Hierarchical hybrid fuzzy-neural networks for modeling of activated carbon preparation for methane storage

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Abstract
Characterization of porous materials has been an interesting issue for researchers. Conditions and operating parameters of preparing porous materials are very important to reach to required charactristics of porous materials. Some methods have been used for estimation of these parameters for instance neural networks. In this paper hierarchical hybrid-fuzzy neural network (HHFNN) is used for approximation of operating parameters of activated carbon preparation as there are mixed input variables, continuous and discrete. The results show that HHFNN approximate the parameters beter than standard neural network (SNN). Also fewer parameters is needed in HHFNN related to SNN.

Keywords:HHFNN, Modeling, activated carbon, Adsorption, Fuzzy systems, Neural networks

Introduction
Storage of natural gas is an important subject for all researchers around the world. Different methods have been invented since now. One of the most important ways is storing natural gas as an adsorbed gas in porous materials which is called ANG. Adsorbents should have high amount of adsorption capacity and rates, high packing density, low adsorption heat and so on. Activated carbon (AC) provides high adsorptive capacity per unit volume.
Several studies have been done for characterization of solid porous materials and finding the proper materials for AC preparation. [1,2,3]
Characterization of porous materials can be seen as a function approximation. Even sometimes optimization is performed to find the best materials and finest conditions for preparation of solid materials.[1,2]
Neural network as a pioneer method is used in new studies. A special class of radial basis function (RBF) neural network known as Regularization network is used by Shahsavand et al. [4] in their paper for characterization of porous materials. Namvar-Asl et al. [5, 6], employed RBF neural networks for modeling of AC preparation. To estimate the preparation conditions of activated carbon, the several neural networks applied because as some parameters are discrete for example agents and precursors.
As shown in figure 1, to use neural networks for approximation of AC preparation parameters, five different networks should be used.

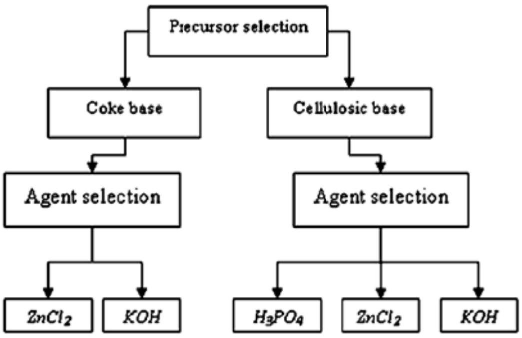

Figure 1: Procedure of effective parameters for the AC preparation [5]

In this paper we used hierarchical hybrid fuzzy neural networks (HHFNN) as a novel method for approximation of system with mixed input variables; discrete and continuous [7, 8, 9, 10]. Precursor and agent are considered as discrete variables and fed to the network. HHFNN is defined in next sections.

Design of Hierarchical hybrid fuzzy-neural network

This section describes the modeling of activated carbon preparation by a novel method. Hierarchical hybrid fuzzy-neural network is used to predict the activated carbon(AC) parameters. We make a new method for modeling of AC preparation parameters by using HHFNN.

First we look briefly to the HHFNN structure. HHFNN consists of two levels as shown in figure 2; First level is fuzzy combination level (FCL) and the upper level is neural network level(NNL). FCL composed of some fuzzy combination sub-systems (FCSS). Each FCSS in lower level aggregates several discrete variables with a few values, linguistic variables or Boolean input variables into one intermediate variable which is then considered as one input variable to the upper NNL [7,8].

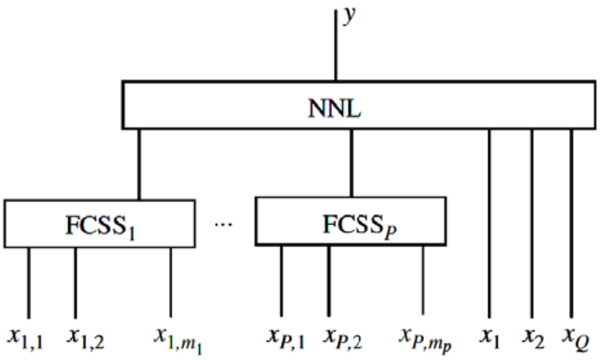

Figure 2: Hierarchical hybrid fuzzy neural networks

The data required for training of the network gathered from various papers specially Namvar-Asl [5,6]. These data consisted of Precusor, Agent, Impregnation ratio, Activation temperature, Activation time and heating rate. Precursor and Agent considered as discrete variables and others as continues variables.

