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Development of a method for comprehensive water quality forecasting and its application in Miyun reservoir of Beijing, China

*Lei Zhang, Zhihong Zou, Wei Shan**

School of Economics and Management, Beihang University, Beijing 100191, China. Email: windyhot@126.com

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A B S T R A C T

Water quality forecasting is an essential part of water resource management. Spatiotemporal variations of water quality and their inherent constraints make it very complex. This study explored a data-based method for short-term water quality forecasting. Prediction of water quality indicators including dissolved oxygen, chemical oxygen demand by $KMnO_4$ and ammonia nitrogen using support vector machine was taken as inputs of the particle swarm algorithm based optimal wavelet neural network to forecast the whole status index of water quality. Gubeikou monitoring section of Miyun reservoir in Beijing, China was taken as the study case to examine effectiveness of this approach. The experiment results also revealed that the proposed model has advantages of stability and time reduction in comparison with other data-driven models including traditional BP neural network model, wavelet neural network model and Gradient Boosting Decision Tree model. It can be used as an effective approach to perform short-term comprehensive water quality prediction.

Introduction

In recent years, natural water bodies suffered varying degrees of pollution. Hence the surface water quality has always been a research hotspot in environmental science. Accurate and effective prediction of water quality is critical to better understand aqueous ecosystems. A variety of methods have been applied in this field (Li, 2006; Zou et al., 2008; Zhu et al., 2007; Bahaa et al., 2012; Kim and Seo, 2015; Deng et al., 2014, 2015). Most researches focused on the prediction of a certain single water quality indicator, few on the whole status. Because of the wide range of physical, chemical, biological factors influencing water quality, the traditional prediction method based on linear relationships is not sufficient for this problem. Several nonlinear mapping methods were used including the weighted Markov chain (Qiu et al., 2007), logistic regression (Zou et al., 2008), genetic algorithm based optimal Back Propagation (BP) neural network (Ding et al., 2014). Zhou (2012) studied water quality attribute data and graphic data and developed water quality prediction system using data management and topology relationship analysis function of the Java platform. Yan and Yang (2015) used the fuzzy comprehensive evaluation and analytic hierarchy process for water quality assessment and proposed the regression model of the inflow and water quality fuzzy comprehensive evaluation index. Forecasting of water quality status remains challenging. Further explorations are needed in order to find suitable methods and increase prediction accuracy.

Wavelet neural network (WNN) combined time-frequency localization character of wavelet transfer and self-study capacity of neural network. With strong approximation ability and fault tolerance, it has been a research hotspot for the last decades and

* *Corresponding author*. E-mail: shanwei@buaa.edu.cn (Wei Shan).

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widely applied in forecast filed such as mid-long-term power load forecasting (He et al., 2012), air temperature prediction (Wang and Gou, 2015) and seawater quality parameter prediction (Mohamad and Mohamad, 2015). Particle swarm optimization (PSO) is a computational method that optimizes a problem by iteratively trying to improve a candidate solution with regard to a given measure of quality. Zhang et al. (2014) proposed a conjunction method of wavelet transform-PSO-support vector machine for stream flow forecasting. Application of PSO based optimal WNN model in power transformer fault diagnosis (Cheng et al., 2014) and parameter optimization in twist spring back process for high-strength sheets (Xie et al., 2015) proved that the PSO algorithm can accelerate the training speed of WNN and improve the accuracy of training. In the comparison made by Azimirad et al. (2015) among three classifiers (PSO based optimal WNN, Artificial Immune System (AIS) based optimal WNN and Genetic Algorithm based optimal WNN), the PSO based optimal WNN results in the best classification accuracy.

In this study, the PSO based optimal WNN model was proposed for comprehensive water quality forecasting. First, water quality indicators including dissolved oxygen (DO), chemical oxygen demand by $KMnO_4$ (COD_{Mn}) and ammonia nitrogen (NH_3-N) were predicted with support vector machine (SVM). Then the PSO based optimal WNN model was adopted to predict the whole status index of water quality. To test the forecasting performance, application of the optimized model was performed to predict water grades of the Gubeikou monitoring section, Miyun reservoir in Beijing, China.

