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Accurate model to predict the diameters of Single Wall Carbon Nanotubes by Using Support Vector Regression

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The support vector regression (SVR) combined with particle swarm optimization (PSO) for parameter optimization was successfully utilized to predict diameters of single wall carbon nanotubes based on nine synthesis process factors. The prediction results strongly support that the generalization ability of SVR model consistently surpasses that of multiple linear regression (MLR) and artificial neural network (ANN) by applying identical training and test samples. For SVR model, the mean absolute error (MAE) is 0.0379, the mean absolute percentage error (MAPE) is only 2.7486% and the correlation coefficient (R^2) is as high as 0.98. The results show that the estimated errors by SVR are all smaller than those achieved by MLR and ANN. This study has proved that the SVR is an effective and practical method to assist design experiments, and is helpful to control diameters of single wall carbon nanotubes via rational process parameters.

1. Introduction

The single wall carbon nanotubes (SWCNTS) with unique properties and potential applications have greatly attracted the interest of scientists since their discovery in 1993 [1]. SWCNTS can be applied in many fields of science and engineering [2-6]. All these widely applications depend on their diameters. How to synthesize SWCNTS of different diameters by adjusting experiment parameters is very difficult. And doing experiments is arduous, spending a lot of money and material resources, and that the effect of interaction between various parameters on diameters of SWCNTS cannot be considered at the same time. In general, the relationship between the process parameters and diameters is very complex and exhibits highly nonlinear. It is difficult to build an accurate theoretical method to predict the diameters of SWCNTS

via conventional regression approaches. Support vector regression (SVR) is an effective method to solve this problem.

Support vector machine (SVM) proposed by Vapnik and co-workers [7] in 1995, is a statistical machine learning approach based on structural risk minimization principle. SVM has been successfully applied to solve classification and regression problems in many areas [8-11]. When SVM was employed to solve the regression problems it is called SVR. In this study, the SVR combined with particle swarm optimization (PSO) for its parameter optimization, is proposed to quantitatively model and predict the diameters of SWCNTS for identical training and test samples, and the predictive errors of SVR were also compared with those of MLR and ANN.

2. Methods and Materials

2.1 Theory of support vector regression

The main idea of SVR is to map the input vector $\boldsymbol{x}$ into a high dimensional feature space $\boldsymbol{F}$ via a nonlinear mapping function $\Phi(x)$, and then to conduct a liner regression in $\boldsymbol{F}$ space. The final regression function of SVR is as follows:

$$f(\boldsymbol{x}) = \sum_{i=1}^{l} (\alpha_i - \alpha_i^*) k(\boldsymbol{x}, \boldsymbol{x}_i) + b, \qquad (1)$$

Where l is the number of support vector, α_i and α_i^* are Lagrange multipliers, $k(\boldsymbol{x}, \boldsymbol{x}_i) = \Phi(\boldsymbol{x}) \cdot \Phi(\boldsymbol{x}_i)$ is a kernel function, b is a bias. In this paper, radial basis kernel was adopted as the kernel function, and it is formulated as equation 2. The detailed principle of SVR can be referred to reference [7,12].

$$k(\boldsymbol{x}, \boldsymbol{x}_i) = \exp(-\gamma \| \boldsymbol{x} - \boldsymbol{x}_i \|^2) \qquad (2)$$

2.2 Choosing of SVR parameters with PSO

The PSO method, proposed by Kennedy and Eberhart in 1995 [13-14], was utilized to search for the optimal parameters (ε, C, γ) for SVR. In this study, root mean square error (REMS), which directly

influences the regression performance of SVR, is chosen as the fitness function:

$$RMSE = \sqrt{\frac{1}{n}\sum_{i=1}^{n}(\hat{y}_i - y_i)^2}, \quad (3)$$

Where n is the number of training samples, $\hat{y}_i$ represents estimated value for the ith training sample and y_i stands for the ith actual measured value.