As shown in figure 3, We apply one sub-fuzzy system to combine the features of Discrete variables (Precursor, Agent) together. Then five input variables (Fuzzy(Precursor, Agent),Impregnation ratio, Activation temperature, Activation time, heating rate) are applied to the upper level neural network where Fuzzy(Precursor, Agent) is the output from the lower combination fuzzy system. Other data which gathered from literatures are surface area and micropore volume. These variables are output of models and utilized them in output layer of HHFNN.

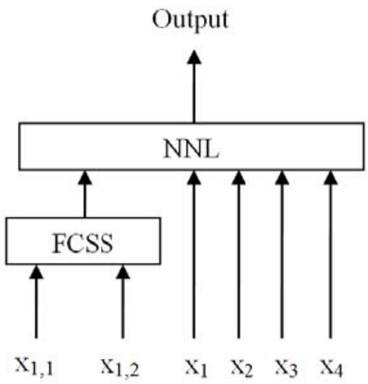

Figure 3: Proposed HHFNN model in this study:
$x_{1,1}$=Precusor, $x_{1,2}$=Agent, x_1=Impregnation ratio,
x_2=Activation temperature, x_3=Activation time, x_4=Heating rate

Around seventy sets of parameters are available in Namvar-Asl [5] which we used them for training and testing of proposed model.
Design of FCSS in lower level: We use triangular membership functions based on the Mamdani fuzzy system for the lower FCl. The edge of one triangular membership function intersects to the middle point of its neighboring triangular membership function. Here we apply triangular membership function to retain the transparency of the lower fuzzy level. Alternative membership functions like Gaussian can also be used. In this paper a commonly used defuzzifier, center average, is applied to evaluate model output of p^{th} FCSS ($\bar{y}_p$) in the lower FCL.
Design of NN in upper level: In the upper level, we use a neural network with one input layer, one hidden layer and one output layer. Sigmoidal activation functions are applied for the hidden neurons.
Training: Parameters updating in the upper neural network level and lower fuzzy combination level are done by gradient-descent algorithm. Weights and bias in hidden neurons, bias in output neuron and THEN part of fuzzy rule are updated in this algorithm.
All relevent formulas are omitted because of page limits.
Number of parameters: The number of parameters needed for this HHFNN model is,

$$\sum_{p=1}^{P} 2^{m_p} + (P + Q + 1) \times H + (H + 1)$$

P = total number of FCSSs , p=1,2,…,P
Q = number of continues input variabeles directly fed to hidden neurons
H = numbers of hidden neurons
m_p = number of inputs to pth FCSS
For a standard neural network, if we assume that H is the number of needed hidden neurons, then the numbers of parameters for SNN is,

$$(n + 1) \times H + (H + 1)$$

n = total number of input variables

We employed a new SNN in this study. All input variables including discrete variables (Precursor and Agent) are supplied to the network otherwise we have to use different networks for each discrete variables.

Simulation and Discussion

As it is described in the last section, we use simulation data set to assess the advantage of HHFNN modeling of AC preparation parameters over Standard Neural Network (SNN) in case of accuracy and number of parameters.

Firstly we use the whole data set for approximation training. The results comparison is reported in Table 1.

Table1: Approximation comparison between HHFNN and SNN using all data set

Method	Hidden neurons	Parameters	Learning rate	MSE1	MSE2
HHFNN	10	75	0.01	0.02206	0.01449
HHFNN	10	75	0.05	0.02305	0.01283
HHFNN	10	75	0.1	0.02154	0.01237
HHFNN	10	75	0.5	0.01695	0.01132
HHFNN	20	145	0.01	0.01829	0.01426
HHFNN	20	145	0.05	0.01869	0.01227
HHFNN	20	145	0.1	0.01432	0.01112
HHFNN	20	145	0.5	0.01324	0.01710
HHFNN	30	215	0.01	0.01178	0.01317
HHFNN	30	215	0.05	0.01056	0.01234
HHFNN	30	215	0.1	0.01127	0.00963
HHFNN	30	215	0.5	0.01167	0.01608
SNN	10	81	0.01	0.02142	0.02087
SNN	10	81	0.05	0.02186	0.01460
SNN	10	81	0.1	0.01629	0.01182
SNN	10	81	0.5	0.01235	0.01263
SNN	20	161	0.01	0.01786	0.01234
SNN	20	161	0.05	0.01467	0.01037
SNN	20	161	0.1	0.01223	0.01012
SNN	20	161	0.5	0.01093	0.01083
SNN	30	241	0.01	0.01480	0.01190
SNN	30	241	0.05	0.01070	0.01336
SNN	30	241	0.1	0.00919	0.01032
SNN	30	241	0.5	0.01874	0.01101

Note: MSE: mean square error, 1: surface area, 2: micropore volume

From table 1, we can see that by using the same number of hidden neurons, HHFNNs in the most of times use fewer parameters respect to SNNs.