1. Methodology

1.1. *Support vector machine*

SVM was first put forward by Vapnik in 1995. It is theoretically based on statistical learning theory, namely approximate implementation of structure risk minimization (Zhang, 2000). It has been commonly used in the pattern recognition and nonlinear regression. SVM has good generality, robustness, effectiveness and simple computation, which gives it great advantage in solving problems of finite sample, nonlinear, over-fitting and pattern recognition with high dimension (Zhang, 2000).

River water quality system is dynamic non-equilibrium composite system with openness, complexity and nonlinearity (Xu et al., 2003). Time series of a certain single factor are seemingly irregular and random, which reduce the likelihood of long-term forecasting. However, inherent regularity of the system makes short-term prediction for the time series feasible. Procedures of regression prediction with SVM are as shown in Fig. 1.

1.2. *The PSO algorithm*

The PSO algorithm solves optimization problems by simulating the birds' predation. In PSO, the population is referred to as a swarm and each individual in the swarm is called a particle. A particle represents a potential optimal solution of the optimization problem. It was characterized by its location, velocity and the fitness value. The fitness value is decided by the objective function of the optimization problem. The optimal or approximately optimal solution can be found from iteration to iteration. Each particle is iteratively updated by its own best fitness value and the best fitness value of the entire swarm so far. Suppose there are n particles in D-dimension space. The position of a particle can be described as $X = (X_1, X_2, \ldots, X_D$. The velocity for the ith particle can be denoted as $V = [V_{i1}, V_{i2},\ldots,V_{iD}]$. The best position so far for the ith particle is represented as $P_i = [P_{i1}, P_{i2}, \ldots, P_{iD}]^T$. The best position so far for the entire swarm can be described as $P_g = [P_{g1}, P_{g2}, \ldots, P_{gD}]^T$. In each iteration, particles change its position and velocity according to the following equations:

$$V_{id}^{k+1} = \omega V_{id}^{k} + c_1 r_1 \left(P_{id}^{k} - X_{id}^{k}\right) + c_2 r_2 \left(P_{gd}^{k} - X_{id}^{k}\right) \quad (1)$$

$$X_{id}^{k+1} = X_{id}^{k} + V_{id}^{k+1} \quad (2)$$

where, ω is the inertia weight; $d = 1, 2, \ldots, D$; $i = 1, 2, \ldots, n$; k is the current generation;c_1 and c_2 are nonnegative constants, controlling the maximum step size; r_1 and r_2 are random numbers in [0,1]. The velocities and positions are normally limited in $[-X_{max}, X_{max}]$ and $[-V_{max}, V_{max}]$ respectively in case of the particles' blind search.

1.3. *Wavelet neural network*

A typical WNN model consists of three layers: input, output and hidden layer. It takes the topology structure of BP neural network as foundation and the wavelet function as the transfer function of the hidden layers. WNN with strong nonlinearity mapping capacity organically combined wavelet analysis and neural network. The wavelet neural network realization process is as followed (Chen et al., 1999):

Set the note number in the input layer, hidden layer and output layer m, n, N respectively. The WNN model can be expressed by the following formulas.

$$y_i(t) = \sum_{j=0}^{n} w_{ij}\, \Psi_{(a,b)} \left(\sum_{j=0}^{n} w_{jk}\, x_{(k)}(t) \right), i = 1, 2, \ldots, N \quad (3)$$

$$E = \frac{1}{2} \sum_{i=i}^{N} \left(y_i(t) - d_{(i)}\right)^2 \quad (4)$$

where, x_k is the input vector; y_i is the predicted output vector; w_{ij} is the connection weight form the ith node of the output layer to the jth node of the hidden layer; w_{jk} is the connection weight from the jth node of the hidden layer to the kth node of the output layer; $\Psi_{(a,b)}$ is the activation function of the hidden layer; a_j, b_j are the expansion parameter and the translation parameter of the wavelet function separately; d_i is the desired output vector; and E is the error function.

