

Review

A Review of the Artificial Neural Network Models for Water Quality Prediction

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Abstract: Water quality prediction plays an important role in environmental monitoring, ecosystem sustainability, and aquaculture. Traditional prediction methods cannot capture the nonlinear and non-stationarity of water quality well. In recent years, the rapid development of artificial neural networks (ANNs) has made them a hotspot in water quality prediction. We have conducted extensive investigation and analysis on ANN-based water quality prediction from three aspects, namely feedforward, recurrent, and hybrid architectures. Based on 151 papers published from 2008 to 2019, 23 types of water quality variables were highlighted. The variables were primarily collected by the sensor, followed by specialist experimental equipment, such as a UV-visible photometer. Five different output strategies, namely Univariate-Input-Itself-Output, Univariate-Input-Other-Output, Multivariate-Input-Other(multi)-output, Multivariate-Input-Itself-Other-Output, and Multivariate-Input-Itself-Other (multi)-Output, are summarized. From results of the review, it can be concluded that the ANN models are capable of dealing with different modeling problems in rivers, lakes, reservoirs, wastewater treatment plants (WWTPs), groundwater, ponds, and streams. The results of many of the review articles are useful to researchers in prediction and similar fields. Several new architectures presented in the study, such as recurrent and hybrid structures, are able to improve the modeling quality of future development.

Keywords: ANNs; feedforward; recurrent; hybrid; water quality prediction

1. Introduction

Water quality plays an important role in any aquatic system, e.g., it can influence the growth of aquatic organisms and reflect the degree of water pollution [1]. Water quality prediction is one of the purposes of model development and use [2], which aims to achieve appropriate management over a period of time [3]. Water quality prediction is to forecast the variation trend of water quality at a certain time in the future [4]. Accurate water quality prediction plays a crucial role in environmental monitoring, ecosystem sustainability, and human health. Moreover, predicting future changes in water quality is a prerequisite for early control of intelligence aquaculture in the future [5]. Therefore, water quality prediction has great practical significance [6].

At present, there are many traditional water quality prediction methods, such as multiple linear regression (MLR) [7], auto-regressive integrated moving average (ARIMA) [8], etc. MLR is not able to detect a nonlinear relationship between water quality parameters because of its linear inherence [9].

The main drawback of ARIMA is the pre-assumption of the linear model [10]. During the model identification phase, the time series data must be checked to see whether they are stationary or not, because it is critical in creating the ARIMA model. In fact, traditional methods are not able to capture the non-linear [11] and non-stationarity [12] of water quality well due to their complex and sophisticated nature.

With the increase in data scale, traditional techniques cannot meet the demand of researchers. Owing to the improvement of computing power, artificial neural network (ANN) models, data-driven models, have been further developed. They can capture functional relationships among the water quality data from the examples [13]. When the underlying relationships of obtained data are difficult to describe, ANN models still work. Moreover, ANNs require fewer prior assumptions [14] and can achieve higher accuracy [15] compared with traditional approaches. In addition, ANNs are suitable for solving the non-linear and uncertain problems due to their similar characteristics with the brain nervous system [4], and have become a hotspot in water quality research [16].

ANNs are a family of models inspired by biological neural networks [17] which specifically refers to the human brain [18], a kind of central nervous system of animals. In general, ANN can be represented as a system of interconnected “neurons” [19] which form the basis of neural network operation. Weight parameters and activation functions are part of the neurons [20]. ANNs are generally divided into three layers of input, hidden and output. When neurons receive information from different inputs, they obtain nonlinearity through activation functions. ANN models depend heavily on the quantity of data [21]. Therefore, it is not recommended to use relatively small data sizes for predictors (inputs). This is because some useful information is lost in short-term data, which may lead to poor prediction results [3]. In addition, data dividing is a necessary step in the modeling process. Furthermore, choosing the training algorithm to calibrate the model parameters (e.g., connection weights) is a vital step so that the network can approximate complicated non-linear input-output relationship [10]. The Levenberg–Marquardt [22] algorithm and the back-propagation (BP) algorithm [23] are the most commonly used algorithms.

ANN models architectures determine the number of connection weights and the way information flows through the network [20]. The most widely used architecture is Multilayer Perceptron (MLPs) with only three layers in many types of feedforward ANNs. Radial Basis Function neural networks (RBFNNs) [24], General regression neural networks (GRNNs) [25] and Extreme learning machines (ELMs) [5] are three typical feedforward ANNs. A Long Short-Term Memory (LSTM) neural network is an improvement of recurrent neural networks (RNNs), which aims to address the well-known vanishing gradient problem [26]. The hybrid models in this review are three classes: model-intensive, technique-intensive, and data-intensive [27]. The emerging frameworks, such as Convolutional Neural Network (CNN) [28], widely used in the field of the image, are also included in this review.

In this review, ANN models for water quality variables prediction are summarized. Previous reviews [20,27,29] about ANNs are more concerned about the water quantity (e.g., flow and rainfall-runoff) prediction, while less attention has been paid to water quality prediction (e.g., Suspended solids (SS)), and the major scenarios they investigated are river systems. At the same time, previous reviews care about the development of the model while ignoring the output strategies between input(s) and output(s) in a given prediction task. To overcome the limitations above, this review focuses on the use of ANNs methods for water quality prediction, with more water quality variables investigated than previous reviews, which are mainly divided into three categories, namely chemical, biological and physical variables [30].

The research scenarios include not only the river system that was the focus of the previous review, but also reservoirs, lakes, wastewater treatment plant (WWTP), groundwater, etc. It must be pointed out that the review did not consider drinking water systems. The reason for this is that drinking water is a system that includes source, treatment, and distribution, and should be considered as an independent branch or subject for systematic research [30]. In addition to the increased number of water quality variables reviewed and broader research scenarios, this review also summarizes five

output strategies. The period of the investigated papers covered was from 2008 to 2019. This period was chosen as it follows on from the period covered in the review by [27] (i.e., 1999–2007). The review is organized as follows. Section 2 presents the process of the paper collection. Section 3 describes three basic model structures in water quality prediction. In Section 4, the applications of artificial neural networks in water quality are surveyed. Then, Section 5 represents the results of this review. Finally, the discussions are given in Section 6. All the abbreviations are mentioned in Table 1.

Table 1. The abbreviations in this review.

Abbreviations	Full Name	Abbreviations	Full Name	Abbreviations	Full Name	Abbreviations	Full Name
AH	air humidity	EC	Electrical conductivity	ORP	Oxidation reduction potential	TCC	total chromium concentration
AODD	August, October, December, data	Evap	evaporation	Q	discharge	TIC	total iron concentration
AP	air pressure	FTT	flow travel time	pH	Pondus Hydrogenii	TAC	total anions and cations
AT	air temperature	Fe	iron	Precip	precipitation	TNs	total nutrients
As	Arsenic	F	flow	P	phosphate	TA	total alkalinity
B	boron	HCO ₃	bicarbonate	RH	relative humidity	TP	total phosphorus
BOD	Biochemical Oxygen Demand;	HA	Hydrogenated Amine	RP	Redox potential	Tur	turbidity
C	carbon	ICs	ionic concentrations	RO	runoff	TDS	total dissolved solids
Cl	chloride	K	potassium	RF	rainfall	TN	total nitrogen
Cu	Copper	Lon	longitude	RainP	Rainy period	TH	total hardness
Ca	calcium	Lat	latitude	SR	solar radiation	TOC	total organic carbon
CO ₃ ²⁻	Carbonate	LV	lake volume	Sth	sunshine time hours	TSS	total suspended solids
Coli	Coliform	MDHM	month, day, hour, minute	SD	transparence	VP	volatile phenol
COD	Chemical Oxygen Demand	Mn	manganese;	SAR	sodium absorption ratio	WL	Water Level
COD _{Mn}	permanganate index	Mg	magnesium	SM	Soil Moisture	WT	water temperature
Chl-a	Chlorophyll a	Na	sodium	ST	soil temperature	WS	wind speed
DO	dissolved oxygen	Ns	nutrients	SO ₄	sulphate	WD	wind direction
DOY	day of year	NO ₂	nitrite	S	salinity	YMDH	the year numbers

