Application of BP neural network based on genetic algorithm optimization in thermal conductivity of nanofluids

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Abstract. In this paper, a hybrid model (BP-GA) including a back propagation network and a genetic algorithm is used to estimate the thermal conductivity of the nanofluids. The genetic algorithm is used to optimize the initial weight and threshold of BP neural network, so that the optimized BP neural network can better predict the function output. In this study, CuO-ZnO hybrid nanofluids with the mass fraction of 0%, 1%, 2%, and 3% were studied at temperatures of 25, 30, 35, 40, 45, 50, 55, and 60 °C, respectively. The thermal conductivity of the hybrid nanofluids base liquid is 20:80, 40:60, 50:50, 60:40, 80:20, and the mass ratio of CuO-ZnO is 50:50. The mass fraction of CuO-ZnO, the temperature and the mixing ratio of different base liquids were used as input parameters, and the thermal conductivity was the output parameter, forming a 3-input ANN neural network. The predicted thermal conductivity results of BP neural network and genetic algorithm optimized BP neural network (GA-BP) were compared with experimental data. The results illustrate that the BP neural network optimized by genetic algorithm exerts a positive influence on the accuracy and stability of the predicted output.

1. Introduction
Nanofluids have potential applications in many important areas, such as advanced heat transfer or cooling, energy harvesting, microelectronics, MEMS, microfluidics, transportation, medical, and numerous thermal management systems [1-7]. Due to the small size and large surface area of nanoparticles, various types of nanofluids have broad application prospects in engineering applications. Therefore, the main goal of the researchers is to estimate the transport parameters of nanofluids called thermal conductivity and viscosity. In the late 1950s, the perceptron network introduced artificial neural networks, which is a powerful statistical tool. In recent years, neural networks, fuzzy logic and genetic algorithms have been introduced as computational methods, therefore, neural network algorithms can be used to predict nanofluids thermal conductivity and viscosity. By reading the relevant literature [8,9], the neural network algorithm has higher prediction accuracy for thermal conductivity and viscosity. Nanofluids have superior heat transfer performance than traditional liquids. One of the main reasons is that nanoparticles significantly increase the thermal conductivity of nanofluids. The thermal conductivity is the main parameter reflecting the heat transfer capacity of the medium and has important theoretical and application significance. So far, there is no molded fluid transient hot wire thermal conductivity tester at home and abroad. In addition, Kurt and Kayfeci [10] predicted the thermal conductivity of ethylene glycol-water-based nanofluids. Emmat Esfe et al. [11] designed an artificial neural network algorithm to estimate the thermal conductivity and dynamic viscosity of ferromagnetic
nanofluids using 72 experimental data. They prepared two sets of relevant data to predict these thermophysical parameters and compared the experimental data with the relevant results. Zhao et al. [12] proposed two neural network models based on radial basis function (RBF) to predict the viscosity of Al2O3-water and CuO-water, evaluated the accuracy of the model by using to the root mean square error (RMSE), mean absolute percentage error (MAPE), the sum of squared errors (SSE), and coefficient of determination (R^2). Hemmat Esfe et al. [13] proposed an artificial neural network to predict the viscosity of TiO2-water nanofluids. They studied various structures of the network and applied a hidden layer and four neuron tansig activation functions to calculate the regression coefficients, the results used for viscosity estimation are compared with experimental data, and the maximum error is 0.5%. Ahmadloo and Azizi [14] used a 776 experiment to establish a 5-input artificial neural network model to estimate Al2O3-water, Al-water, TiO2-water, Cu-water, CuO-water, ZrO2-water, Al2O3-EG The thermal conductivity of Cu-EG, CuO-EG, Mg(OH)2-EG, Al2O3-Oil, Al-Oil, CuO-Oil and Cu-Oil is evaluated by the average absolute error and correlation coefficient. Afrand et al. [15] used experimental data to estimate the relative viscosity of MWCNTs-SiO2/AE40 nano-lubricants, and used 80 experiments to establish an artificial neural network with temperature and nanoparticle volume fraction as input variables, the number of hidden layer neurons, the transfer function, and the repetition of the training step size determine the optimal network. Esfe et al. [16-23] measured the thermal conductivity of other different types of nanofluids based on experimental methods. On this basis, the effectiveness of the multilayer perceptual feedforward network model in the prediction of thermal conductivity of nanofluids was verified. Hemmat and Esfe et al. [24] evaluated the accuracy of the artificial neural network model in predicting the thermal conductivity of Al2O3/EG-W. The volume fraction of 0~1.5% nanoparticle and the temperature range of 20~60°C are input data, and the measured thermal conductivity is the output data, the number of neurons with different transfer functions is evaluated to determine the optimal model of the number of neurons in the hidden layer. The results show that the artificial neural network structure has high simulation accuracy. The paper is arranged in the following structure. Section 1 argues the influence of base mixing ratio, temperature and mass fraction on thermal conductivity. Section 2 introduces the use of GA-BPNN and BPNN model to establish a thermal conductivity prediction model. Section 3 describes the prediction of the thermal conductivity between the GA-BPNN model and the BPNN model and the experimental data, and characterizes the influence of different factors (temperature, nanoparticle mass fraction, base-liquid mixing ratio) on the thermal conductivity. Based on the experimental results, it is found that the GA-BPNN model has higher prediction accuracy than the BPNN model.