The number of parameters for HHFNN and SNN are computed by former formulas. As shown in table 1, the number of parameters for HHFNN is 75 for 10 hidden neurons but for SNN is 81 parameters.
When we use 20 hidden neurons, the HHFNN needs 145 parameters and SNN needs 161 parameters.
When using 3 hidden neurons, The HHFNN requires 215 parameters and SNN needs 241 parameters.

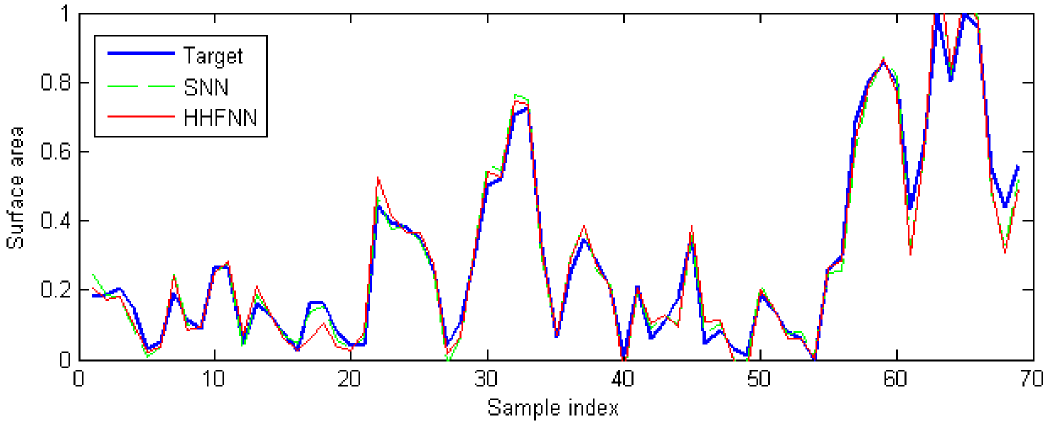

Figure 4: Approximation for surface area using all data set (learning rate=0.1, H=30)

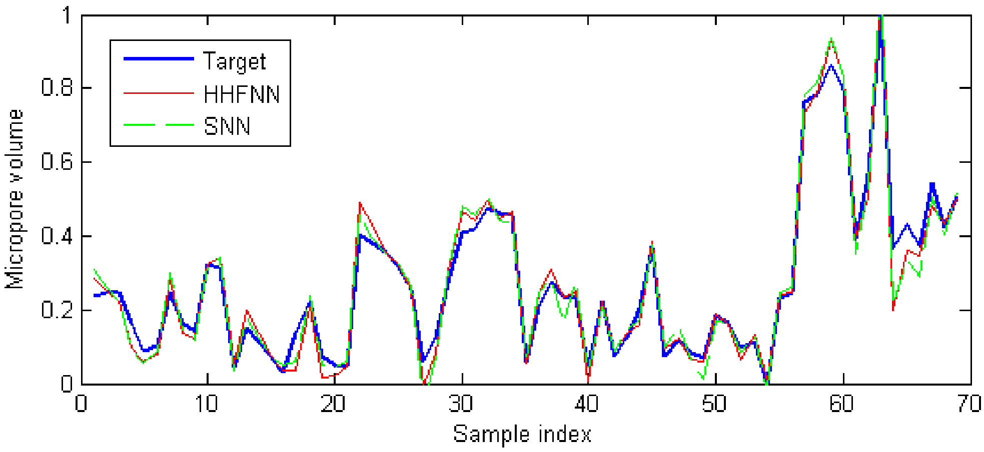

Figure 5: Approximation for Micropore volume using all data set (learning rate=0.1, H=30)

In addition, by using the same number of hidden neurons, HHFNNs in most of the cases have more accuracy than SNN. Training has been done for HHFNN and SNN several times by changing learning rate to achieve optimal ones in each case.
When using 30 hidden neurons, the HHFNN obtains the errors of 0.0105631 and 0.0123447 for learning rate 0.05 while SNN has the errors of 0.017099 and 0.0133644.
Figures 4 and 5 show the accuracy of HHFNNs and SNNs for estimation of related parameters. It is understandable from the figures that HHFNN approximate the AC parameters slightly better than SNN.
If we use 50 data instances for training and remaining 20 instances for testing, then the resulting comparison is shown in Table 2 and figures 6 to 9.