2. Methods

This review focuses on the application of ANNs to water quality variables prediction excluding drinking water from 2008 to 2019. The papers to be reviewed were selected using the following steps:

1. First, we identified ANN-related papers in influential water-related and environmental-related journals to ensure that high-quality papers are included in the review. These papers are mainly from journals whose subjects are environmental science and ecology, water resources, engineering and application.
2. Thereafter, a keyword search of the ISI Web of Science was then conducted for the period 2008–2019 using the keywords; water quality, river, lake, reservoir, WWTP, groundwater, pond, prediction, and forecasting, accompanied by the names of ANN methods (one or more), such as neural network, MLP, RBFNN, GRNN, RNN, to name but a few.
3. Then, through the search process from 1 to 2, 151 articles in English relevant to our focus were selected. The basic information of the papers, including authors (year), locations, water quality variables, meteorological factors, other factors, output strategy, data size, time step, data dividing, methods, and prediction lengths are provided in Appendix A.

3. Three Basic Model Structures in Water Quality Prediction

In this review, the model architecture refers to the overall structure and manner of how information flows from one layer to another. The three model architectures include feedforward, recurrent networks, and hybrid models (see Figure 1) [31]. In addition to categorizing each architecture, Table 2 summarizes the foundation and advantage(s) of the development model structure.

3.1. Feedforward Architectures

The term ‘feed-forward’ means that a neuron connection only exists from a neuron in the input layer to other neurons in the hidden layer or from a neuron in the hidden layer to neurons in the output layer. However, the neurons within a layer are not interconnected [9]. MLPs with only three layers are the most widely used architectures [59] in many types of feedforward ANNs (see Figure 2), followed by BPNNs [37] which use the back-propagation algorithms to train networks. Other commonly used feed-forward network architectures in water quality prediction include TDNNs [36], RBFNNs [60], GRNNs [61], WNNs [62], ELMs [5], CCNN [63] and MNN [50].

Feedforward	<ul style="list-style-type: none"> MLPs, RBFNNs, GRNNs, ELMs, Wavelet neural networks (WNNs), Cascade correlation neural network (CCNN), Modular neural networks (MNNs), Time Delay Neural Networks (TDNNs)
Recurrent	<ul style="list-style-type: none"> RNN, LSTM, Elman, Nonlinear Autoregressive with exogenous input (NARX),SRU, Time-lag recurrent network (TLRN), Echo state network (ESN), Ridge regression echo state network (RESN)
Hybrid	<ul style="list-style-type: none"> model intensive: e.g. fuzzy wavelet neural network (FNN-WNN), LSTM-RNN technique intensive: e.g. ARIMA-RBFNNs, ARIMA-ANN data-intensive: e. g. wavelet-artificial neural network (WANN), Principal component analysis with back-propagation networks(PCA-BPNN), K-means-MLP, empirical mode decomposition(EMD)-BPNN, particle swarm optimization(PSO)-BPNN
Emerging methods	<ul style="list-style-type: none"> CNN, Deep belief network(DBN), Self-organizing deep belief network (SODBN)

Figure 1. Three main model architectures in the reviewed papers.

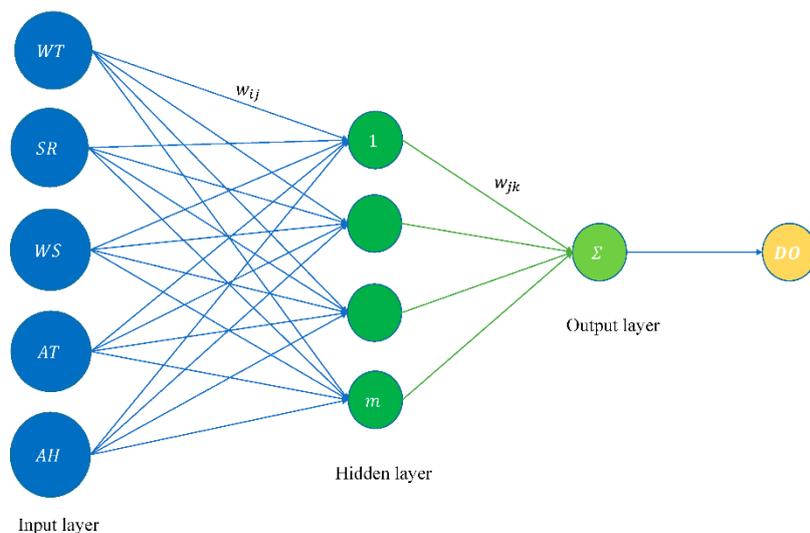


Figure 2. The common architectures of MLPs.

Table 2. The developments and advantages of different ANNs architectures.

Categories	Structure(s)	Advantage(s)	Reference(s)
MLPs	They are based on an understanding of the biological nervous system	Solving the nonlinear problems	[19,23,30,32–35]
TDNNs	They are based on the structure of MLPs	Using time delay cells to deal with the dynamic nature of sample data	[36]
RBFNNs	The structure of RBFNNs is similar to the MLPs The radial basis activation function is in the hidden layer	To overcome the local minimum problems	[5,18,37,38]
GRNNs	A modified form of the RBFNNs model There is a pattern and a summation layer between the input and output layers	Solving the small sample problems	[24,39–43]
WNNs	Wavelet function replace the linear sigmoid activation functions of MLPs	Solving the non-stationary problems	[16,44]
ELMs	The structure of ELMs is similar to the MLPs Only need to learn the output weight	Reducing the computation problems because the weights of the input and hidden layer need not be adjusted	[31,45–48]
CCNN	Start with input and output layer without a hidden layer	A constructive neural network that aims to solve the problems of the determination of potential neurons which are not relevant to the output layer	[49]
MNNs	A special feedforward network Choosing the neural network which have the maximum similarity between the inputs and centroids of the cluster	Solving the problem of low prediction accuracy	[30,50]
RNNs	The RNNs are developed with the development of deep learning	Solving the problems of long-term dependence which are not captured by the feedforward network	[12,31,38,51,52]
LSTMs	Its structure is similar to RNNs Memory cell state is added to hidden layer	Addressing the well-known vanishing gradient problem of RNNs	[15,26,45,53,54]
TLRN	Its structure is similar to MLPs It has the local recurrent connections in the hidden layer	Reducing the influence of the noise and owning the advantage of adaptive memory depth	[55]
NARX	Sub-classes of RNNs Their recurrent connections are from the output	Solving the problems of long-term dependence	[12]
Elman	A context layer that can store the internal states is added besides the traditional three layers	It is useful in dynamic system modeling because of the context layer	[3]
ESN	Different from the above recurrent neural networks The three layers are input, reservoir, and readout layer	To overcome the problems of the local minima and gradient vanishing	[3]
RESN	They are based on the structure of ESN which has a large and sparsely connected reservoir	To overcome the ill-posed problem existing in the ESN	[3]
Hybrid methods	The combination of conventional or preprocess methods with ANNs The internal integration of ANN methods or	Exploring the advantages of each methods	[56]
CNN	Input, convolution, fully connection, and output layers	An emerging method to solve the dissolved oxygen prediction problem	[57]
SODBN	They are based on the structure of DBN whose visible and hidden layers are stacked sequentially	Investigating the problem of dynamically determining the structure of DBN	[58]

TDNNs is a subclass of MLPs that learns temporal behavior from continuous past and present signals [36]. The major difference between RBFNNs and MLPs is that the hidden layer of RBFNNs is self-organizing while the latter is not, although the structure of RBFNNs is similar to MLPs. As the center of RBF, the training weights can be defined by a clustering algorithm. For example, the k-means algorithm is a commonly used one [24]. GRNNs is a modified form of the RBFNNs model, but it differs from RBFNNs in structure. Pattern and summation layers are located between the input and output layers [27]. The training between the input and pattern layer of GRNNs is equivalent to the research on the input and hidden layer of the RBFNNs. WNNs have made some changes based on the traditional MLPs, in which the non-linear sigmoid activation functions is replaced by the Morlet wavelet function commonly used in the WNNs hidden layer. Therefore, WNNs are suitable for solving non-stationary time series problems [64]. The biggest innovation of ELMs is the random selection of hidden nodes and the use of a least squares method to determine the output layer weight. CCNN is different from the above feedforward networks because it constructs the neural network without a hidden layer at first and automatically adds hidden units instead of fixing the network architectures and then training the weights and thresholds. The first step of MNN, a special feedforward network, is data clustering using the fuzzy c-means method [65]. The second step is updating the clusters by adding the new datasets. To achieve better prediction accuracy, a neural network with the maximum similarity between the inputs and centroids of the cluster is chosen.

