

A novel nonlinear regression model of SVR as a substitute for ANN to predict conductivity of MWCNT-CuO/water hybrid nanofluid based on empirical data

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HIGHLIGHTS

- Propose a nonlinear regression model of Support Vector Regression (SVR).
- A substitution for ANN to predict the thermal conductivity.
- According to the empirical data of MWCNT-CuO/water hybrid nanofluid.

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ABSTRACT

An ideal regression method should have several characteristics including precision, accuracy and generalization. In many studies in the field of nanofluid, the precision of models is more highlighted. Nevertheless, a lack of generalization may lead to over fitted models. In this paper, two nonlinear regression methods, namely the ANN and SVR are employed to predict the thermal conductivity of MWCNT-CuO/water hybrid nanofluid with temperature and volume fraction. It is seen that precision of SVR & ANN approaches are able to be compared. However, SVR generalization is more convenient, compared to ANN because SVR method utilizes less parameters. Hence SVR can show better persistence to overfitting in little-size datasets compared to ANN. Therefore, SVR is more authentic approach for the regression with little-size datasets.

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1. Introduction

Several examples can be mentioned for the substances at nano scales level such as electronic devices, medicine, ventilation and MEMS. Metal or non-metal nanoparticles are usually added to the base fluids to produce a mixture called nanofluid. These mentioned nanoparticles must be dispersed through the base liquid in a suitable way to generate a homogeneous mixture. Higher amount of nanoparticles thermal conductivity leads to increase the mixture thermal conductivity which it can be estimated as the main reason of using nanofluid. This fact causes the significant increase in conduction heat transfer through the mixture; however the nanofluid convection heat transfer can be invigorated due to Brownian motions of nanoparticles. Better quality of producing the nanofluid in aspect of thermal conductivity, encourage

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Table 1
The input-target dataset, k ($\frac{W}{mK}$) [14].

| | $T(^{\circ}C)$ | | | | | | |
|------------|----------------|-------|-------|-------|-------|-------|-------|
| | 25 | 30 | 35 | 40 | 45 | 50 | |
| ϕ (%) | 0.05 | 0.655 | 0.662 | 0.670 | 0.684 | 0.696 | 0.707 |
| | 0.1 | 0.674 | 0.685 | 0.693 | 0.705 | 0.723 | 0.730 |
| | 0.15 | 0.689 | 0.701 | 0.710 | 0.723 | 0.737 | 0.751 |
| | 0.2 | 0.705 | 0.717 | 0.728 | 0.744 | 0.758 | 0.770 |
| | 0.4 | 0.736 | 0.748 | 0.763 | 0.780 | 0.799 | 0.809 |
| | 0.6 | 0.766 | 0.777 | 0.788 | 0.810 | 0.829 | 0.840 |

researchers to apply the hybrid nanoparticles. Less concentration of hybrid nanoparticles also leads to less cost beside more efficiency. Moreover various types of the base liquids can be examined which it depends on the working conditions. It should be mentioned that surfactant substances should be used as the hydrophilic factor for the some nanoparticles dispersed through the base liquid layers [1–15].

The working temperature of nanofluid beside the shape, diameter and volume fraction of nanoparticles can affect its behavior; as a regard the type of the base fluid should also be involved. However each one of these mentioned factors might have a significant influence on the mixture thermal and hydrodynamic properties such as viscosity, thermal conductivity and density. A large number of works can be addressed in this way [16–31].

As a result it is necessary to have a complete knowledge of a nanofluid thermo-physical properties especially for the new types. Thermal efficiency, pumping power and heat transfer rate are some examples for the nanofluid usage which usually are reported though the literature. Due to high cost of experimental studies concerned nanofluid, several works can be referred using the numerical approaches. Propose a correlation and then validation of its performance, are the favorite topics for the researchers in the field of nanofluids & composites [32–49].

The experimental studies encounter some difficulties which implies several specified points usually would be evaluated. Therefore the numerical optimization/interpolation approaches should be employed to present the fluid behavior at each desired condition. Commonly the “Artificial Neural Network” (ANN) method is used to estimate the thermo-physical conditions of nanofluid according to the experimental results [50–72].

It is well known that Artificial Neural Network (ANN) is the most famous regression approach because of its universal approximation capability. A multi-layer feed-forward artificial neural network with finite amount neurons in hidden-layer, can predict each relationship between the dependent and independent parameters of a desired variable. ANN involves several disadvantages as follows in addition of its appropriate performance:

- Select ANN structure and desired training algorithm would be empirical.
- Results would be affected significantly by the initial conditions.
- Much amount of model variables (weights and biases) would be necessary.
- Models of the resultant would not be same.
- Great value of dataset would be necessary to satisfy the training stage.
- Overfitting would happen simply and frequently which decreases model generalization.