The wavelet neural network adopts the gradient descent algorithm to correct the connection weight, thus minimize the network error. The parameters are changed using Eq. (5).

$$w_{jk}(t+1) = -\eta \frac{\partial E}{\partial w_{jk}} + w_{jk}(t) \quad (5)$$

where, η is the learning rate. w_{ij}, a_j, b_j can be adjusted in the same way. When the maximum number of iterations is exceeded or the targeted error is less than the predetermined threshold, the WNN training is stopped; otherwise, the WNN training should be continued (Li et al., 2015).

1.4. PSO based optimal WNN model

Compared with BP neural network and Radial basis function (RBF) neural network, WNN is faster in convergence and has more effective function approximation ability. However, as it also takes the gradient descent method, the premature convergence problem and local optimal problem are hardly evitable for it. Therefore the PSO algorithm is introduced to tackle the parameter optimization problem of WNN. It can avoid the requirement of differentiability and derivability for excitation function and the process of derivation of the function. It has shown excellent performance in optimization and overcome the drawbacks of falling in to local extremes. The procedures of PSO optimizing WNN can be concluded as follows:

Steps 1: Set up a WNN model with the structure of N–M–L, where N, M, and L represent the node number of the input layer, the hidden layer and the output layer respectively. Map the parameters of the WNN model to the location of particles in the PSO algorithm, therefore the dimension of particles can be calculated using Eq. (6).

$$D = (N+1) * M + (L+1) * M \tag{6}$$

Step 2: Initialize particles with a randomized velocity and position.
Step 3: Input the training sample data to the WNN model, calculate E according to Eq. (4) and set it as the fitness value of particles. The best position so far for the particle until the current iteration is represent as Pbest. The best position so far for the entire swarm until the current iteration is denoted as Gbest.
Step 4: Update the velocity and position for each particle according to Eqs. (1)–(2).
Step 5: If the stopping iteration condition is met, output Gbest as parameters of the WNN model; if not, loop to step 3.

2. Development of the method

2.1. Frame of the method

The comprehensive water quality forecasting model based on SVM and optimized WNN using PSO is described in Fig. 2.

As illustrated in Fig. 2, the selected water quality indicators are firstly predicted with SVM separately. The WNN model is improved with PSO and trained with sample data generated by the random number generator. The predictions of water quality indicators are used as the inputs of the WNN model to forecast the whole status index of water quality in the next period.

2.2. Selection of water quality indicators

Water quality covers a wide range of physical, chemical, and biological indicators such as DO, temperature, electrical conductivity, salinity, turbidity, alkalinity, ammonia, total dissolved solids, nitrate, sulfate and phosphate (Mohamad and Mohamad, 2015). According to the availability to the monitoring data and Standard GB 3838-2002, this paper selected DO, COD_{Mn} and NH_3-N as single factor indexes.

2.3. Sample data analysis

According to Standard GB 3838-2002, water quality is divided into six classes, namely I, II, III, IV, V and V minus. According to monitoring data from the Ministry of Environmental

