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Prediction of multi-inputs bubble column reactor using a novel hybrid model of computational fluid dynamics and machine learning

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Abstract

The combination of artificial intelligence algorithms and numerical methods has recently become popular in the prediction of macroscopic and microscopic hydrodynamics parameters of bubble column reactors. The multi inputs and outputs machine learning can cover small phase interactions or large fluid behavior in industrial domains. This numerical combination can develop the smart multiphase bubble column reactor with the ability of low-cost computational time. It can also decrease case studies for the optimization process when big data is appropriately used during learning. There are still many model parameters that need to be optimized for a very accurate artificial algorithm, including data processing and initialization, the combination of inputs and outputs, number of inputs and model tuning parameters. For this study, we aim to train four inputs big data during learning process by an adaptive neuro-fuzzy inference system or adaptive-network-based fuzzy inference system (ANFIS) method, and we consider the superficial gas velocity as one of the input variables, while for the first time, one of the computational fluid dynamics (CFD) outputs named gas velocity is used as an output of the artificial algorithm. The results show that the increasing number of input variables improves the intelligence of the ANFIS method up to $R = 0.99$, and the number of rules during learning process has a significant effect on the accuracy of this type of modeling. The results also show that propper selection of model parameters results in more accuracy in prediction of the flow characteristics in the column structure.

Keywords: machine learning, computational fluid dynamics (CFD), hybrid model, adaptive neuro-fuzzy inference system (ANFIS), artificial intelligence, big data, prediction, forecasting, optimization, hydrodynamics, fluid dynamics, soft computing, computational intelligence, computational fluid mechanics

1. Introduction

As multiphase contactors and reactors, bubble columns have an extensive application in chemical, biochemical and petrochemical industries(Masood & Delgado, 2014; Masood, Khalid, & Delgado, 2015; Rabha, Schubert, & Hampel, 2013; Şal, Gül, & Özdemir, 2013). Bubble columns have various advantages including simple structure for phase interactions (liquid-gas or liquid-gas-solid interactions), high transfer rates of mass and heat and compactness during operation and maintenance and the simple structure of sparging mechanism (Kumar, Degaleesan, Laddha, &

Hoelscher, 1976; Pino et al., 1992; Shah, Kelkar, Godbole, & Deckwer, 1982). In reaction engineering, three-phase bubble column reactors have an extensive application. For instance, to manufacture industrially valuable bioproducts, gas-liquid-solid interaction reactors are the frequency used in biochemical applications (Essadki, Nikov, & Delmas, 1997; Lopez de Bertodano, Lahey Jr, & Jones, 1994; Sokolichin & Eigenberger, 1994). To understand better about complex behavior of mas and heat transfer rate, hydrodynamic characteristics such as gas-liquid interactions, bubble coalescence, and break-up, it is required to investigate design parameters and optimization of the process in bubble column reactors (Dhotre, Ekambara, & Joshi, 2004; Krishna & Van Baten, 2003; Maalej, Benadda, & Otterbein, 2003; S. Wang et al., 2003).

These type of reactors are produced in different shapes such as cylindrical and rectangular and different sizes, and they are a suitable domain for phase interactions such as liquid-gas, liquid-gas, and solid reactors. (Behkish, Men, Inga, & Morsi, 2002; Cho, Woo, Kang, & Kim, 2002; H. Li & Prakash, 2002; Michele & Hempel, 2002; Ruzicka, Zahradnık, Drahoš, & Thomas, 2001). The gas distributors are also located at the bottom of the domain and sparge gas phase as a dispersed phase into the matrix phase as liquid phase or liquid-solid phase. When there are solid materials in the matrix (continuous phase), bubble column reactors are broadly called a slurry bubble column reactors (Bouaifi, Hebrard, Bastoul, & Roustan, 2001; Deen, Solberg, & Hjertager, 2000; Luo, Lee, Lau, Yang, & Fan, 1999; Shimizu, Takada, Minekawa, & Kawase, 2000). Bubble columns have an extensive application in different industries such as chemical, biochemical and pharmaceutical, where the interaction of different phases are very crucial, or the chemical reactions during production are sometimes required (Degaleesan, Dudukovic, & Pan, 2001). For instance, they are also used in biochemical processes including biological wastewater treatment as well as

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fermentation (Prakash, Margaritis, Li, & Bergougnou, 2001; Shah et al., 1982). They also have an extensive application for large-scale aerobic fermentations in the bioprocessing industry (Doran, 1995; Masood & Delgado, 2014; Şal et al., 2013). Furthermore, they are utilized for performing a range of reactions in the chemical industry (Anabtawi, Abu-Eishah, Hilal, & Nabhan, 2003; Maalej et al., 2003; Shah et al., 1982).

There has been a strong interest in modeling bubble columns by (CFD) since their industrial applications are diverse (Krishna, Urseanu, Van Baten, & Ellenberger, 1999; Rampure, Kulkarni, & Ranade, 2007; Sanyal, Vásquez, Roy, & Dudukovic, 1999). There have been various numerical, experimental, and mathematical approaches developed to estimate and measure the flow pattern and bubbles dynamics (Besbes, El Hajem, Aissia, Champagne, & Jay, 2015; Islam, Ganesan, & Cheng, 2015; W. Li, Zhong, Jin, Lu, & He, 2014; Liu & Hinrichsen, 2014; Masood & Delgado, 2014; Masood et al., 2015; McClure, Aboudha, Kavanagh, Fletcher, & Barton, 2015; M Pourtousi, Sahu, & Ganesan, 2014; H. Wang et al., 2014; Xiao, Yang, & Li, 2013; Xing, Wang, & Wang, 2013; Thomas Ziegenhein, Rzehak, Krepper, & Lucas, 2013; T Ziegenhein, Rzehak, & Lucas, 2015). Nevertheless, there are a number of difficulties in making a complete prediction for the fluid structure and the interaction between phases during the bubbling process.(K. Chau & Jiang, 2002) Besides, the optimization of bubble column reactors for different operational conditions (superficial gas velocity, pressure, and temperature of continuous phase size of the reactor and time of mixing process) is required expensive computational time and efforts. The measurement of fluid properties for each node in a 3D bubble column requires very fine mesh in the computational methods and also causes the disturbance in experimental methods. Additionally, The significant disadvantage of the computational methods for simulating the large reactor (more

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than 2 m) with several operational parameters/inputs is computation time and computer capability(K.-w. Chau, 2017; Faizollahzadeh Ardabili et al., 2018; Simonnet, Gentric, Olmos, & Midoux, 2007, 2008; Tabib, Roy, & Joshi, 2008). Due to these disadvantages, soft computing approaches, particularly the ANFIS method has been developed for estimating the fluid properties in the column for different conditions which have not been experimented in the lab or simulated by numerical methods (Burns, Frank, Hamill, & Shi, 2004; Cheng & Chau, 2002; Moazenzadeh, Mohammadi, Shamshirband, & Chau, 2018; Pfleger & Becker, 2001; M Pourtousi, Sahu, Ganesan, Shamshirband, & Redzwan, 2015; Taherei Ghazvinei et al., 2018; Yaseen, Sulaiman, Deo, & Chau, 2018). These algorithms are used to mimic the hydrodynamics of the bubble column reactor for a specific condition. However, they cannot feel the exact physics, and they are capable based on their understanding (training data)(Panella & Gallo, 2005; M. Pourtousi, Zeinali, Ganesan, & Sahu, 2015; Ryoo, Dragojlovic, & Kaminski, 2005; Schurter & Roschke, 2000).

The pattern of a neural network for the learning process and the fuzzy logic framework for decision are both combined in the ANFIS structure(J.-S. Jang, 1996; Panella & Gallo, 2005). One of the most remarkable characteristics of this structure is its capability for learning complex relationships according to the pattern data(K.-W. Chau & Albermani, 2002; K. Chau & Albermani, 2003; Chen & Chau, 2016; Lei, He, Zi, & Hu, 2007; Nabavi-Pelesaraei, Bayat, Hosseinzadeh-Bandbafha, Afrasyabi, & Chau, 2017; Schurter & Roschke, 2000; Yun et al., 2008). This model categorizes the domain into different regions for modeling nonlinear and complex case studies (Ben-Nakhi, Mahmoud, & Mahmoud, 2008; Lei et al., 2007; Varol, Avci, Koca, & Oztop, 2007; Varol, Koca, Oztop, & Avci, 2008). A general local model is then extended for each local region according to linear functions or even adjustable factors(J.-S. Jang, 1993, 1996; J.-S. R. Jang, Sun, & Mizutani,

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1997). This feature of the model enables the method to thoroughly learn the process and predict the missing local nodes in the prediction domain (Avila & Pacheco-Vega, 2009; Yun et al., 2008).

The ANFIS approach has been employed in several papers to learn data from CFD database and then predict the bubbling flow including flow pattern, amount of gas, and turbulent kinetic energy(Abd Fatah et al., 2015; Azwadi, Zeinali, Safdari, & Kazemi, 2013; W.-c. Wang, Chau, Qiu, & Chen, 2015; Zeinali, Mazlan, Fatah, & Zamzuri, 2013). Moreover, this model was applied for predicting the microscopic parameters including bubble formation, detachment and rising. Pourtousi et al. (Mohammad Pourtousi, 2012; M. Pourtousi et al., 2015) recommended the new integration of the CFD data-set with artificial algorithms such as ANFIS method for prediction of the fluid flow recognition in the bubble column reactor. They trained their CFD database and simulated the new flow pattern, including turbulent kinetic energy liquid pattern and the interface of the dispersed and continuous phase in the reactor (M Pourtousi et al., 2015; M. Pourtousi et al., 2015). This study aims to use the methodology of Pourtousi et al. (Mohammad Pourtousi, 2012; M. Pourtousi et al., 2015) in the prediction of gas velocity in the bubble column reactor. Additionally, the different pattern of input parameters has been examined for various tuning parameters of the ANFIS method.

2. Methodology

2.1. Geometrical structure

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In this research, an industrial two-phases reactor with 2.6m was utilized. The ring sparger is embedded at the end of the bubble column reactor, and the diameter of the orifice hole is 0.7 mm.

2.2. CFD

In CFD, the single size eulerian-eulerian approach has been employed for simulating the homogeneous bubble column reactor hydrodynamics. The continuity equation is the first equation to be considered which is employed for calculating the volume of available gas or volume of the available liquid. The continuity equation is presented as:

$$\frac{\partial}{\partial t}(\rho_k \epsilon_k) + \nabla(\rho_k \epsilon_k u_k) = 0 \quad (1)$$

The momentum transfer calculation is provided, and the amount of gas and liquid phase can be calculated by this equation. The momentum transfer calculation is written as:

$$\frac{\partial}{\partial t}(\rho_k \epsilon_k u_k) + \nabla(\rho_k \epsilon_k u_k u_k) = -\nabla(\epsilon_k \tau_k) - \epsilon_k \nabla p + \epsilon_k \rho_k g + M_{I,k} \quad (2)$$

For interactions between the main liquid and gas phase, the total interfacial force defines the main forcing scheme for the accurate dynamics of bubbles, and the total force between bubbles and matrix phase is expressed as:

$$M_{I,L} = -M_{I,G} = M_{D,L} + M_{TD,L} \quad (3)$$

All forcing schemes between gas bubbles and liquid phase and the $k-\epsilon$ turbulence model are consistent with Tabib et al (Tabib et al., 2008).

