Water Quality Modeling and Prediction Method Based on Sparse Recurrent Neural Network*

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Abstract. It is an important prerequisite for scientific management and maintenance of water resources to accurately predict all kinds of indices that affect water quality. This paper propose a method of forecasting water quality index and rank based on sparse recurrent neural network (SRNN). The learning algorithm of the network is designed based on the principle of minimum mean square recursive error.A prediction model for predicting water quality index and rank is constructed by using the neural network.The validity of the model is verified by predicting the water quality parameters and water quality rank of a river in Zhejiang Province.

Keywords: Water quality modeling · Water quality prediction · Recurrent neural network.

1 Introduction

Along with the rapid development of economy and population growth, sewage and wastewater generate by the production and living of human are posing a serious threat to the water quality of lakes and rivers[16].There are various problems such as water shortage, water pollution and deterioration of water ecological environment in all parts of China[16], which have become the main bottleneck restricting the sustainable development of economy and society. In order to solve this problem efficiently, the rational planning of water resources is particularly important[10, 9]. Accurately detecting and reasonably predicting of water quality parameters future trend are essential prerequisites for scientific planning of water resources[2]. Water quality prediction is the process of constructing a water quality model by using already existing data and then estimating the future water quality parameters of via the model. Common prediction models can be divided into two categories: Principle Driven Model (PDM) and Data Driven Model (DDM).

PDM is generally modeled by domain experts who construct the hydrodynamic motion and energy equations of water, taking into account the interactions between water components and their own biochemical effects[12, 3]. Typical principle driven water quality models include: the Streeter Phelps(SP) model

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for quantifying oxygen balance[1], which is often applied to simple water self-purification; QUAL model, which can simulate up to 15 water quality components, is often used to study the effect of inflow sewage load on the water quality of receiving rivers; the Water Quality Analysis Simulation Program(WASP) model of pollutant interaction[3] and the BASINS model combined with geographic information system[12, 13]. The above prediction models have been widely used in water pollution control and early warning, water quality planning and other fields because they can accurately describe the relationship between various components of water.For PMD,however,once the factors affecting water quality changed, it is necessary for domain experts to redesign the model. The application of this type of water quality model lacks sufficient flexibility.

Unlike PDM, building DDM does not necessarily require the involvement of domain experts. It only needs to input a large amount of water quality data into the learning model, and then adjust the parameters of the learning model according to the algorithm to obtain a mapping between the input data and the data to be predicted. The learning model with adjusted parameters can be used for water quality prediction. Common learning models include the various regression analysis based on statistical principles[5, 23, 22, 20] and the artificial neural network (ANN)[14, 6, 18, 8, 15, 19]. Because these models have a learning process, they can be applied to various water quality predictions under a scene where the environment changes frequently.

In order to obtain higher prediction accuracy, the ANN commonly used in DDM often needs a large number of historical water quality data, and then automatically learns the water quality prediction model to meet the demand according to the historical data. However, the back propagation (BP) network which is commonly used in ANN often has the disadvantage of slow convergence speed. In addition, BP network is a typical feedforward structure neural network, but water quality data is often a time series[21]. BP network is difficult to simulate the time correlation between water quality data. To this end, this study is based on the latest theoretical research results of the prefrontal cortex in neuroscience[17, 4], through the construction of a sparse connection large-scale recurrent neural network which used the least mean square recursive error algorithm to quickly learn the patterns between water quality data. The accuracy of the model is verified by predicting the water quality indices such as ammonia nitrogen (AN), dissolved oxygen (DO), permanganate index (PI), total phosphorus (TP) and total nitrogen (TN) in a reservoir.

2 Water quality model

We use a sparse recurrent neural network (SRNN) to simulate the temporal correlation between water quality data. SRNN which is unlike common recurrent neural networks contains a large number of neurons. The positive and negative connection weights between neurons are roughly the same. In particular, when the intensity coefficient of weighted connections between neurons in SRNN exceeds a certain threshold, the spontaneous activity of the recurrent network will exhibit chaotic characteristics[15]. This feature makes the network has strong state coding capabilities. SRNN has been widely used in cognitive modeling of neuroscience. Some theoretical neuroscientists even speculate that SRNN is similar to the function of the prefrontal cortex of the brain[19].

2.1 SRNN network structure

As shown in Figure 1, the SRNN contains three layers, an input layer y, a recurrent layer x and an output layer z. Vector y $=[y_1, y_2, ..., y_m]^T$ represents the input layer neuron activity, where y_i is the input water quality indices and the superscript T is the transpose.