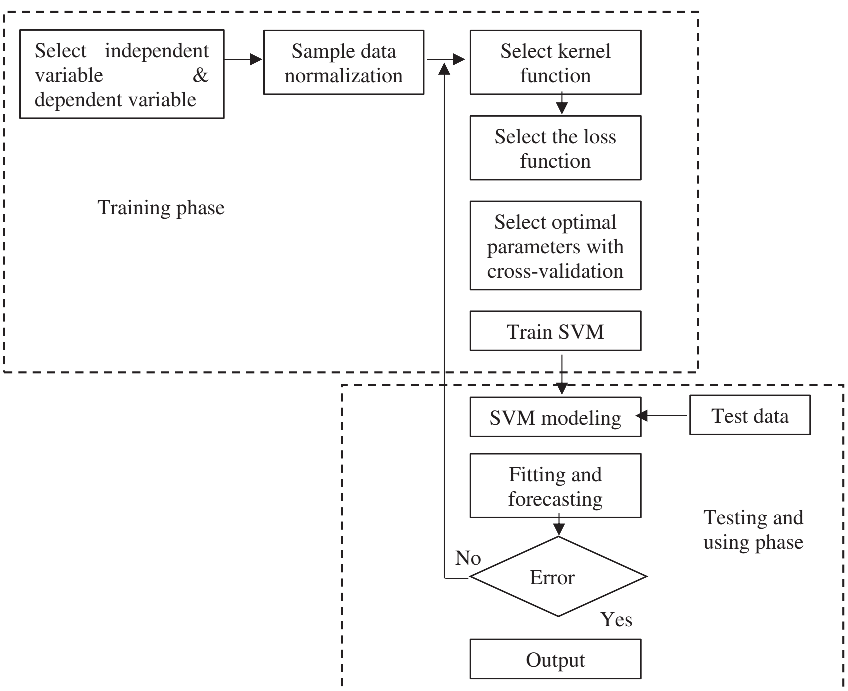

Fig. 1 – Diagram for regression prediction algorithm process with SVM. SVM: support vector machine.

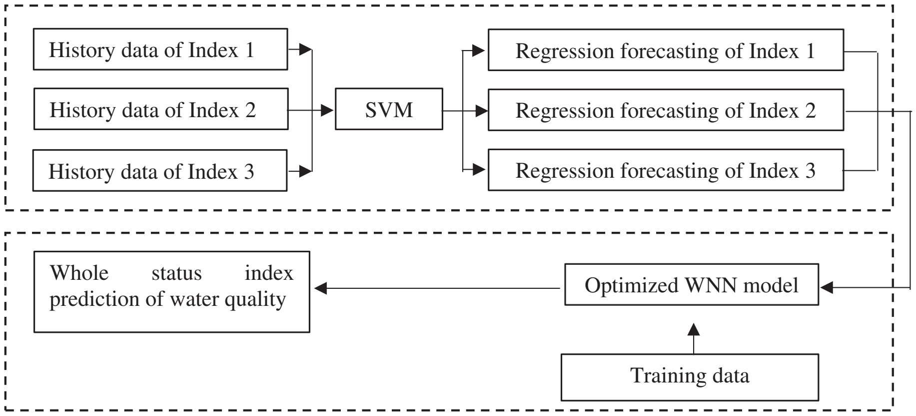

Fig. 2 – Schematic of the comprehensive water quality forecasting model.

Protection, over 90% of 145 water quality automatic monitoring section in China's main water systems belong to Classes I–IV. Hence Classes V and V minus are not taken under consideration in this study.

A large number of sample data are required to ensure the accuracy of neural network training. In order to get enough samples, values of chosen single factor indexes generated by the random number generator according to Standard GB 3838-2002 are taken as inputs when training the optimized WNN. According to the attribution of every indicator, the whole status index is proposed as output of the model. It can be calculated according to the following equations:

$$A = \frac{COD_{Mn} * NH_3\text{–}N}{DO} \tag{7}$$

$$W = (A_{normalized} + i\text{–}1) * 0.25 \tag{8}$$

where, DO, COD_{Mn}, and NH_3-N (in mg/L) are values of the indicators respectively; and *i* is water quality class. According to the attribution of each indicator, these indicators can be divided into two types: efficiency type and cost type. Efficiency type means it is best when the indicator value is the biggest; cost type means it is best when the value is the smallest. DO is efficiency type, and the other two indicators are cost type. Therefore, normalized value of *A* was brought to corresponding location in [0,1] with Eq. (8). Range of inputs and outputs are shown in Table 1. 5000 groups of data were generated using the random number generator, including 4900 groups as training samples and 100 groups as testing samples. Inputs are also needed to be normalized for better training effect.

Table 1 – Range of samples for the optimized WNN model.

Single factor index	Water quality class			
	I	II	III	IV
DO (mg/L)	7.5–12	6–7.5	5–6	3–5
COD_{Mn} (mg/L)	0–2	2–4	4–6	6–10
NH_3-N (mg/L)	0.05–0.15	0.15–0.5	0.5–1	1–1.5
W	0–0.25	0.25–0.5	0.5–0.75	0.75–1

WNN: Wavelet neural network; DO: dissolved oxygen; COD: chemical oxygen demand; NH_3-N: ammonia nitrogen.