2.3 Data set and Modeling

The data set consist of 44 samples splitting into training set of 34 and test set of 10 was selected form reference [20]. The results was list in the following table 1. In this modeling process, buffer gas pressure (P), discharge current (I), Ni concentration (Ni), Y concentration (Y), Fe concentration (Fe), ratio of Ho gas (Ho), ratio of He gas (He), ratio of H_2 gas ($H_{2)}$ and ratio of N_2 gas (N_2) act as nine input variables, while the diameter of SWCNT is as the output variable. For comparison with the previous work in reference [20], the modeling and prediction were conducted by using the 44 samples based on SVR for the identical training and test sets.

Table1. Measured diameters about different samples.

No.	P	I	Ni	Y	Fe	Ho	He	H2	N2	D
1	500	100	0.3	0.3	0	0	1	0	0	1.25
2	500	40	1.0	1.0	0	0	1	0	0	1.30
3	700	40	1.5	1.5	0	0	1	0	0	1.13
4	500	80	2.5	0	0	0	1	0	0	1.30
5	100	70	2.5	0	2.5	0	1	0	0	1.27
6	300	60	2.5	0	2.5	0	1	0	0	1.27
7	500	60	2.5	0	2.5	0	1	0	0	1.27
8	200	100	4.2	0	1	0	1	0	0	1.24
9	600	70	0	0	0	0	1	0	0	1.28
10	50	70	0	0	0	0	1	0	0	1.00
11	500	90	1.0	0.25	0	0	1	0	0	1.52
12	500	90	3.0	0.75	0	0	1	0	0	1.52

13	500	90	4.0	1.0	0	0	1	0	0	1.52
14	500	90	6.0	1.5	0	0	1	0	0	1.52
15	600	90	1.0	0	0	1	1	0	0	1.49
16	600	90	2.0	0	0	1	1	0	0	1.50
17	600	90	3.0	0	0	1	1	0	0	1.49
18	600	90	4.0	0	0	1	1	0	0	1.49
19	600	90	5.0	0	0	1	1	0	0	1.51
20	600	90	2.0	0	0	0.5	1	0	0	1.49
21	600	90	2.0	0	0	1	1	0	0	1.50
22	600	90	2.0	0	0	2	1	0	0	1.50
23	600	90	2.0	0	0	3	1	0	0	1.48
24	600	90	2.0	0	0	4	1	0	0	1.49
25	200	50	0	0	1	0	0	3	2	1.10
26	200	50	0	0	1	0	0	1	1	1.01
27	200	50	0	0	1	0	0	2	3	1.01
28	200	50	0	0	1	0	0	3	7	1.06
29	200	50	0	0	1	0	0	3	2	1.10
30	200	90	4.2	1.0	0	0	0	0	0	1.54
31	200	60	0	0	1	0	0	2	0	1.65
32	199.5	10	0	0	1	0	0	2	0	0.80
33	199.5	25	0	0	1	0	0	2	0	1.10
34	199.5	55	0	0	1	0	0	2	0	0.90
35	200	50	0	0	1	0	0	0.4	0.6	1.01
36	200	50	0	0	1	0	0	0.3	0.7	1.06
37	200	90	4.2	1	0	0	0	0	0	1.54
38	200	60	0	0	1	0	0	0.4	0	1.65
39	200	10	0	0	1	0	0	0.4	0	0.80
40	200	25	0	0	1	0	0	0.4	0	1.10
41	200	55	0	0	1	0	0	0.4	0	0.90

42	660	100	40	1.0	0	0	1	0	0	1.60
43	500	100	4.2	1.0	0	0	1	0	0	1.30
44	600	30	4.0	1.0	0	0	1	0	0	1.86

2.5 Evaluation of Model's Generalization Performance

Three parameters, *i.e.*, the mean absolute error (MAE), mean absolute percentage error (MAPE) and correlation coefficient (R^2), were adopted for generalization performance evaluation:

$$MAE = \frac{1}{m}\sum_{j=1}^{m}\left|\hat{y}_j - y_j\right|, \tag{4}$$

$$MAPE = \frac{1}{m}\sum_{j=1}^{m}\left|\frac{\hat{y}_j - y_j}{y_j}\right|, \tag{5}$$

$$R^2 = \frac{\left[\sum_{j=1}^{m}(y_j - \bar{y})(\hat{y}_j - \bar{\hat{y}})\right]^2}{\sum_{j=1}^{m}(y_j - \bar{y})^2 \sum_{j=1}^{m}(\hat{y}_j - \bar{\hat{y}})^2}, \tag{6}$$

Where m means the number of test samples, y_j is the jth target value, $\hat{y}_j$ stands for predicted value for the jth test sample and $\bar{y}$ is the mean target value for all test samples.