Now the problem is to find a substitution approach for ANN with the higher capability and less disadvantages. Present work claims that SVR seems to have more suitable performance between too many developed machine learning approaches.

2. Problem definition: goal of the proposed model

In many studies in the field of nanofluid, the precision of models is more highlighted. Nevertheless, a lack of generalization may lead to overfitted models. In this paper, two nonlinear regression methods, namely the ANN and SVR are employed to predict the thermal conductivity of MWCNT-CuO/water hybrid nanofluid with temperature and volume fraction. Hence A new nonlinear regression model is proposed to predict the nanofluid thermal conductivity according to temperature and nanoparticles volume fraction.

Two independent variables of temperature & volume fraction of nanoparticles and one dependent variable of thermal conductivity $k(W/(mK))$ are included through the model. The input-goal has 36 samples shown in Table 1 at $T = 25, 30, 35, 40, 45, 50 (^{\circ}C)$ and $\phi = 0.5, 0.1, 0.15, 0.2, 0.4, 0.6$ (%) [14].

3. Numerical approach: SVR concept

SVM is a supervised learning approach for the classification and regression steps; in which input space is mapped through the feature domain and then it is resolved by the optimization method. SVM involves the powerful theoretical concepts and suitable generalization, accuracy and precision which works with nonlinear conditions [28]. The type of SVM called Support Vector Regression (SVR) was presented to estimate the function [29]. SVR implies the nice resistance on overfitting and good in little-size datasets beside the suitable generalization. As a result, it can be considered as the best approach to regression.

In the following parts, a short glance on SVR is provided at first; then SVR is applied to predict the present sample nanofluid thermal conductivity. At the end, the incomes of SVR and ANN are evaluated with one another.

Assume the training input-goal dataset of (x_i, y_i) for $i = 1, \dots, n$ while $x_i \in \mathfrak{R}^d$ & $y_i \in \mathfrak{R}$. A linear regression approach is presented as [30]:

$$y = \omega \cdot x + b \tag{1}$$

In which $\omega \in \mathfrak{R}^d$ & $b \in \mathfrak{R}$. The goal is to estimate the linear regression for the last equation with highest flatness and deviation ε from y_i at $i = 1, \dots, n$ which means,

$$\begin{aligned} \min: & \frac{1}{2} \|\omega\|^2 \\ \text{s.t.}: & \begin{cases} y_i - \omega \cdot x_i - b \leq \varepsilon \\ \omega \cdot x_i + b - y_i \leq \varepsilon \end{cases} \text{ for } i = 1, \dots, n \end{aligned} \tag{2}$$

In some cases, it may not practical to gain an answer for the previous optimization object. Hence precision condition of ε is able to be relaxed with the variables of ξ_i & ξ_i^* . It should be mentioned that variables must not be let to be increased in order to keep the precision,

$$\begin{aligned} \min: & \frac{1}{2} \|\omega\|^2 + \gamma \sum_{i=1}^n (\xi_i + \xi_i^*) \\ \text{s.t.}: & \begin{cases} y_i - \omega \cdot x_i - b \leq \varepsilon + \xi_i \\ \omega \cdot x_i + b - y_i \leq \varepsilon + \xi_i^* \\ \xi_i \geq 0 \\ \xi_i^* \geq 0 \end{cases} \text{ for } i = 1, \dots, n \end{aligned} \tag{3}$$

In which $\gamma > 0$ implies to agreement among the flatness and suitable deviations. Now the optimization approach is followed by presenting the Lagrange multipliers as $\alpha_i > 0, \alpha_i^* > 0, \eta_i > 0$ & $\eta_i^* > 0$:

Lagrangian:

$$\begin{aligned} L = & \frac{1}{2} \|\omega\|^2 + \gamma \sum_{i=1}^n (\xi_i + \xi_i^*) \\ & - \sum_{i=1}^n \alpha_i (\varepsilon + \xi_i - y_i + \omega \cdot x_i + b) - \sum_{i=1}^n \alpha_i^* (\varepsilon + \xi_i^* + y_i - \omega \cdot x_i - b) \\ & - \sum_{i=1}^n \eta_i \xi_i - \sum_{i=1}^n \eta_i^* \xi_i^* \end{aligned} \tag{4}$$

