments and $y_1^r, \ldots, y_F^r$ are the intermediate ones of the layer r;

2) the operators of the kind

$$\begin{vmatrix} y_i^{r+1} = f\left(y_i^r, y_j^r\right), i = 1,2,\ldots,C_i^2, \ i,j = \overline{1,F}, \\ y_i^{r+1} = f\left(y_i^r, x_j\right), i = 1,2,\ldots,Fm, \ i = \overline{1,F}, \ j = \overline{1,m} \end{vmatrix}$$

may be applied on the layer $r+1$ to construct linear, bilinear and quadratic partial descriptions:

$$z = f(u,v) = a_0 + a_1 u + a_2 v; \quad (1)$$

$$z = f(u,v) = a_0 + a_1 u + a_2 v + a_2 uv; \quad (2)$$

$$z = f(u,v) = a_0 + a_1 u + a_2 v + a_2 uv + a_4 u^2 + a_5 v^2; \quad (3)$$

3) for any description, the optimal structure is searched by combinatorial algorithm (see below equations)

$$z = f(u,v) = a_0 d_1 + a_1 d_2 u + a_2 d_2 v; \quad (4)$$

$$z = f(u,v) = a_0 d_1 + a_1 d_2 u + a_2 d_2 v + a_2 d_4 uv; \quad (5)$$

$$z = f(u,v) = a_0 d_1 + a_1 d_2 u + a_2 d_2 v + a_2 d_4 uv + a_5 d_6 v^2, \quad (6)$$

where $d_k \in \{0,1\}$ are the elements of the binary structural vector d and values 1 or 0 mean inclusion or not a relevant argument. Then the best model will be described as $f(u,v,d_{opt})$, where $d_{opt} = \arg\min_{i=\overline{1,q}} CR_i$, $q = 2^p - 1$, $f_{opt}(u,v) = f(u,v,d_{opt})$;

4) the algorithm stops when the condition $CR^r > CR^{r-1}$ is true. Here CR^r, CR^{r-1} are criterion values for the best models of $(r-1)$-th and r-th layers respectively. If the condition holds, then stop, otherwise jump to the next layer.

The GIA structure is schematically represented in the Fig. 1.

Table 1. **Comparison of algorithms measures for test noisy linear model**

Measure \ Algorithms	MLP	GIA	GIGA	MIGA
MAPE	0,116	0,035	0,041	0,051
R2	–1,331	0,906	0,935	0,949
MSE	0,085	0,028	0,025	0,01
Time,sec,	15,47	14,312	11,711	8,752

Table 2. **Comparison of algorithms measures for test nonlinear data**

Measure \ Algorithms	MLP	GIA	GIGA	MIGA
MAPE	0,178	0,135	0,128	0,118
R2	–0,215	0,742	0,776	0,810
MSE	0,320	0,172	0,17	0,126
Time,sec	18,045	17,17	20,37	5,389

Currently, GIA GMDH is one of the most effective GMDH NN, but it still needs to increase the speed and simplify the calculation schemes. Forthispurpose, thefollowing 2 modificationsofitwerecreated.

Construction of a new class of GMDH neural networks with active neurons using genetic algorithm

The general workflow of the first modification of the generalized GMDH (Generalized Iterative Genetic Algorithm or GIGA)

1) Only partial descriptions of the full form (3) are considered.

2) The parameters of each node are evaluated using Least Squares Algorithm. Using direct search,the best m candidates from each layer are selected

3) The structure of these nodes is optimized according to the equation (6) using genetic optimization.

The general workflow of the second modification of the generalized GMDH(Meta-generalized Iterative Genetic Algorithm or MIGA)

Let us have m outputs on the current layer of the neural network. We optimize all functions of the form (6) of the layer simultaneously using the genetic algorithm. It is proposed to encode each function in the form of a binary vector of length 7. The first two components determine input variables that we include into the function, the next 5 components determine the values of *d*2-*d*6. For example, if we have 5 outputs $x_1, x_2, \ldots, x_5$, the function can be specified by the vector (3,4,1, 1,1,0,0) which is decoded as the function $a_0 + a_1 x_2 + a_2 x_4 + a_2 x_2 x_4$. The first two components have to be integers in the interval $\overline{1,m}$, while the other components are binary.

We use mean squared error as a fitness function of each individual [1–3]. We use standard GA [19–22] only with mutation operator and elite selection operator.

Computational experiments and results

The purpose of these experiments is to compare the efficiency of such algorithms: Multilayered perceptron, GIA, proposed GIGA, and proposed MIGA. These algorithms are compared using such measures [8]:

1) Mean squared error;
2) Mean average percentage error
3) R2 score
4) Working time of the algorithm (sec.)

We split the data into three subsets: training (60%), checking (30%), validation(10%). We estimate the coefficients of GIA, GIGA, and MIGA algorithms using training data, and select the best models using testing data. Classical neural network uses both training and checking data during fit procedure. We validate and compare results in this chapter using validation data.

The research was carried out for noisy linear and nonlinear models with artificially generated data. Both datasets consist of 110 observations and 20 variables. All independent variables are from uniform distribution with zero mean value and unity standard deviation. Dependent variable of the linear noisy model has 10% of uniformly distributed noise [17]. Optimal model include 9linear terms

(for nonlinear model we add three nonlinear terms, namely x_2x_4, $x_8x_9x_{10}$, x_{18}^2.