2.4. Model evaluation criterion

Root-mean-square error (RMSE), mean absolute error (MAE) and error rate of water quality prediction are chosen as criterion to evaluate the effectiveness and forecast the performance of the model. RMSE is very sensitive to the maximum and minimum error, which enables it effectively reflect the accuracy of the prediction results. Since the deviation is absolute in MAE, it can preferably reflect the actual situation of prediction error (Zhang, 2000). The indexes are defined as follows:

$$RMSE = \sqrt{\frac{1}{n}\sum_{1}^{n}\left(W_{i(predicted)} - W_{i(calculated)}\right)^2} \tag{9}$$

$$MAE = \frac{1}{n}\sum_{1}^{n}\left|W_{i(predicted)} - W_{i(calculated)}\right| \tag{10}$$

$$\text{Error rate} = \frac{\text{Error count}}{n} \tag{11}$$

where *n* is the forecasting times.

3. Water quality prediction of Miyun reservoir inlet

3.1. Prediction object and data source

Miyun reservoir is located at the downstream of Chaohe River which originated in Hebei Province. Miyun reservoir serves as Beijing's largest source of drinking water, with a catchment area of 188 km^2 and a storage capacity of 4×10^9 m^3. Chaohe River is of great importance for Miyun reservoir, accounting for about 60% of its water inflow. Therefore, water quality of the Miyun reservoir inlet (Gubeikou monitoring section) was chosen as the research target. The data of Miyun reservoir inlet for 104 weeks from January 2014 to December 2015 were selected as sample data, week 1 to week 94 for in-sample simulation and week 95 to week 104 for out-of-sample

Table 2 – Characteristics of the experiments and prediction results.

No.	Input	Output	Data size	RMSE	MAE
1	DO(t − 1), DO(t − 2), DO(t − 3)	DO(t)	91	1.2256	0.2346
2	DO(t − 1), DO(t − 2), DO(t − 3)	DO(t)	41	1.1511	0.3162
3	$COD_{Mn}(t-1)$, $COD_{Mn}(t-2)$, $COD_{Mn}(t-3)$	$COD_{Mn}(t)$	91	0.1998	0.2001
4	$COD_{Mn}(t-1)$, $COD_{Mn}(t-2)$, $COD_{Mn}(t-3)$	$COD_{Mn}(t)$	41	0.2227	0.2228
5	NH_3-N(t − 1), NH_3-N(t − 2), NH_3-N(t − 3)	NH_3-N(t)	91	0.0452	0.0551
6	NH_3-N(t − 1), NH_3-N(t − 2), NH_3-N(t − 3)	NH_3-N(t)	41	0.0372	0.0370
7	DO(t − 1),DO(t − 2),DO(t − 3),DO(t − 4)	DO(t)	90	1.3125	0.6348
8	DO(t − 1),DO(t − 2),DO(t − 3),DO(t − 4)	DO(t)	40	1.2900	0.9793
9	$COD_{Mn}(t-1)$, $COD_{Mn}(t-2)$, $COD_{Mn}(t-3)$, $COD_{Mn}(t-4)$	$COD_{Mn}(t)$	90	0.2041	0.2223
10	$COD_{Mn}(t-1)$, $COD_{Mn}(t-2)$, $COD_{Mn}(t-3)$, $COD_{Mn}(t-4)$	$COD_{Mn}(t)$	40	0.2029	0.2653
11	NH_3-N(t − 1), NH_3-N(t − 2), NH_3-N(t − 3), NH_3-N(t − 4)	NH_3-N(t)	90	0.0435	0.0540
12	NH_3-N(t − 1), NH_3-N(t − 2), NH_3-N(t − 3), NH_3-N(t − 4)	NH_3-N(t)	40	0.0369	0.0380

RMSE: root-mean-square error; MAE: mean absolute error.

forecasting. It should be mentioned that the value of the week is mean value of the seven daily data in the week. Data used in this paper were collected from the network of the Ministry of Environmental Protection of the People's Republic of China.

3.2. Forecasting of single factor indexes

Forecasting of single factor indexes using SVM was carried out by Library for Support Vector Machines (LIB-SVM) toolkit in MATLAB 14.0. To test the efficiency of SVM, experiments with different characteristics were conducted. Characteristics of the experiments and results are shown in Table 2.