2.2.1. Grid

In this study, the non-uniform meshes are used for CFD analysis in the bubble column reactor. This mesh structure is similar to that of the study conducted by Laborde-Boutet et al. (Laborde-Boutet, Larachi, Dromard, Delsart, & Schweich, 2009).

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2.3. ANFIS

The ANFIS approach is a useful tool which can be used to predict physical and biological phenomena that are found in nature. In various studies such as a study conducted by Takagi and Sugeno, the ANFIS approach has been described (Takagi & Sugeno, 1985). To start the learning process, learning data is first categorized at several levels of membership formations (MFs). As indicated in Figure 1, according to AND law, the first feedback from the learning step multiplies. The function ith rule can be defined as follows:

$$w_i = \mu_{Ai}(x)\,\mu_{Bi}(y)\mu_{ci}(z)\mu_{di}(v_{as}) \tag{4}$$

Where w_i refers to the output of learning feedback and μ_{Ai}, μ_{Bi} , μ_{Ci} and μ_{di} also express the input of learning feedback.

Figure 1

In the third step of learning, the relative firing strengths of each rule are defined according to the following formula. The weight fraction of each layer is specified by:

$$\overline{w_i} = \frac{w_i}{\sum(w_i)} \tag{5}$$

Where $\overline{w}_i$ is normalized firing strengths. In the fourth step of learning, Takagi and Sugeno (Takagi & Sugeno, 1985) used the if-then rule function. The mesh formula in the ANFIS can be modified as follows:

$$\overline{w_i}f_i = \overline{w_i}(p_i x + q_i y + r_i z + S_i v_{as} + t_i) \tag{6}$$

In the above formula p_i , q_i , $r_{i,}$, s_i and t_i are parameters related to "if-then rules".

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3. Result and discussion

Simulation of a cylindrical bubble column (BCR) reactor by CFD resulted in various fluid parameters as the output of the CFD. From among such CFD outputs, coordinates in x, y, and z-direction, as well as superficial air velocity and air velocity could be mentioned. In this study, the information generated by the CFD will be investigated using ANFIS method.

In the study implementing the ANFIS method, part of the CFD output is used as input and the rest as output. The description of the system studied here is as follows; there are four inputs used in this study with coordinates in x-direction used as input 1, coordinates in y-direction used as input 2, and coordinates in z-direction used as input 3, while superficial air velocity was taken as input 4. This is while air velocity is the only output studied in this research. The following conditions are presumed for the initiation of the learning process by machine learning (ANFIS):

- A maximum of 600 for an epoch.
- A total of 5000 data.
- 65% as the value for p which indicates the percentage of data (from the whole data) used in the training process.
- 65% of the data used in training, and 100% of the data used in the testing process.
- gbellmf type chosen as the type of membership functions (MFs)

With the abovementioned assumptions and considering one input, being coordinates in the x-direction, and air velocity as output, training, and testing processes were carried out for each number of membership functions (2, 4, 6, and 8) separately. As shown in figures 2 (a and b), R(Regression) amounts to 0.52 at best which indicates ANFIS methods are devoid the proper

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intelligence and changing the number of members functions led to no significant improvement in the intelligence of ANFIS method.

Figure 2(a)

Figure 2(b)

Increasing the number of inputs was studied as a way of increasing the system intelligence, and coordinates in x and y directions were taken as inputs and air velocity as output, meanwhile, the testing and training processes were carried out separately for numbers of membership functions (2, 4, 6, 8). Figures 3(a and b) shows an increase in the value of R from 0.52 to 0.76 which is an indication of improvement in the ANFIS method. When the number of membership functions is 4, the best value for R (R= 0.76) is reported, which is a proper rise but still not adequate, and there is a need for more investigation. That is why changing the membership functions; including gbellmf, gaussmf, gauss2mf, trimf, dsigmf, psigmf, pimf, with the number of membership functions being 4 was studied.

Figure 3(a)

Figure 3(b)

Training and testing processes were conducted separately for each type of MFs, and in the training process, 65% of the data was used. For the testing process, however, the sum of all data used in the training process plus the remaining 35% were evaluated by the ANFIS method.

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According to figures 4 (a and b), there was no considerable improvement in system intelligence.

Considering the fact that two inputs ultimately resulted in an increase of R to 0.75, it was decided to increase the number of inputs from 2 to 3 in order to enhance the system intelligence. Coordinates in x, y, and z directions were considered inputs while air velocity was the output.

Figure 4(a)

Figure 4(b)

Having two as the number of membership functions, the learning process was also carried out. This increase in the number of inputs led to a substantial enhancement in the intelligence of the ANFIS method, and R-value rose to 0.92. The appropriate increase in the intelligence of the ANFIS method took place when the number of (MFs) was 2. Moreover, increasing the number of membership functions to 4 also demonstrated acceptable results and R rose to 0.992 (see figures 5 (a and b)).

Figure 5(a)

Figure 5(b)

In the rest of this research, one of the air superficial velocity parameters was particularly added to the system as input number 4. Under the new circumstances, with the position of meshes (nodes) and superficial air velocity as input parameter and air velocity as an output parameter, the learning

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process was performed separately with the number of (MFs) being 2 and 4 (see figures 6(a and b)).

Figure 6(a)

Figure 6(b)

With 2 as the number of membership functions, R amounted to 0.97, whereas with the number of MFs being 4 R rose to 0.998 which is perfectly suitable for the ANFIS method, and represents a proper agreement between the ANFIS outputs and CFD outputs (See figures 7(a, b, c, d, e and f)).

Figure 7(a)

Figure 7(b)

Figure 7(c)

Figure 7(d)

Figure 7(e)

Figure 7(f)

The use of air superficial velocity as input led to particularly suitable results, and with this intelligence in the ANFIS method, parts of BCR can also be predicted (Figure 8).

Points can be predicted that had no participation in the learning process, and this indicates the considerable ability of the machine learning in prediction (see figures 9 (a, b, c, d, e, and f)).

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Combining machine learning (ANFIS method) and CFD means a substantial reduction in the time required for making calculations, and also obviates the need for complex CFD.

Figure 8

Figure 9(a)

Figure 9(b)

Figure 9(c)

Figure 9(d)

Figure 9(e)

Figure 9(f)

4. Conclusions

In this study, the machine learning method of ANFIS is combined with CFD data to predict the macroscopic parameters such as gas velocity in the multiphase reactor. Four input parameters are

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elected as inputs of the multiphase reactor for the learning process, and then one output such as gas velocity is also considered in the input parameters. To understand the behavior of AI in learning CFD data, the different number of inputs, number of rules and membership functions have been examined. This study shows that one of the main advantages of artificial intelligent modeling is a combination of input with output parameters, and also replacement of outputs with inputs matrix. This replacement does not feel with smart method as it is data-based modeling, but we can understand the effect of outputs parameters on the input variables. The number of inputs has a significant impact on the accuracy of the method to capture the whole behavior of Fluid flow in the column.

Additionally, the combination of numerical methods and AI algorithms enable us to reduce the computational time and number of simulation time during the optimization process. However, this type of modeling should be considered as an assistance tool besides the numerical method. This framework is also limited to the amount of data, and it can only show the process behavior based on the input data. For future study, we will specifically use more input data based on the clustering algorithm and parallel code implementation.

Abbreviation

g	[m s^{-2}]	Gravitational force
k	[m^2 s^{-2}]	Turbulent kinetic energy for modelling of dispersed phase
M_I	[N m^{-3}]	Interfacial force
M_D	[N m^{-3}]	Drag force for modelling of dispersed phase
P	[N m^{-2}]	The pressure in the reactor
MFs		Membership functions for ANFIS

Greek Symbols

ε	[m^2 s^{-3}]	Turbulent energy dissipation rate per unit mass
$\in$	[-]	phase hold-up (-)

$\overline{\in}$	[-]	Average phase hold-up (-)
ρ	[kg m^{-3}]	Density of phases
μ_T	[Pa s^{-1}]	Turbulent viscosity
τ_k	[Pa]	Shear stress of phase k
ϵ_g	[-]	The volume of the dispersed phase
Subscripts		
G		Dispersed phase
L		Matrix/Continuous phase

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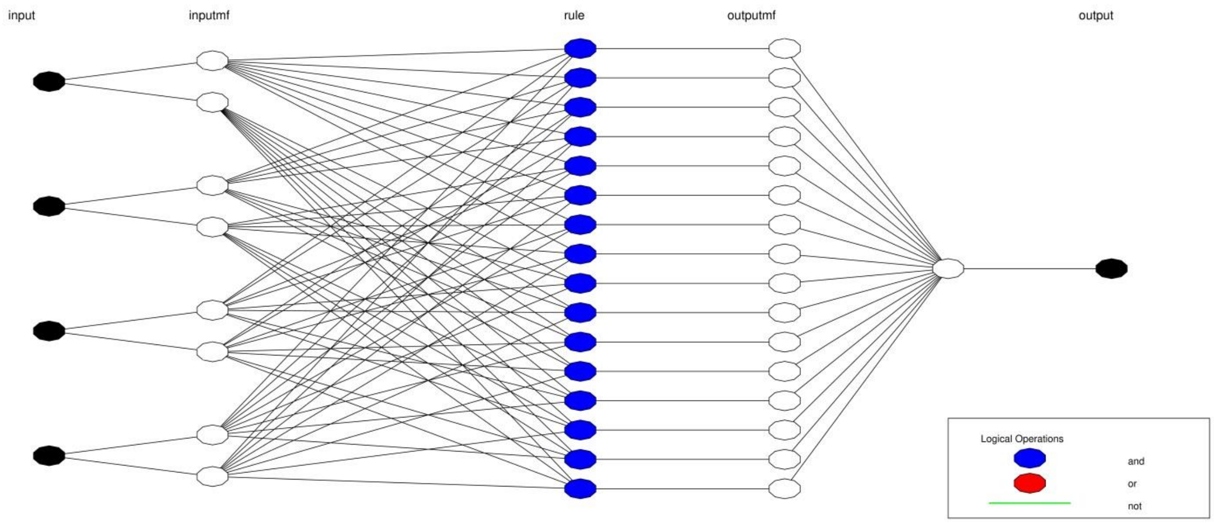

Figure1: Schematic of the ANFIS structure.