3.2. Recurrent Architectures

Compared with feedforward ANNs, RNNs differs in that neurons within a layer are interconnected and allow feedback [53]. Different types of RNNs are developed so that the neural networks have better memory ability (see Figure 1). LSTM, an improvement over RNN, adds a processor called “memory cell state” to its hidden layer to determine whether the information is useful or not [66], and this is also suitable for SRU (Simple Recurrent Unit) [67]. Furthermore, the forget gate also determines what information should be discarded from the cell state [66]. TLRN has a similar structure to MLPs, but has local recurrent connections in the hidden layer (see Figure 3), with the advantages of low noise sensitivity and adaptive storage depth [55]. NARX networks are also sub-classes of RNNs and can be utilized to establish a long-term temporal relationship. The recurrent connections of NARX networks come from the output (see Figure 3) [12]. In addition to the input, hidden, and output layers, the Elman neural network has a context layer to store the internal states [3]. The Elman neural network is sensitive to the historical information of inputs because of the self-connections of the context nodes (see Figure 3). The three layers of ESN are different from the above recurrent neural networks. The three layers are input, reservoir, and readout layer. The feature of the reservoir layer is randomly and sparsely connected. The echo state property whose internal states are particularly dependent on the inputs is the key to the ESN. To overcome the ill-posed problem existing in the ESN, an RESN method using the ridge regression algorithm instead of linear regression to calculate output weights is proposed [38].

3.3. Hybrid Architectures

There is a growing tendency to use hybrid ANNs models, which play a huge role in modeling, for their ability to integrate with other conventional and more advanced modeling techniques [68], to create flexible and efficient models in recent years (see Figure 1). Hybrid models are divided into three categories, namely model-intensive, technique-intensive, and data-intensive [27]. The model-intensive approaches model the sub-components of the whole physical system and aggregate the overall response of each model. Relevant forms, such as LSTM-RNN [26] or FNN-WNN [69], are model-intensive methods. The core of the technique intensive methods is to develop a modeling framework that is able to take advantage of different technologies. Methods that combine ensemble approaches [32] or time series models that remove trends or periodicities like Autoregressive Integrated Moving Average-Radial Basis Function neural networks (ARIMA-RBFNNs) [70] or ARIMA-ANN [71] are

technique-intensive methods. In this review, data-intensive approaches are to combine different technologies to preprocess the data. Wavelet analysis approaches such as WANN [72] can provide some useful information about the physical structure of the data. ANNs models the approximation and details component from the discrete wavelet transformation (see Figure 4). Dimensionality reduction methods such as PCA can reduce the dimension of the input data space to prevent redundancy [73]. Then, ANNs models some aggregative indices obtained by PCA (see Figure 4). Clustering methods [50] such as K-means-MLP [43] identify the data belonging to a particular class. Other data-intensive approaches include decomposition [5] and evolution-related [16] methods. ANN models the Intrinsic Model Function (IMF) obtained from the decomposition of complicated signals.

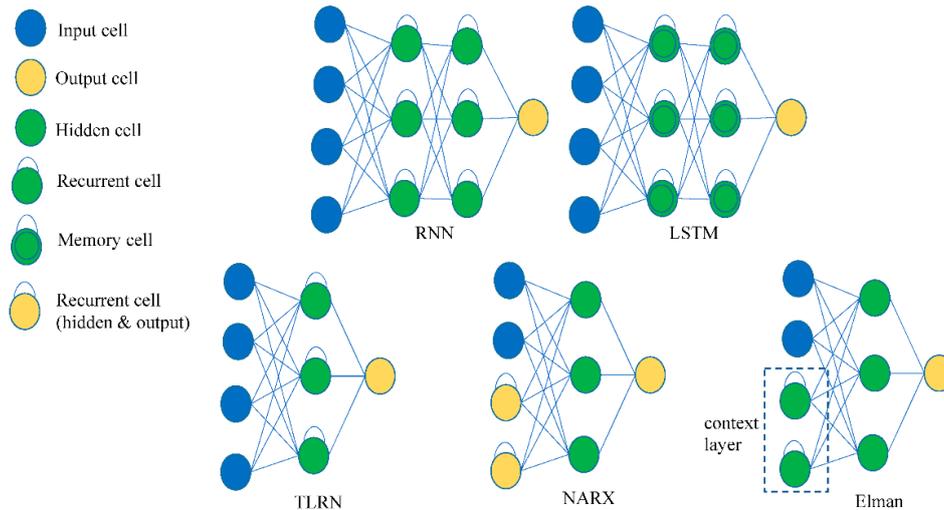


Figure 3. Five categories of recurrent model architectures.

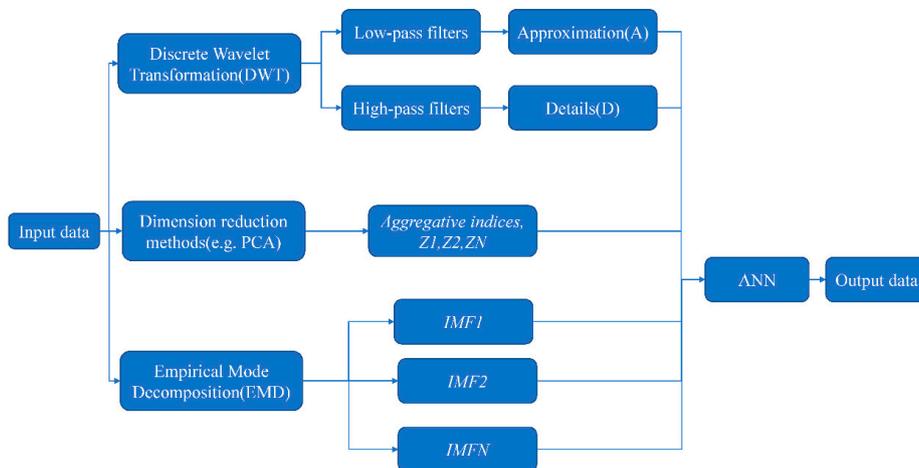


Figure 4. The modeling process of three data-intensive approaches.

3.4. Emerging Methods

CNN is a feed-forward neural network, primarily used in the image field. Input, convolution, pooling, full connection, and output layers are the basic elements of the traditional CNN. In recent years, CNN has been used as an emerging method in water quality prediction. The operation of convolution can be implemented more than one time to reveal the relationship between the parameters hidden in the input matrix [57]. However, since the purpose of the prediction model is to extract potential factors rather than simply raise the convolutional layer’s results to a higher level, the pooling layer is removed (see Figure 5). In the meantime, the number of calculations can be reduced.

