Multi-layered GMDH-type Neural Network Algorithm Using Principal Component-Regression Analysis and PSS Criterion

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Abstract

In this study, a hybrid Group Method of Data Handling (GMDH)-type neural network algorithm using principal component-regression analysis is proposed and applied to the nonlinear system identification. The architectures of the GMDH-type neural networks are automatically organized using heuristic self-organization method which is a kind of evolutionary computation. In the heuristic self-organization method, many nonlinear combinations of the input variables are generated and new neurons are constructed from these combinations. Only desirable neurons which fit the characteristics of the nonlinear system, are selected and these neurons are combined again in next layer. These procedures are iterated and a multi-layered neural network architectures are automatically organized. In the GMDH-type neural network, the multi-collinearity of the variables generates and the prediction output values of the neural network become unstable. In this study, the principal component-regression analysis is used for estimating the parameters of the neurons and stable and accurate multi-layered architectures of the GMDH-type neural networks are organized using the heuristic self-organization.

1 Introduction

In this study, a revised Group Method of Data Handling (GMDH)-type neural network algorithm using principal component-regression analysis is proposed and applied to the nonlinear system identification. The GMDH-type neural network algorithms and their applications have been proposed in our early works [1]-[4]. GMDH-type neural networks can automatically organize neural network architecture by heuristic self-organization method [5],[6] and they can also determine such structural parameters as the number of layers, the number of neurons in hidden layers and useful input variables so as to minimize the prediction error criterion defined as Akaike's information criterion (AIC) [7] or Prediction sum of squared (PSS) [8]. The heuristic self-organization method can be used for organizing the multi-layered architecture but the multicollinearity in the partial polynomials of the neurons is generated. The nonlinear models which contain the multicollinearity in the partial polynomials is very unstable

and can not be used in the prediction problem. In the conventional GMDH-type neural networks [1]-[4], the stepwise regression analysis [9] is used to avoid the multicollinearity and stable parameters in the neurons can be estimated. In this paper, the revised GMDH-type neural network algorithm is proposed and the principal component-regression analysis [10] is used for estimating the parameters of the neurons and stable and accurate multi-layered architectures of the GMDH-type neural networks are organized using the heuristic self-organization. This algorithm is applied to the identification problem of the nonlinear system and the identification results are compared with feedback GMDH-type neural network [3], GMDH [8] and conventional neural network trained using the back propagation algorithm. It is shown that the revised GMDH-type neural network algorithm is very accurate for the nonlinear system identification.

2 Heuristic self-organization

Architectures of GMDH-type neural network are automatically organized by the heuristic self-organization method. First, the procedures of the heuristic self-organization method are shown because it plays very important roles for organization of GMDH-type neural network. Heuristic self-organization method is a kind of the evolutionary computation.

Heuristic self-organization method is constructed by the following six procedures:

1) Separating original data into training and test sets

Original data is separated into training and test sets. Training data is used for estimating parameters of partial descriptions which describe partial relationships of the nonlinear system. Test data is used for organizing complete description which describes complete relationships between input and output variables of the nonlinear system.

2) Generating combinations of input variables in each layer

All combinations of two input variables (x_i, x_j) are generated in each layer. The number of combinations is $\frac{p!}{(p-2)!2!}$. Here, p is the number of input variables.

3) Calculating partial descriptions

For each combination, partial descriptions of the nonlinear system can be calculated by applying regression analysis to training data. Output variables of partial descriptions are called as intermediate variables.

4) Selecting intermediate variables

L intermediate variables which give L smallest test errors calculated using test data are selected from generated intermediate variables.

5) Iterating calculations from procedure 2) to 4)

Selected L intermediate variables are set to input variables of the next layer and calculations from procedure 2) to 4) are iterated. The multi-layered architecture is organized.

6) Stopping multi-layered iterative calculations

When errors of test data in each layer stop decreasing, iterative calculation is terminated. Finally, complete description of the nonlinear system is organized by partial descriptions generated in each layer.

3 Revised GMDH-type neural network algorithm

The revised GMDH-type neural network has a common feedforward multilayered architecture. Figure 1 shows architecture of the revised GMDH-type neural network. This neural network is organized by the heuristic self-organization method.

Fig.1 Architecture of revised GMDH-type neural network

Procedures for determining architecture of revised GMDH-type neural network conform to the following:

3.1 The first layer

$$u_j = x_j \quad (j=1,2,\dots,p) \quad (1)$$

where x_j ($j=1,2,\dots,p$) are input variables of the nonlinear system, and p is the number of input variables. In the first layer, input variables are set to output variables.