3. Results and discussions

Table 2 gives a comparison between the experimental diameters and estimated values predicted by MLR, ANN and SVR. From Table 2, it can be observed that, the prediction results of all samples estimated by SVR are closer to experimental values than those achieved by MLR and ANN in the case of using the same test samples. The absolute percentage errors of solubility predicted by SVR model are all smaller than those calculated by MLR and ANN model. The maximum absolute percentage error does not exceed 7.80% while the others are within the range of 0~2.69% calculated by SVR. However, for MLR model, the maximum absolute percentage error is -38.73% and there are 70% samples with absolute percentage errors exceeding 3%. For ANN model, the maximum absolute percentage error is -41.68% and there are 90% samples with absolute percentage errors exceeding 3%. These results reveal that the SVR model is a more effective and powerful tool for predicting the diameters than MLR and ANN model, and also suggests that modeling ability of SVR is superior to that of MLR and ANN model.

Table 2. Comparison of experimental values and calculated results by using MLR, ANN and SVR models.

No.	Exp.	Diameter (nm)					
		MLR	Error(%)	ANN	Error(%)	SVR	Error(%)
1	1.01	1.038	2.77	1.136318	12.51	1.037209	2.69
2	1.06	1.0215	-3.63	1.13468	7.05	1.081159	2.00
3	1.54	1.546	0.39	1.526322	-0.89	1.538625	-0.09
4	1.65	1.2569	-23.82	1.229979	-25.46	1.532844	-7.10
5	0.80	0.9304	16.30	1.133407	41.68	0.798069	-0.24
6	1.10	1.02835	-6.51	1.153161	4.83	1.099191	-0.07
7	0.90	1.22425	36.03	1.215165	35.02	0.970210	7.80
8	1.60	1.62876	1.80	1.540107	-3.74	1.600069	0.00
9	1.30	1.5486	19.12	1.536623	18.20	1.298916	-0.08
10	1.86	1.1396	-38.73	1.448118	-22.14	1.722320	-7.40

Table 3 lists the statistical results about MAE, MAPE, RMSE and R^2 for MLR, ANN and SVR models. Table 3 indicates that for the test errors, the MAE (0.0379), MAPE (2.7486%) and RMSE (0.0623) of the SVR model are more smaller than those calculated via MLR (0.1990, 14.9111%, 0.2942) and ANN (0.2045, 17.1512%, 0.2531) model respectively. The correlation coefficients (0.98) achieved by SVR is also more bigger than those calculated by MLR (0.30) and ANN (0.43) models. It shows once again that the regression performance of SVR model is superior to that of MLR and ANN model.

Table 3. Comparison of prediction performances of MLR, ANN and SVR models.

Regression method	RMSE	MAE	MAPE%	R^2
MLR	0.2942	0.1990	14.9111	0.30
ANN	0.2531	0.2045	17.1512	0.43
SVR	0.0623	0.0379	2.7486	0.98

Figure 1 present the pairwise comparison between experimental results and predicted results estimated by MLR, ANN and SVR models. From figure 1, one can see that the vast majority of points estimated by SVR lie on or very close to the best-line. But majority of points estimated by MLR and ANN scatter at both sides of the best-fit line for the test sets.

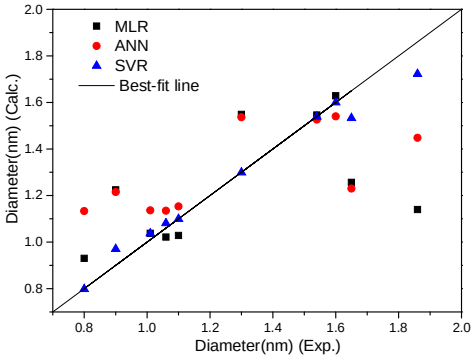

Figure 1. Comparison of experimental values vs. calculated values predicted by MLR, ANN and SVR models for the test sets.