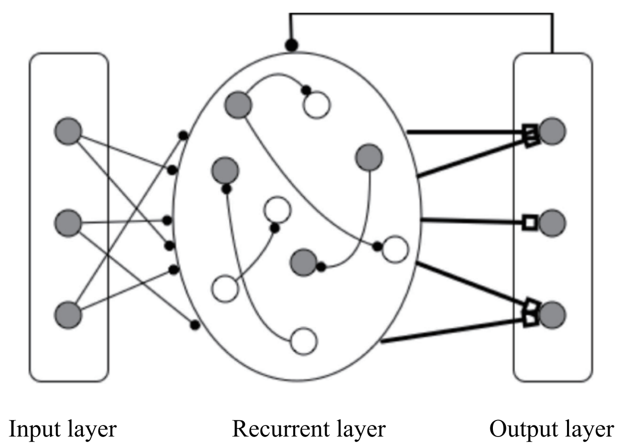

Fig. 1. Structure of SRNN

The activity of recurrent layer neurons is represented by x, whose activity is calculated by the formula:

$$\tau \frac{d_x}{d_t} = -x + w^{RNL} r + w^{in} y + w^{fb} z, \tag{1}$$

where $r = \tanh(x)$represents the rate of release of recurrent layer neurons. *tanh* is a hyperbolic tangent function as the activation function of recurrent layer neurons. $\tau = 0.01$ is the neuron activity decay constant.

w^{RNL} represents the recurrent connection matrix between neurons in the recurrent layer. Since the recurrent layer has $N = 1000$ neurons,w^{RNL} is a matrix of 1000×1000 size.The element w_{ij}^{RNL} in the matrix represents the connection weight among the i-th neuron and the j-th neuron in the recurrent layer. The recurrent layer is a sparse connection, and w_{ij}^{RNL} sets the probability of $p =$

0.1 to a non-zero value and the probability of $1-p=0.9$ to zero.This means that there are only a few connections between recurrent layer neurons. The value of the non-zero element of w_{ij}^{RNL} is randomly selected from the Gaussian distribution $Norm(0, g^2/pN)$, where g is the intensity coefficient of weight. When $g=1.5$, the recurrent layer neurons will have the spontaneous activity of chaotic characteristics[15].

w^{in} represents the connection matrix among the input layer and the recurrent layer. The weights are randomly selected according to the Gaussian distribution $Norm(0, 0.5)$.w^{fb} is the connection weight of the output neuron feedback back to the recurrent layer neurons. It is still a sparse connection.90% of the weights are set to 0, and other non-zero elements are still randomly selected according to the Gaussian distribution $Norm(0, 0.5)$. z is the output layer neuron activity, corresponding to the predicted output, and its calculation is determined by:

$$z = wr \tag{2}$$

where w represents the connection matrix between the recurrent layer and the output layer. The recurrent layer and the output layer are fully connected, and the weights are randomly assigned according to a uniform distribution between $[-1, 1]$. w is different from w^{RNL}, w^{in}, and w^{fb}, and its element values need to be updated during the learning phase, while the values of w^{RNL}, w^{in}, and w^{fb} remain unchanged during the learning phase.

As can be seen from the structure of SRNN, it is similar to the Echo State Network (ESN) [11]. They all have a recurrent layer and the learning process only adjusts the weight between the recurrent layer and the output layer. However, SRNN and ESN also have the following differences. First of all, the SRNN's recurrent layer connection weight does not need to be specially set, but the ESN needs to have a weight matrix with a spectral radius greater than or equal to 1 in order to achieve reverberation. Secondly, the training of ESN is a kind of offline learning. It needs to wait for the network to pre-calculate for a period of time before starting to adjust the weight, but SRNN can update the weight immediately according to the current input.

2.2 SRNN learning algorithm

According to the description of SRNN in the previous section, the recurrent layer connection weights only need to be randomly selected according to a given probability distribution and use the online learning mode. These features require a learning algorithm that quickly determines how the output weight should be updated so that the network output is equal to the value of the real output.

