A new water quality state estimation method with an unknown state model

Daxing Xu*, Hailun Wang, Lu Zhang

College of Electrical and Information Engineering, Quzhou University, Quzhou 324000, China, emails: daxingxu@163.com (D. Xu), 18968098195@126.com (H. Wang), zhanglu90573@163.com (L. Zhang)

ABSTRACT

Water quality estimation is a basic task in regional water environment planning, evaluation, and management. This paper studies the water quality state estimation problem of the nonlinear system with an unknown state model. The existing algorithms based on nonlinear filtering and neural networks have limited accuracy in state estimation. To solve this problem, a new estimation method based on high-degree cubature Kalman filtering and neural networks is proposed. First, neural network is used to establish the state-space model for the nonlinear system. Then, the weights of the neural network and the system state variables are combined as a new state variable. Meanwhile, the real-time state update is performed by high-degree cubature Kalman. Moreover, the neural network can achieve the true approximation of the nonlinear system model and the accurate estimation of the state value. Finally, water quality estimation simulation shows the effectiveness of the proposed algorithm.

Keywords: Nonlinear system; Unknown state model; High-degree cubature Kalman filtering; Neural network; Water quality estimation

1. Introduction

With the application of the internet, the internet of things, and smart sensors and other technical means, rapid and real-time monitoring of water indicators can be achieved [1]. Accurately predicting the trend of water quality changes in important water bodies is of great significance for taking governance measures and establishing decision-making early warning mechanisms [2]. The water environment is a system full of uncertain factors, which is susceptible to climate change, ecological changes in river basins, and human activities. Research on the changing characteristics and trends of key water quality indicators can help to interpret the internal mechanism of the water environment system, and have guiding significance for the prevention and control of water pollution.

In 1980s, an error back-propagation algorithm based on forward neural networks was proposed by Rumelhard.

Due to its simple structure, easy implementation, and strong nonlinear mapping capabilities, it has been widely used in aerospace, intelligent transportation, pattern recognition, and medical engineering [3,4]. However, the model of the actual system is sometimes unknown, such as the water quality model of a region is often unknown. Under this case, it is a simple and effective method to use a neural network to approximate the model nonlinearly. The neural network determines the non-linear function of the network approximation according to the actual data set. However, when the state variables of the actual system are not fully measurable, the neural network cannot establish a model of the process. The state-space model method describes the change relationship between the internal state of the system and the external observable output variables. Since this method can estimate and predict the complex state inside the system, it has been widely used in the processing of dynamic systems. After the state-space model of the system

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* Corresponding author.

is established, it is necessary to estimate the state of the system by using an appropriate method, where the system input and output observation data in the state space are used to make an optimal estimation of the system state [5]. This filtering method can not only estimate the state, but also identify the parameters of the neural network system.

Non-linear filtering algorithms have made considerable progress in parameter estimation, especially in the parameter identification of neural networks, which treat the weight coefficient parameters of the network as special states for estimation. Singhal and Wu [6] first established a state-space model using a neural network, where the network weight coefficient is used as the state variable of the system, and then updated the state variable in real-time based on the extended Kalman filter algorithm. Simulation experiments show that the effect is significantly better than the traditional error back-propagation algorithm, especially in the presence of obvious noise interference. It can achieve higher estimation accuracy. Extended Kalman filtering is currently the most widely used nonlinear filtering method. However, when the degree of nonlinearity of the system is high, the first-order approximation will bring a very large truncation error, which will cause the estimated performance of the extended Kalman filter algorithm to be greatly reduced, or even divergent [7,8]. Due to the shortcomings of extended Kalman filtering, such as poor stability and low accuracy, Julier et al. proposed unscented Kalman filtering, which uses an unscented transformation to handle the non-linear transfer of mean and variance [9,10]. Many researchers have used unscented Kalman filtering and neural networks to solve the nonlinear system state estimation problem with an unknown system model. Zha and Xu [11] proposed the application of an unscented Kalman filtering algorithm to an online estimation of neural network weight coefficients. Wu and Wang [12] carried out an experimental comparison of neural networks based on extended Kalman filtering and unscented Kalman filtering, and the results show that neural networks based on unscented Kalman filtering are significantly better than neural networks based on extended Kalman filtering algorithm. Nevertheless, the accuracy of unscented Kalman filtering is still limited, and its estimation performance is significantly reduced when the system dimension is high. In order to further improve the state estimation accuracy, Jia et al [13] proposed a high-degree volume Kalman filtering using the Genz integration method and moment matching method to derive spherical rules and phase diameter rules of any order. Then high-degree spherical-phase diameter volume rules to calculate Gaussian integrals can be constructed, and high-degree cubature Kalman filtering algorithm can be established. Zhang et al. [14] compared the accuracy and applicable range of the unscented Kalman filter algorithm and the high-degree cubature Kalman filter algorithm. The results showed that the high-degree cubature Kalman filter algorithm was more applicable to high-dimensional systems. Recently, Zhang et al. [15–17] proposed "a high order unscented Kalman filtering method", "interpolatory cubature Kalman filters", "embedded cubature Kalman filter with the adaptive setting of free parameter". It has been proven that these algorithms can achieve higher filtering accuracy than existing fifth-degree