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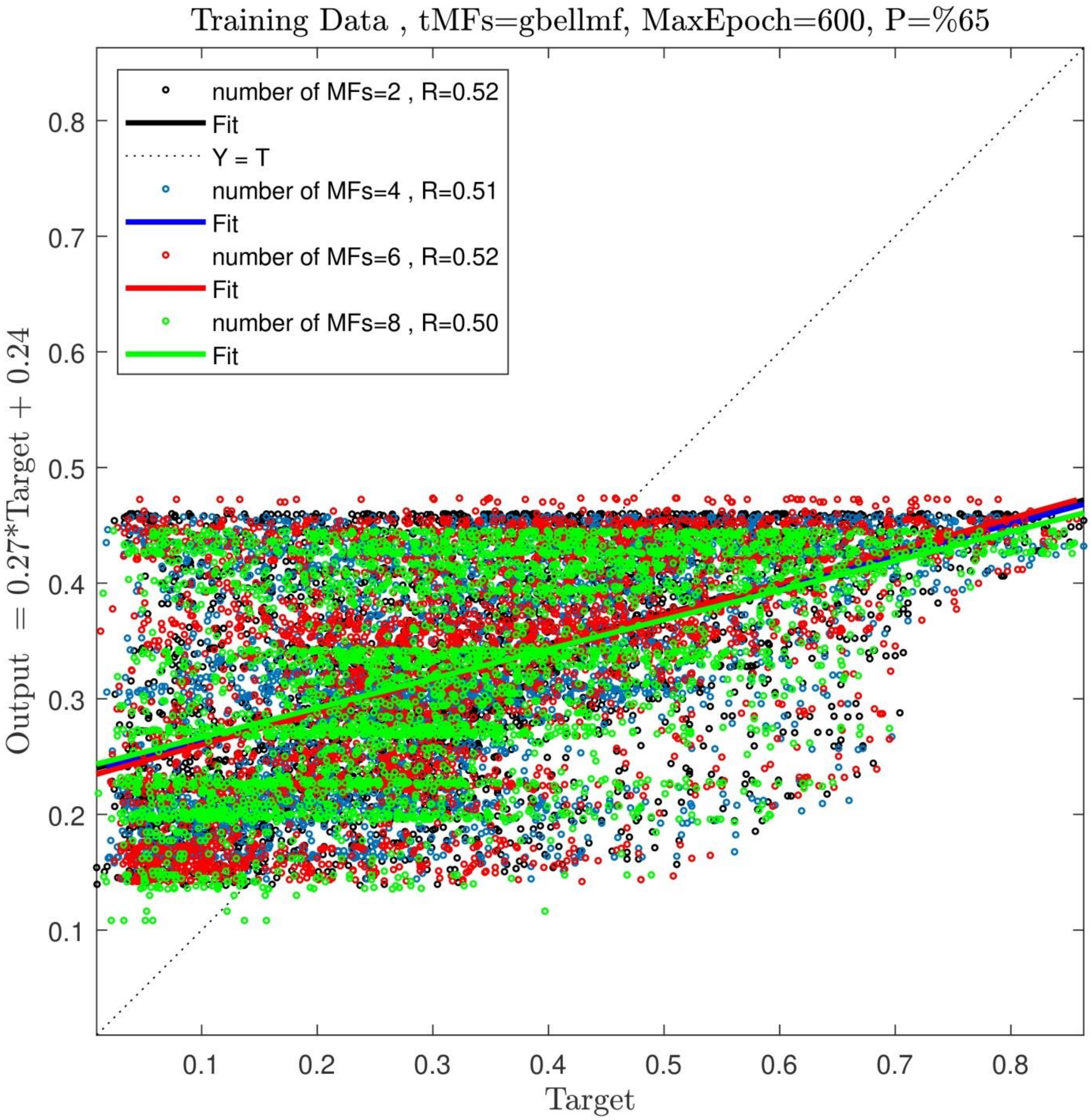

Figure 2(a): Training with using one input and different number of MFs (ANFIS method).

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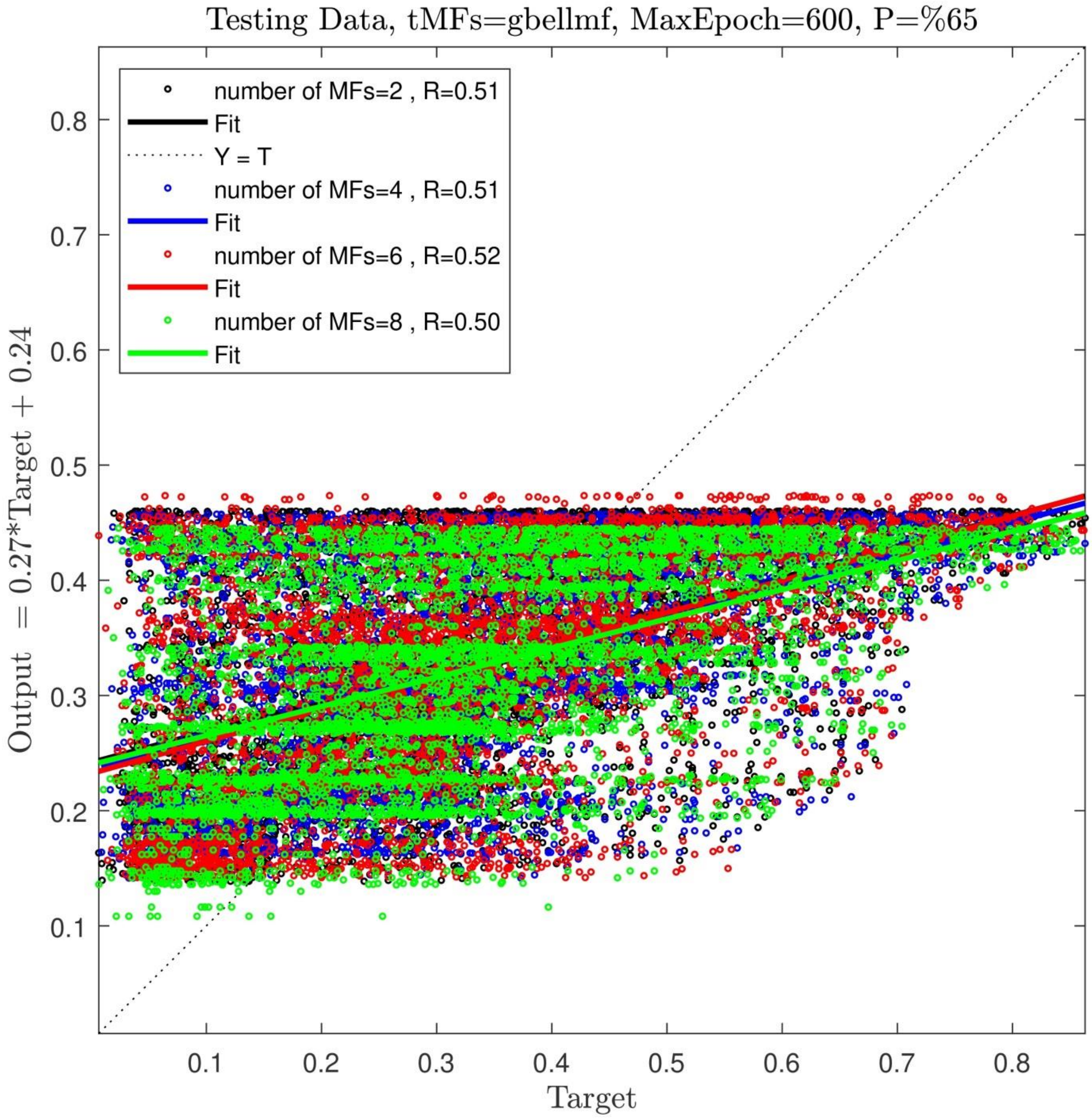

Figure 2(b): Testing with using one input and different number of MFs (ANFIS method).

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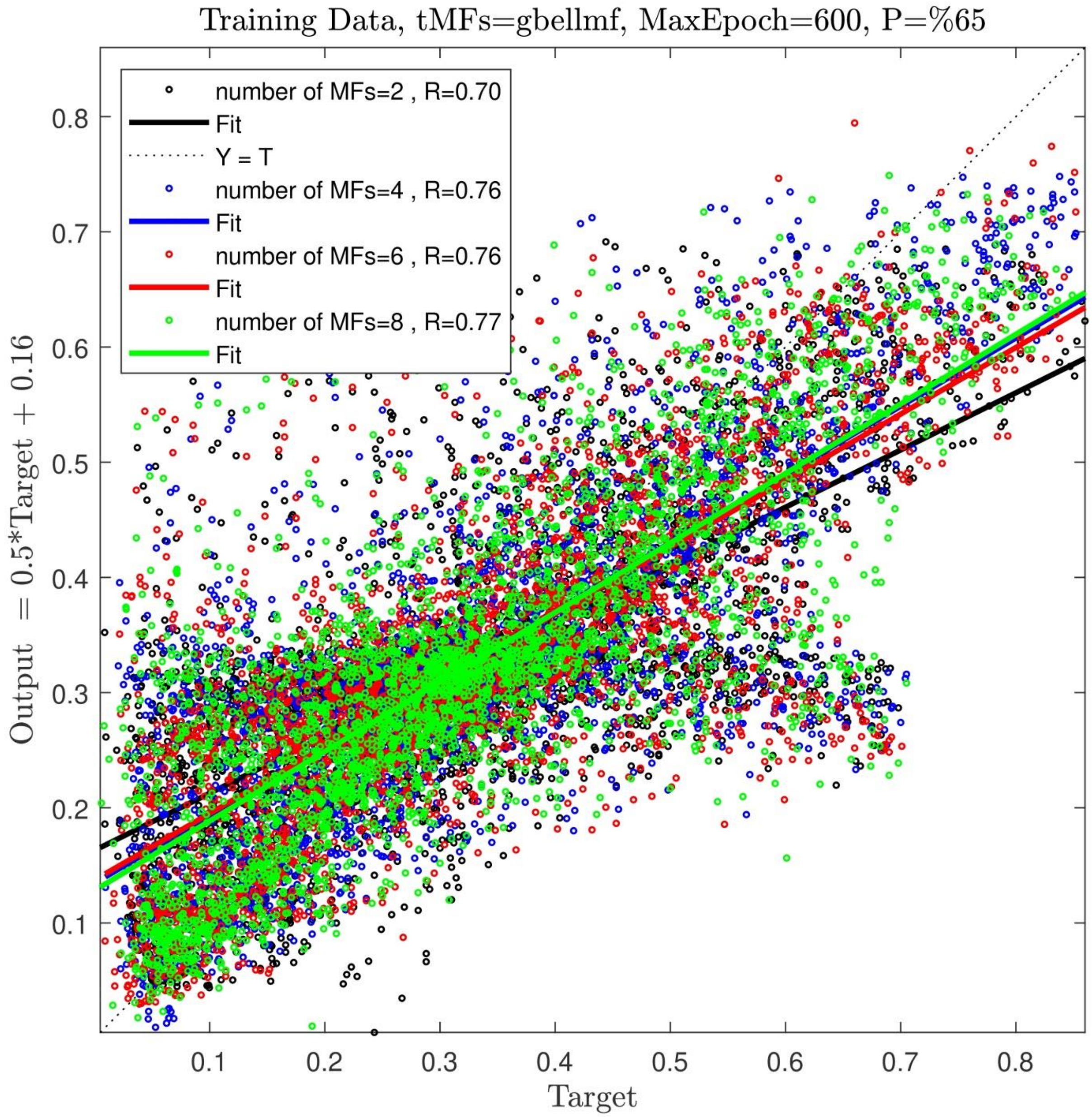

Figure 3(a): Training with using two inputs and different number of MFs (ANFIS method).