The target output expected at time t is $f(t)$. The real output of the network is $w^T(t-\Delta t)r$.The error between them is $e(t)$.

$$e(t) = w^T(t-\Delta t)r - f(t) \tag{3}$$

The learning algorithm is to adjust the output weight from $w^T(t-\Delta t)$ to $w^T(t)$ so that the error $e(t)$ is gradually reduced. After the output weight is updated, the output error of the network becomes:

$$e_+(t) = w^T(t)r - f(t) \tag{4}$$

After the algorithm converges, the value of $e(t)/e_+(t)$ should go to 1 and $e(t) > e_+(t)$. This means that the adjustment of the output weights will not further reduce the output error. In order to achieve fast learning, the weight adjustment of the output requires a quick reduction in the error value during the previous learning. To this end, according to the recurrent least mean square error algorithm [7], the output weights are adjusted as follows:

$$w(t) = w(t - \Delta t) - e(t)P(t)r(t) \tag{5}$$

Equation 5 shows that the decision to update the output weight is the error $e(t)$, the firing rate r of neurons in the recurrent layer, and the matrix $P(t)$.

The matrix $P(t)$ can be seen as the learning rate, which is used to determine the size and scale of connection weights adjustment. However, it is unlike the general learning rate, this learning rate is a matrix. It means that each output weight has its own learning rate, which is one of the main reasons that the algorithm can converge quickly.

The computation of the learning rate matrix $P(t)$ is carried out in the following way:

$$P(t) = P(t - \Delta t) - \frac{(P(t - \Delta t)r^T(t)P(t - \Delta t))}{(1 + r^T(t)P(t - \Delta t)r^T)} \tag{6}$$

$P(t)$ needs to have an initial value in the first step, and then update it every step according to Equation 6. The initial value of $P(t)$ is set to $\frac{1}{\alpha}$, where I is a unit matrix of 1000×1000, and α is a constant.

3 Experimental result

3.1 Water quality data preparation

We select the water data of a reservoir in Zhejiang from May 2012 to May 2015. The data source is the actual value which detected by the automatic monitoring station every 4 hours. Dissolved oxygen, permanganate index, ammonia nitrogen, total phosphorus and total nitrogen, are selected to evaluate the water quality rank. In addition, in order to reduce the influence of daytime illumination and human activity factors, only the water data at 4 o'clock in the morning is selected. Considering the possible abnormalities of the water quality parameters in the measurement, the data is preprocessed to remove some obvious abnormal data. It uses the Grubbs criterion for outlier detection. First of all, the data is sorted in ascending order. The outliers are sequentially removed from both ends until the data set meets the requirements. In order to determine the abnormal data, it need to be calculated:

$$G_i = \frac{|X_i - \bar{x}|}{S} \tag{7}$$

where G_i is the characteristic data of the Grubbs criterion test. X_i is the data to be tested. $\bar{x}$ is the arithmetic mean of the data set. S is the standard deviation of the data set.If G_s is bigger than $G_p(n)$, it is judged that the data is an abnormal value. The critical value $G_p(n)$ is determined by the Grubbs table. It is related to the detected rank $\sigma = 0.05$ and the number n of data of the test data set.

Since the data and the detection range of the water indices are not uniform, the input data need to be normalized. The value of the input data x is mapped between 0.2 and 0.8. The normalization formula is as follows:

$$y = 0.6 * \frac{x - min(x)}{max(x) - min(x)} + 0.2 \tag{8}$$

The minimum time unit of the data set is day T. T is taken form 7 days, 14 days, and 30 days. They respectively generate 3 sets of training and testing data sets. The water quality data from May 1, 2012 to April 30, 2014 are selected as training data. The water quality data from May 1, 2014 to April 30, 2015 are selected as testing data. Ammonia nitrogen, dissolved oxygen, permanganate index, total phosphorus and total nitrogen are selected as the measured parameters to verify the effectiveness of SRNN.

3.2 Water quality parameter prediction

Water quality data for several days are used as input to predict water quality afterwards parameters. Network performance is quantified by calculating the root mean square (RMS) error:

$$RMS = \frac{1}{t_e - t_s} \sum_{i=t_s}^{t_e} \sqrt{(\bar{y}(i) - y(i))^2} \tag{9}$$

where $\bar{y}(i)$ and $y(i)$ are network estimated value and actual value. t_e and t_s are the start time and end time. The training results of the ammonia nitrogen index were selected to examine the convergence of SRNN. The number of recurrent layer neurons is set to 1000. The weight intensity coefficient g is set to 1.5. The step size of Equation 1 is set to 0.05. The constant α of the learning rate matrix P is set to 1.5.