As shown in Table 2, there is no significant difference between the prediction results of SVM with various data size and time lag. Therefore, values of the first three days were selected as independent variables, the 4th day as dependent variable for prediction of single factor indexes and the data size was set 91. To illustrate prediction effect of SVM, results of DO is shown as an example.

Distribution of regression forecasting error is illustrated in Fig. 3. The fitting errors are clustered around 0.001213, which is in the allowable range. Fig. 4 presents the DO time series of Gubeikou monitoring section and regression predictions. DO in this section is basically located in the range of 6 to 13 mg/L. DO is an important index of water self-purification ability. In this regards, water quality of this section has remained at high level.

3.3. Comprehensive water quality prediction

Different parameter settings are examined to get the best model performance. The optimized WNN model parameter values were ultimately set as: N is 3; M is 4; L is 1; maximum number of iterations were 500, 1000 and 2000 successively; population size is 30; c_1 and c_2 are 1.5; initial inertia weight and final inertia weight are 0.9 and 0.4, respectively. Different data-driven models including traditional BP neural network, WNN model and Gradient Boosting Decision Tree (GBDT) model using the same data were introduced to compare with the optimized WNN model. The BP neural network model parameter values were set as: N is 3; M is 5; L is 1; learning rate is 0.2; maximum number of iterations were 2000, 3000, 4000 and 5000 successively. The WNN model parameter values were set as: N is 3; M is 4; L is 1; learning rate is 0.1; maximum number of iterations were 1000, 1500, 2000 successively. The GBDT model parameter values were set as: estimator is 200; maximum depth is 25, learning rate is 0.01. A large number of simulation experiments indicated that models with the above

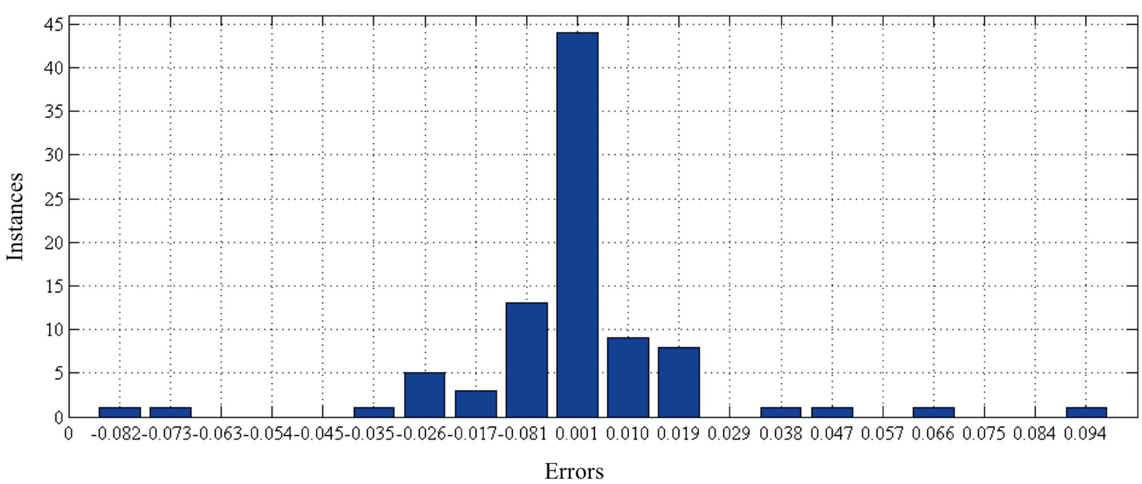

Fig. 3 – Frequency statistics of regressing forecasting errors for DO in Gubeikou monitoring section.