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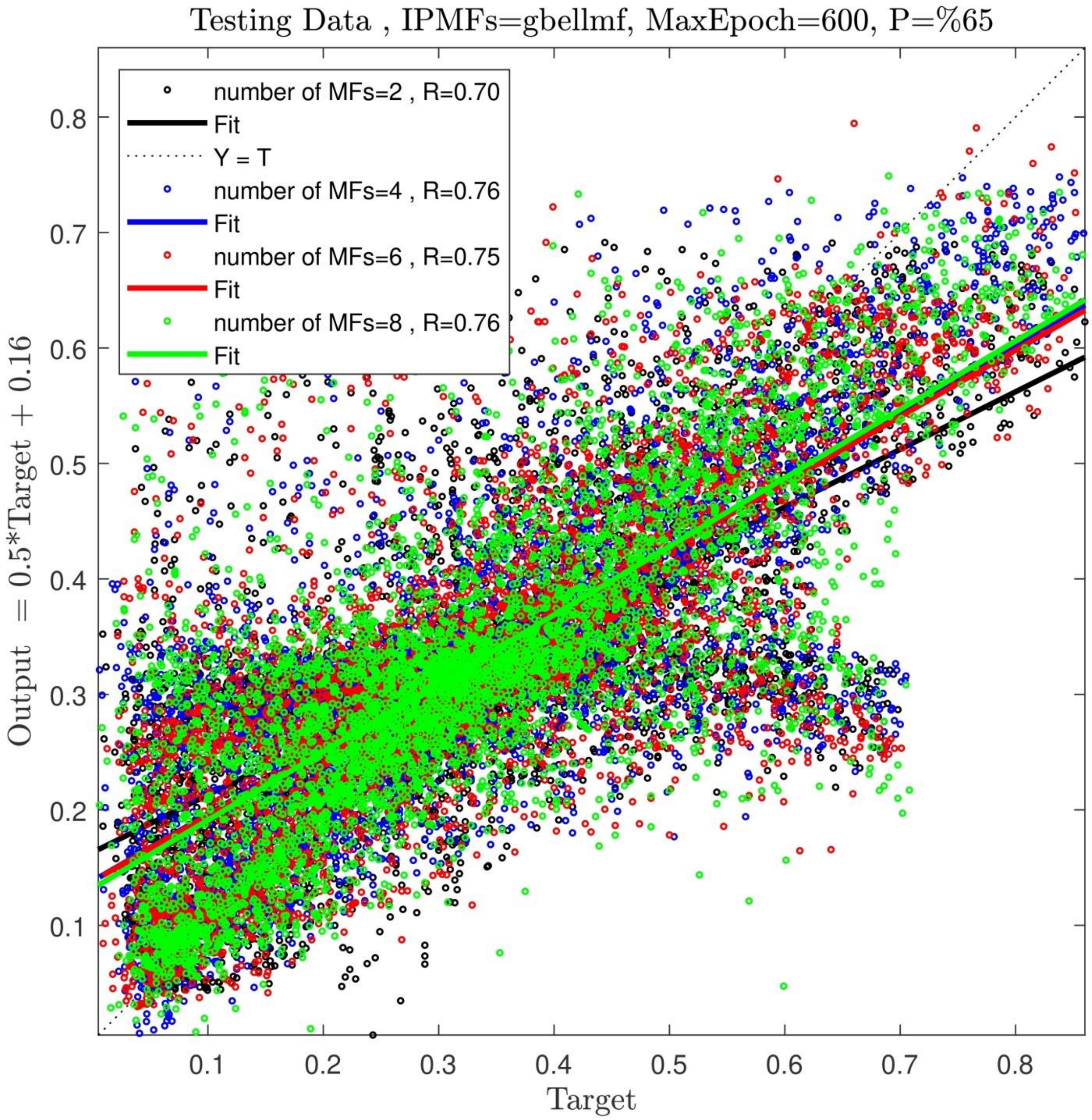

Figure 3(b): Testing with using two inputs and different number of MFs (ANFIS method).

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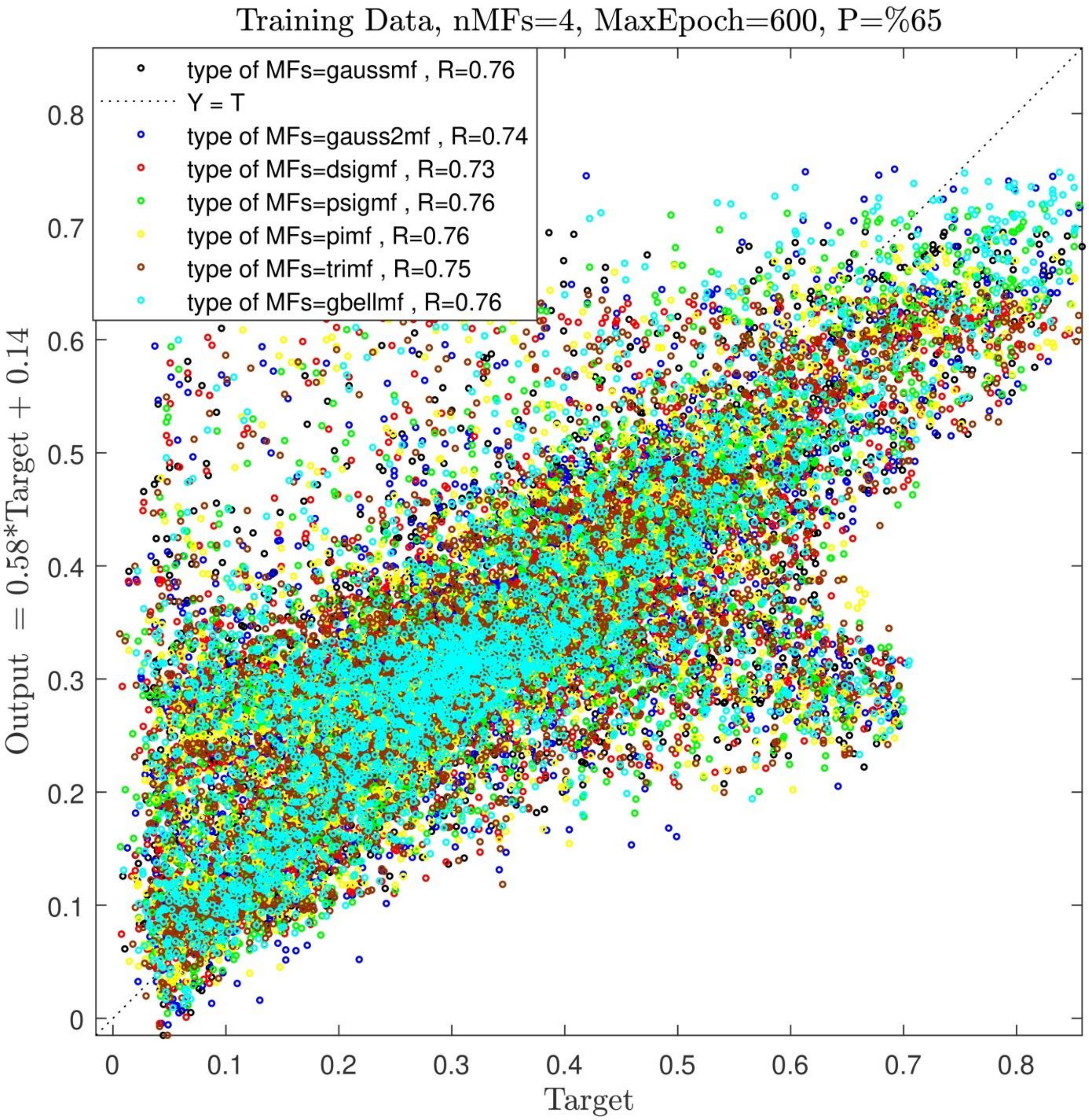

Figure 4(a): Training with using two inputs and different type of MFs (ANFIS method).

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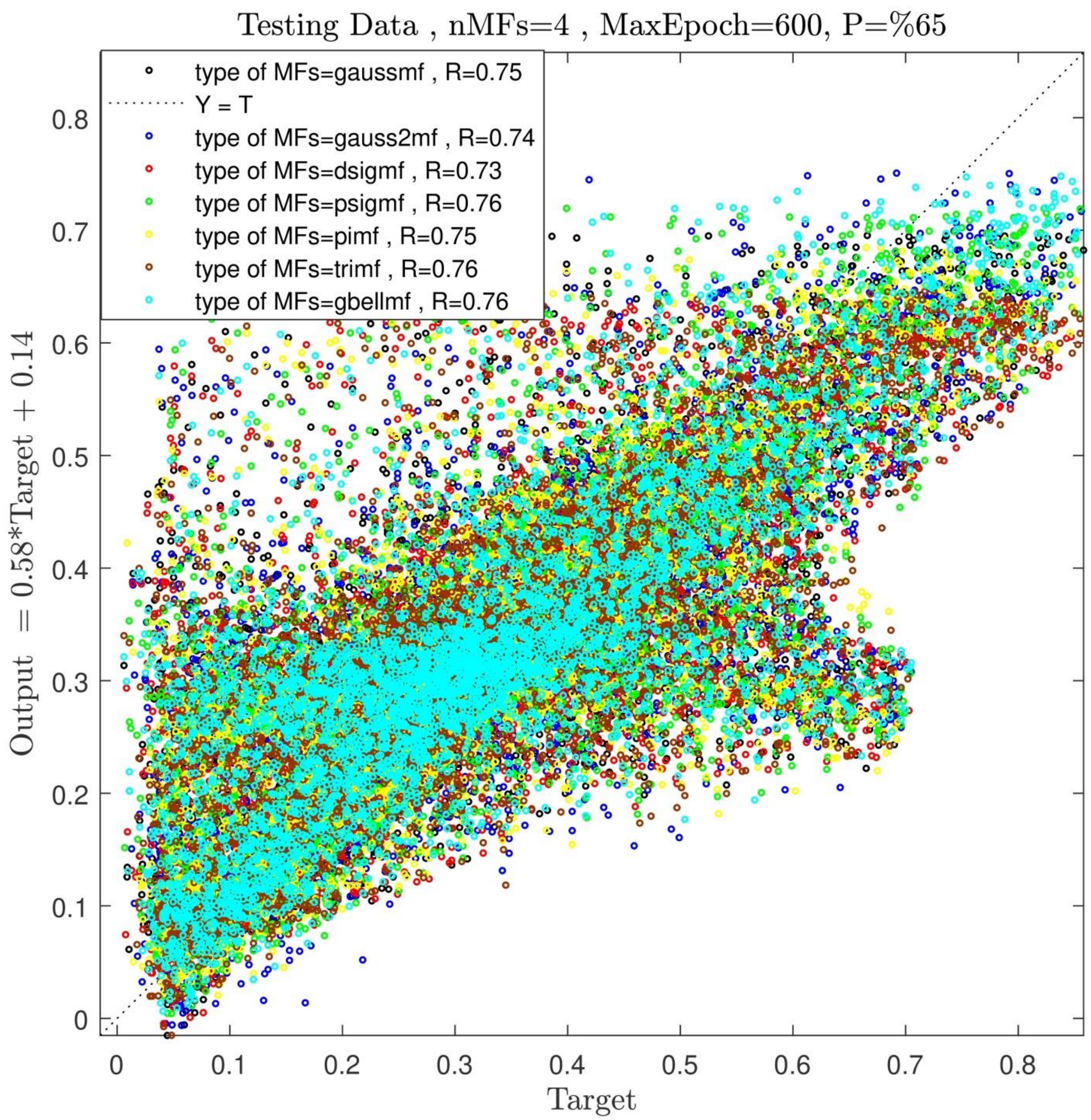

Figure 4(b): Testing with using two inputs and different type of MFs (ANFIS method).