Figure 2 shows the learning curve of SRNN, that is the changes of RMS with the number of iterations. The data in the figure is the result of repeating 10 training sessions. It can be seen from the figure that the value of RMS gradually decreased with the number of iterations. It converge after about 15 iterations, which indicates that the training speed of SRNN is faster.

Although the SRNN training converge faster, it is necessary to calculate the prediction result of SRNN under the test data in order to characterize the prediction ability of SRNN. We test the prediction results of SRNN on ammonia nitrogen and dissolved oxygen in water quality. The prediction result is shown in Figure 3. The solid line is the measured data of ammonia nitrogen and dissolved oxygen, while the dashed line is the prediction result given by SRNN. Ammonia

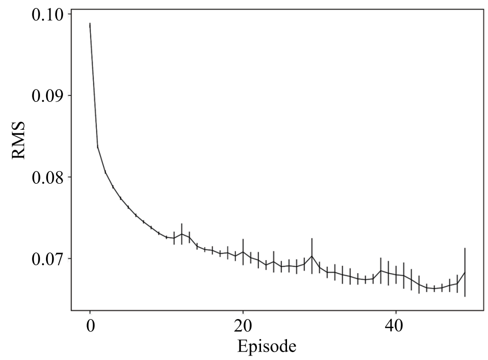

Fig. 2. RMS error for SRNN

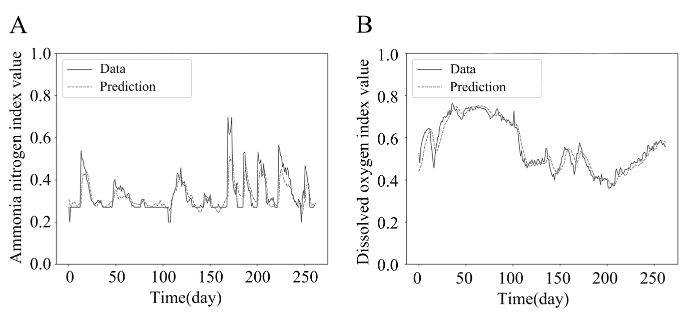

Fig. 3. Prediction results for ammonia nitrogen and dissolved oxygen using SRNN

nitrogen refers to nitrogen in the form of free ammonia (NH_3) and ammonium ions (NH_4^+) in water. The ammonia nitrogen wastewater is mainly derived from chemical fertilizer, coking, petrochemical, pharmaceutical, food, landfill and so on. The discharge of a large amount of ammonia nitrogen wastewater into the water not only causes eutrophication of the water, but also causes black odor in the water. The trend of the change of ammonia nitrogen in time in Figure 3 indices (solid line) that the change of ammonia nitrogen in water is extremely unstable and there are often mutations. The dissolved oxygen content in the water is closely related to the partial pressure of oxygen in the air and the temperature of the water. Compared with the ammonia nitrogen index in water, the change of dissolved oxygen index is relatively flat. It is not difficult to find from the prediction results in Figure 3 (dashed line) that SRNN can accurately predict these two water quality indices whether it is for the ammonia nitrogen index with mutation (Figure 3(A)) or for the relatively stable dissolved oxygen (Figure 3(B)). The prediction errors (RMS) of the two water quality indices under the test data set in Fig3 are 0.065 and 0.057, respectively.

Determining the model prediction results are often free parameters in the model, such as the number of BP network hidden layer neurons as well as the initial value of the weight and the strength coefficient g of the SRNN recurrent layer weight. The generalization ability of the SRNN network is verified by calculating the RMS under repeated tests. Let the intensity coefficient g be equal to 0.5, 1.0 as well as 1.5 and run 10 replicates for each parameter. Each repeated experiment includes two phases of training and testing. The weight of each repeated experiment SRNN is randomly selected according to a given distribution. As shown in Figure 4(A), the mean values of the test RMS under the three intensity coefficients are less than 0.08. Their respective variances are 0.0042, 0.0001 and 0.0006. This shows that SRNN can obtain better prediction results under different weight intensity coefficients. In particular, when the intensity coefficient g is equal to 1.5, the spontaneous activity of the SRNN recurrent network has chaotic characteristics [15]. But SRNN can still obtain better prediction results.