cubature Kalman filtering methods by properly choosing free parameters. Since the framework of these algorithms is similar to high-degree cubature Kalman filter algorithm, thus the idea of this paper can be extended to these work for further improvement. However, this paper focuses more on high-degree cubature Kalman filter and provides a simpler model-free water quality prediction framework.

In this paper, for the nonlinear system with an unknown state model, we use a neural network to build a state-space model. Then, the network weight coefficients and the system state are combined as an expanded state variable. Moreover, high-degree cubature Kalman filter algorithm is used to estimate the state of the neural network system. Thus, the adaptive adjustment of the network weight coefficients and the real-time update of the state are realized. Finally, the proposed algorithm is used to predict water quality and the estimation accuracy is greatly improved. The contributions of this paper are summarized as follows: (1) we construct the state estimation model based on high-degree cubature Kalman filter and neural network. (2) we also provide the analytical iterative steps for the estimation algorithm. (3) To the best of our knowledge, this is the first work to apply this type of algorithm to water quality state estimation with an unknown state model.

2. State-space model of neural network

Structural models of neural networks can generally be divided into feed-forward neural network models, feedback neural network models, and stochastic neural network models. At present, the feedforward neural network model is most widely used in various industries. The model structure of its state space is shown in Fig. 1.

The neural network model structure has three node layers, namely input layer, hidden layer, and output layer. It is connected by weight coefficients, the input, and output layers are at both ends, and the number of nodes in the middle hidden layer is selected according to actual requirements.

3. High-degree cubature Kalman filtering principle

Consider the following discrete nonlinear systems:

$$x_k = f(x_{k-1}) + w_k \tag{1}$$

$$z_k = h(x_k) + v_k \tag{2}$$

where x_k is a n-dimensional state vector. z_k is a m-dimensional observation vector. Functions f, h are known nonlinear functions. $\{w_k\}$ and $\{v_k\}$ are independent zero-mean Gaussian white noise.

For general nonlinear systems, under the Gaussian hypothesis, the basic theory of Bayesian estimation can be combined with any order cubature rule to derive a high order cubature Kalman filter. Similar to the unscented Kalman filter structure, it is also divided into two steps: state prediction (time update) and measurement update. The high-degree cubature Kalman filter uses the phase difference cubature rule to solve the problem of a
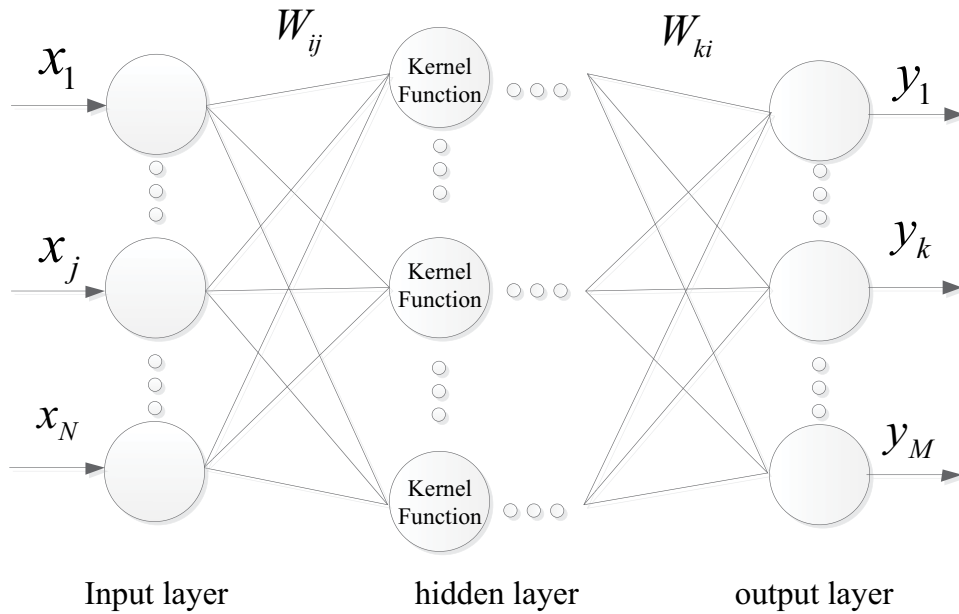
Fig. 1. Model structure of neural network where $x_1, x_2, \ldots, x_n$ represent the input sample nodes, and W_{ij}, W_{ki} stand for the weight coefficients among all layers. $y_1, y_2, \ldots y_m$ denote the output sample nodes.