Figure 2 depict the percentage errors distribution of diameters calculated by MLR, ANN and SVR models. From figure 2, it can be seen that the calculated percentage errors of diameters predicted by SVR are all smaller than MLR and ANN. About 70% of the samples the percentage errors predicted by SVR are not exceeding 3%, while there are 70% samples for MLR and 90% samples for ANN exceeding 3%. These demonstrate that the predicted values of SVR are in good agreement with the experimental values, and also illustrates that the constructed SVR model possess good generalization ability.

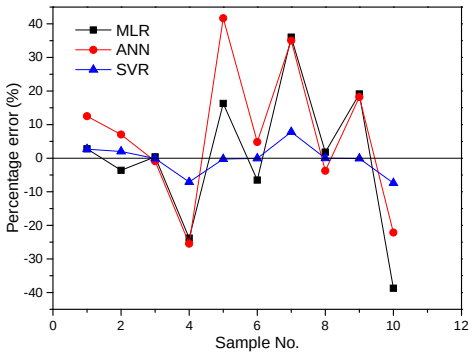

Figure 2. Plot of the percentage errors distribution of diameters calculated by MLR, ANN and SVR models for the test sets.

Figure 3 is the statistical analysis of the differences between the experimental and calculated values via the established SVR model against the experimental values. Let $e = r_p - r$ be the difference between the experimental value and the predicted value. Where r_p stands for the predicted value, r is the

experimental value. Figure 3 shows the graph of the difference between the actual data and the calculated data by SVR model against the actual value. The degree of agreement between the two values can be evaluated by the mean difference $\bar{e}$ and the standard deviation of the difference $\delta_{\bar{e}}$. For the test set, the mean difference $\bar{e} = -0.01414$ and the standard deviation $\delta_{\bar{e}} = 0.06395$. One would expect that most of the differences lie between $\bar{e} - 2\delta_{\bar{e}}$ and $\bar{e} + 2\delta_{\bar{e}}$. The lower limit of agreement is $\bar{e} - 2\delta_{\bar{e}} = -0.14204$, and the upper limit of agreement is $\bar{e} + 2\delta_{\bar{e}} = 0.11376$. From figure 3 it can be seen that all of the differences for the test sets lie within the limit scope between ($\bar{e} - 2\delta_{\bar{e}}$) and ($\bar{e} + 2\delta_{\bar{e}}$). This illustrates a good agreement between the experimental data and the estimated value via the established SVR model.

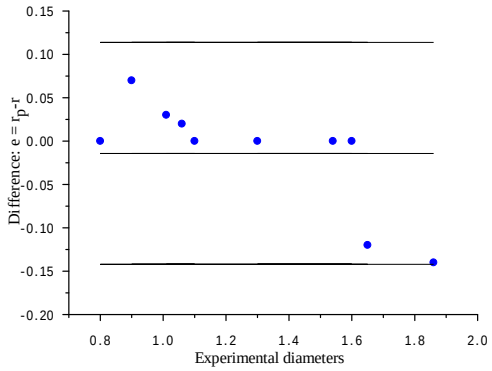

Figure 3. Differences between the experimental value and predicted value via SVR against the experimental value for the test sets.

Overall, the results above illustrate that the constructed SVR model possesses excellent performance which has the merits of fast-learning and excellent generalization ability for small size sample to solve nonlinear regression issues. The SVR is an effective and powerful technique for forecasting the diameters of SWCNTS.

4. Conclusions

In this paper, the model for predicting the diameters of SWCNTS under nine different parameters was built by using SVR combined with PSO, and the prediction results are compared with those of MLR and ANN model. The predicted errors of SVR are all smaller than those of MLR and ANN for the identical

samples. The prediction results show that the correlation between the diameters of SWCNTS and the nine different parameters is nonlinear. The SVR model is more attractive and more competitive than MLR and ANN model because the predicted values of SVR are consistent quite well with the experimental values. These indicate that SVR has a theoretical significance and potential application in predicting the diameters of SWCNTS and guiding the experiments.

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