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

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ABSTRACT

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.

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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 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 widely applied in forecast filed such as mid-long-term power

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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 ($\text{NH}_3\text{-N}$) 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 $X = (X_1, X_2, \dots, X_D)$. The velocity for the i th particle can be denoted as $V = [V_{i1}, V_{i2}, \dots, V_{iD}]$. The best position so far for the i th particle is represented as $P_i = [P_{i1}, P_{i2}, \dots, P_{iD}]^T$. The best position so far for the entire swarm can be described as $P_g = [P_{g1}, P_{g2}, \dots, P_{gD}]^T$. In each iteration, particles change its position and velocity according to the following equations:

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

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

where, ω is the inertia weight; $d = 1, 2, \dots, D$; $i = 1, 2, \dots, n$; 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 $[-X_{\text{max}}, X_{\text{max}}]$ and $[-V_{\text{max}}, V_{\text{max}}]$ 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 node number in the input layer, hidden layer and output layer m, n, N respectively. The WNN model can be expressed by the following formulas.

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

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

where, x_k is the input vector; y_i is the predicted output vector; w_{ij} is the connection weight from the i th node of the output layer to the j th node of the hidden layer; w_{jk} is the connection weight from the j th node of the hidden layer to the k th node of the output layer; $\Psi_{(a,b)}$ is the activation function of the hidden layer; a, b 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, b 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).

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