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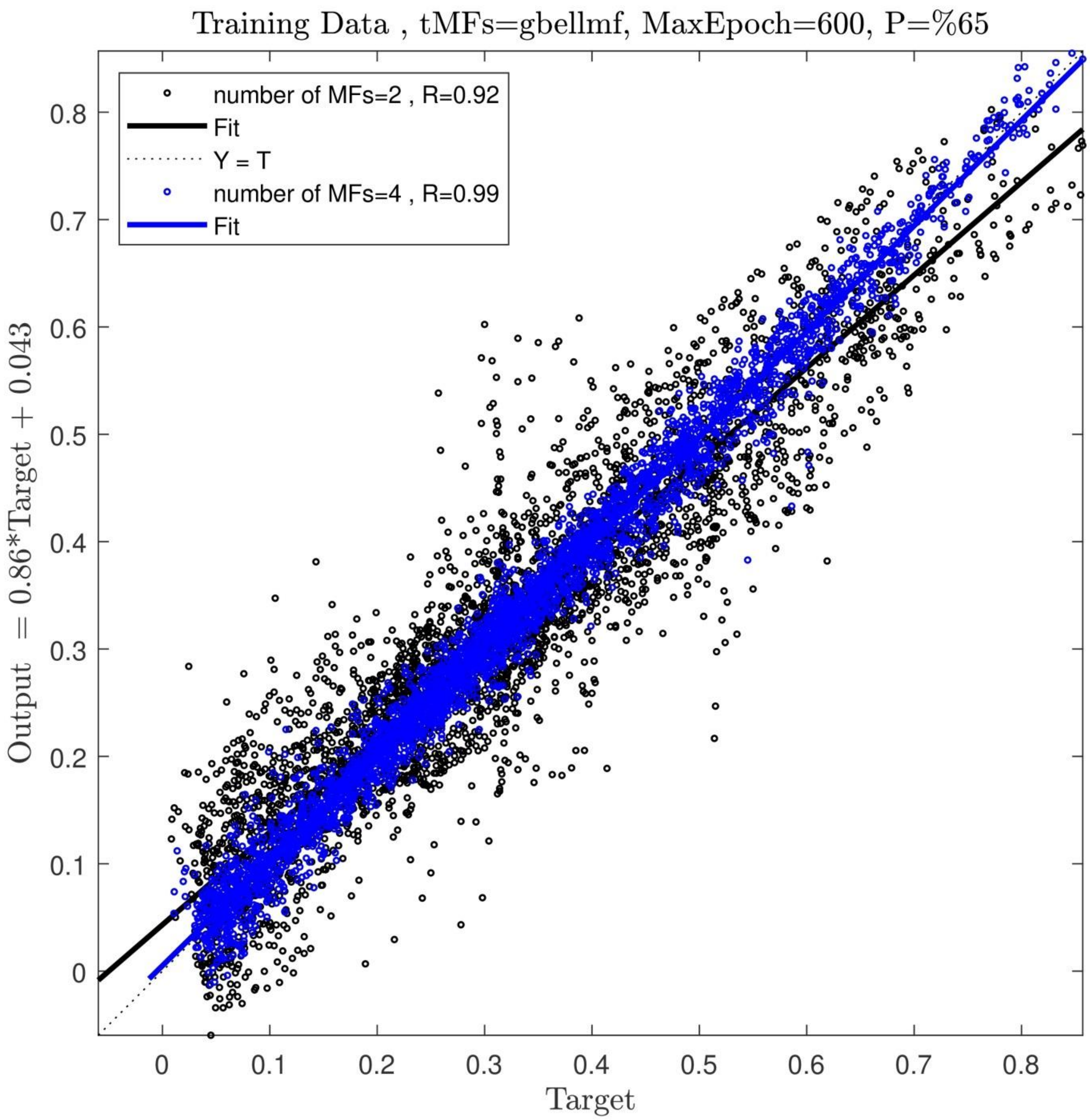

Figure 5(a): Training with using three inputs and different number of MFs (ANFIS method).

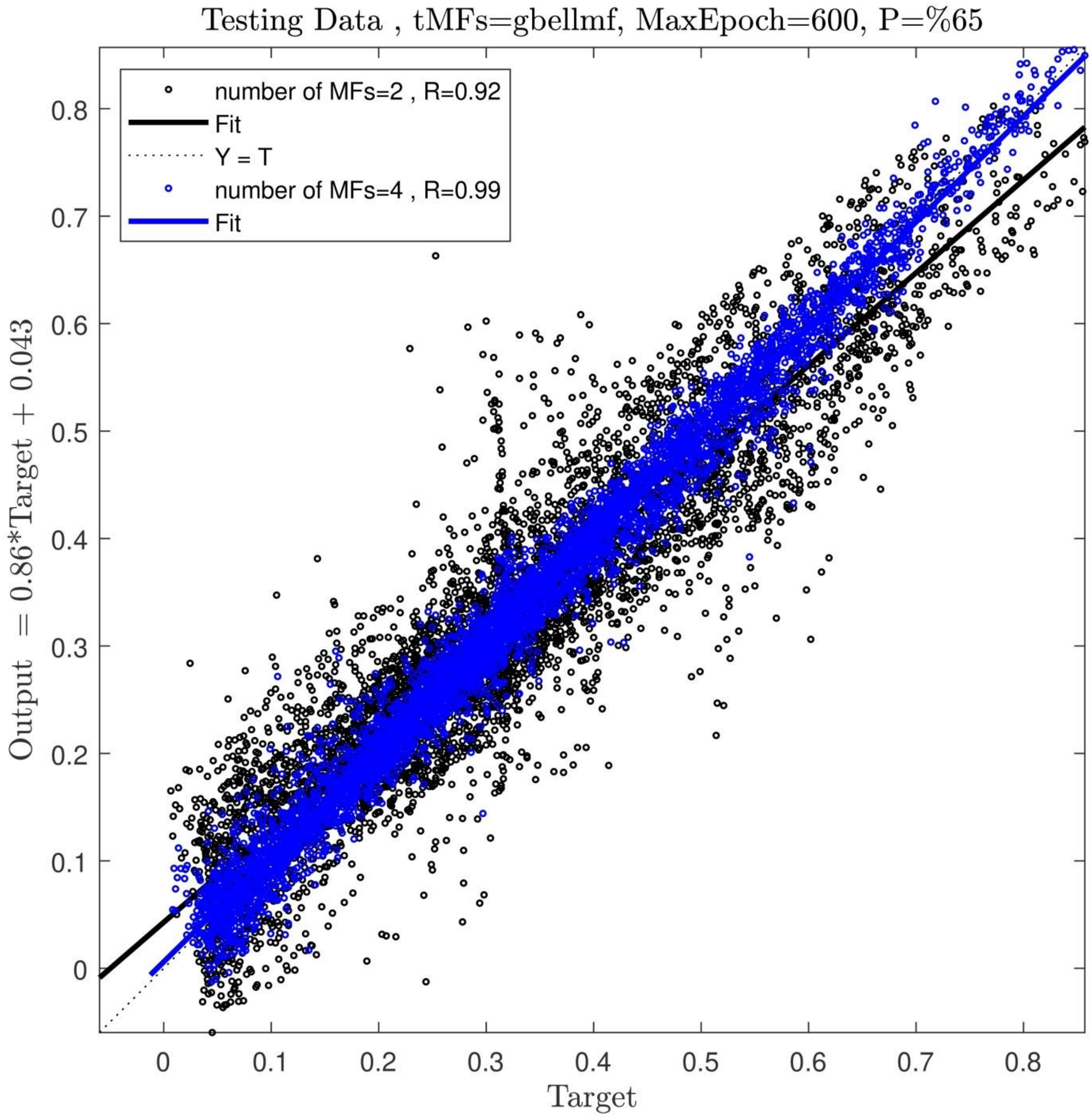

Figure 5(b): Testing with using three inputs and different number of MFs (ANFIS method).

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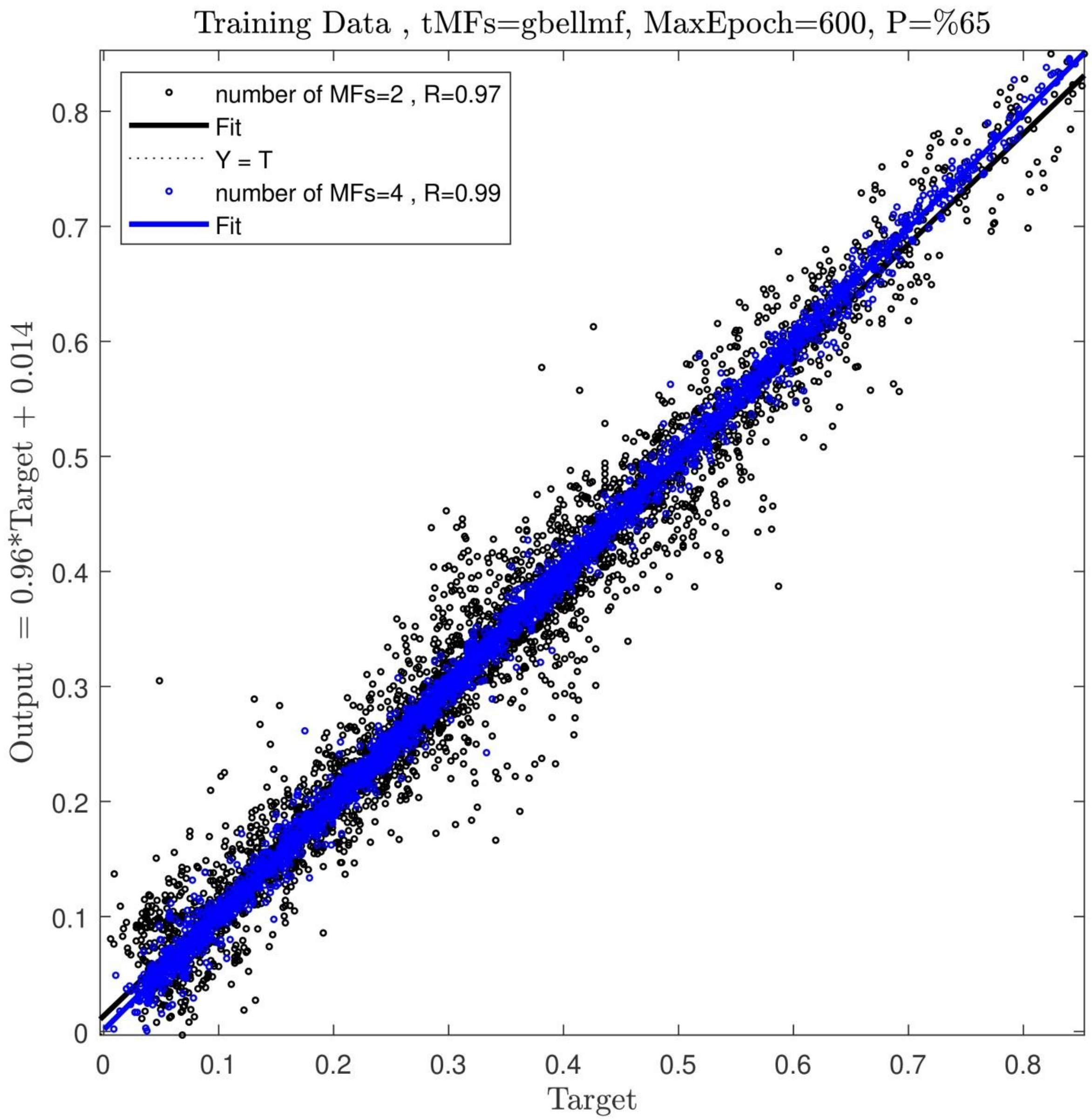

Figure 6(a): Training with using four inputs and different number of MFs (ANFIS method).