3.2 The second layer

All combinations of r input variables are generated. For each combination, optimum neuron architectures are automatically selected from the following two neurons.

Architectures of the first and second type neurons are shown in Fig.2 and Fig.3 respectively. Optimum neuron architecture for each combination is selected from the first and second type neuron architectures.

Fig.2 Neuron architecture of the first type neuron

Fig.3 Neuron architecture of the second type neuron

Revised GMDH-type neural network algorithm can select optimum neural network architecture from three neural network architectures such as sigmoid function neural network, RBF neural network and polynomial neural network.

3.2.1 Neuron architectures

Neuron architectures of the first and second type neurons in each neural network architecture are shown as follows.

1) Sigmoid function neuron

a) The first type neuron

Σ : (Nonlinear function)

$$z_k = w_1 u_i + w_2 u_j + w_3 u_i u_j + w_4 u_i^2 + w_5 u_j^2 - w_0 \theta_l \quad (2)$$

f : (Nonlinear function)

$$y_k = \frac{1}{1 + e^{(-z_k)}} \quad (3)$$

Here, $\theta_l = 1$ and w_i ($i=0,1,2,\dots,5$) are weights between the first and second layer. Value of r , which is the number of input variables u in each neuron, is set to two for the first type neuron.

b) The second type neuron

Σ : (Linear function)

$$z_k = w_1 u_1 + w_2 u_2 + w_3 u_3 + \dots + w_r u_r - w_0 \theta_l \quad (r < p) \quad (4)$$

f : (Nonlinear function)

$$y_k = \frac{1}{1 + e^{(-z_k)}} \quad (5)$$

Here, $\theta_l = 1$ and w_i ($i=0,1,2,\dots,r$) are weights between the first and second layer. Value of r , which is the number of input variables u in each neuron, is set to be greater than two and smaller than p for the second type neuron. Here p is the number of input variables x_i ($i=1,2,\dots,p$).

2) Radial basis function neuron

a) The first type neuron

Σ : (Nonlinear function)

$$z_k = w_1 u_i + w_2 u_j + w_3 u_i u_j + w_4 u_i^2 + w_5 u_j^2 - w_0 \theta_l \quad (6)$$

f : (Nonlinear function)

$$y_k = e^{(-z_k^2)} \quad (7)$$

Here, $\theta_l = 1$ and w_i ($i=0,1,2,\dots,5$) are weights between the first and second layer. Value of r , which is the number of input variables u in each neuron, is set to two for the first type neuron.

b) The second type neuron

Σ : (Linear function)

$$z_k = w_1 u_1 + w_2 u_2 + w_3 u_3 + \dots + w_r u_r - w_0 \theta_l \quad (r < p) \quad (8)$$

f : (Nonlinear function)

$$y_k = e^{(-z_k^2)} \quad (9)$$

Here, $\theta_l = 1$ and w_i ($i=0,1,2,\dots,r$) are weights between the first and second layer. Value of r , which is the number of

input variables u in each neuron, is set to be greater than two and smaller than p for the second type neuron. Here p is the number of input variables x_i ($i=1,2,\dots,p$).

3) Polynomial neuron

a) The first type neuron

Σ : (Nonlinear function)

$$z_k = w_1 u_i + w_2 u_j + w_3 u_i u_j + w_4 u_i^2 + w_5 u_j^2 - w_0 \theta_l \quad (10)$$

f : (Linear function)

$$y_k = z_k \quad (11)$$

Here, $\theta_l = 1$ and w_i ($i=0,1,2,\dots,5$) are weights between the first and second layer. Value of r , which is the number of input variables u in each neuron, is set to two for the first type neuron.

b) The second type neuron

Σ : (Linear function)

$$z_k = w_1 u_1 + w_2 u_2 + w_3 u_3 + \dots + w_r u_r - w_0 \theta_l \quad (r < p) \quad (12)$$

f : (Linear function)

$$y_k = z_k \quad (13)$$

Here, $\theta_l = 1$ and w_i ($i=0,1,2,\dots,r$) are weights between the first and second layer. Value of r , which is the number of input variables u in each neuron, is set to be greater than two and smaller than p for the second type neuron. Here p is the number of input variables x_i ($i=1,2,\dots,p$). Weights w_i ($i=0,1,2,\dots$) in each neural network architecture are estimated by the principal component-regression analysis [10].

3.2.2 Estimation procedure of weight w_i

First, values of z_k^{**} are calculated for each neural network architecture as follows.