dimensional explosion in high-dimensional systems. High-degree cubature rules satisfy:

$$I_{U_n} = \bar{w}_{s1} \sum_{j=1}^{n(n-1)} \left(g_s(s_j^+) + g_s(-s_j^+) + g_s(s_j^-) + g_s(-s_j^-) \right) +$$

$$\bar{w}_{s2} \sum_{j=1}^{n} \left(g_s(e_j) + g_s(-e_j) \right) \tag{3}$$

where, $s = [s_1, s_2, \ldots, s_n]^T$, $U_n = \{ s \in R^n : s_1^2 + s_2^2 + \ldots + s_n^2 = 1 \}$, and e_j is the j-th column of the unit vector matrix of n-dimensional space R^n. $g_s()$ is a general nonlinear function that has different forms in different filtering steps. s_j^+ and s_j^- are the sets of points as shown below:

$$\{ s_j^+ \} = \left\{ \sqrt{1/2} (e_k + e_l) : \quad k < l, \ k, l = 1, 2, \ldots, n \right\} \tag{4}$$

$$\{ s_j^- \} = \left\{ \sqrt{1/2} (e_k - e_l) : \quad k < l, \ k, l = 1, 2, \ldots, n \right\} \tag{5}$$

The weight coefficients $\bar{w}_{s1}$ and $\bar{w}_{s2}$ are:

$$\bar{w}_{s1} = \frac{A_n}{n} (n + 2) \tag{6}$$

$$\bar{w}_{s2} = \frac{(4 - n) A_n}{(2n(n + 2))} \tag{7}$$

where $A_n = 2\sqrt{\pi^n} / \Gamma(n/2)$ is the surface area of the unit sphere and $\Gamma(z) = \int_0^\infty \exp(-\lambda) \lambda^{z-1} d\lambda$. According to the moment matching method, when $n = 2$, the weight is:

$$\begin{cases} w_1 = \Gamma(n/2) / (n + 2) \\ w_2 = n\Gamma(n/2) / (2(n + 2)) \end{cases} \tag{8}$$

4. State estimation based on high-degree cubature Kalman filter and neural network

When the model of the system is unknown, the neural network is used to approximate the system model, then the optimal network node weight coefficients need to be solved. Meanwhile, the state is also unknown, and the state and weight coefficients are related. Therefore, we combine the state and weight coefficient of the system as a new state. Then, the original system equation and the augmented equation of the weight coefficient equation are considered as a new system model. Further, the state and weight coefficients are estimated in real time using a high-degree cubature Kalman filter algorithm. The specific system principle is shown in Fig. 2.