We observed from these figures the performance of HHFNN and SNN. It is clear that the performance of HHFNN is better than SNN in the most of the cases with the same hidden neurons and learning rate.

Table2: Training and testing comparison between HHFNN and SNN

Method	Hidden neurons	Parameters	Learning rate	Training		Testing	
				MSE1	MSE2	MSE1	MSE2
HHFNN	10	75	0.05	0.01997	0.01291	0.02371	0.01701
HHFNN	10	75	0.1	0.01866	0.00676	0.02156	0.01070
HHFNN	20	145	0.05	0.01911	0.01004	0.02321	0.01525
HHFNN	20	145	0.01	0.00881	0.00917	0.01211	0.01407
HHFNN	30	215	0.05	0.01735	0.01096	0.02001	0.01460
HHFNN	30	215	0.1	0.01152	0.00669	0.01082	0.00969
SNN	10	81	0.05	0.01968	0.01363	0.02100	0.01744
SNN	10	81	0.01	0.01756	0.01209	0.01876	0.01790
SNN	20	161	0.05	0.01601	0.01290	0.02011	0.01599
SNN	20	161	0.1	0.01221	0.00916	0.01820	0.01366
SNN	30	241	0.05	0.01773	0.01520	0.02177	0.02221
SNN	30	241	0.01	0.01611	0.00838	0.02188	0.01138

Note: MSE: mean square error, 1: surface area, 2: micropore volume

It is obvious from figures 6 to 9 that HHFNN and SNN can approximate the properties of AC better than SNN but in this case study the difference is not impressive.

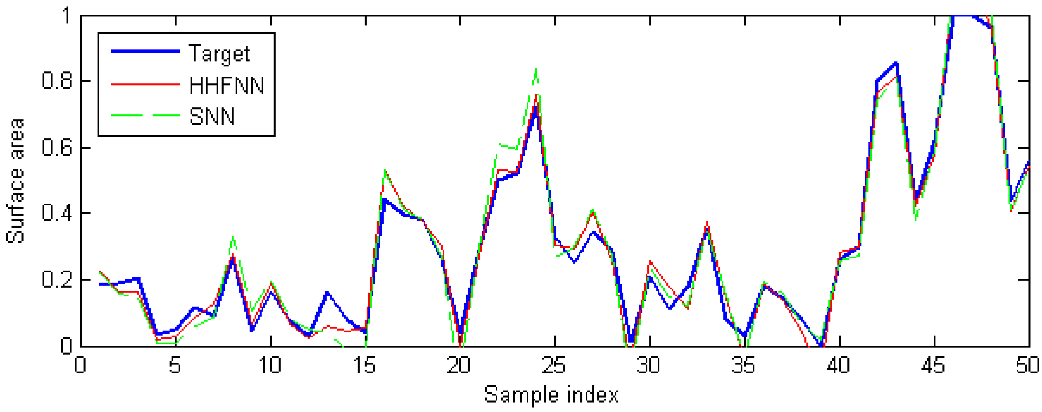

Figure 6: Performance comparison for the training data set (learning rate=0.1, H=30)

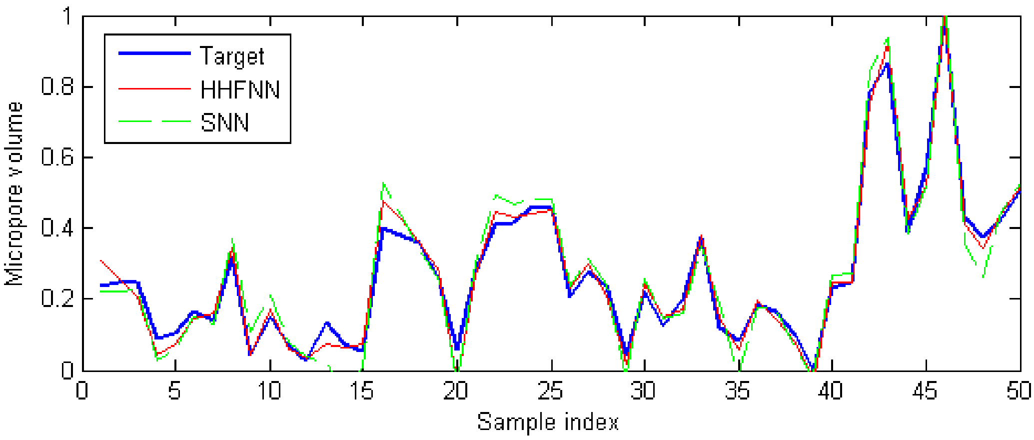

Figure 7: Performance comparison for the training data set (learning rate=0.1, H=30)