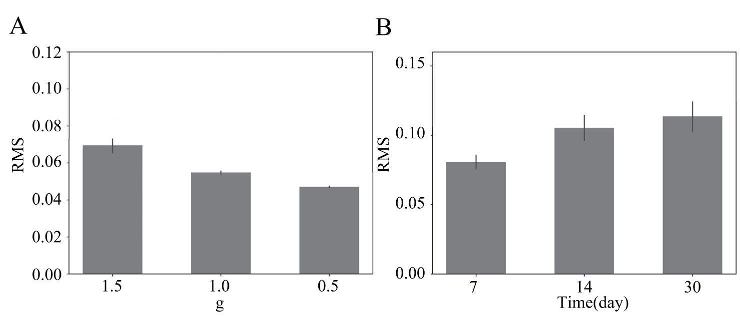

Fig. 4. Generalization ability for SRNN

The length of the SRNN input sequence has a different impact on the prediction results. As shown in Figure 4(B), the prediction results based on the time series of the previous 7 days are significantly better than the prediction results based on the time series of the first 14 days or the first 30 days.

In addition, SRNN is used to test the three water quality indices of permanganate index, total nitrogen and total phosphorus in water. The test results are shown in Figure 5. It is not difficult to see that SRNN's predictions for these three water quality indices are equally accurate.

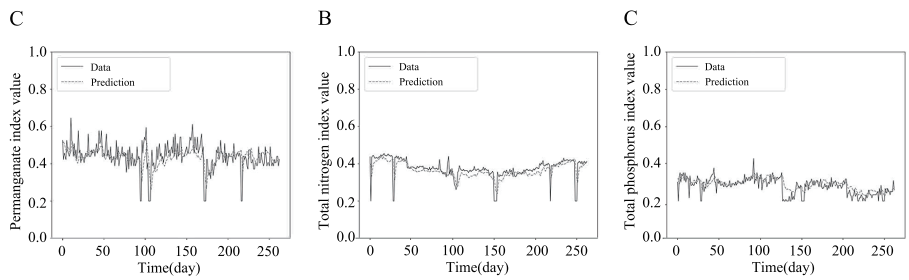

Fig. 5. Prediction results for other water quality indices

3.3 Water quality rank prediction

After successfully predicting water quality indices, SRNN will be further used to predict water quality ranks. According to the National Surface Water Environmental Quality Standard (GB3838-2002): the surface water quality rank (L) is divided into five ranks from I to V. Class I-III water meets urban drinking water standards. In order to correspond to the five ranks of water quality, the output of SRNN is modified to 5 neurons. Each neuron corresponds to a rank. The five neurons with the highest rate of release are set to the output of SRNN:

$$L = argmax_i[z_1, z_2, z_3, z_4, z_5](i = 1, 2, 3, 4, 5) \tag{10}$$

When the output result $z = [0.001, 0.089, 0.2, 1.23, 0.5]^T$ and the index i of the largest element in z is 4, then the water quality rank L predicted by SRNN is IV. In order to more accurately describe the relationship between the predicted rank and the actual rank, the relative distance D between the two ranks is also calculated to represent $e(t)$. The setting of $e(t)$ is shown in Table 1.

We use a total of 368 data sets with a 7-day monitoring interval from May 1, 2012 to April 30, 2014 during training process. We use a total of 200 data sets with a 7-day monitoring interval from May 1, 2014 to April 30, 2015 during testing process. Through 20 repeated experiments, the best correct rate of water rank prediction was 89%, as well as the average correct rate was 85.6%. At the same time, this study also tests the SRNN predict to reach the water quality

Table 1. Training error setting

D	0	1	2	3	4
$e(t)$	0	0.15	0.25	0.35	0.45

rank in the next 2 to 6 days. As shown in Figure 6, the correct rate of prediction results is above 80%.