In Fig. 2, at time k–1, the state x_{k-1} of the original system is combined with the weight coefficient W_{k-1} into a new augmented state vector $[x_{k-1} W_{k-1}]$, which is input into the neural network. Then the high-degree cubature Kalman filter makes the time update step according to the augmented state and the output results of the neural network. Finally, the high-degree cubature Kalman filter performs time update according to the time update result and the measured output structure to obtain the system augmented state value $[x_k W_k]$ at time k, which is used as the input state of the system at next time. The specific algorithm is given as follows:

First, combining the state of the system with the weight coefficients of the neural network to form an augmented state $x^a = [xW]^T$, a non-linear system can be established as follows:
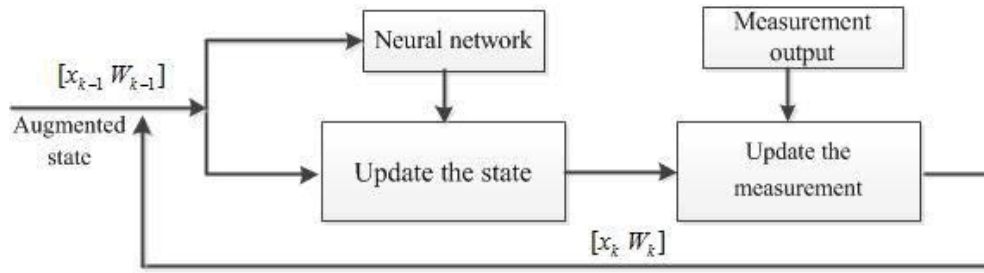
Fig. 2. State estimation system.

$$x_k^a = \begin{bmatrix} x_k \\ W_k \end{bmatrix} = \begin{bmatrix} f^1(x_k) \\ f^2(x_k) \\ . \\ . \\ . \\ W_k \end{bmatrix} + w_k = \begin{bmatrix} f(x_k) \\ . \\ . \\ . \\ W_k \end{bmatrix} + w_k \tag{9}$$

$$z_k = h(x_k^a) + v_k \tag{10}$$

where $f^j(x_k)$ is the mathematical model established by the neural network for the nonlinear system:

$$f^j(x_k) = \sum_{l=i}^{L} \left(W_{j,l}^2 \left(g\left(\sum_{i=1}^{N} x_{i,k} W_{i,l}^1 \right) \right) \right), \quad j = 1,2,...,N \tag{11}$$

where $g(x)$ is the Sigmod kernel function of the neural network, W_k is the weight coefficient of the neural network. The process noise w_k and observation noise v_k of the new system are independent zero-mean Gaussian white noise, and the corresponding covariance matrices are Q_k and R_k.

Update the state:

- At time k, assume that the error covariance $P_{k-1|k-1}$ at time k–1 is known, the factorization is:

$$P_{k-1|k-1} = S_{k-1|k-1} S_{k-1|k-1}^T \tag{12}$$

where the vector $S_{k-1|k-1}$ is the Cholesky factorization of $P_{k-1|k-1}$.

- Compute the cubature points

$$X_{i,k-1|k-1}^a = S_{k-1|k-1} \xi_i + \hat{x}_{k-1|k-1}^a \quad (i = 1,2,...,m) \tag{13}$$

where $m = 2n$, and the vector ξ_i is:

$$\xi_i = \begin{cases} [0 \quad 0,...,0]^T, \quad i = 0 \\ \beta s_i^+, \quad i = 1,2,...,n(n-1)/2 \\ -\beta s_{i-n(n-1)/2}^+, \quad i = n(n-1)/2+1, n(n-1)/2+2,...,n(n-1) \\ \beta s_{i-n(n-1)}^-, \quad i = n(n-1)+1, n(n-1)+2,...,3n(n-1)/2 \\ -\beta s_{i-3n(n-1)/2}^-, \quad i = 3n(n-1)/2+1, 3n(n-1)/2+2,...,2n(n-1) \\ \beta e_{i-2n(n-1)}, \quad i = 2n(n-1)+1, 2n(n-1)+2,...,n(2n-1) \\ -\beta e_{i-n(2n-1)}, \quad i = n(2n-1)+1, n(2n-1)+2,...,2n^2 \end{cases} \tag{14}$$

where $\beta = \sqrt{n+2}$, e_i represents an n-dimensional unit vector and its i-th element is 1. s_j^+, s_j^- are:

$$\begin{cases} s_j^+ = \sqrt{1/2}(e_p + e_q), \quad p < q, p,q = 1,2,...,n \\ s_j^- = \sqrt{1/2}(e_p - e_q), \quad p < q, p,q = 1,2,...,n \end{cases} \tag{15}$$