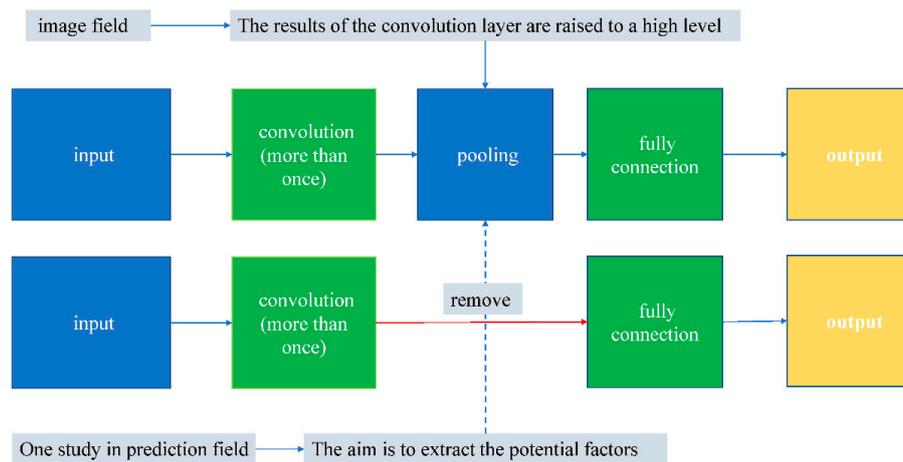


Figure 5. The architecture of a Convolutional Neural Network.

Deep belief network (DBN) is a kind of neural network based on deep learning which is similar to feedforward structure and has been widely used in recent years. The blue virtual box in Figure 6 shows several visible and hidden layers, stacked in order to make up the DBN [74]. However, the researches about dynamically determining the structure are seldom investigated. To overcome the limitations above, a SODBN has been proposed. The structure of the SODBN is not determined by artificial experience but the automatic growing and pruning algorithm (AGP) [58]. Especially, the hidden layers and neurons are changed by the AGP at first. Then, the weights of the SODBN are continuously adjusted in the process of self-organization. Finally, some aspects of network performance, such as running time and prediction accuracy have been improved.

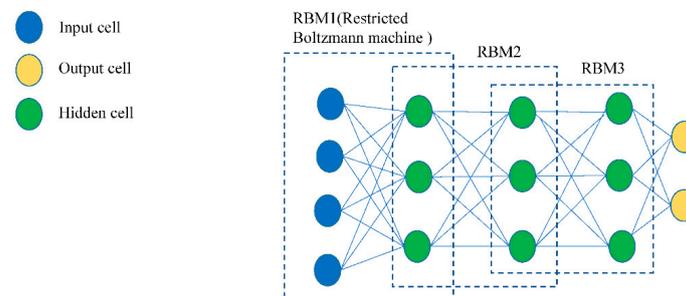


Figure 6. The architecture of deep belief network.

4. Artificial Neural Networks Models for Water Quality Prediction

From 2008 to 2019, the use of the ANN technique has been very popular in the field of water quality prediction. Many researchers have utilized ANNs to model and predict water quality. Dogan et al. [75] adopt ANN to predict the BOD, which is difficult to measure and needs at least five days to get the final results in WWTP. Results showed that COD was the most effective variables on BOD estimation after conducting the sensitivity analysis. Elhatip and K m r [76] revealed that ANN techniques depend on using more input data to solve the water quality problems, although they did not illustrate the size of the appropriate datasets. Palani et al. [40] tested MLP and GRNN models with various input selected by stepwise constructive methods for multistep prediction of S, DO, and Chl-a. They pointed out that the limited data set was one of the drawbacks of their research and encouraged others to collect more data to recalibrate and revalidate the model. Wang et al. [19] employed a typical three-layer of MLP structure [77–89] with the BP algorithm to achieve Chl-a prediction. They divided the dataset into training (75%) and testing parts (25%). Results indicated that ANNs could establish a stable and effective model for Chl-a prediction. This result is also suitable for other parameters

prediction. Yeon et al. [90] evaluated ANN, MNN, and adaptive neuro-fuzzy inference system (ANFIS) performance in 1-h and 2-h ahead prediction of DO and TOC. They added Q to inputs because rainfall affected the water quality prediction. It was found that using the Levenberg–Marquart algorithm to train the MNN could provide the least error and better results. Dogan et al. [91] divided the data into training (60%), validation (20%), and testing sets (20%). They adopted a sensitivity analysis method to find out the important water quality parameters and excluded fewer influence variables, resulting in a compact network. Miao et al. [92] used BPNN to COD and ammonia nitrogen (NH₃-N) prediction. The whole datasets were normalized at first and then divided into training (80%) and testing (20%) sets. The sigmoid transfer function that can establish the random nonlinear map between inputs and outputs were adopted. Oliveira Souza da Costa et al. [93] divided the data into training (50%), validation (25%), and testing sets (25%). Shen et al. [94] employed a golden section method to select the hidden layer nodes of BPNN. Singh et al. [95] investigated the partition approach in evaluating the relative importance of eleven environmental variables to the output layer. They divided the datasets into training (60%), validation (20%), and testing sets (20%). Results showed that the predicted values of the ANN model were close to the measured value. Yeon et al. [96] combined Precip and Q to realize a one-step prediction of Q. Then, the connected system utilized the prediction value of Q and historical TOC to fulfill the one-step prediction of TOC. Finally, the connected system had better performance than a single ANN model. Zuo and Yu [97] pointed out that ANN models could process complex and multivariable problems. Akkoyunlu and Akiner [98] verified the feasibility of ANN technique, data-driven models, in predicting DO. Results showed that the ANN method was superior to the nonlinear regression (NLR) technique. Chen et al. [99] scaled the datasets to lie between 0 and 1 [9,16,59,62,100–104] so that it could be compatible with the sigmoid transfer functions used in the hidden layer and applied the constructive and pruning of stepwise methods that aim to maximize the model's performance through a constant adjustment to surface water quality prediction. Markus et al. [105] purely relied on a trial-and-error approach to determine the model structure and dividing the data into training (50%) and testing sets (50%). Result found that ANN could improve the forecast accuracy of NO₃ compared with previous studies. Merdun and Çinar [106] preprocessed the data set by normalization and moving average techniques. They improved the representation of the acquisition data through a data preprocessing technique. Ranković et al. [107] used a sensitivity analysis method to determine the influence of input variables on outputs and found out that 15 hidden neurons gave the best choice. Zhu et al. [108] not only predicted the water quality using ANN models but also introduced a remote wireless monitoring system. Banerjee et al. [109] checked that ANN models were an accurate alternative to the numerical methods. They used quick propagation algorithm to realize super linear convergence speed. Han et al. [110] demonstrated the effectiveness of a flexible structure RBFNN which using neuron activity and mutual information (MI) to add or remove hidden neurons to reduce network complexity and improve computational efficiency. The connected weights are trained by an online learning algorithm. Zare et al. [10] used a UV-visible photometer to measure the NO₃ concentration in the laboratory.

Asadollahfardi et al. [111] utilized Q to forecast TDS when TDS was not available. Al-Mahallawi [77] revealed that the reason why ANN models could model complex water quality phenomena was that they provided a non-linear function mapping from input to corresponding network outputs. Ay and Kisi [112] divided the data into training (50%), validation (25%), and testing sets (25%). In the three parts of data division, the validation set can be implemented more than once to monitor whether the model is overfitting or not. Comparison results showed that the RBNN model performed better than MLP in DO prediction. Baek et al. [50] chose the neural network of MNN, which has the maximum similarity between the inputs and centroids of the cluster, to solve the problem of low prediction accuracy. They introduced Gradient descent with momentum and Levenberg–Marquardt backpropagation (TRAINLM) to train the neural network. Bayram et al. [79] used the one-year Tur data whose time step is fortnightly to achieve the prediction of SS. Gazzaz et al. [113] scaled the data into the scope between 0 and 1 and utilized cross-validation to improve the generalization ability