2. Experiments
The specific preparation of the hybrid nanofluids, firstly, according to the mass fraction of (CuO-ZnO), calculate the corresponding mass of 40nm CuO and 30nm ZnO nanoparticles and the corresponding deionized water and ethylene glycol mass, secondly, weighed and mixed together in accordance with the ratio of ethylene glycol to deionized water. Finally, the mixture was stirred for 30 min with a magnetic stirrer and ultrasonically shaken for 45 min to form a uniformly dispersed nanofluids.

Preparation of nanofluids, used for CuO-ZnO(ethylene glycol: deionized water) nanofluids with the equal mass fraction (1:1) nanofluids under different temperature and nanoparticle mass fraction and different basic mixing ratio under experimental evaluation. The nanoparticle mass fraction of CuO-ZnO was 0%, 1%, 2%, 3%,... At temperatures of 25,30,35,40,45,50,55 and 60 °C, ethylene glycol and deionized water at different mixing ratio (20:80, 40:60, 50:50, 60:40, 80:20) with a Hot disk 2500 s thermal constant analyzer repeated four times, each sample taken four times the average thermal conductivity as the final measured values.

As shown in figure 1, the mass fraction of 0%, 1%, 2%, and 3%, depicts the temperature of 20,25,30,35,40,45,50,55 and 60 °C, ethylene glycol and deionized water at different mixing ratio (20:80, 40:60, 50:50, 60:40, 80:20) effect on the thermal conductivity, and through the experiment measuring the thermal conductivity of 3 d surface figure.
Figure 1. Three dimensional scatter surface of thermal conductivity under different mass fraction

It can be seen from Figure 1 that, when the temperature and nanoparticle mass fraction are constant, the ratio of ethylene glycol to deionized water (that is, the mass fraction of ethylene glycol to ethylene glycol and deionized water) increases. The decrease in thermal conductivity is chiefly due to the fact that the thermal conductivity of ethylene glycol is lower than that of deionized water.

When the temperature and the ratio of ethylene glycol to deionized water are constant, as the mass fraction increases from 0% to 1%, the thermal conductivity increase greatly. The primary reason is that the addition of nanoparticles is the main factor affecting the thermal conductivity. When the mass fraction increases from 1% to 3%, the thermal conductivity increases with the increase of the mass fraction. The cause is that the increase of the content of nanoparticles per unit volume leads to the increase of the heat exchange area, and the probability of collision between particles greatly improves the heat exchange efficiency.

When the mass fraction and the ratio of ethylene glycol to deionized water are constant, the thermal conductivity increases as the temperature rises. The cause for this is that the Brownian motion velocity increases, which contributes to the increase of the thermal conductivity of the nanofluids.

2.1 Creating an BP neural network model

The BP neural network is a multi-layer feedforward neural network. The main feature of this neural network is that the signal is transmitted forward and the error is transmitted backward. The BP neural network consists of three layers of input layer, hidden layer and the output layer, as shown in Figure 2. BP neural network usually uses sigmoid function (log-sigmoid or tan-sigmoid) as the transfer function. The so-called reverse propagation learning algorithm is that input information is passed from the input layer through the hidden layer to the output layer. If the output error is large, the error signal is returned along the original path for reverse learning. During the return process, the new output error is obtained by modifying the connection weight and threshold between the neurons until the error signal is minimum. As shown in Figure 1, the input values are the mass fraction W, temperature T, the ratio of ethylene glycol to deionized water R, and the output value is the thermal conductivity. Seen from the topology results graph, BP neural network is equivalent to a nonlinear function, mapping the input value to the output value.

