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

**Abstract:** It is an important prerequisite for scientific management and maintenance of water resources to accurately predict all kinds of indicators that affect water quality. *This paper proposed a method of forecasting water quality index and rank based on sparse recurrent neural network (SRNN). Based on the principle of minimum mean square recursive error, the training algorithm of the network was designed. The neural network was used to construct a water quality prediction model.* The experimental results showed that the model can be used to predict the trend of water quality in ZheJiang province.

**Keywords:** water quality modeling; water quality prediction; sparse recurrent neural network; learning algorithm

**Introduction**

With the rapid economic development and population growth, sewage and wastewater generated by the production and living of human are posing a serious threat to the water quality of lakes and rivers.[1]。There are various problems such as water shortage, water pollution and deterioration of water ecological environment in all parts of China [1], which has become the main bottleneck restricting the sustainable development of economy and society. In order to effectively solve this problem, the rational planning of water resources is particularly important. In order to effectively solve this problem, the rational planning of water resources is particularly important[2, 3]. Accurate detection of water quality parameters of rivers and lakes, as well as reasonable prediction of future changes in water quality parameters [4], is a necessary prerequisite for scientific planning of water resources. Water quality prediction is the process of constructing a water quality model using existing data and then estimating the future water quality parameters of the predicted point via the model. Common predictive models can be divided into two categories: Principle Driven Model (PDM) and Data Driven Model (DDM).

PDM is generally based on the principle of mass and energy conservation, and considers the interaction between water quality components and its own biochemical effects, and then through the construction of hydrodynamic motion and energy equations of water [5, 6]. Typical principle driven water quality models include the Streeter Phelps(SP) model for quantifying oxygen balance[7], which is often applied to simple water body self-purification; a QUAL model capable of simulating up to 15 water quality components [5], which is often used to study the impact of influent wastewater load on the water quality of the receiving river; the Water Quality Analysis Simulation Program(WASP) model of pollutant interaction[6] and the BASINS model combined with geographic information system[5, 8]. The above prediction model has been widely used in water pollution control and early warning, water quality planning and other fields because it can accurately describe the relationship between various components of water. For PMD, however, once the factors affecting water quality change, it is often necessary for domain experts to redesign the model, resulting in the lack of flexibility in the application of such water quality models.

The construction of DDM which is different from PDM does not necessarily require the participation of domain experts. It only needs to input a large amount of water quality data into a learning model, and then adjust the parameters of the learning model according to the algorithm to obtain the 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 various regression analysis based on statistical principles[9-12] and artificial neural network model[13-18] Artificial Neural Network(ANN). Because of the learning process of these models, they can be applied to various water quality prediction under the changeable environment scenarios.

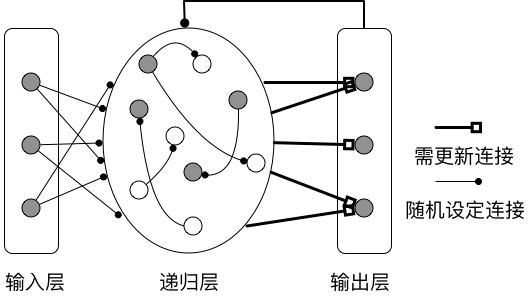
In order to obtain higher prediction accuracy, the ANN model commonly used in DDM often needs a large number of historical water quality data, and then automatically learns the water quality prediction model to meet the demand according to the historical data. However, the Back Propagation(BP) network 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[19]. BP network is difficult to simulate the time correlation between water quality data. To this end, this study based on the latest theoretical research results of the prefrontal cortex in neuroscience[20, 21], through the construction of a sparsely connected large-scale recurrent neural network and the recursive least mean square error algorithm to quickly learn the water quality data mode. The accuracy of the model was verified by predicting the water quality indicators such as ammonia nitrogen, dissolved oxygen, permanganate index, total phosphorus and total nitrogen in a reservoir.

**1 Water quality model**

This study used a sparsely connected 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 recursive network will exhibit chaotic characteristics [17]. This feature makes the network have 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 [18].

**1.1 SRNN network structure**

As shown in Figure 1, the SRNN contains three parts, an input layer y, a recursive layer x, and an output layer z. Vector **y** = [*y*1, *y2,…, y*m]Trepresents the input layer neuron activity, where *yi* is the input water quality indicator and the superscript T is the transpose.