- Calculate the cubature points after propagation of state equation ($i = 1,2,...,m$):

$$X_{i,k|k-1}^{a*} = f(X_{i,k-1|k-1}^a) \tag{16}$$

- Compute one-step state prediction:

$$\hat{x}_{k|k-1}^a = \sum_{i=1}^{m} w_i X_{i,k|k-1}^{a*} \tag{17}$$

where the weights w_i are:

$$w_i = \begin{cases} 2/n+2, \quad i = 0 \\ 1/(n+2)^2, \quad i = 1,2,...,2n(n-1) \\ (4-n)/(n+2)^2, \\ i = 2n(n-1)+1, 2n(n-1)+2,...,2n^2 \end{cases} \tag{18}$$

- Calculate the one-step prediction error covariance matrix:

$$P_{k|k-1} = \sum_{i=1}^{m} w_i X_{i,k|k-1}^{a*} X_{i,k|k-1}^{a*T} - \hat{x}_{k|k-1}^a (\hat{x}_{k|k-1}^a)^T + Q_{k,k-1} \tag{19}$$

Update the measurement:

- Factorization as follows:

$$P_{k|k-1} = S_{k|k-1} S_{k|k-1}^T \tag{20}$$

- Calculate the state cubature point after update:

$$X_{i,k|k-1} = S_{k|k-1} \xi_i + \hat{x}_{k|k-1}^a \quad (i = 1,2,...,m) \tag{21}$$

- Compute the cubature point after the measurement equation has propagated:

$$Z_{i,k|k-1} = h(X_{i,k|k-1}^a) \tag{22}$$

- Calculate one-step measurement and prediction at time k:

$$\hat{z}_{k|k-1} = \sum_{i=1}^{m} w_i Z_{i,k|k-1} \tag{23}$$

- Calculate the innovation covariance matrix:

$$P_{zz,k|k-1} = \sum_{i=1}^{m} w_i Z_{i,k|k-1} Z_{i,k|k-1}^T - \hat{z}_{k|k-1} \hat{z}_{k|k-1}^T + R_k \tag{24}$$

- Compute the one-step prediction cross covariance matrix:

$$P_{xz,k|k-1} = \sum_{i=1}^{m} w_i X_{i,k|k-1} Z_{i,k|k-1}^T - \hat{x}_{k|k-1}^a \hat{z}_{k|k-1}^T \tag{25}$$

- Calculate the gain matrix:

$$K_k = P_{xz,k|k-1} P_{zz,k|k-1}^{-1} \tag{26}$$

- Update state as follows:

$$\hat{x}_{k|k} = \hat{x}_{k|k-1}^a + K_k \left(z_k - \hat{z}_{k|k-1} \right) \tag{27}$$

- Error covariance matrix can be obtained by:

$$P_{k|k} = P_{k|k-1} - K_k P_{zz,k|k-1} K_k^T \tag{28}$$

For the known nonlinear system described in Eqs. (9) and (10), given the initial state of the state, the high-degree cubature Kalman filtering can be performed according to the above two steps of time update and measurement update to obtain an expanded state vector value.

5. Simulation example

Assume that the real model of water quality is the following non-linear system, where the water quality state model is unknown to us, but only for comparison.

$$x(k+1) = \begin{bmatrix} 0.5 + 0.05\sin(0.01k) & 0.06 \\ 0.1 & -0.2 + 0.2\sin(0.01k) \end{bmatrix} x(k) + w(k) \tag{29}$$

$$y(k) = x_1(k) + x_2(k) + v(k) \tag{30}$$

where states $x(k)$ represent the dissolved oxygen amount and biochemical oxygen demand (BOD) value, respectively. The BOD value represents the amount of oxygen consumed by the decomposition of organic matter in the water. $w(k)$ process noise and observation noise $v(k)$ are independent zero-mean Gaussian white noise, with the variances are $Q(k) = \begin{bmatrix} 1.5784 & 0.5124 \\ 0.5124 & 1.4539 \end{bmatrix}$ and $R(k) = 0.5$, respectively. The initial state is $x_0 = \begin{bmatrix} 3.1 & 2.5 \end{bmatrix}^T$, and its estimate is set as $\hat{x}_0 = \begin{bmatrix} 3.8 & 1.2 \end{bmatrix}^T$. The initial state error covariance matrix is $P_0 = \begin{bmatrix} 0.1 & 0 \\ 0 & 0.1 \end{bmatrix}$. The neural network model has two

input nodes, two output nodes, and two hidden nodes. The number of weights is 8, and the kernel function is chosen as Sigmod. The initial weight is selected as random noise with variance 0.2. The simulation environment is Intel i5 CPU, 4G memory, and the simulation software uses Matlab R2013a.