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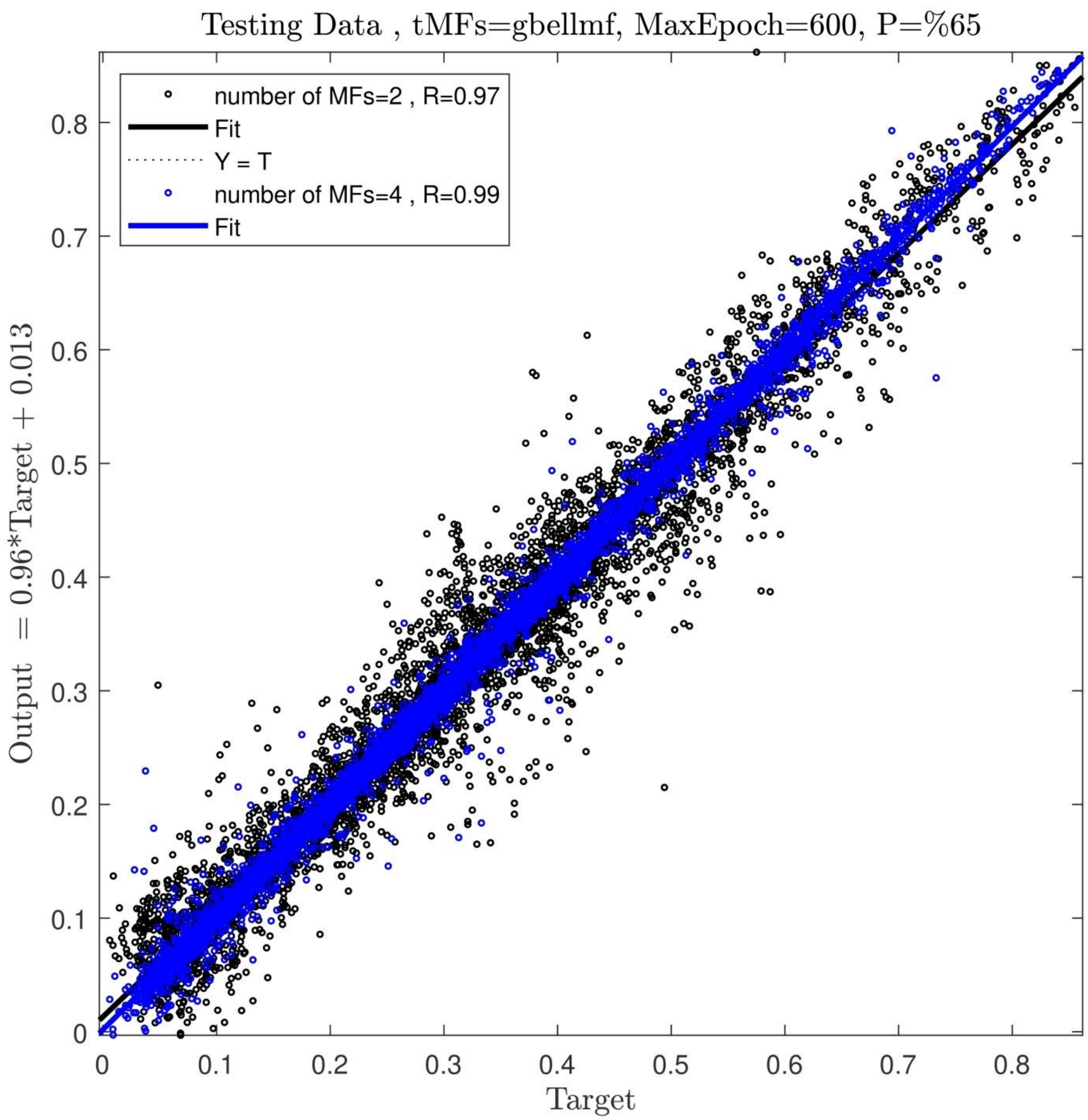

Figure 6(b): Testing with using four inputs and different number of MFs (ANFIS method).

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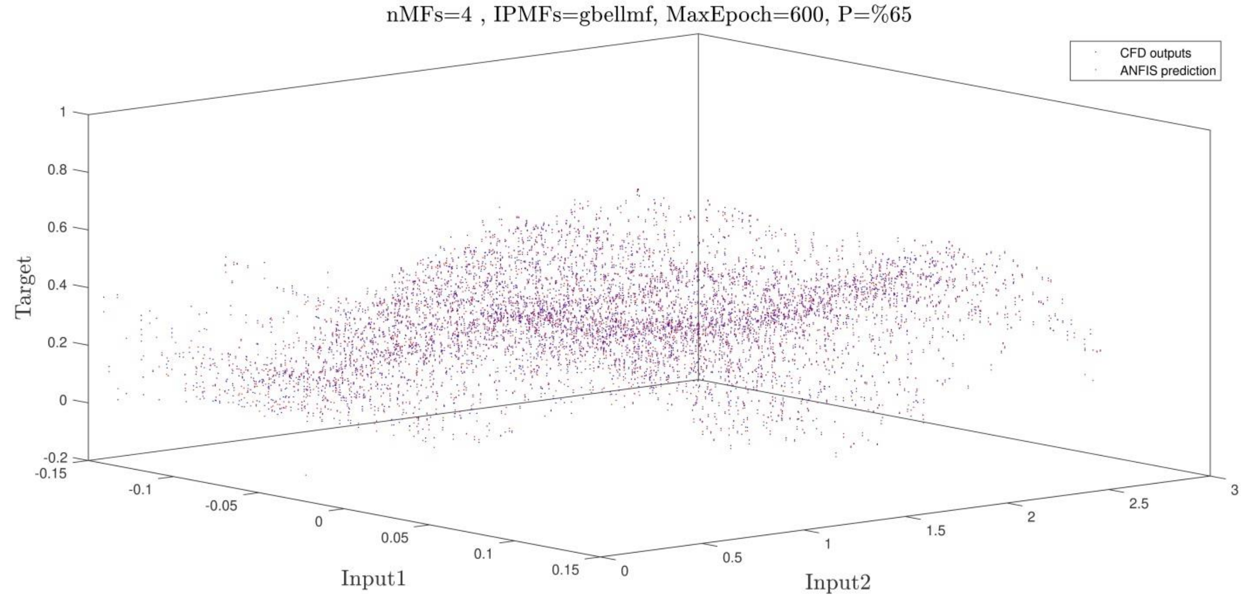

Figure 7(a): Compare CFD output and ANFIS method prediction using inputs 1 and 2.

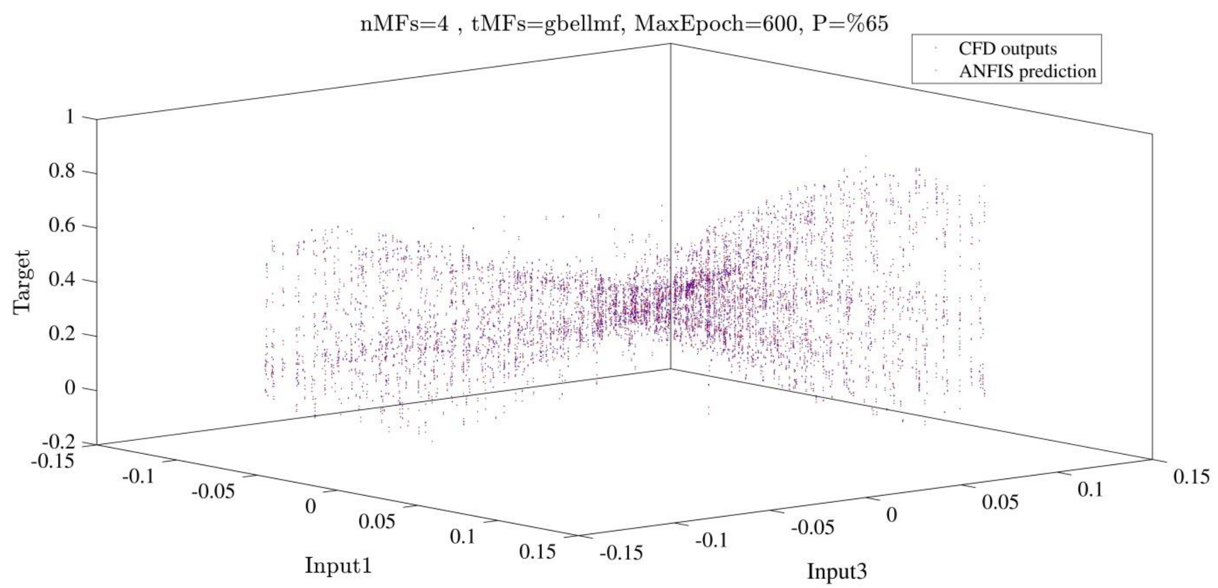

Figure 7(b): Compare CFD output and ANFIS method prediction using inputs 1 and 3.

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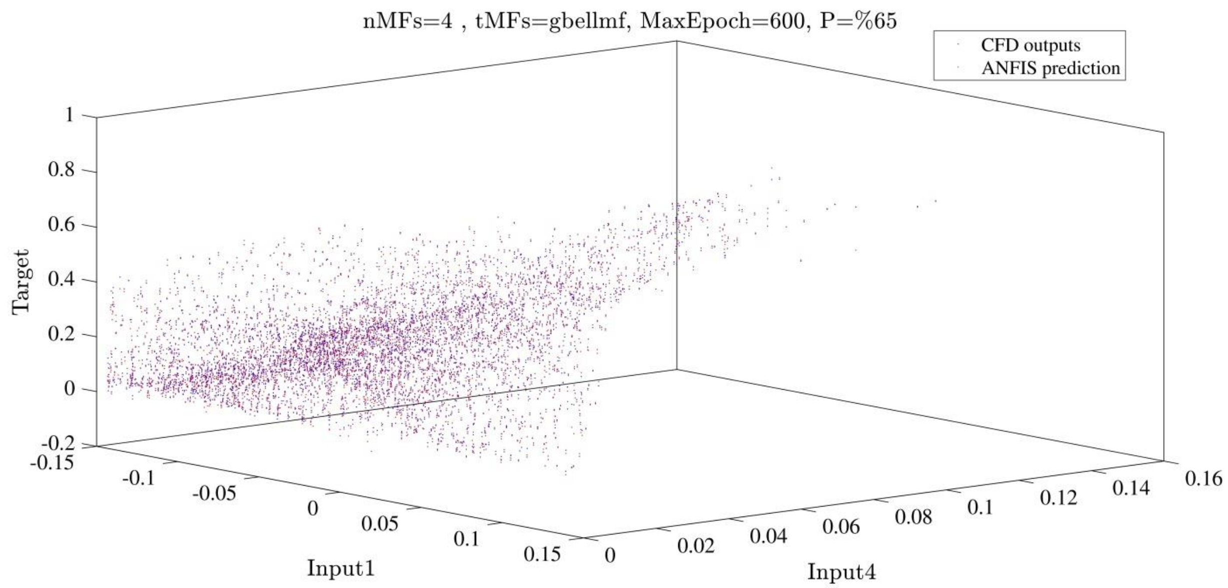

Figure 7(c): Compare CFD output and ANFIS method prediction using inputs 1 and 4.