and limit the overfitting problem. Cross-validation was suitable for the situation where the size of the training data was small or the number of parameters in the model was large. Overfitting refers to the situation that when the error on the training set is driven to a very small value, the test data are presented to the network with a large error. That means the network has memorized the training examples, but it has not learned to generalize to new situations. Hong [78] took the AT, AP, WD, and WS variables measured by meteorological station into account. They divided the data samples into training (70%) and testing (30%) sets. Results indicated that MLP also could deal with large data samples. Liu and Chen [114] recorded the location information to complete the three-dimensional DO prediction. Tota-Maharaj and Scholz [22] assessed the influence of bp, Levenberg–Marquardt, Quasi-Newton, and Bayesian Regularization algorithms on BOD prediction. Results showed that the combination of bp and ANN had low minimum statistical errors. Kakaei Lafdani et al. [115] firstly used M-test to obtain several data points through the winGamma software. Then, the genetic algorithm (GA) method was implemented to make the best combination which extracted from a list of possible inputs as inputs. Karakaya et al. [116] conducted research, namely temporal partitioning, to divide the data into diel, diurnal, and nocturnal in order to obtain continuous records, and chose MLP as a prediction model. Antanasijević et al. [117] utilized Monte Carlo simulation (MCS), a sensitivity analysis method that involves repeatedly generating a probability distribution of random input values, to ultimately create an ANN model with fewer inputs. Moreover, other input selection techniques include correlation analysis and genetic algorithm were tested. Chen and Liu [118] utilized sigmoid and linear transfer function in the hidden and output layer, respectively. Results showed that ANFIS and BPNN could predict DO with reasonable accuracy. Han et al. [119] adopted linear interpolation whose data increment was calculated by the slope of the assumed line to fill the missing data. Then, hierarchical ELM based on a hierarchical structure was chosen to model the DO, pH, and SS. The advantage of hierarchical ELM is able to learn sequential information online. Results demonstrated the effectiveness of the proposed methods. Researchers tended to divide the training set data into 70% to 90% of the total data [39,42,49,52,72,120–127]. Iglesias et al. [35] divided the data into training (90%) and testing sets (10%). Then, they applied three typical MLP architectures to complete the Tur prediction whose inputs were $\text{NH}_3\text{-N}$, EC, DO, pH, and WT. Kılçaslan et al. [128] randomly divided the datasets and pointed out that when the data tended to be roughly periodic after a year, the time length of data acquisition, covering a long period such as a year or more was highly recommended in order to capture long-term variation. Yang et al. [129] found the most significant parameters by using analysis of variance (ANOVA) techniques. Result indicated that rainfall records were the most significant parameters for turbidity forecasting. Khashei-Siuki and Sarbazi [130] took the normalization step to control the scale of each feature, in the same range in case the difference of the order of magnitude will lead to the dominance of larger attributes thereby slowing down the iterative convergence. However, they did not give clear details about normalization. Gholamreza et al. [36] used time delay cells of TDNNs, designed based on the structure of MLPs, to deal with the dynamic nature of sample data. Then, they applied factor analysis to select the model inputs. Results illustrated that TDNN with 2 hidden layers of 15 neurons in each of the layers was the best architecture. Nourani et al. [9] provided a new solution to EC and TDS prediction. When the predictive variables were not available, researchers could realize the final predictions through modeling other relevant variables. They utilized monthly meteorological data RF, RO, and WL to forecast EC and TDS due to the lack of historical records of outputs. Zounemat-Kermani [82] introduced a Quasi-Newton method, Broyden–Fletcher–Goldfarb–Shanno (BFGS), to train the parameters of MLP in SS forecasting. Hameed et al. [60] conducted the sensitivity analysis of the obtained data and scaled it to between 0.1 to 0.9. Results indicated that RBFNN could achieve high-performance accuracy. Heddami and Kisi [47] utilized open-source data from Eight United States Geological Survey stations (USA) and preprocessed the data by standardization method. Several ELM models are applied for DO prediction. Yousefi [131] discussed the Garson method to find the relative importance of each input variable. Results indicated that including meteorological and hydrologic variables could improve the accuracy of the models

with fewer influential variables. Elkiran et al. [32] and Najah et al. [132] demonstrated the feasibility of the ANFIS method in predicting river water quality. This model overcame the shortcomings of ANN models such as overfitting and local minima, and combined fuzzy logic with ANN to provide a method to solve uncertain problems. Sinshaw et al. [133] took interrelated and easily measurable parameters of pH, EC, and Tur, as inputs to realize TN and TP predictions.

Liu et al. [3] pointed out that if more historical data were available [15], ANN models may provide better predictions than a relatively small data set. Antanasijević et al. [41] tested the performance of RNN, GRNN, and MLP in small samples prediction. Results indicated that the error of RNN in test data was less than 10%. Besides, the error of GRNN was lower than MLP. Evrendilek and Karakaya [55] deleted the missing data directly. Then, discrete wavelet transforms (DWT) with the orthogonal wavelet families was applied to denoise the data measured by proximal sensors. The result indicated that the modeling effect of using TLRN to the data after noise reduction was superior to TLRN, TDNN, and RNN. Chang et al. [12] attempted to use NARX, a dynamic neural network, to model ten-year seasonal water quality data. Then, 42-fold cross-validation was used to divide the data. Results demonstrated that the NARX network outperformed BPNN because it could capture the important dynamic features of TP data. Wang et al. [6] tested the prediction performance of LSTM, BPNN, Online sequential (OS)-ELM in DO, and TP. The results indicated that LSTM was more accurate and generalizable than the above feedforward ANNs. Zhao et al. [38] used an improvement of the ESN, namely RESN, to predict the BOD and TP. This new method used the ridge regression algorithm to calculate the output weights to solve the ill-posed problem existing in the ESN. Hu et al. [66] fully preprocessed the acquired water quality data. They firstly imputed, corrected, and denoised the data by using linear interpolation, smoothing which could attenuate high-frequency signals, and moving average filtering techniques. Then, correlation analysis, which belongs to analytical methods, was carried out. The LSTM was adopted for model establishment. Experimental results showed that the prediction accuracy was high and could reach 98.97% and LSTM was suited for long-term prediction. J. Liu [67] introduced Back-propagation through time (BPTT) to train the SRU model. The main difference between SRU and RNN is the “cell state” part added in the hidden layer. They proposed an Improved mean value method to solve the breakpoint phenomenon of the mean value method and the linear interpolation method. Results showed that the prediction error was small, within the range of 1%. Lim et al. [53] converted the irregular data into daily data by using a linear interpolation method and provided a solution to abnormal data identification. They used a fixed threshold method to set the upper and lower threshold ranges and proved that linear interpolation had better robustness than spline interpolation, nearest-neighbor interpolation, and cubic interpolation according to model results when water quality changed dramatically. Results showed that the removal of abnormal data beyond the threshold value could preliminarily improve the data convergence.

Partal and Cigizoglu [134] decomposed the measured SS data into wavelet components via DWT. The DWT-ANN method could more accurately approximate the peak values, which have lesser distributions compared with non-peak values. Anctil et al. [135] applied MLP to forecast daily SS and NO₃ without considering missing data. They applied a self-organizing map (SOM), a stratified method, to construct a topological map to visualize the clustered input variables, thereby ensuring that the statistical properties of the subsets were similar. Levenberg–Marquardt algorithm [24,136–139] and Bayesian methods were conducted to train the network. Results showed that ANN models could achieve high accuracy. Sahoo et al. [140] used the SR and AT meteorological data to achieve the WT prediction. They introduced micro-genetic algorithms (u GA), a creep mutation in small populations, to update the weights. Wu et al. [141] reported that the GA-BP algorithm whose relative errors were below 35% was more suitable for TP, TN, and Chl-a prediction than simple multivariate regression analysis. Kişi [142] utilized neural differential evolution (NDE) models, a combination of neural networks and differential evolution approaches, to model SS. The result showed that NDE has a low mean square error. Ömer Faruk [71] investigated the performance of ARIMA-ANN in WT, DO, and B prediction. Afshar and Kazemi [143] combined PSO and ANN methods in water quality parameter