R² and MSE are considered to be the two main parameters for determining the best mode of the neural network. In fact, when the error measurement standard reaches a predetermined amount, the training of the BP neural network ends. The error measurement criteria include mean square error (MSE) and Coefficient of determination (R-square). The values are defined as follows:
Figure 2. BP neural network extension structure

$R^2$ and MSE are considered to be the two main parameters for determining the best mode of the neural network. In fact, when the error measurement standard reaches a predetermined amount, the training of the BP neural network ends. The error measurement criteria include mean square error (MSE) and Coefficient of determination (R-square). The values are defined as follows:

$$R^2 = 1 - \frac{\sum_{i=1}^{n} (T_i - P_i)^2}{\sum_{i=1}^{n} (T_i - \bar{T})^2} / n$$

$$MSE = \frac{1}{n} \sum_{i=1}^{n} (T_i - P_i)^2$$

(1)

(2)

In these equations, $T_i$ is the actual value and $P_i$ is the value of the model. $\bar{T}$ is the average experimental value of $n$ sets of test data. MSE (Mean Squared Error) refers to the expected value of the square of the difference between the parameter estimate and the true value of the parameter. MSE can evaluate the degree of change of the data. The smaller the MSE value, the more accurate the prediction model describing the experimental data. $R^2$ is statistically used to represent the goodness of fit of the model. The larger the R-square is, the better the effect of our model is. The maximum value is 1.

2.2 BP neural network prediction model construction

All the data of the 112 groups after the pretreatment were normalized with reference to the equation (3), and distributed between 0 and 1.

The normalized data is divided into the training group and the prediction group. The BP neural network is established by using the newff function in Matlab, and the predictable result of the newly established neural network model is normalized to obtain the final result. This paper uses a three-layer BP neural network structure of the input layer, the output layer and the hidden layer. After normalization, the three key parameters, in other words, temperature, nanoparticle mass fraction, the mixing ratio of different base liquids are used as the input layer, and the thermal conductivity is used as the output layer, so the number of neurons in the input layer and the output layer is 3, respectively, and 1. The choice of the number of hidden layer nodes is given by equation (4).
In the equations, \( m \): The number of nodes for the input layer. 
\( n \): The number of nodes for the output layer.

It can be known from equation (4) that the number of hidden layer nodes of the neural network is between 3 and 12. The new data is trained by using the newff function to build a BP neural network model. The BP neural network predictive model selects 70% of the data as training, 15% of which is used for verification, and the remaining 15% is used to test the accuracy of the predicted sample model.

2.3 Genetic algorithm optimization BP neural network

Genetic algorithm (GA)-a parallel random search optimization method that simulates the natural genetic mechanism and biological evolution theory. Based on the biological evolution principle of "survival of the fittest, survival of the fittest", the coding series is formed by optimizing parameters. The selected fitness function is used to screen individuals through selection, crossover and mutation in the inheritance, so that individuals with good fitness values are retained, individuals with poor fitness are eliminated, and new groups inherit the information of the previous generation. Superior to the previous generation, repeated cycles until the conditions are met. If the optimal initial weights and thresholds obtained by genetic algorithm optimization can be given to the BP neural network and training is started, BP can be improved. The flow chart of the prediction accuracy and stability of the neural network model is as follows.

The main optimization process is as follows:
Step 1: encode weights or thresholds and randomly generate connection weights or thresholds between a group of neurons.
Step 2: input the training sample, calculate its error, and define the sum of the absolute error as the fitness function.
Step 3: if the error is smaller, screen out the individuals with small sum of absolute error and directly pass them on to the next generation.
Step 4: evolve the current population and produce the next generation population through crossover, mutation and other operations.
Step 5: The initial weight or threshold of the BP neural network is continuously updated until the final condition is met, and the accuracy of the model is verified.
3. Results and Discussion

3.1 BP neural network model prediction results

The predicted sample data were substituted into the BP neural network prediction model, and the predicted absolute and relative thermal conductivity errors were calculated according to equations (3) and (4), and then the number of neurons in different hidden layers and different transfer functions were calculated. MSE and R², as shown in table 1, BP neural network prediction model has the best thermal conductivity when the hidden layer is 10 neurons and tansig transfer function. BP neural network predicted the thermal conductivity.