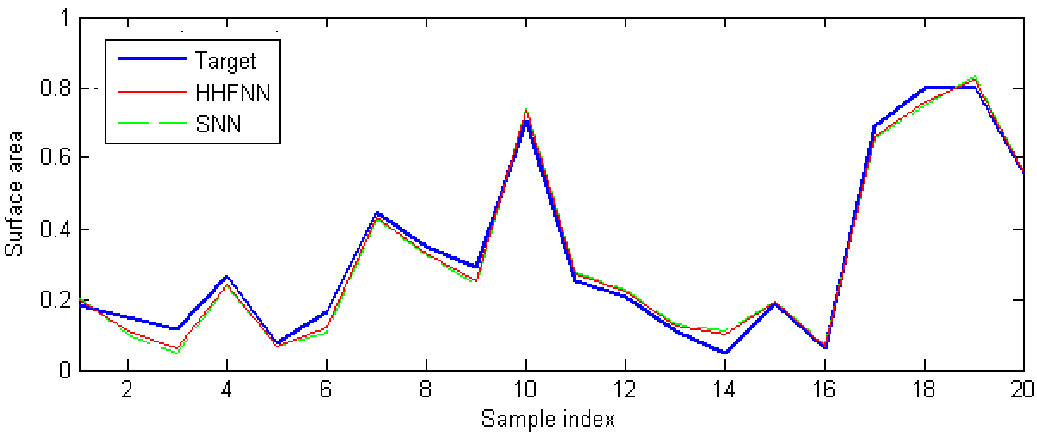

Figure 8: Performance comparison for the testing data set (learning rate=0.1, H=30)

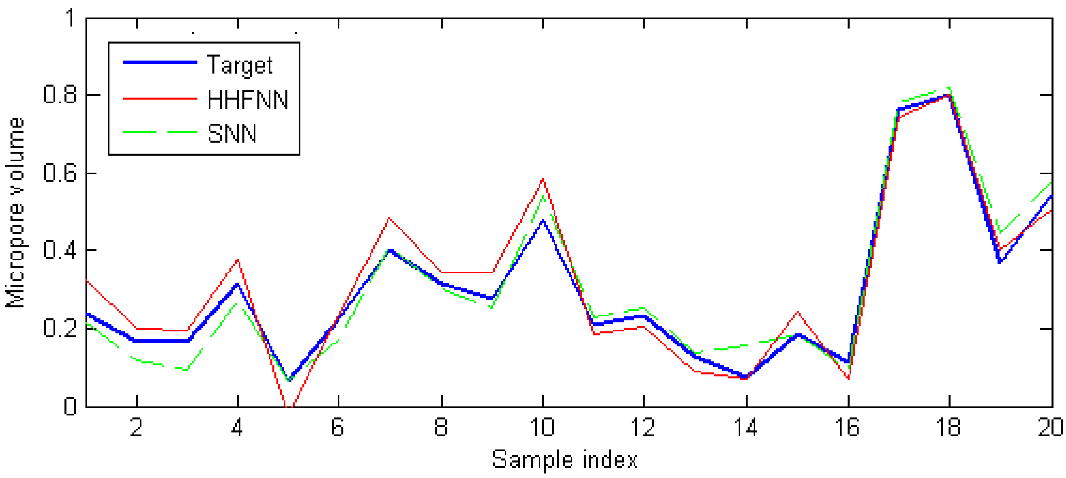

Figure 9: Performance comparison for the testing data set (learning rate=0.1, H=30)

Conclusions

Hierarchical hybrid fuzzy-neural network was used for approximation of activated carbon preparation parameters and results compared with SNN. SNN in this study is a different network which we applied all variables including discrete variables as inputs. HHFNN consists of two layers, first is fuzzy layer and second one is NN. Although neural networks can work with discrete variables, but fuzzy systems are better at presenting of linguistic or discrete input variables. The results shows that HHFNN obviously approximate AC preparation parameters with more accuracy than SNN. The results also show that performance differences between the HHFNN and SNN in our case study are not as high as reported in other case studies. Furthermore with the same number of hidden neurons, HHFNN needs fewer parameters than SNN.

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