prediction. Han et al. [1] used cross-correlation and mutual information to select the input to achieve the prediction of BOD and DO, respectively. The conjugate gradient algorithm was carried out to train the model. Areeerachakul et al. [144] presented two cluster technique, namely K-means, fuzzy c-means (FCM) in DO prediction. Results indicated that the performance of hybrid methods was better than single models. Y. Wang [64] designed a missing–refilling scheme which divided the data into incidental missing (ID) and structural missing (SD). Then, a temporal exponentially moving average was applied to fill the missing data. They investigated the time relationship of the DO, NH₃-N univariate time series using a bootstrapped wavelet neural network (BWNN). Aleksandra and Antanasijevi [42] used the databases of the European Statistical Office and World Bank to complete the BOD prediction. Ay and Kisi [43] integrated k-means clustering and MLP in daily COD concentration modeling by using SS, pH, and WT. Result indicated that this hybrid methods performed better than MLP, RBFNN, and two different ANFIS approaches (subtractive clustering and grid partition). Ding et al. [120] collected 23 water quality parameters and considered the problems of data dimensionality. Therefore, the PCA techniques was used to compress the original data into 15 aggregative indices. Then, the GA approach was applied to optimize the parameters of BPNN. The result showed that the average prediction accuracy was up to at least 88%. Gazzaz et al. [145] developed a data mining method, namely re-sampling, to solve the unbalance problem. Heddam [146] recommended collecting more than one-year water quality data, because they wanted to include all four seasons in the validation and testing phases. Liu et al. [147] proposed a hybrid model, namely empirical mode decomposition (EMD)-BPNN. BPNN predicted each sub-series which are IMFs and the residue decomposed by EMD. The results demonstrated that a hybrid model could capture the non-stationary characteristics of WT after EMD. Qiao et al. [44] scaled the datasets between -1 and 1 and then used phase space reconstruction (PSR) of chaos theory to extract much more information from BOD datasets. Results showed that the hybrid model, namely chaos theory-PCA-ANN, had high prediction accuracy. Sakizadeh et al. [73] applied early stopping which is fit for small networks and datasets to determine the model structure.

Yu et al. [148] utilized 5-fold cross-validation to divide the data and applied RBFNN to fuse data from multiple sensors. The convergence rate and the solution accuracy could be improved through the variant of PSO (IPSO). The comparison of prediction results validated the effectiveness of the hybrid model. Zhao et al. [149] converted the signal into an output linear system by the Kalman filter. The result showed that this hybrid method was a good and effective approach to water quality prediction. Huang et al. [69] simulated the nonlinearity of data by the combination of the neural network, fuzzy logic, wavelet transform, and the GA. Results showed that this hybrid model could handle the problems of data fluctuation. Li et al. [123] adopted the most extreme form of K-fold cross-validation, namely leave-one-out cross-validation to divide the datasets. Zhang et al., 2017 [16] divided the dataset into training (98%) and testing sets (2%) and adopted the PSO algorithm to accelerate the training speed of WNN. Karaboga proved that artificial bee colony (ABC) algorithms were more precise than GA and PSO [150]. Chen et al. [4] proposed an improved method of ABC (IABC) which added the optimal and global optimal solution to the updated formulas. The result indicated that the limitation of the method above was that water quality data needed to obey the normal distribution appropriately. Li et al. [54] used sparse auto-encoder (SAE) to pre-train the hidden layer data because SAE contained deep latent features. Qiao et al. [58] determined the structure of DBN by growing and pruning algorithms instead of artificial experience (SODBN). Results showed that SODBN could short running time and improve accuracy. Ta and Wei [57] applied Adam optimization method which could handle sparse gradients on noisy problems to train the parameters of CNN. Zhou et al. [151] focused on the Improved Grey Relational Analysis (IGRA) method which calculated the similarity and proximity by relative area change ratio. Fijani et al. [5] used variational mode decomposition (VMD) algorithm to decompose the highest frequency component produced by a complete ensemble empirical mode decomposition algorithm with adaptive noise (CEEMDAN). ELM was applied for modeling. Results indicated that this hybrid model could reduce error whether in root mean square or mean absolute error. Jin et al. [152] proposed an improvement variant namely

improved genetic algorithm (IGA) to avoid the situation where excellent individuals are discarded by the GA. Li et al. [15] introduced evidence theory, that has good data fusion ability, since it is able to reason with uncertainty to synthesize the evidence from SRU, Gated Recurrent Unit (GRU), LSTM sources in DO, pH, TP prediction, and eventually reached a certain level of belief. The improved probability assignment function of the evidence theory, designed based on the softmax function, could solve the failure of weight allocation problems existing in the traditional probability assignment function. As a general framework of uncertain reasoning, the application of evidence theory can be further extended. Tian et al. [153] combined transfer learning (TL) and ANNs approaches which do not require a large amount of training data because TL has the ability to transfer knowledge from past tasks to predict Chl-a dynamics. The biggest difference between TL and traditional ANNs methods is that the former does not need to learn each task from scratch while the latter does. Results indicated that the hybrid models enhanced the generalization ability compared with the dropout and parameter norm penalties methods in the long-term application. At the same time, the impact of mutable data distribution on the models was decreased. Yan et al. [154] utilized mean value method using a median of k data before and after to correct wrong data and got the missing data by the values of model prediction of other water quality variables at the missing point. The restricted condition of the model was that the data were appropriately and normally distributed. Therefore, it is uncertain whether the above method can be applied to other prediction tasks that do not meet the above conditions. Yan et al. [68] proposed a hybrid optimized algorithm, namely PSO and GA, to optimize BPNN with reasonable accuracy. Y. Liu [45] investigated the DO prediction, which considered a temporal and spatial relationship. Spatial relationship refers to the spatial correlations between external variables instead of the geographic distributions. The newly proposed attention-RNN model achieved excellent performance whether in short-term and long-term prediction. Zounemat-Kermani et al. [63] tested the performance of decomposition approaches, DWT and VMD, in DO prediction. They concluded that these two methods are an alternative tool for accurate prediction when the input was combination III and model was MLP.

5. Result

The year of the publication is analyzed at first. Figure 7 plots the number of articles published from 2008 to 2019 each year. There is a growing number of publications since 2008 that use the ANN models to predict the water quality, including above 50% of the papers published since 2015, despite the fact that there are some fluctuations in the quantity of papers—which was in decline in 2010 and 2011. The increasing popularity of ANNs in the field of water resources [155] and environmental engineering [16] may be explained by the major advantage of the ANNs—that researchers can utilize them to model nonlinear and complex phenomena even if they do not fully understand the underlying mechanisms [156]. The popularity of ANNs above is also in agreement with the observations of other researchers [27,30]. Moreover, the number of papers for different prediction variables is summarized in Figure 8. The majority of the reviewed papers used chemical water quality variables, such as DO, BOD, and COD as outputs [30] in the systems of the river, lake, and WWTP. Furthermore, attention was also directed towards physical variables like pH, WT, and biological variables such as Chl-a.

The number of diverse forecast lengths is shown in Figure 9. The forecast length in this review refers to the length of time to predict in advance. For example, if researchers used the historical data of the previous three days to predict the values of the current day, then the forecast length would be 1 [157]. However, 107 papers did not provide details about the forecast length which cast ambiguity and doubts to researchers in parameter settings [31]. It seems ideal to utilize ANN models to capture short-term (length = 1) relationships, as the process was carried out 30 times in 44 papers which provide details about the forecast length, while only 10 papers consider long-term (length > 1) forecasting.