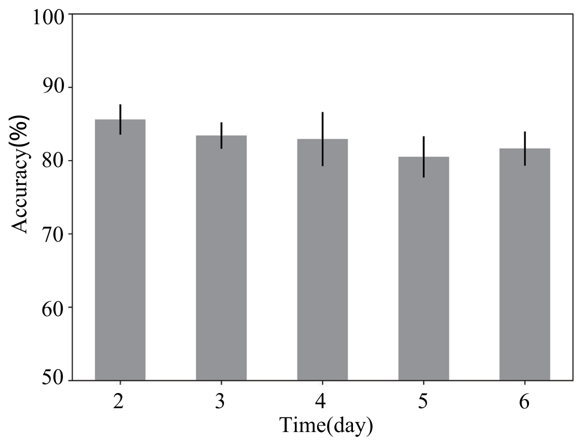

Fig. 6. Water quality rank prediction accuracy

3.4 Model comparison

The effectiveness of SRNN has been demonstrated by predicting different water quality indices and water quality ranks in a river. In the following, we will further explain that SRNN is more suitable for the prediction of water quality indices and ranks with time correlation by comparing with the prediction results of BP neural network. BP neural network model structure is a three-layer structure BP. The number of neurons in the input layer corresponds to the input length of the data. The time scale of the input data is converted together into the input of the BP network. The number of hidden layer neurons is taken as 13, and the number of neurons in the output layer is set to 1 or 5 according to the prediction task. The experiment was repeated 10 times. The comparison between the BP network and the SRNN prediction results is shown in Table 2.

Table 2. Comparison on prediction results between BP network and SRNN network

Model	RMS error value					Accuracy of next day
	AN	DO	PI	TP	TN	
SRNN	0.0342	0.0234	0.0468	0.0241	0.0244	85.6%
BP	0.066	0.1082	0.0943	0.0441	0.0662	51.75%

4 Discussion

In this study, a recurrent neural network with sparse connection features is designed to model the water quality data. The mean square recursive error algorithm is used to train the network to predict various indices of water quality and water quality ranks. The simulation results show that SRNN has better prediction ability. In particular, SRNN has few free parameters. The three weights of w^{RNL}, w^{in}, and w^{fb} only need to be randomly set according to the distribution to obtain better prediction results. This makes SRNN easier to apply to environmentally variable water quality predictions.

SRNN which is similar to Echo State Network (ESN) training only needs to adjust the weight between recurrent layer and output layer. This greatly improves the operational efficiency of the recurrent network. Since there is no need to adjust the connection weights between the neurons in the recurrent layer during learning, the recurrent layer of SRNN and ESN can be considered as a general-purpose computing unit similar to the function of the prefrontal cortex of the brain[17, 4]. Although SRNN and ESN are similar in structure, there are also essential differences between them. Firstly, SRNN's recurrent layer connection weight does not require special settings. In order to achieve reverberation, ESN requires a weight matrix with a spectral radius greater than or equal to 1. Secondly, ESN training is a kind of offline learning, that is, it needs to wait for the network to pre-calculate for a period of time before adjusting the output weight. But SRNN can update the output weights on the fly based on the current input. This feature is especially important in situations where the amount of training data is insufficient.

The good predictive performance of SRNN is not only related to its structure, but also closely related to the learning algorithm. It is not difficult to see from Equation 5 and 6 that the learning algorithm of SRNN is the same as the BP network error back propagation algorithm. However, compared to the error backpropagation algorithm, the learning process of SRNN can quickly make the network output close to the target output which mainly in the calculation of the matrix P. The matrix P is equivalent to the inverse of the correlation matrix in estimating the recurrence rate of the recurrent layer [7]. Intuitively, SRNN's algorithm can accurately adjust the weights between the neurons and the output neurons based on the activity of the recurrent layer neurons, so that the output of the output neurons quickly approaches the actual output value. In addition, SRNN has better predictive performance than BP networks commonly used for water quality prediction. Because the BP network is just a feedforward neural network, which cannot model the correlations that may existing in the input data over time. SRNN which is different from BP networks is a recurrent neural network. The existence of the recurrent layer makes it possible to establish the temporal correlation of the input data.

The prediction model proposed in this study belongs to the data-driven water quality prediction model(DDM). Compared with PDM, DDM can adapt to water quality prediction under changeable environment. However, the model constructed in DDM mode is difficult to interpret from the perspective of actual biochemical reaction between water quality indices. This makes it possible to overfit the data when applying DDM. Therefore, when applied to the prediction of water quality indices, considering the integration of PDM into DDM is a problem that needs to be studied in the future. In addition, there are many factors affecting water quality parameters and ranks, such as seasons and climate. However, this study has not add these factors to the model. Therefore, how to integrate more variables into SRNN to improve the accuracy of model prediction is a problem worthy of further study.

5 Conclusion

We design a recurrent neural network with sparse connection features for modeling water quality data. This study uses the mean square recurrent error algorithm to train the network to predict various indices of water quality and water quality ranks. The simulation results show that the method has the characteristics of wide adaptability to the model parameters and fast convergence ability. This method can be used to predict the future trends of water quality parameters and water quality ranks of rivers and lakes. The method can play an active role in intelligent modeling of river water quality, watershed planning and pollution control.

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