For convenient of comparison, we simply marks the following algorithms as follows:

- *Algorithm 1*: estimation algorithm based on high-degree cubature Kalman filter and neural network.
- *Algorithm 2*: estimation algorithm Based on Unscented Kalman filter and neural network.

The simulation results are shown in Figs. 3–7 and Table 1.

From the estimation curves of Figs. 3 and 4, both algorithms 1 and 2 can perform a good tracking estimation on the original water quality state, indicating that both algorithms are effective. From the estimation error curves of Figs. 5 and 6, the errors of the two algorithms quickly stabilize. But the error curve of algorithm 2 is generally above algorithm 1, which means that the error of algorithm 2 is obviously greater than that of algorithm 1. From the statistics of Table 1, it can be seen that the time consuming of the two algorithms is comparable, but the accuracy of the state estimation of algorithm 1 is much higher than that of algorithm 2. For the estimation accuracy of dissolved oxygen and BOD, the estimation error of algorithm 2 is more than three times that of algorithm 1. This is mainly because the estimation accuracy of the high-degree cubature Kalman filtering algorithm is higher than that of the unscented Kalman filtering algorithm. As shown in Fig. 7, the weights of the neural network are an adaptive adjustment process in the whole estimation process. These demonstrate the effectiveness of cubature Kalman filtering and neural network estimation algorithms.

6. Conclusion

This paper proposed a state estimation algorithm based on high-degree cubature Kalman filter algorithm and neural network for nonlinear systems with unknown state
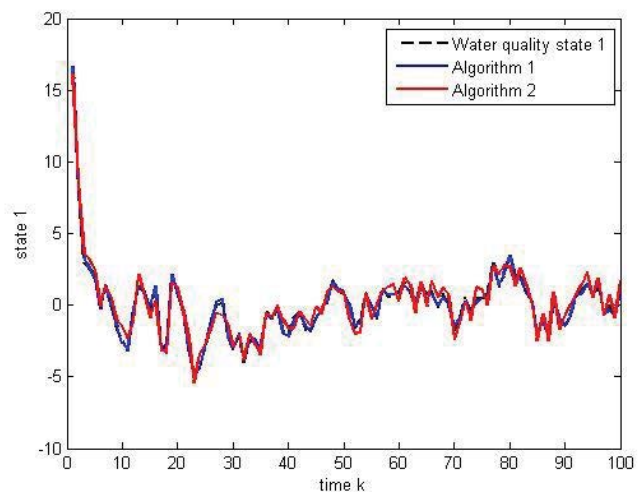