1) Sigmoid function neural network

$$z_k^{**} = \log_e \left(\frac{\phi'}{1 - \phi'} \right) \quad (14)$$

2) RBF neural network

$$z_k^{**} = \sqrt{-\log_e \phi'} \quad (15)$$

3) Polynomial neural network

$$z_k^{**} = \phi \quad (16)$$

where ϕ' is the normalized output variable whose values are between 0 and 1. ϕ' is calculated using following equation.

$$\phi' = \frac{\phi - \phi_{\min}}{\phi_{\max} - \phi_{\min}} \quad (17)$$

Here, $\phi_{\max}$ is the maximum value of the output variable (ϕ), and $\phi_{\min}$ is the minimum value of ϕ .

Weights w_i ($i=0,1,2,\dots$) in each neural network architecture are estimated by the principal component-regression analysis.

3.2.3 Principal component-regression analysis.

Multicollinearity is generated in the function Σ of the neurons because heuristic self-organization method is used. In this study, the function Σ is calculated using the principal component-regression analysis.

In the case of Eq.(2), orthogonal vector $\underline{v}$ is calculated .

$$\underline{v} = C \cdot \underline{u} \quad (18)$$

Here,

$$\underline{v} = (v_1, v_2, \dots, v_5)$$

$$\underline{u} = (u_i, u_j, u_i u_j, u_i^2, u_j^2)$$

$\underline{v}$ is orthonormal vectors and C is orthonormal matrix. C is calculated using the following eigenvalue problem .

$$R \cdot C = C \cdot \Lambda \quad (19)$$

Here, R is a correlation matrix. Then, variable z_k is calculated using orthogonal regression analysis.

$$z_k = \underline{w}^T \cdot \underline{v}$$

$$= w_1 v_1 + w_2 v_2 + \dots + w_5 v_5 \quad (20)$$

Using the principal component-regression analysis, variable z_k in the function Σ is calculated without multi-collinearity. In (20), useful orthogonal variables v_i ($i=1,2,\dots,5$) are selected using PSS criterion[8] as the variable selection criterion [9].

PSS is described by the following equations:

$$PSS = \sum_{\alpha=1}^n (z_{\alpha}^{**} - z_{k\alpha}^*)^2 \quad (21)$$

where

$$z_{k\alpha}^* = w_1 v_{1\alpha} + w_2 v_{2\alpha} + \dots + w_5 v_{5\alpha} \quad \alpha=1,2,\dots,n \quad (22)$$

n is the number of training data, z_{α}^{**} is the α -th observed value of z^{**} , $v_{i\alpha}$ is the α -th observed value for the input variable (v_i), and $z_{k\alpha}^*$ is the α -th estimated value obtained by the multiple regression analysis of all the data except the α -th datum. In order to calculate PSS in (21), the multiple regression analysis must be repeated n times, and the amount of calculations increases in the number of data. But PSS in (21) can be reduced as follows,

$$PSS = \sum_{\alpha=1}^n \left\{ \frac{z_{\alpha}^{**} - z_{k\alpha}^*}{1 - \underline{v}_{\alpha}^T (V^T V)^{-1} \underline{v}_{\alpha}} \right\}^2 \quad (23)$$

where

$$z_{k\alpha}^* = w_1 v_{1\alpha} + w_2 v_{2\alpha} + \dots + w_5 v_{5\alpha} \quad \alpha=1,2,\dots,n \quad (24)$$

$$\underline{v}_{\alpha}^T = [v_{1\alpha}, v_{2\alpha}, \dots, v_{5\alpha}], \quad \alpha=1,2,\dots,n \quad (25)$$

$$V^T = [\underline{v}_1, \underline{v}_2, \dots, \underline{v}_n] \quad (26)$$

$z_{k\alpha}^*$ is the α -th estimated value obtained by the multiple regression analysis of all the data. With this procedure, we need not repeat the regression analysis n times. PSS criterion does not contain the statistical assumption in the regression model.

For each combination, three neuron architectures which are sigmoid function neuron, RBF neuron and polynomial neuron, are generated and L neurons which minimize PSS are selected for each neuron architecture. From these L selected neurons for each neuron architecture, estimation errors of L neurons are calculated. Then, neural network architecture which has minimum estimation error is selected as revised GMDH-type neural network architecture from three neural network architectures such as sigmoid function neural network, RBF neural network and polynomial neural network.

After the type of revised GMDH-type neural network architecture is selected, output variables y_k of L selected neurons are set to input variables of neurons in the third layer.