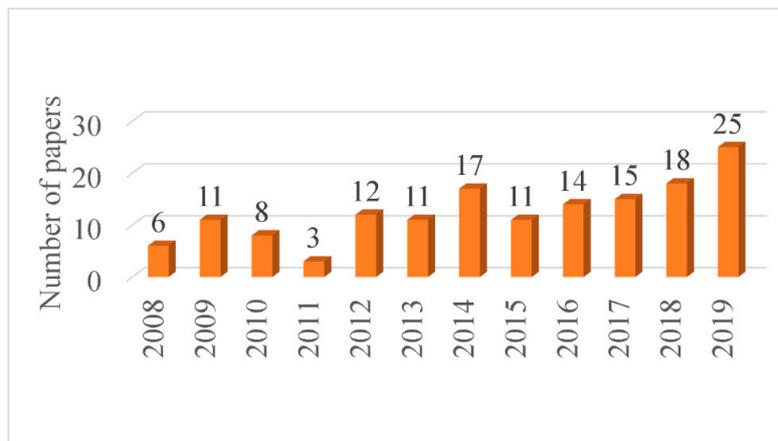


Figure 7. The distribution of papers between 2008 and 2019.

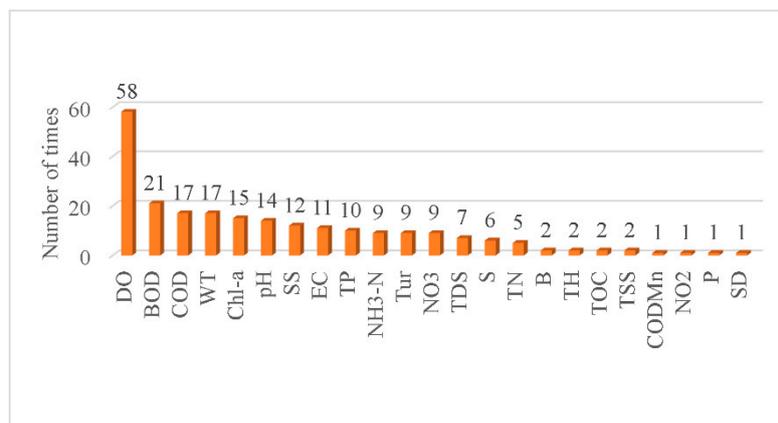


Figure 8. Number of papers for different prediction variables.

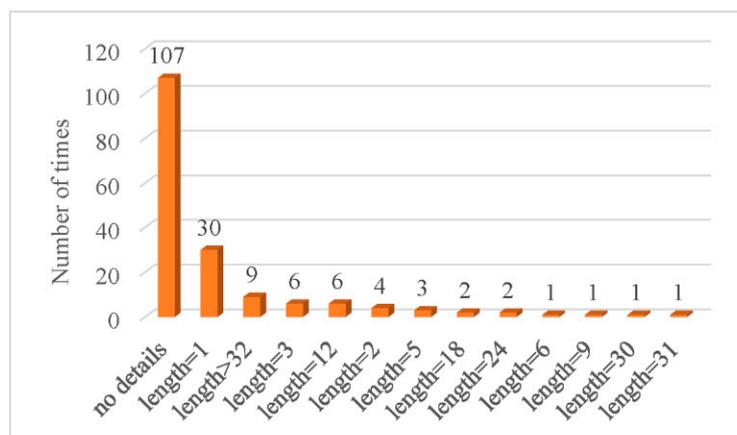


Figure 9. The distribution of prediction lengths.

As mentioned in the Introduction, this review not only includes more water quality parameters but also more extensive research scenarios compared with the previous reviews. On the whole, there are 23 types of water quality variables examined in this review. They are mainly physical, chemical, and biological variables. In the field of water quality prediction, relatively mature sensors include DO, WT, Chl-a, pH, EC, and NH₃-N. There are different application scenarios among the investigated water quality variables. Table 3 summarizes the main application scenarios of various water quality variables. Researchers conducted more prediction studies on DO, WT, Chl-a, pH, EC, NH₃-N, Tur, and S than other water quality variables. It can be seen from Table 3 that there are simple and practical

sensors that can measure these water quality variables. Therefore, the extensive research of the above variables may benefit from the wide application of these sensors [148].

Table 3. Basic information of water quality variables.

Water Quality Variables	Categories	Unit	Major Sensors	Research Scenarios
DO	chemical	mg/L	✓	river, lake, reservoir, WWTP, ponds, coastal waters, creek, drain
BOD	chemical	mg/L	-	river, lake, WWTP, mine water experimental system
COD	chemical	mg/L	-	river, lake, reservoir, WWTP, groundwater, mine water
WT	physical	°C	✓	river, lake, ponds, catchment, stream, coastal waters
Chl-a	biological	µg/L	✓	lake, reservoir, surface water, coastal waters
pH	physical	none	✓	river, lake, WWTP, stream, coastal waters
SS	physical	mg/L	-	river, stream, coastal waters, creek, catchment
EC	physical	us cm ⁻¹	✓	river, lake, reservoir, groundwater, stream
TP	physical	µg/L	-	river, lake, WWTP
NH ₃ -N	chemical	mg/L	✓	river, lake, reservoir, groundwater experimental system
Tur	physical	FNU	✓	river, stream
NO ₃	chemical	mg/L	-	river, groundwater, catchment, wells, aquifer experimental system
TDS	physical	mg/L	-	river, groundwater, drain
S	physical	psu	✓	groundwater, coastal waters
TN	chemical	mg/L	-	lake, WWTP, coastal waters
B	physical	mg/L	-	river
TH	physical	mg/L	-	river
TOC	chemical	mg/L	-	river
TSS	physical	mg/L	-	river
COD _{Mn}	chemical	mg/L	-	river
NO ₂	chemical	mg/L	-	groundwater
P	physical	mg/L	-	experimental system
SD	physical	cm	-	lake

Table 4 summarizes the data set sizes of feedforward and recurrent neural networks involved in this review. According to Table 4, the number of samples applied for water quality prediction varies from 28 [39] to 45,594 [78] which illustrates the fact that ANN models are capable to deal with different size of the dataset. However, there has been no research studying the optimal amount of data required for each ANN model. As can be seen from Table 4, the recurrent neural networks [55] generally need more datasets compared with feedforward neural networks [139]. Research into the water quality parameter prediction have focused on rivers, WWTP, lake, and reservoir. In contrast, researchers have done little on artificial facilities, such as stream and pond. In the river system, most researchers use feed-forward neural networks for modeling, which may be due to the fact that the river system can be well analyzed using only the feed-forward neural network. This result also applies to WWTP systems. In the lake system, recurrent neural networks have shown significant results. These two kinds of neural networks have applications in reservoirs. In contrast, feed-forward neural network can predict water quality with relatively little data. In addition to being able to perform prediction tasks, GRNN is also suitable for small data sets (28, 32, 61, 151, 159, 265 samples) compared with other types of ANNs [24,39–43], so researchers should pay some attention to it.

Table 4. Datasets of feedforward and recurrent neural networks.