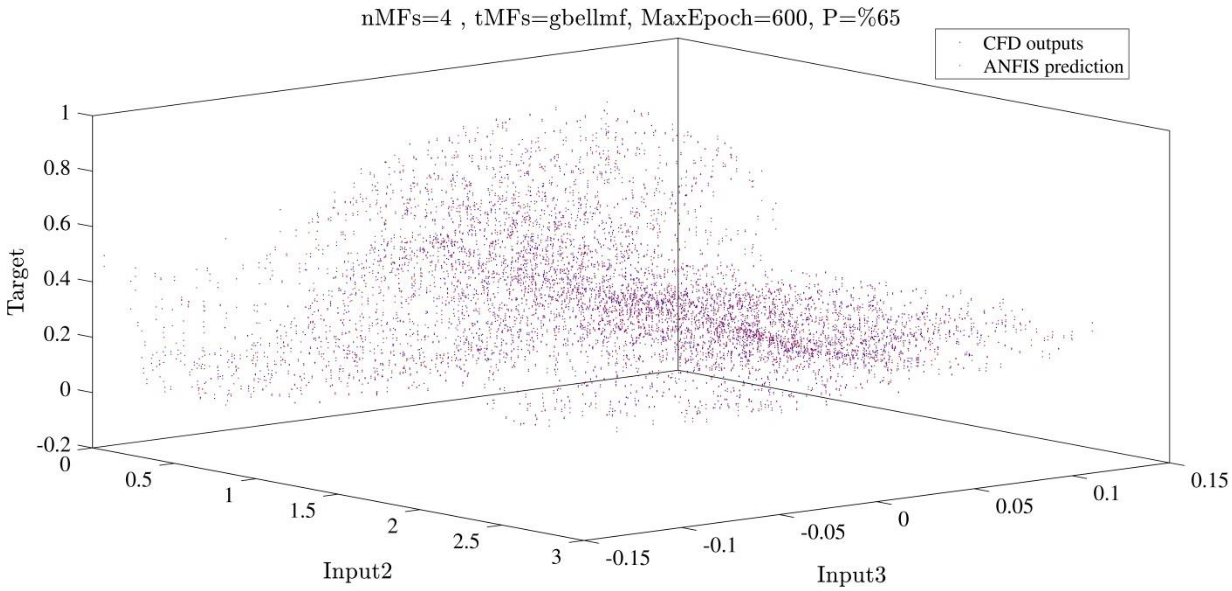

Figure 7(d): Compare CFD output and ANFIS method prediction using inputs 2 and 3.

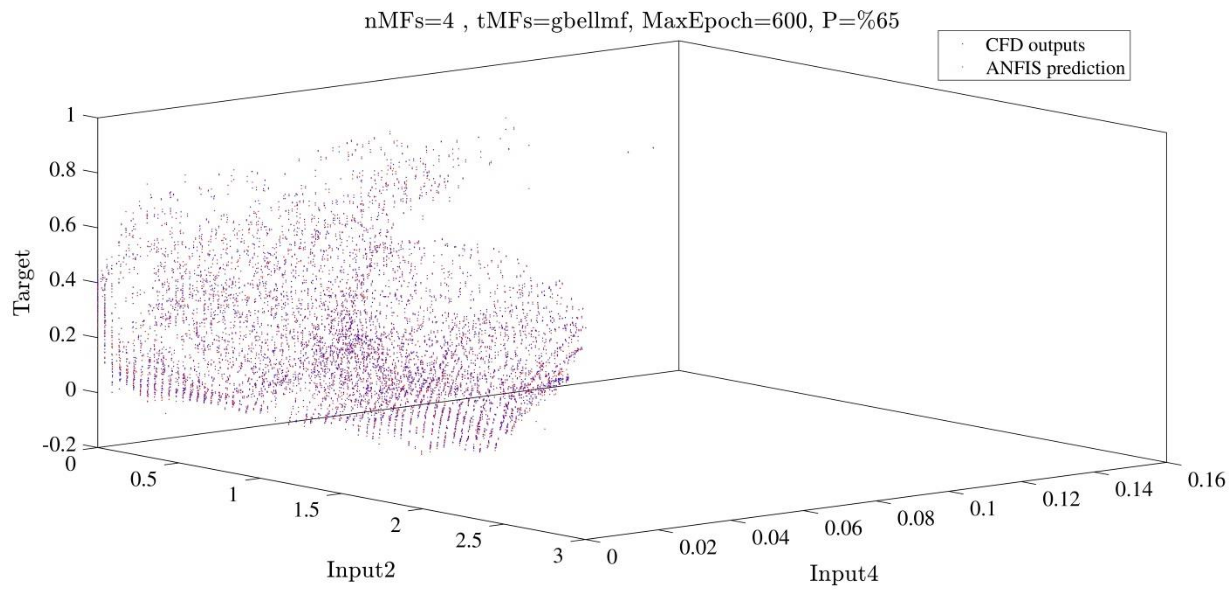

Figure 7(e): Compare CFD output and ANFIS method prediction using inputs 2 and 4.

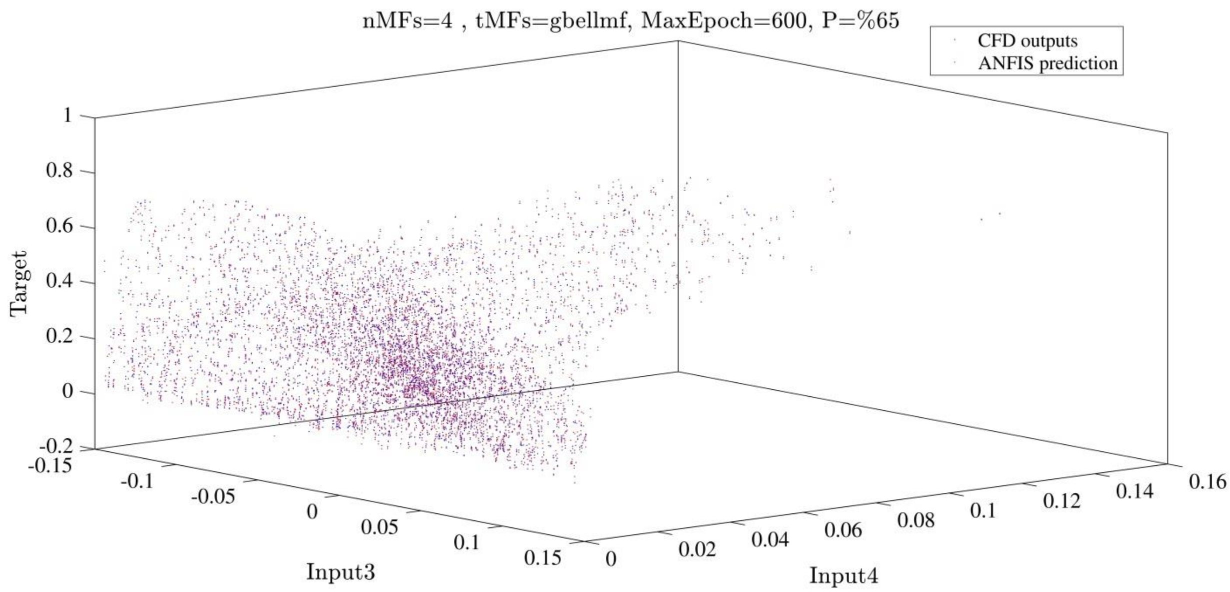

Figure 7(f): Compare CFD output and ANFIS method prediction using inputs 3 and 4.

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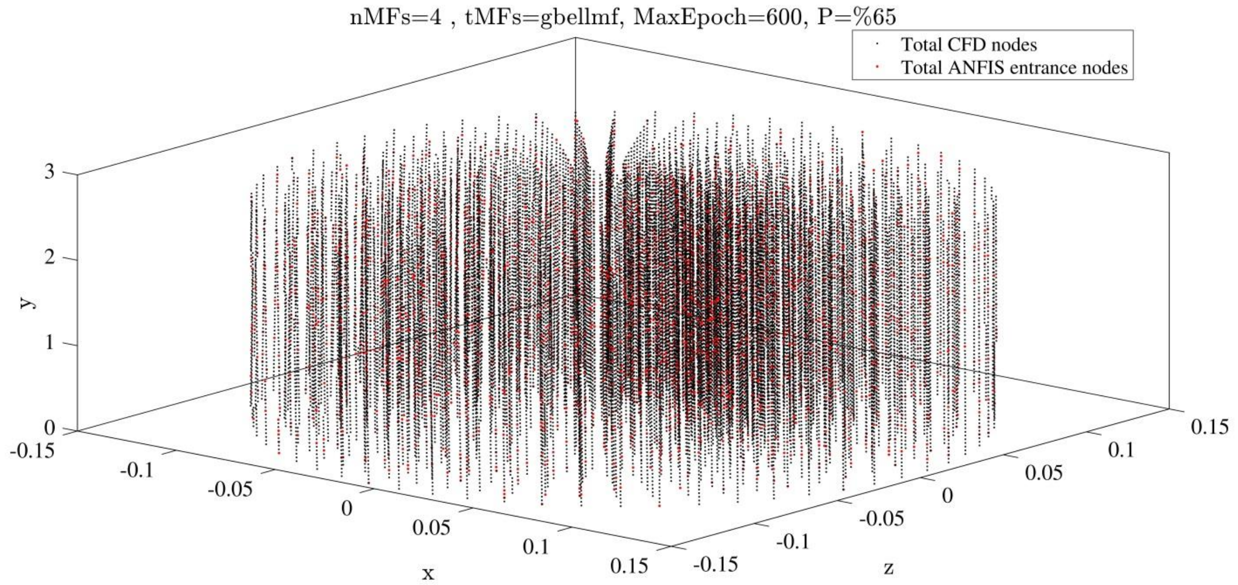

Figure 8: Points of the bubble column that were in the ANFIS learning process.