Table 1. BP neural network results for all data

| Candidate topology num | Number of hidden layers | Transfer Function | MSE      | R-square |
|------------------------|-------------------------|-------------------|----------|----------|
| 1                      | [3]                     | tansig            | 2.7720E-04 | 0.99763  |
| 2                      | [3]                     | logsig            | 4.3312E-04 | 0.99229  |
| 3                      | [4]                     | tansig            | 6.6516E-04 | 0.992806 |
| 4                      | [4]                     | logsig            | 3.0390E-03 | 0.98958  |
| 5                      | [5]                     | tansig            | 2.6150E-04 | 0.99775  |
| 6                      | [5]                     | logsig            | 8.3406E-04 | 0.99839  |
| 7                      | [6]                     | tansig            | 2.437E-03  | 0.99736  |
| 8                      | [6]                     | logsig            | 4.2303E-04 | 0.99832  |
| 9                      | [7]                     | tansig            | 3.5047E-04 | 0.99836  |
| 10                     | [7]                     | logsig            | 1.1381E-04 | 0.99887  |
| 11                     | [8]                     | tansig            | 1.4523E-04 | 0.99898  |
| 12                     | [8]                     | logsig            | 3.5191E-03 | 0.99899  |
| 13                     | [9]                     | tansig            | 7.8411E-04 | 0.99834  |
| 14                     | [9]                     | logsig            | 1.8542E-03 | 0.99716  |
| 15                     | [10]                    | tansig            | 8.9056E-04 | 0.99913  |
| 16                     | [10]                    | logsig            | 5.1475E-04 | 0.99793  |
| 17                     | [11]                    | tansig            | 4.0209E-03 | 0.99887  |
| 18                     | [11]                    | logsig            | 1.7804E-03 | 0.99841  |
| 19                     | [12]                    | tansig            | 3.9780E-04 | 0.99892  |
| 20                     | [12]                    | logsig            | 3.7639E-03 | 0.99663  |

Figure 4. BP neural network predicts the ratio of thermal conductivity data to experimental data.

Figure 5. BP neural network predicts thermal conductivity regression.
There were 160 sets of data, 112 of which were used for training data. Of the 112 data sets, 70% was used for training, 15% for validation, 15% for testing, the remaining 48 data sets were used for new data, and the original training neural network was used for testing to ensure the stability of the model and prevent overfitting phenomenon. It can be seen from Table 1 that the number of neurons under the hidden layer is 10, and the transfer function is an s-type function, and the prediction performance is the best. From Figure 4, it can be seen that when the experimental data and the predicted data are equal, the line with the slope of 1 is detected on the graph, when the predicted data is larger than the experimental data, it will be revealed above the line, Forecast data is less than experimental data and will be reflected below this line. It can be seen from Figure 5 that the BP neural network algorithm predicts the regression coefficient of the thermal conductivity coefficient as 0.99913.

3.2 Analysis of prediction results of BP neural network model optimized by genetic algorithm

In view of the disadvantage of BP neural network algorithm falling into local optimization when optimizing weights and thresholds, this study used the genetic algorithm to optimize the initial weights and thresholds of BP neural network, determined the optimal initial weights and thresholds, eliminated the randomness of BP neural network results, and improved the accuracy and stability of the model.

This study uses the genetic algorithms to perform 10 generations of evolution, with a crossover probability of 0.3 and a mutation probability of 0.1, to obtain the optimal individual fitness curve, as shown in Figure 6. It can be seen from the figure that the optimal individual fitness obtained is 1.3189, and the corresponding evolutionary algebra is 7, and the fitness does not change any more. Therefore, it can be determined that the optimal fitness of the individual has been reached at this time. The initial weights and thresholds obtained from the optimization results are given to the BP neural network for model training, and the prediction results of the multiple training are completely consistent.