3.3 The third and successive layers

In the second layer, optimum neural network architecture is selected from three neural network architectures. In the third and successive layers, only one neuron architecture, which is sigmoid function neuron or

RBF neuron or polynomial neuron, is used for calculation and the same calculation of the second layer is iterated until PSS values of L neurons with selected neuron architecture stop decreasing. When iterative calculation is terminated, neural network architecture is produced by L selected neurons in each layer.

By using these procedures, the revised GMDH-type neural network using the principal component-regression analysis is organized. Figure 4 shows the flowchart of the revised GMDH-type neural network. Revised GMDH-type neural network has an ability of self-selecting optimum neural network architecture. Therefore, neural network architecture is automatically selected from three neural network architectures. Furthermore, structural parameters such as the number of layers, the number of neurons in hidden layers and useful input variables are automatically selected to minimize prediction error criterion defined as PSS.

Fig.4 Flowchart of the revised GMDH-type neural network

4 Application to nonlinear system identification

To verify the performance of the revised GMDH-type neural network, it is applied to the nonlinear system identification problem. In this application, PSS was used as the prediction error criterion.

4.1 Nonlinear system identification problem

The nonlinear system is assumed to be described by the following equations:

$$\phi_1 = (1.0 + 1.1x_1 + 1.2x_2 + 1.3x_3)^4 + \varepsilon_1 \quad (27)$$

$$\phi_2 = (1.0 + 1.4x_1 + 1.5x_2 + 1.6x_3)^4 + \varepsilon_2 \quad (28)$$

$$\phi_3 = (1.0 + 1.7x_1 + 1.8x_2 + 1.9x_3)^4 + \varepsilon_3 \quad (29)$$

$$\phi_4 = (1.0 + 2.0x_1 + 2.1x_2 + 2.2x_3)^4 + \varepsilon_4 \quad (30)$$

Here, $\phi_1 \sim \phi_4$ show output variables and $x_1 \sim x_3$ show input variables. $\varepsilon_1 \sim \varepsilon_4$ are Gaussian white noise, i.e., $N(0, 0.005^2)$. Furthermore, x_4 is added as the input variable of the neural network in order to check that the revised GMDH-type neural network can eliminate the useless input variables. The neural network is organized by using twenty training data. The prediction is carried out by using twenty testing data so as to check the generalization ability.

4.2 Identification results obtained using the revised GMDH-type neural network

1) Input variables

Four input variables were used but the useless input variables x_4 was automatically eliminated.

2) Number of selected neurons

Four neurons were selected in the hidden layer.

3) Selection of the neural network architecture

The polynomial neural network architecture was selected as the revised GMDH-type neural network architecture.

4) Structure of the neural network

The calculation of the GMDH-type neural network was terminated at the sixth layer.

5) Estimation accuracy

The estimation accuracy was evaluated by using the following equation:

$$J_1 = \frac{\sum_{i=1}^{20} |\phi_i - \phi_i^*|}{\sum_{i=1}^{20} |\phi_i|} \quad (31)$$

where ϕ_i ($i = 1, 2, \dots, 20$) were the actual values and ϕ_i^* ($i = 1, 2, \dots, 20$) were the estimated values by the revised GMDH-type neural network. The values of J_1 for four output variables are shown in Table1.

6) Prediction accuracy

The prediction accuracy was evaluated by using the following equation:

$$J_2 = \frac{\sum_{i=21}^{40} |\phi_i - \phi_i^*|}{\sum_{i=21}^{40} |\phi_i|} \quad (32)$$

where ϕ_i ($i = 21, 22, \dots, 40$) were the actual values and ϕ_i^* ($i = 21, 22, \dots, 40$) were the predicted values by the revised GMDH-type neural network. The values of J_2 for four output variables are shown in Table1.

7) Variation of PSS and estimated values

The variation of PSS in (23) of the output variables ϕ_1 is shown in Fig.5. It decreased gradually through layers and converged at the sixth layer. The estimated values of ϕ_1 by the revised GMDH-type neural network is shown in Fig.6. We can see that the estimated values are very accurate.