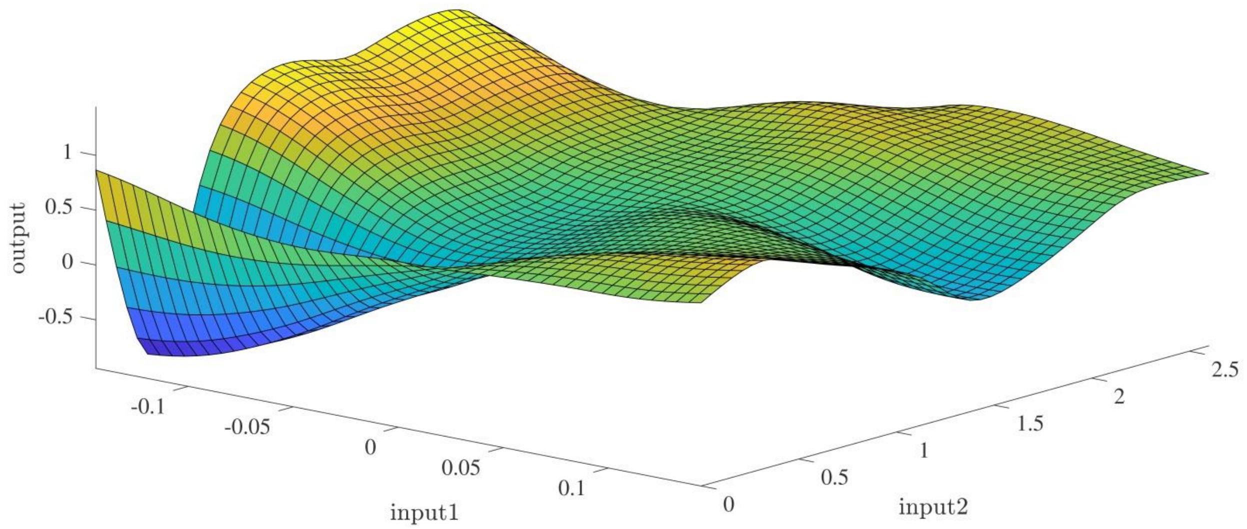

Figure 9(a): Output prediction in Full intelligence of ANFIS method using inputs 1 and 2.

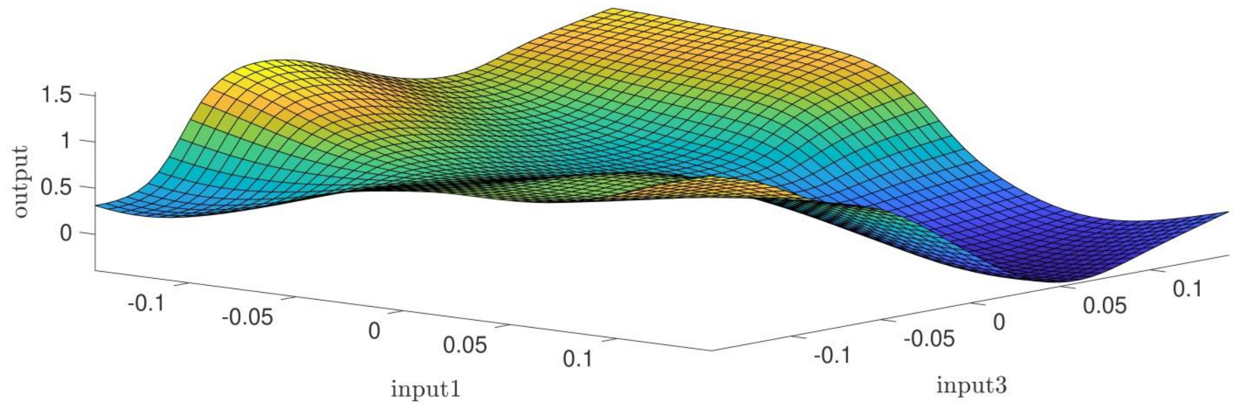

Figure 9(b): Output prediction in Full intelligence of ANFIS method using inputs 1 and 3.

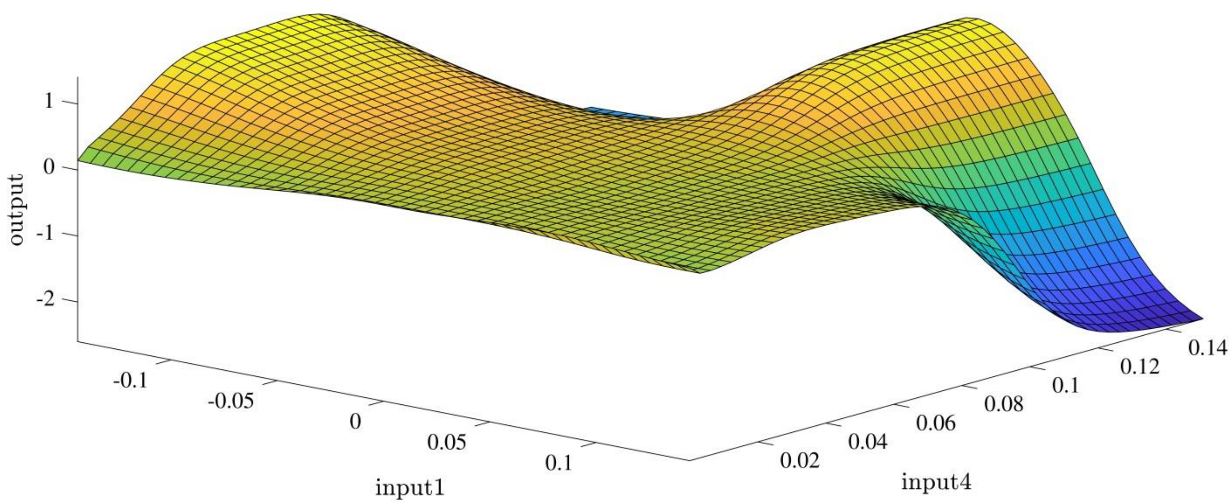

Figure 9(c): Output prediction in Full intelligence of ANFIS method using inputs 1 and 4.

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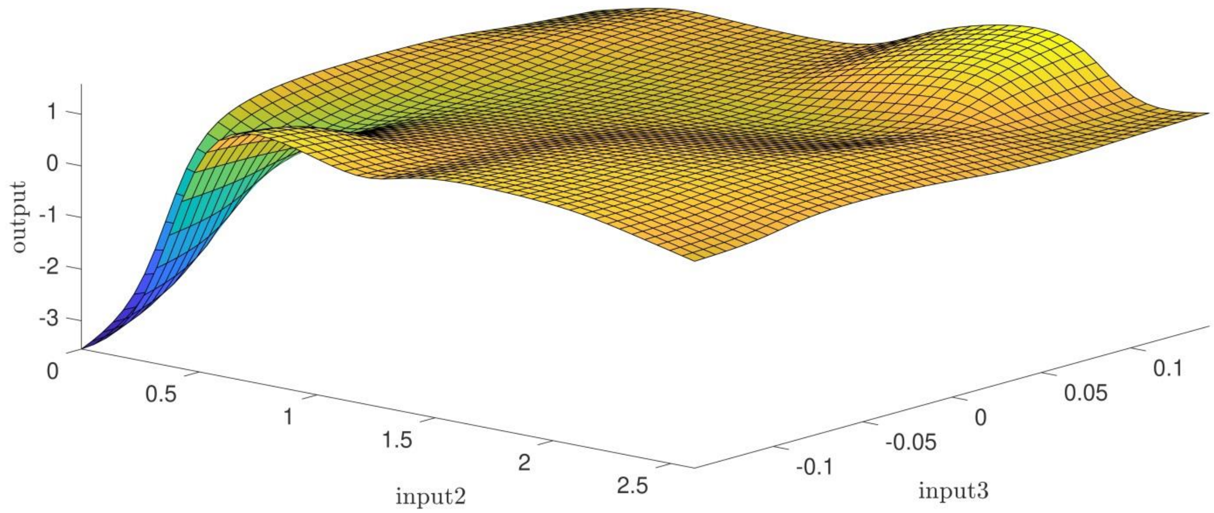

Figure 9(d): Output prediction in Full intelligence of ANFIS method using inputs 2 and 3.

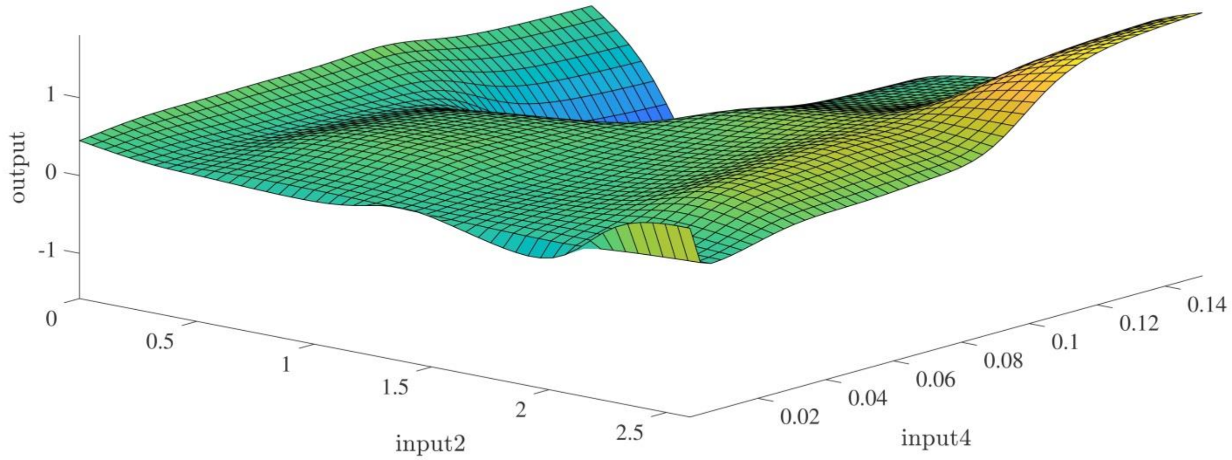

Figure 9(e): Output prediction in Full intelligence of ANFIS method using inputs 2 and 4.

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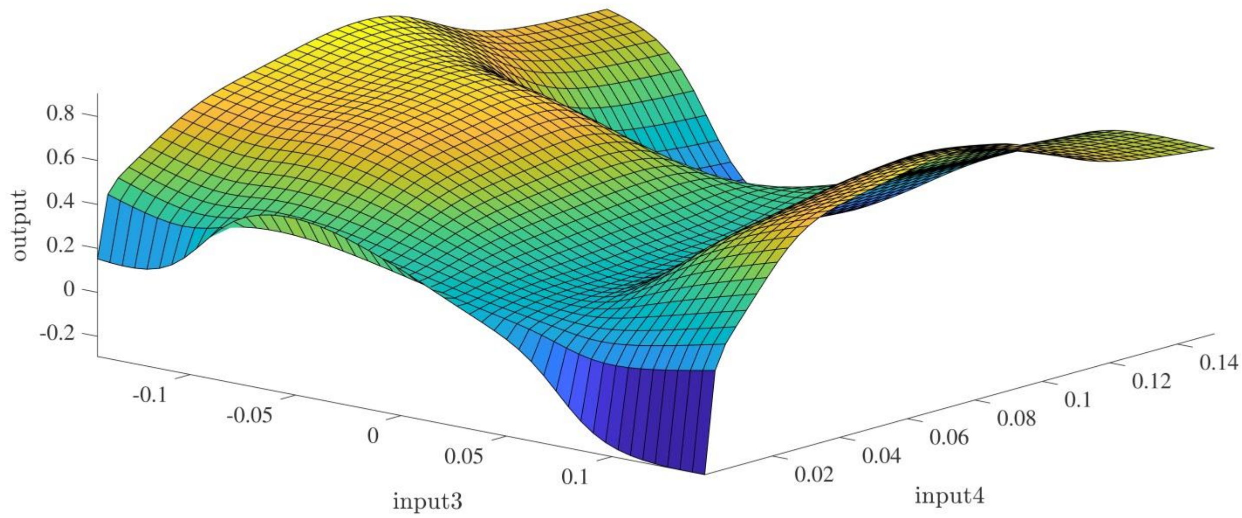

Figure 9(f): Output prediction in Full intelligence of A