Partial deviations must be omitted from the Lagrangian, considering the parameters of ω, b, ξ_i & ξ_i^* ,

$$\begin{aligned} \frac{\partial L}{\partial \omega} &= \omega - \sum_{i=1}^n (\alpha_i^* - \alpha_i) x_i \\ \frac{\partial L}{\partial b} &= \sum_{i=1}^n (\alpha_i^* - \alpha_i) \\ \frac{\partial L}{\partial \xi_i} &= \gamma - \alpha_i - \eta_i \\ \frac{\partial L}{\partial \xi_i^*} &= \gamma - \alpha_i^* - \eta_i^* \end{aligned} \tag{5}$$

Eq. (6) is achieved for the optimization object by substitution of Eq. (5) in (4) [30],

$$\begin{aligned} \min: & -\frac{1}{2} \sum_{i,j=1}^n (\alpha_i - \alpha_i^*) (\alpha_j - \alpha_j^*) (x_i \cdot x_j) - \varepsilon \sum_{i=1}^n (\alpha_i + \alpha_i^*) + \sum_{i=1}^n y_i (\alpha_i - \alpha_i^*) \\ \text{s.t.}: & \begin{cases} \sum_{i=1}^n (\alpha_i - \alpha_i^*) = 0 \\ 0 \leq \alpha_i \leq \gamma \\ 0 \leq \alpha_i^* \leq \gamma \end{cases} \end{aligned} \tag{6}$$

Table 2
Error percentage of original experimental results versus those of SVR model for $k \left(\frac{W}{mK} \right)$.

| | | $T(^{\circ}C)$ | | | | | |
|------------|------|----------------|------|------|------|------|------|
| | | 25 | 30 | 35 | 40 | 45 | 50 |
| ϕ (%) | 0.05 | 0.01 | 0.08 | 0.14 | 0.20 | 0.05 | 0.09 |
| | 0.1 | 0.01 | 0.27 | 0.03 | 0.06 | 0.47 | 0.09 |
| | 0.15 | 0.20 | 0.00 | 0.26 | 0.33 | 0.43 | 0.00 |
| | 0.2 | 0.13 | 0.17 | 0.05 | 0.26 | 0.07 | 0.23 |
| | 0.4 | 0.07 | 0.07 | 0.05 | 0.05 | 0.05 | 0.14 |
| | 0.6 | 0.00 | 0.17 | 0.24 | 0.09 | 0.04 | 0.01 |

The variables corresponded to Eq. (1), are achieved from the last optimization equation,

$$\omega = \sum_{i=1}^n (\alpha_i - \alpha_i^*) x_i \quad (7)$$

$$b = \frac{1}{2} \{ \min (y_i - \omega \cdot x_i) + \max (y_i - \omega \cdot x_i) \}$$

Now it is assumed a nonlinear object, which means the input x is primary moved from the input domain to the feature domain by the function of $\phi(x)$. Then, input–output relationship is corresponded by the linear regression as follows:

$$y = \omega \cdot \phi(x) + b \quad (8)$$

By the same procedure, the next optimization expression is achieved:

$$\min: -\frac{1}{2} \sum_{i,j=1}^n (\alpha_i - \alpha_i^*) (\alpha_j - \alpha_j^*) K(x_i, x_j) - \varepsilon \sum_{i=1}^n (\alpha_i + \alpha_i^*) + \sum_{i=1}^n y_i (\alpha_i - \alpha_i^*) \quad (9)$$

$$\text{s.t.:} \begin{cases} \sum_{i=1}^n (\alpha_i - \alpha_i^*) = 0 \\ 0 \leq \alpha_i \leq \gamma \\ 0 \leq \alpha_i^* \leq \gamma \end{cases}$$

K represents the kernel function which must contains the specified characteristics. Various types of kernel functions can be found through the literature, however the Radial Basis Function (RBF) Kernel can be addressed as the suitable one among them,

$$K(x_i, x_j) = \exp\left(-\frac{\|x_i - x_j\|^2}{2\sigma^2}\right) \quad (10)$$

where σ^2 represents the kernel variable. A quadratic programming problem was shown in Eq. (9). The most famous approach to solve it, would be the Least Squares-Support Vector Machine (LS-SVM) among the various available methods. LS-SVM corresponds to the linear objects instead of quadratic ones. Moreover an optimization method of simplex can be employed for it which leads to achieve the variables of Eq. (8):

$$\omega = \sum_{i=1}^n (\alpha_i - \alpha_i^*) \phi(x_i) \quad (11)$$

$$b = \frac{1}{2} \{ \min (y_i - \omega \cdot \phi(x_i)) + \max (y_i - \omega \cdot \phi(x_i)) \}$$

4. Results

At first step, SVR is applied by the simplex optimization approach and using RBF kernel. The variables of σ^2 & γ are demonstrated using Coupled Simulated Annealing (CSA). Fig. 1 shows the present model obtained results for the input-target dataset. Moreover the regression of original experimental data versus proposed numerical model of SVR are illustrated in Fig. 2. The regression slope and bias are around one and zero respectively, which implies the model can closely trace the goal data through the trained objects. Table 2 involves the deviation percentage between the original experimental results and those of proposed model of SVR. It is observed that SVR shows the nice precision.