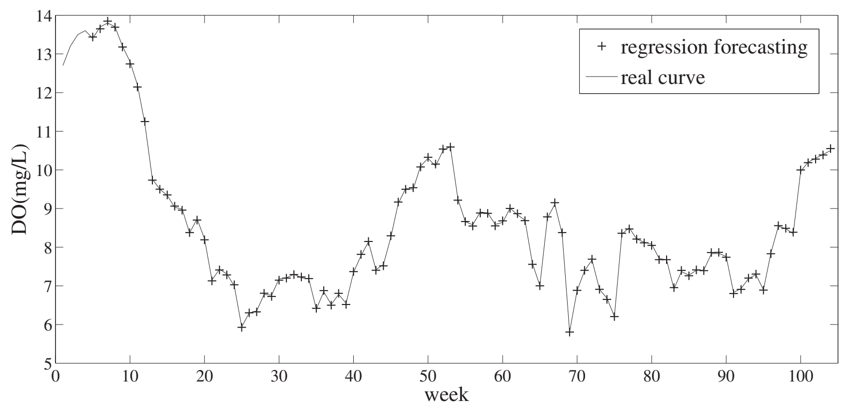

Fig. 4 – Plots from the real value and regressing forecasting results of DO in Gubeikou monitoring section.

settings gained stable performance and good generalization ability. The forecasting results with four different models are shown in Table 3.

Based on the data from the website, Gubeikou monitoring section remained in Class II during 2014 and 2015. Prediction results in Table 3 indicate that the four models all achieved accurate predicting outcomes, which proved the effectivity of the model proposed in this paper. The prediction results gained by the optimized WNN model are acceptable and reliable. The model proposed in this paper enhances the water quality forecasting system. It can be regarded as a useful and innovative tool to perform comprehensive water quality prediction.

Table 3 – Forecasting results of the optimized WNN model and other data-driven models.

Week	Real value	Optimized WNN	WNN	BP neural network	GBDT
95	0.4315	0.3404	0.3294	0.3192	0.3217
96	0.3976	0.3095	0.3149	0.3132	0.2901
97	0.5000	0.3470	0.3420	0.3723	0.3198
98	0.4480	0.3295	0.3295	0.3511	0.3074
99	0.2800	0.2967	0.2630	0.2773	0.2633
100	0.2592	0.2762	0.2562	0.3110	0.2567
101	0.2500	0.2780	0.2523	0.3175	0.2565
102	0.3068	0.2934	0.2853	0.3752	0.2759
103	0.2599	0.2805	0.2602	0.3213	0.2581
104	0.2670	0.2795	0.2649	0.3320	0.2577

WNN: Wavelet Neural Network; BP: Back Propagation; GBDT: Gradient Boosting Decision Tree.

Table 4 – Evaluation of optimized WNN model and other data-driven models.

Index	Optimized WNN	WNN	BP neural network	GBDT
RMSE	0.0701	0.0739	0.2556	0.0740
MAE	0.0546	0.0508	0.0738	0.0596

WNN: Wavelet Neural Network; BP: Back Propagation; GBDT: Gradient Boosting Decision Tree.

Performance of the optimized WNN model is shown in Table 4, together with that of the other three data-driven models for comparison. As can be seen in Table 4, the optimized WNN model has better prediction accuracy (RMSE = 0.0701), especially when compared to the BP neural network model (RMSE = 0.2556). In addition, the optimized WNN model can get acceptable results within 1000 epochs while the WNN model within 2000 epochs and the BP neural network model within 5000 epochs, which indicated that the optimized WNN model has the potential to accelerate convergence rate and reduce errors in prediction. The results demonstrate that the PSO technique is a good tool to solve parameter optimization problems.

4. Conclusions

This paper proposed a new framework to improve the forecasting of water grades. It was based on SVM and optimized WNN using PSO. First, water quality indicators including DO, COD_{Mn}, NH_3-N were predicted with SVM. Then the predictions were used as the inputs of the trained WNN model to forecast the whole status index of water quality in the next time.

The experiments of the Gubeikou monitoring section, inlet of Miyun reservoir, verified the effectivity of the model. It can be applied on short-term water quality forecasting, precaution basin water pollution accidents and providing more objective reference for water quality management. Experiments also show that the optimized WNN model has the potential to accelerate convergence rate and reduce errors in prediction when compared to other data-driven models. This study provided novel ideas about exploration of methods for comprehensive water quality forecasting. Methods of reducing forecast error and enhancing the generalization ability will be discussed in the future study.

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