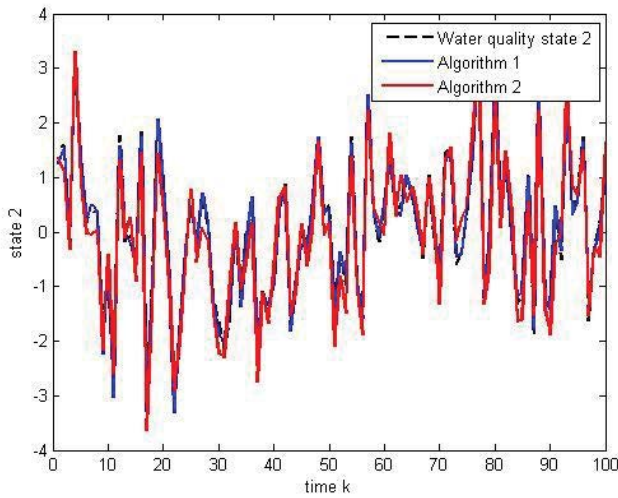Fig. 3. Estimation curve for dissolved oxygen.
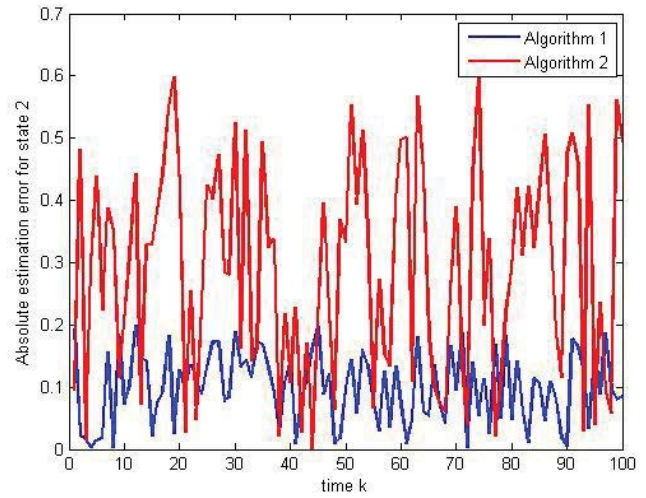
Fig. 4. Estimation curve for BOD.
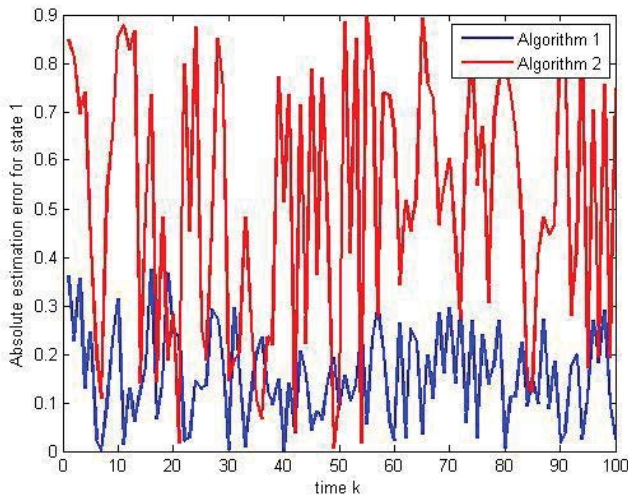

Fig. 6. Estimation error curve for BOD.

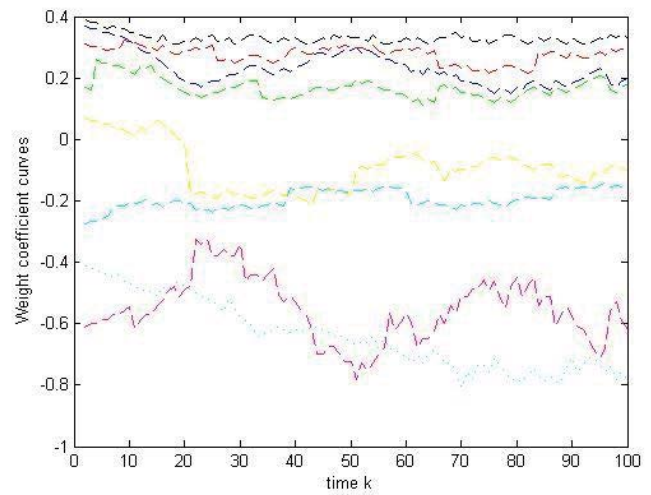Fig. 5. Estimation error curve for dissolved oxygen.

Fig. 7. Weight coefficient curves.

Table 1
Comparison of estimation errors and time-consuming

Algorithm	Mean absolute estimation error of dissolved oxygen	Mean absolute estimation error of BOD	Algorithm time-consuming
Algorithm 1	0.1543	0.0886	0.686
Algorithm 2	0.5079	0.2891	0.652

model. The system state model is constructed by using neural network. And we use the high-degree cubature Kalman filter algorithm to estimate the state in real time. The proposed algorithm made up for the shortcomings of existing algorithms and improved the accuracy of state estimation based on neural networks. Water quality estimation simulation showed the effectiveness of the proposed algorithm. Actually, although we assume that the model can be described as Eq. (9), the system model is still inaccurate in practice, which means that there is model uncertainty. Under this case, robust filters can be used to deal

with this problem. Some related methods can be used for reference, such as literature [18–21], these robust Kalman filters based on non-Gaussian modeling exhibit good performance for addressing the model uncertainty. This is also our future work.

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