Figure 1 Structure of SRNN

Neuronal activity level is represented by recursion x, whose activity was calculated by the formula:

(1)

Among them, **r** = tanh(**x**) represents the rate of release of recurrent layer neurons and tanh is a hyperbolic tangent function as well as the activation function of recursive layer neurons. is the neuron activity decay constant.

represents the recursive connection matrix between neurons in the recursive layer. Since the recursive layer has *N*=1000 neurons, is a matrix of size 1000×1000. The element in the matrix represents the connection weight between the i-th neuron and the j-th neuron in the recursive layer. The recursive layer is a sparse connection, and sets the probability of to a non-zero value and the probability of to zero.

This means that only a few of the reciprocal layer neurons have a mutual connection. The value of the non-zero element of is randomly selected from the Gaussian distribution Norm(0, g^2/pN), where is the intensity coefficient of weight. When , the recursive layer neurons will have the spontaneous activity of chaotic characteristics [17].

represents the connection matrix between the input layer and the recursive layer.

The weights are randomly selected according to the Gaussian distribution *Norm*(0, 0.5). is the connection weight of the output neuron feedback back to the layered neuron, 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 .

**z** is the output layer neuron activity, corresponding to the predicted output, and its calculation is determined by:

(2)

represents the connection matrix between the recursive layer and the output layer. The recursive layer and the output layer are fully connected, and the weights are randomly assigned according to a uniform distribution between [-1, 1]. is different from , , and . Its element values need to be updated during the learning phase, while the values of , 、, and remain unchanged during the learning period.

As can be seen from the structure of SRNN, it is similar to the Echo State Network (ESN) [22].

They all have a recursive layer and the learning process only adjusts the weight between the recursive layer and the output layer. However, SRNN and ESN also have the following differences. First of all, the SRNN's recursive 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.

**1.2 SRNN learning algorithm**

According to the description of SRNN in the previous section, the recursive 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 ，r. The error between them is .

(3)

The learning algorithm is to adjust the output weight from to so that the error is gradually reduced. After the output weight is updated, the output error of the network becomes:

***.*** (4)

After the algorithm converges, the value of should go to 1 and . 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 recursive least mean square error algorithm [23], the output weights are adjusted as follows:

(5)

Equation 5 shows that the decision to update the output weight is the error , the distribution rate ***r*** of recurrence of the recursive network neurons, and the matrix ***P***(*t*).

The function of matrix ***P***(*t*) is equivalent to the learning rate, which is used to determine the size and scale of weight 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 is carried out in the following way:

(6)

needs to have an initial value in the first step of the algorithm, and then update it every step according to Equation 6. The initial value of is set to **I**/α where **I** is a unit matrix of 1000 x 1000, and α is a constant.

**2 Experimental result**

**2.1 Water quality data preparation**

This paper selects the water body data of a reservoir in Zhejiang from May 2012 to May 2015. The data source is the actual value of the water detection by the automatic monitoring station every 4 hours. Dissolved oxygen, permanganate index, ammonia nitrogen, total phosphorus and total nitrogen, were selected to evaluate the water quality grade. 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 when the water body is most stable 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 anomaly data, it need to calculate:

(7)

Where is the characteristic data of the Grubbs criterion test. is the data to be tested. is the arithmetic mean of the data set. S is the standard deviation of the data set If is bigger than , it is judged that the data is an abnormal value. The critical value is determined by the Grubbs table. It is related to the detected level σ = 0.05 and the number n of data of the test data set.

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

(8)

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

**2.2 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 error RMS:

(9)