As shown in Table 2, the BP neural network optimized by the genetic algorithm has different transfer functions and the number of neurons is also different. For comparison with BP neural network, the selected transfer function is S type (tansig) and the number of hidden layer neurons is 10. The prediction model (GA-BP) obtained by BP neural network optimized by genetic algorithm is used to predict the thermal conductivity, and the prediction results are compared with the experimental data, as shown in Figure 7. It can be seen from the figure that the overall trend of the BP neural network model optimized by genetic algorithm is in good agreement with the experimental data, and there is basically no predicted value with large deviations, and the maximum error limit is 2%.

As shown in Figure 8, the maximum error of the relative error is 4%. Therefore, whether from the accuracy of prediction results or the stability of prediction, the BP neural network prediction model optimized by genetic algorithm can play a good predictive effect.
Table 2. BP neural network optimized by genetic algorithm results for all data

| Candidate topology num | Number of hidden layers | Transfer Function | MSE       | R-square |
|------------------------|-------------------------|-------------------|-----------|----------|
| 1                      | [3]                     | tansig            | 2.7184E-04| 0.99861  |
| 2                      | [3]                     | logsig            | 4.0989E-05| 0.99745  |
| 3                      | [4]                     | tansig            | 9.4888E-05| 0.99889  |
| 4                      | [4]                     | logsig            | 3.8722E-04| 0.99815  |
| 5                      | [5]                     | tansig            | 1.1465E-04| 0.99864  |
| 6                      | [5]                     | logsig            | 2.7019E-04| 0.99796  |
| 7                      | [6]                     | tansig            | 6.5392E-04| 0.99902  |
| 8                      | [6]                     | logsig            | 3.1106E-04| 0.99865  |
| 9                      | [7]                     | tansig            | 1.4937E-04| 0.99927  |
| 10                     | [7]                     | logsig            | 1.7827E-04| 0.99849  |
| 11                     | [8]                     | tansig            | 6.8901E-05| 0.99917  |
| 12                     | [8]                     | logsig            | 7.7350E-04| 0.99894  |
| 13                     | [9]                     | tansig            | 2.2214E-04| 0.99927  |
| 14                     | [9]                     | logsig            | 8.1118E-05| 0.99859  |
| 15                     | [10]                    | tansig            | 4.1656E-05| 0.99947  |
| 16                     | [10]                    | logsig            | 6.4236E-05| 0.99798  |
| 17                     | [11]                    | tansig            | 4.3754E-04| 0.99941  |
| 18                     | [11]                    | logsig            | 5.9504E-04| 0.99863  |
| 19                     | [12]                    | tansig            | 5.5396E-04| 0.99919  |
| 20                     | [12]                    | logsig            | 2.3979E-04| 0.99877  |

4. Conclusions

Based on the experimental data in CuO-ZnO/(EG:DW) nanofluids with the same mass ratio (1:1), the CuO-ZnO mass fraction, temperature, and different base-liquid mixing ratios were used as input parameters, corresponding thermal conductivity is used as the output to apply the BP neural network optimized by genetic algorithm to construct the thermal conductivity prediction model. The results illustrate that the BP neural network optimized by genetic algorithm can establish a predictive model that can accurately predict the thermal conductivity, using 30% of the experimental data. Model
verification, the predicted thermal conductivity maximum error limit is 2%, MSE is 0.000041656, and R2 is 0.99947. Compared with the unoptimized BP neural network, the genetic algorithm can not only solve the BP problem, but also improve the prediction accuracy. The neural network randomly selects the problem that the prediction result caused by the initial weight and threshold is unstable, and it can also give BP neural network the accuracy of the model by parallel random search optimal initial weight and threshold.

5. Appendices

| Symbols | Units | meaning |
|---------|-------|---------|
| $R^2$   | 1     | Coefficient of determination |
| MSE     | 1     | Mean Square Error Normalized value |
| $X$     | 1     | Actual input value. |
| $X_{nor}$ | 1     | Normalized value. |
| $X_{max}$ | 1     | The maximum of the actual input value. |
| $X_{min}$ | 1     | The minimum of the actual input value. |
| $m$     | 1     | The number of nodes for the input layer. |
| $n$     | 1     | The number of nodes for the output layer. |
| $T_i$   | 1     | The actual value |
| $P_i$   | 1     | The value of the model |
| $\bar{T}$ | 1     | The average experimental value of n sets of test data. |
| $T$     | °C    | Temperature |
| $R$     | (W/(m·°C)) | ethylene glycol and deionized water at different mixing ratio |
| $W$     |       | The mass fraction |

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