Table 1 Prediction and estimation accuracy

Model	J	ϕ_1	ϕ_2	ϕ_3	ϕ_4
Revised GMDH-NN	J1	0.007	0.007	0.007	0.007
(PSS)	J2	0.011	0.009	0.009	0.008
Feedback GMDH-NN	J1	0.029	0.029	0.013	0.013
(PSS)	J2	0.038	0.037	0.017	0.017
GMDH(PSS)	J1	0.08	0.082	0.083	0.081
	J2	0.083	0.084	0.085	0.094
NN	J1	0.119	0.133	0.108	0.11
	J2	0.114	0.133	0.102	0.109

Fig.5 Variation of PSS values in the layers

Fig.6 Estimated values of ϕ_1 by revised GMDH-type neural network

4.3 Comparison of the revised GMDH-type neural network and other models

The identification results were compared with those of the conventional GMDH-type neural network which is called as feedback GMDH-type neural network, GMDH algorithm, conventional multilayered neural network trained using the back propagation algorithm.

1) Feedback GMDH-type neural network [3]

We have developed the feedback GMDH-type neural network algorithm and applied to the nonlinear system identification problem [3]. In this algorithm, feedback loop calculations are carried out and the GMDH-type neural network architecture is organized using the feedback loop calculations. In the neuronal calculation, the stepwise regression analysis is used in order to estimate the parameters of the neurons. The values of J_1 and J_2 are shown in Table1.

2) GMDH algorithm

The identification results were referred from [11]. Four input variables were used but the useless input variable x_4 was automatically eliminated. Four intermediate variables were selected. The calculation was terminated at the fifth layer. The values of J_1 and J_2 are shown in Table1.

3) Conventional multilayered neural network trained using the back propagation algorithm

The neural network had three layered structures. Four input variables were used in the input layer and eight neurons were used in the hidden layer. The estimated values of ϕ_1 by the conventional neural network are shown in Fig.7. The values of J_1 and J_2 are shown in Table1.

Fig.7 Estimated values of ϕ_1 by the conventional multilayered neural network

5 Discussions

From the identification results, we can say the following:

1) Both estimation and prediction errors of the revised GMDH-type neural network were smallest in the four identified models. We can see that the revised GMDH-type neural network is a very accurate identification method for the nonlinear system.

2) In the revised GMDH-type neural network, PSS values at the second layer were not small but it was gradually decreased through layers and the small PSS values were obtained at the sixth layer.

3) In the revised GMH-type neural network, the complexity of the neural network increases through the layers and the calculation of the revised GMDH-type neural network is terminated when the complexity of the neural network fits the complexity of the nonlinear system. We consider that the nonlinear combinations of the input variables are very important in the complex nonlinear system and the influence of the high order terms of the input variables must be contained in the neural network architectures. In the conventional neural network, the influence of high order terms of the input variables is not considered. Furthermore, it does not have the ability of self-selecting useful input variables. So the accuracy of the neural network was not good.

4) In the revised GMDH-type neural network, many nonlinear combinations of the input variables are generated and the optimum neuron architectures are calculated for these combinations. The learning calculations using the principal component-regression analysis with PSS criterion, are carried out for all neurons. In these learning calculations, the computation times are very short because the sizes of the neuron architectures in Eq.(2), (4), (6), (8), (10) and (12) are very small. The calculation time of the nonlinear system identification in this study is about two seconds. On the other hand, in the conventional sigmoid function neural network, the calculation time of the back propagation algorithm is long and it is about a few minutes in this study, and furthermore, we must repeat the calculations of the back propagation many times in order to fine out the optimum neural network architecture changing the structural parameters of the neural network.

5) The revised GMDH-type neural network can organize the conventional neural network architectures (sigmoid function type and radial basis function type architectures) and the GMDH architecture (polynomial type architecture). This algorithm contains the characteristics of the conventional neural networks and the GMDH algorithm and it is a very flexible method for the identification problem of the complex nonlinear system.

6 Conclusions

In this paper, the revised GMDH-type neural network algorithm using the principal component-regression analysis was proposed. This algorithm can automatically organize a multilayered neural network architecture fitting the complexity of the nonlinear system using the heuristic self-organization method. In this algorithm, the parameters of the neurons are estimated using the principal component-regression analysis and the multicollinearity dose not generate. Therefore, very stable multi-layered neural network architecture can be organized. Furthermore, optimum neural network architecture is automatically selected from three types of neural network architectures, such as, sigmoid function neural network, RBF neural network and polynomial neural network. The structural

parameters such as the number of hidden layers, the number of neurons in hidden layers and useful input variables are automatically selected to minimize prediction error criterion defined as PSS. This algorithm was applied to the nonlinear system identification and it is shown that revised GMDH-type neural network algorithm is a valuable method for the nonlinear system identification since the neural network architectures are automatically organized using the revised GMDH-type neural network algorithm.

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