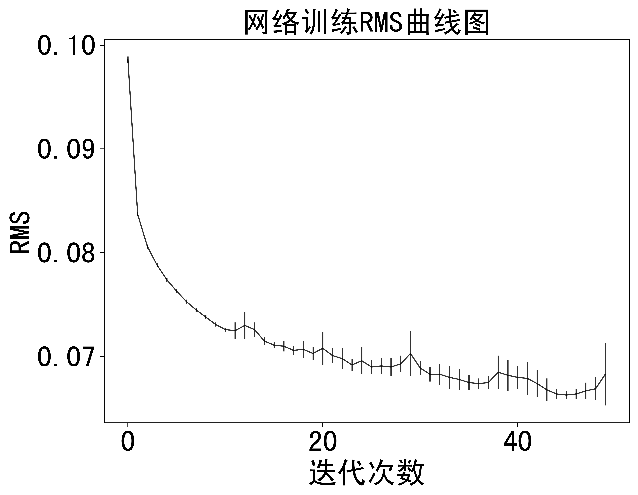


Figure 2 Learning curve for SRNN

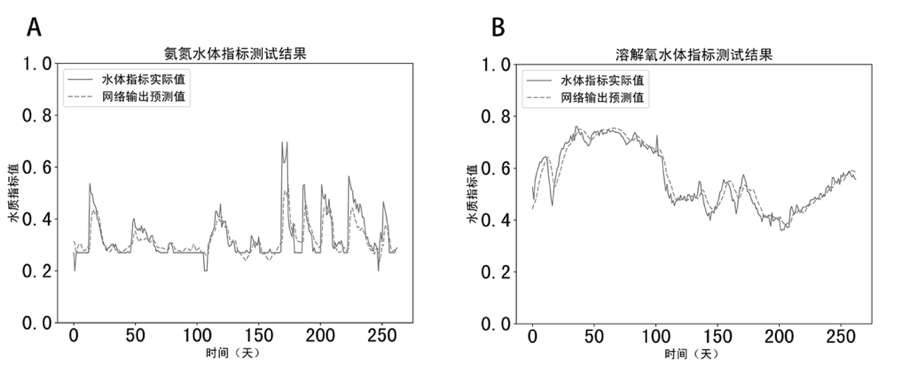


Figure 3 Prediction results for ammonia and dissolved oxygen using SRNN

and are network estimates and real values. *te* and *ts* are the start time and end time. The training results of the ammonia nitrogen index are selected to examine the convergence of SRNN. The number of recursive 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 change 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 decreases with the number of iterations. It converges after about 15 iterations, which indicates that the training speed of SRNN is faster.

Although the SRNN training converges faster, it is necessary to calculate the prediction result of SRNN under the test data in order to characterize the prediction ability of SRNN. To this end, we test the prediction results of SRNN on ammonia nitrogen and dissolved oxygen in water quality. The predicted result is shown in Figure 3. The solid line is the measured data of ammonia nitrogen and dissolved oxygen, while the dotted line is the predicted result given by SRNN. Ammonia nitrogen refers to nitrogen in the form of free ammonia (NH3) and ammonium ions (NH4+) 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 body, but also causes black odor in the water. The trend of the change of ammonia nitrogen in time in Figure 3 indicates (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 indicators 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) for the two water quality indicators in Figure 3 against the test data set were 0.065 and 0.057.

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 recursive 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 recursive network has chaotic characteristics [17]. But SRNN can still obtain better prediction results.