Second step is provided by the results from SVR in comparison with ANN composed of one hidden layer and an output layer. Hidden layer involves fifteen “tansig” neurons and output layer involves the linear neurons while Levenberg–Marquardt backpropagation algorithm is applied as the learning algorithm. Fig. 3 represents the regression of ANN and also the deviation between original experimental results versus those of ANN are presented in Table 3. It is seen that ANN involves the appropriate precision through the trained samples which implies that SVR & ANN precisions are comparable.

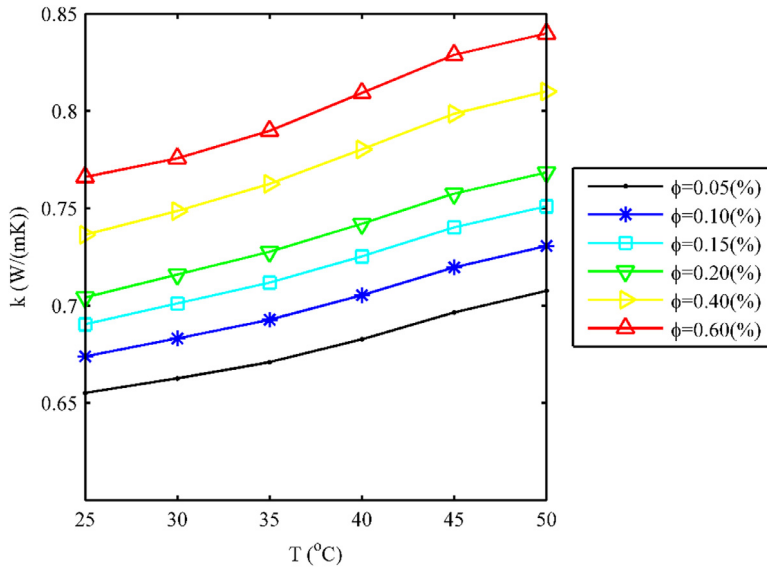


Fig. 1. Validation of SVR obtained data for input-target dataset.

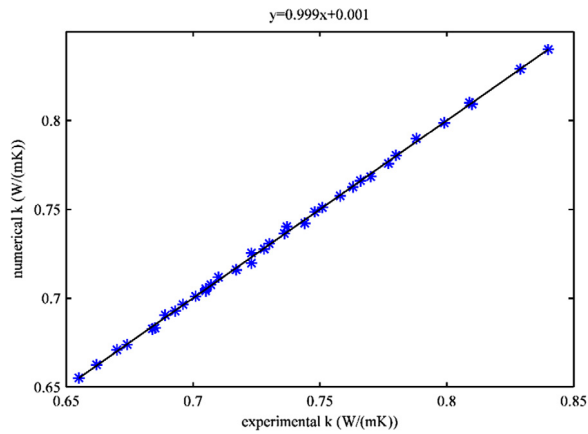


Fig. 2. Regression of original experimental results versus those of SVR numerical model.