The results of compared algorithms on the test linear noisy data are given in the Table 1. The worst algorithm is undoubtedly MLP neural network. It can be explained by the fact that MLP neural networks has a lot of parameters (weights) which causes model overfitting. The best algorithm is MIGA, which is closely followed by GIGA algorithm. It is faster and more efficient. Classical GIA algorithm works not so efficient because during the optimization we consider only the full form of the neuron functions, which slows down convergence to the optimal model.

The obtained corresponding results are given in Table 2 and show similar results to ones presented in the previous table. As nonlinear model is more complex, efficiency measures for all algorithms are worse than in previous case. However, relative efficiency still follows the same order: MIGA is the best algorithm, GIGA is the second best one.

Conclusion

Results presented above demonstrated improving the efficiency of complex systems modeling based on hybridization of architecture of GIA GMDH algorithm and genetic algorithm. Effectiveness of the developed improvements has been confirmed by numerical experiments on artificial linear noisy and nonlinear tasks.

Detection of advantages and drawbacks of GIA algorithm with active neurons has resulted in two reasonable ways to increase effectiveness of solving the model construction problems. The two versions of Generalized Genetic Iterative Algorithm GMDH with Active Neurons are implemented. The first one is based on the genetic optimization of partial descriptions of the best models. The second one optimizes all partial model structures simultaneously using GA.

Numerical experiments show that MIGA algorithm demonstrates highest performance when solving noisy and nonlinear problems in comparison to other algorithms such as MLP, GIA and GIGA. High performance speed of MIGA algorithm is the consequence of the GA usage in model optimization, which is much faster than direct search.

This fact once again confirms that hybridization with a genetic algorithm approach can significantly improve the efficiency of a neural network.

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Received 31.07.2022

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Надійшла 31.07.2022

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ПРОБЛЕМА КОНСТРУЮВАННЯ МГУА НЕЙРОННИХ МЕРЕЖ З АКТИВНИМИ НЕЙРОНАМИ

Вступ. Нейронні мережі на основі багаторядного ітераційного алгоритму групового врахувння аргументів (БІА МГУА) є ефективними інструментами для вирішення актуальних проблем прогнозування, аналізу даних, розпізнавання образів, кластеризації, класифікації тощо. Існує багато типів нейронних мереж МГУА, розробка яких спрямована на підвищення ефективності індуктивної побудови моделей складних систем за статистичними даними. Основними недоліками класичної нейронної мережі МГУА є: можливість втрати інформативних аргументів, якщо вони були втрачені на початку пошуку; можливість фіксації неінформативних аргументів, якщо вони були включені на початку пошуку; експоненційне зростання степеня полінома в квадратичному описі; зі збільшенням кількості ітерацій вихідні вектори кращих моделей стають все більш корельованими, що погіршує обумовленість систем рівнянь для оцінки параметрів.

Для усунення недоліків класичного алгоритму МГУА було розроблено узагальнений ітераційний алгоритм МГУА, який базується на поєднанні ідей щодо збереження початкової бази моделювання та застосування оптимізації складності до частинних моделей з використанням так званих «активних нейронів» з різною структурою, яка оптимізується комбінаторним алгоритмом МГУА. Його окремими випадками є алгоритми багаторядкового та релаксаційного типів, а також деякі типи ітераційно-комбінаторних (гібридних) алгоритмів.

У цій роботі досліджуються переваги та недоліки існуючих архітектур нейронних мереж на основі МГУА з активними нейронами задля подальшого удосконалення алгоритмів їх побудови. Також у роботі розроблено та досліджено два алгоритми оптимізації узагальненої нейромережі МГУА з активними нейронами з використанням генетичного алгоритму.

Метою статті є дослідження переваг та недоліків наявних архітектур нейромереж МГУА з активними нейронами та підвищення їхньої ефективності при індуктивній побудові моделей складних систем за статистичними даними на основі їхньої гібридизації з гентичними алгоритмами.

Методи. У роботі представлено опис основних нейромереж МГУА з активними нейронами.

Результати. Подано характеристику наявних нейромереж МГУА з активними нейронами, проаналізовано їх основні переваги та недоліки. Серед основних недоліків нейромережі МГУА виявлено такі: експоненційний ріст степеня полінома в квадратичному частинному описі, можливість втрати інформативних і закріплення неінформативних аргументів в моделі.

Запропоновано два підходи до підвищення ефективності узагальненого алгоритму МГУА з використанням генетичного алгоритму.

Висновки. У статті наведено результати аналізу основних переваг та недоліків існуючих нейронних мереж МГУА з активними нейронами. Їхнім основним недоліком є використання детермінованих методів оптимізації нейронів, що призводить до використання великої кількості обчислювальних і часових ресурсів. Для її усунення розроблено два підходи до підвищення ефективності індуктивної побудови моделей складних систем. Ці підходи базуються на застосуванні генетичних алгоритмів до задачі пошуку оптимальної структури узагальненого алгоритму МГУА з «активними нейронами».

Ключові слова: *індуктивне моделювання, нейромережа МГУА, активні нейрони, обчислювальний інтелект, генетичні алгоритми.*