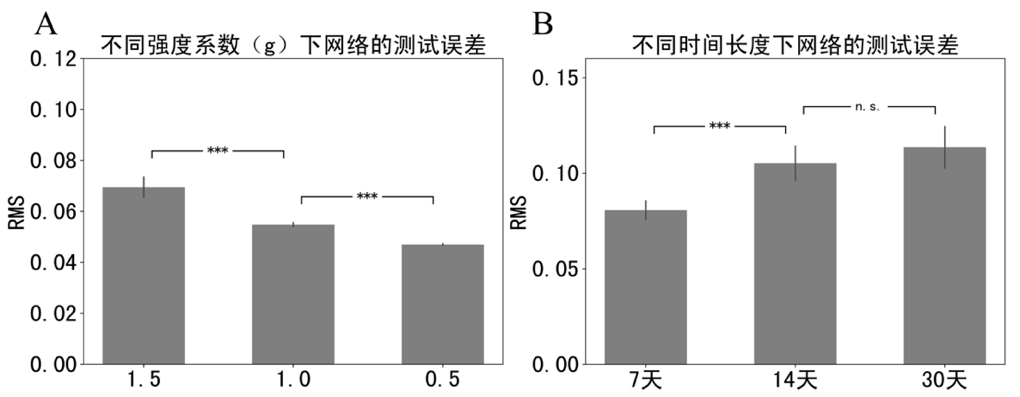


Figure 4 Generalization for SRNN

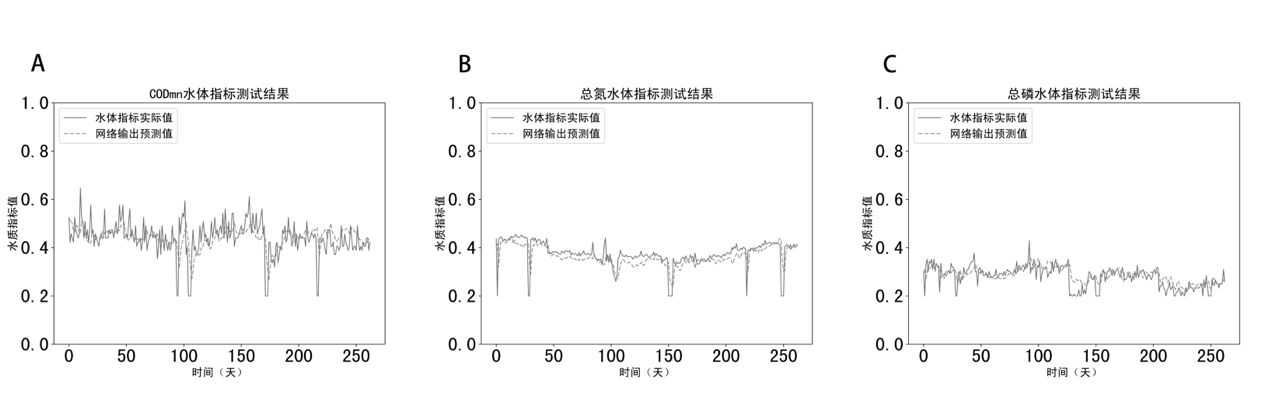


Figure 5 Prediction results for other water quality indicators

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 was used to test the three water quality indicators 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 indicators are equally accurate.

**2.3 Water quality level prediction**

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

(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 level *L* predicted by SRNN is IV. In order to more accurately describe the relationship between the predicted level and the true level, the relative distance *D* between the two levels is also calculated to represent . The setting of is shown in Table 1.

Table1 Training error setting

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| *D* | 0 | 1 | 2 | 3 | 4 |
|  | 0 | 0.15 | 0.25 | 0.35 | 0.45 |

使用2012年5月1日至2014年4月30日监测区间为7天的数据集共368组进行训练，再使用2014年5月1日至2015年4月30的数据集共200组进行测试验证。通过20次重复实验，得到水体等级预测的最佳正确率为89%，平均正确率为85.6%。同时，还测试了SRNN预测未来2天到6天之后到水质等级，预测结果的正确率都在80%以上（如图6所示）。

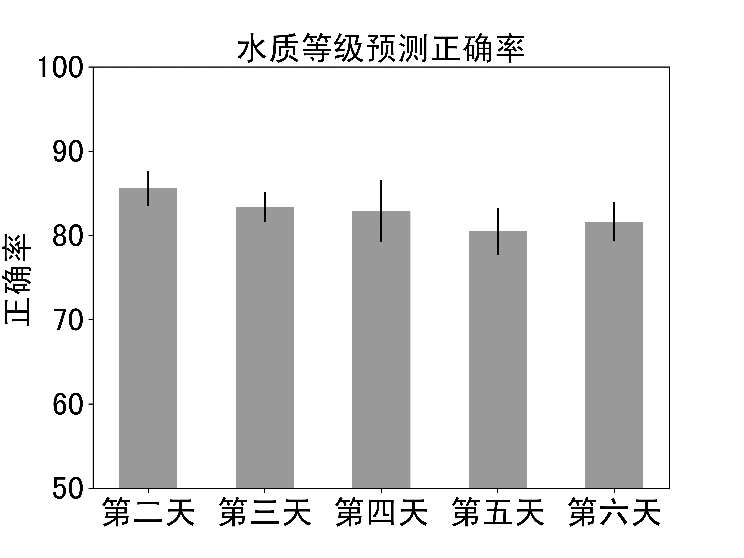


图6 SRNN预测水质等级

Figure 6 Predict water quality level using SRNN

**2.4 模型比较[[1]](#footnote-1)**

通过预测水体中不同的水质指标和水质等级，已经证明了SRNN的有效性。下面将通过与BP神经网络的预测结果的比较，进一步说明SRNN更适用于具有时间相关性的水质指标和等级的预测。BP神经网络模型结构为三层结构，输入层的神经元个数对应数据的输入长度。这里将输入数据的时间尺度一起转化为BP网络的输入。隐藏层神经元个数取为13，而输出层的神经元个数根据预测任务分别设为1或者5。重复10次实验，得到BP网络与SRNN预测结果的比较如表2所示。