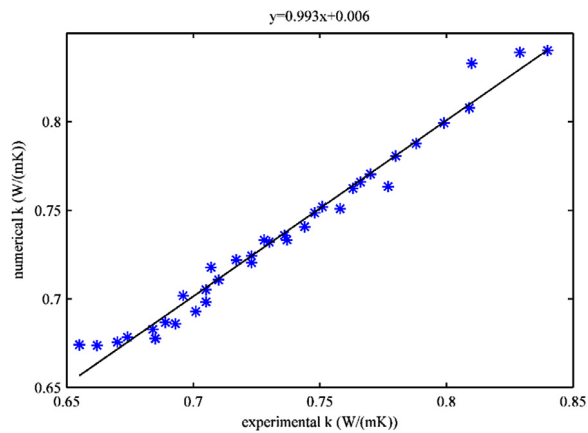
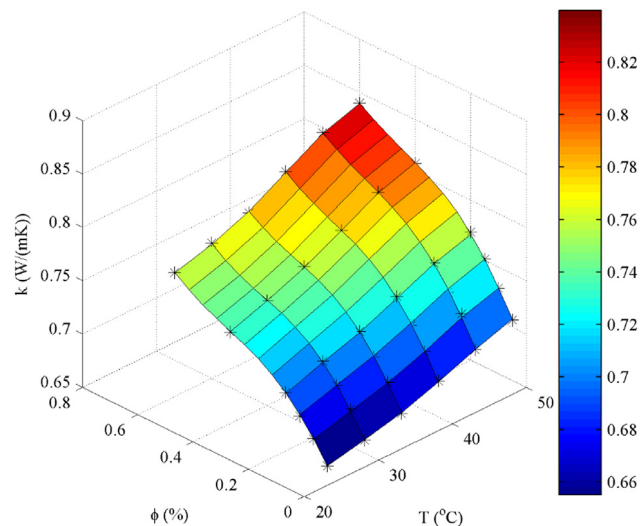
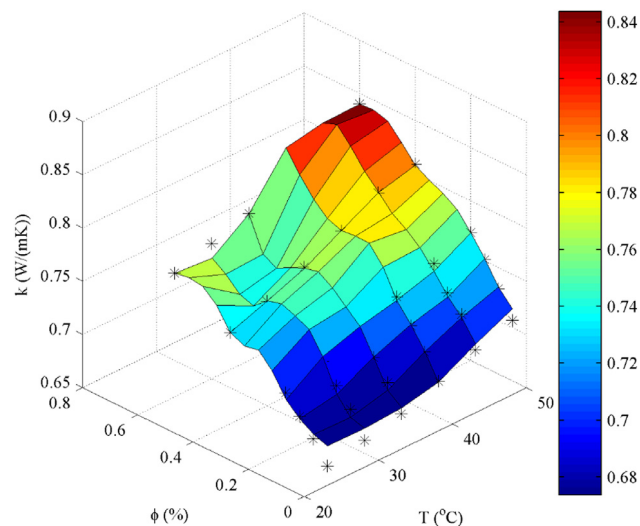


Fig. 3. Regression of original experimental results versus those of ANN numerical model.

Table 3Error percentage of original experimental results versus those of ANN model for k ($\frac{W}{mK}$).

| | | $T(^{\circ}C)$ | | | | | |
|------------|------|----------------|------|------|------|------|------|
| | | 25 | 30 | 35 | 40 | 45 | 50 |
| ϕ (%) | 0.05 | 2.83 | 1.74 | 0.83 | 0.18 | 0.82 | 1.50 |
| | 0.1 | 0.65 | 1.10 | 1.02 | 0.03 | 0.35 | 0.28 |
| | 0.15 | 0.33 | 1.17 | 0.10 | 0.17 | 0.51 | 0.13 |
| | 0.2 | 0.97 | 0.69 | 0.70 | 0.45 | 0.94 | 0.05 |
| | 0.4 | 0.03 | 0.08 | 0.09 | 0.07 | 0.04 | 0.16 |
| | 0.6 | 0.01 | 1.79 | 0.04 | 2.75 | 1.20 | 0.02 |

**Fig. 4.** Nanofluid thermal conductivity from SVR versus temperature and nanoparticles volume fraction (asterisks: input-target dataset).**Fig. 5.** Nanofluid thermal conductivity from ANN versus temperature and nanoparticles volume fraction (asterisks: input-target dataset).

At the end, trained SVR and ANN are applied to evaluate the non-trained inputs to examine the model generalization. The predicted thermal conductivity by SVR and ANN at various temperature and nanoparticles volume fraction are presented in Figs. 4 and 5. It is seen that SVR produces a smooth surface; however ANN makes a distorted one. ANN involves the generalization object due to surface distortion that would not physically sensible. This fact is because of the acquired ANN overfitting which is commonly happens in ANN with little-size training and much amount of variables. It should be

mentioned that it is possible for ANN to decrease the approach variables with no losing of accuracy. Hence, it is not easy to keep ANN precision and generalization with little-size datasets. It means SVR can present higher accurate outcomes because of using the less amounts of variables in LSR. Therefore SVR can be estimated as the better reliable approach for the regression schemes with little-size datasets.

5. Conclusion

In this paper, two nonlinear regression methods, namely the ANN and SVR were employed to predict the thermal conductivity of MWCNT-CuO/water hybrid nanofluid with temperature and volume fraction. Hence A new nonlinear regression model was proposed to predict the nanofluid thermal conductivity according to temperature and nanoparticles volume fraction.

It was seen that precision of SVR & ANN methods can be compared together. SVR generalization was more suitable than ANN because SVR approach used less parameters. Hence SVR could demonstrate further resistance to overfitting in small-size datasets compared with ANN. Hence, SVR was more reliable method for the regression of small-size datasets.

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