**3 讨论**

本研究通过设计具有稀疏连接特征的递归神经网络，用于对水质数据的建模，利用均方递归误差算法训练网络从而预测水质的各种指标和水质等级。仿真结果表明，SRNN具有较好的预测能力。尤其是， SRNN的自由参数少，且、和这三组权重只需要按照分布随机设置就能获得较好的预测结果，这使得SRNN更易于应用于环境多变的水质预测。

SRNN与回声网络ESN类似，网络的训练都只需要调整递归层与输出层之间的权重，这大大提高了递归网络的运行效率。由于不需要在学习的时候调整递归层内部神经元之间的连接权重，可以将SRNN与ESN的递归层看作与大脑前额叶皮层的功能类似的通用计算单元[20, 21]。尽管SRNN与ESN在结构上有相似的地方，但它们之间也存在本质的不同。首先，SRNN的递归层连接权重并不需要特别设置，而ESN为了实现回响需要权重矩阵的谱半径大于等于1。其次，ESN的训练是一类离线学习，即需等待网络预先运算一段时间后才可调整输出权重，而SRNN则可根据当前的输入即时更新输出权重。这一特性在训练数据量不足的情况尤其显得重要。

SRNN所具备的良好预测性能，不仅与它的结构有关，更与它采用的学习算法密切相关。从式(5)和式(6)不难看出，SRNN的学习算法与BP网络误差反向传播算法一样都属于监督学习。然而，相比较于误差反向传播算法，SRNN的学习过程能很快的使得网络输出接近目标输出，主要在于矩阵***P***的计算。矩阵***P***相当于在估计递归层发放率的相关矩阵的逆[23]，直观而言就是SRNN的算法能精确根据递归层神经元的活性，调整它们与输出神经元之间的权重，从而使得输出神经元的输出快速接近实际输出值。此外， SRNN比常应用于水质预测的BP网络有更好的预测性能。这主要是由于BP网络只是一个前馈神经网络，它不能对输入数据在时间上可能存在的相关性进行建模。与BP网络不同，SRNN是递归神经网络，递归层的存在使得它能建立输入数据在时间上的相关性。

本研究提出的预测模型属于数据驱动的水质预测模型DDM。相比较于PDM，DDM能适应环境多变情况下的水质预测。然而，DDM模式下构建的模型难以从水质指标间真实的生化反应这一角度进行解读。这使得在应用DDM时，存在过度拟合数据的可能。因此，在应用于水质指标预测时，考虑将PDM融入到DDM中是今后需要研究的问题。此外，影响水质参数和等级的因素众多，比如季节和气候等。然而，本研究并未将这些因素加入到模型中，因此如何融入更多的变量到SRNN中，从而提

表2 BP网络与SRNN网络预测结果比较

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

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| 模型 | RMS误差值 | | | | | 第二天水质等级预测正确率 |
| 氨氮 | 溶解氧 | 高锰酸盐 | 总磷 | 总氮 |
| SRNN网络 | 0.0342 | 0.0234 | 0.0468 | 0.0241 | 0.0244 | 85.6% |
| BP网络 | 0.066 | 0.1082 | 0.0943 | 0.0441 | 0.0662 | 51.75% |

高模型预测的准确性是值得进一步研究的问题。

**4 结论**

本研究通过设计具有稀疏连接特征的递归神经网络，用于对水质数据的建模，利用均方递归误差算法训练网络，从而预测水质的各种指标和水质等级。仿真结果表明，该方法具有对模型参数设定适应范围广和收敛速度快的特点。采用该方法可对河流、湖泊的水质参数和水质等级的未来变化趋势进行预测，该方法可在河流水质的智能化建模、流域规划和污染控制等方面发挥积极作用。

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1. 本文SRNN代码公开在https://github.com/weather319/SRNN. [↑](#footnote-ref-1)