Categories	Authors (Year)	Methods	Scenario (s)	Time Step	Dataset (Samples)
Feedforward	[39]	GRNN, BPNN, RBFNN	lake	weekly	28 (6 months)
	[40]	ANN(MLP), GRNN	coastal waters	No details	32 (5 months)
	[59]	BPNN	river	No details	39 (3 days)
	[158]	ANN	mine water	No details	73
	[97]	ANN	groundwater	No details	97
	[106]	ANN(MLP)	surface water	No details	110
	[159]	MLP	river	No details	110 (8 hours)
	[130]	ANN(MLP)	plain	No details	122
	[128]	ANN	groundwater	monthly	124 (1 year)
	[80]	ANN(MLP)	stream	No details	132 (11 months)
	[79]	ANN(MLP)	basin	fortnightly	144 (1 year)
	[131]	ANN(MLP)	river	monthly	144 (12 years)
	[121]	RBFNN	river	weekly	144
	[24]	GRNN, ANN(MLP), RBFNN, MLR	river	monthly	More than 151 samples (6 years)
	[42]	GRNN, MLR	Open-source data	No details	159 (9 years)
	[160]	ANN(MLP)	river	monthly	164 (over 6 years)
	[107]	ANN	reservoir	No details	180 (3 years)
	[22]	ANN	system	No details	195 (4 years)
	[161]	ANN(MLP), RBFNN	river	monthly	200 (17 years)
	[139]	ANN	river	No details	200 (16 years)
	[93]	ANN	river	No details	232 (3 years)
	[63]	CCNN, MLP	river	half a month	232 (12 years)
	[122]	ANN	river	No details	252 (21 years)
	[113]	ANN(MLP)	river	No details	255 (7 months)
	[43]	ANN(MLP), RBFNN, GRNN	WWTP	daily	265 (3 years)
	[119]	ELM	WWTP	daily	360
	[75]	ANN	WWTP	daily	364 (1 year)
	[118]	BPNN	reservoir	No details	400 (20 years)
	[94]	BPNN	NA	No details	500
	[95]	ANN	river	monthly	500 (10 years)
	[10]	ANN	groundwater	30 minutes	818 (nearly 17 days)
	[162]	BPNN	river	No details	969
	[77]	MLP, RBE, GRNN	Well	No details	975 (16 years)
	[163]	ANN(MLP)	stream	daily	982 (6 months)
	[88]	MLP	lake	No details	1087 (6 years)
	[133]	ANN	lake	No details	1217
	[127]	RBFNN, GRNN, MLR	river	No details	More than 1300 samples (6 years)
	[36]	RBFNN, TDNN	river	monthly	1320 (10 years)
	[117]	GRNN	river	No details	1512 (9 years)
	[50]	MNN	WWTP	No details	1900
	[83]	ANN(MLP), RBFNN	river	daily	2063 (6 years)
	[137]	ANN	river	No details	3001
	[112]	RBFNN, ANN(MLP), MLR	upstream and downstream	daily	2063 and 4765 samples (18 years)
	[115]	ANN	river	daily	more than 3000 samples (11 years)
	[116]	ANN	lake	15 minutes	6674 (86 days)
	[164]	ANN	river	No details	13,800 (5 years)
	[25]	GRNN	river	No details	more than 32,000 samples
	[47]	ELM, ANN(MLP)	Open-source data	hourly	35,064 (4 years)
[78]	ANN(MLP)	power station	10 minutes	45,594 (2 years)	

Table 4. Cont.

Categories	Authors (Year)	Methods	Scenario (s)	Time Step	Dataset (Samples)
Recurrent	[41]	Elman, GRNN, BPNN, MLR	river	monthly or semi-monthly	61
	[12]	NARX, BPNN, MLR	river	monthly	280 (11 years)
	[26]	LSTM	river	12 hours	460 (14months)
	[6]	LSTM, BPNN	lake	monthly	657 (7 years)
	[66]	LSTM, RNN	Mariculture base	5 minutes	710 (21 days)
	[67]	SRU	Mariculture base	No details	710
	[3]	Elman	pond	No details	816 (34 days)
	[153]	RNN, LSTM	reservoir	5 minutes	1440 (5 days)
	[15]	RNN, BPNN	river	No details	1448
	[165]	LSTM	lake	No details	1520
	[54]	LSTM, BPNN	pond	10 minutes	2880 (20 days)
	[38]	RESN	WWTP	No details	5000
	[45]	RNN	Freshwater	10 minutes	5006 (1 year)
	[55]	TLRN, RNN, TDNN	lake	15 minutes	13,744 (573 days)
[154]	LSTM	WWTP	hourly	23,268 (4 years)	

The artificial neural network has been widely used in water quality prediction. If researchers only look at the modeling process, various studies follow some of the steps of the modeling framework below (see Figure 10).

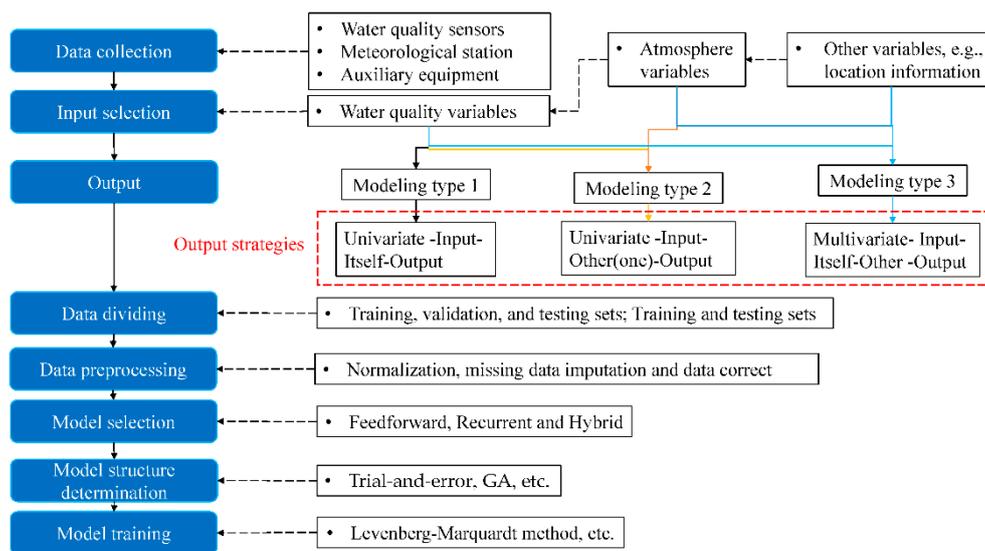


Figure 10. General framework for water quality modeling.

5.1. Data Collection

The data collection process is not easy due to the requirement of costly measuring instruments (e.g., water quality sensors, meteorological stations), laboratory equipment, and good operating conditions. Water quality variables are primarily collected by the sensors. Meteorological variables, such as AT, WS, RF, SR, Precip, and AP, often influence water quality. Therefore, some researchers took the meteorological station to obtain the data. In addition, some parameters, such as BOD, COD, need to be measured by auxiliary laboratory equipment [44]. Location information is essential when researchers want to make a three-dimensional prediction of water quality. In the above case, the required data is obtained through the device (see Figure 10). In some studies [42,47], the researchers conduct studies based on an open-source dataset.

Based on the obtained data, researchers can perform three modeling types. The first type of modeling is where the researcher models only historical information about the output variable.

The second type of modeling is when the output variables are difficult to measure, and the researchers can use easily measured water quality or meteorological data to complete the prediction. In the first two modeling types, the researchers utilized univariate historical information. However, for the third type of modeling, the researchers used multivariable historical information. Overall, the researchers utilized water quality, atmosphere, and other variables such as location data for the prediction task. The above three modeling types are analyzed from the perspective of data. If analyzed from the perspective of studying the temporal and spatial relationship between input and output, the above modeling types can be further divided.

5.2. Output Strategy

The output strategies can be further divided into five categories based on the three modeling types (see Figure 10). Temporal relationship refers to the relationship learning in the time dimension. Spatial relationship [45] refers to the spatial correlations between external variables (see Figure 11). The black origin describes a variety of input variables. Table 5 summarized the detailed descriptions of the five output strategies. Simply speaking, external variables are the other variables (more than one) in Multivariate-Input-Itself-Other(multi)-Output. Univariate-Input-Itself-Output [64] and Univariate-Input-Other(one)-Output [79] refer to the univariate case, while Multivariate-Input-Other (multi)-Output [35], Multivariate-Input-Itself-Other-Output [52], and Multivariate-Input-Itself-Other (multi)-Output are multivariate [45] (see Table 5). The model learns the temporal relationship from five output strategies, while the spatial relationship is only considered in Multivariate-Input-Itself-Other (multi)-Output. The distinctions between Univariate-Input-Other (one)-Output and Multivariate-Input-Other (multi)-Output are not only the number of input variables, but also the fact that the former’s output strategy focuses on time series data while the latter contains more. The main difference between Multivariate-Input-Itself-Other-Output and Multivariate-Input-Other (multi)-Output is that the former uses the historical information of the output variable, while the latter does not.

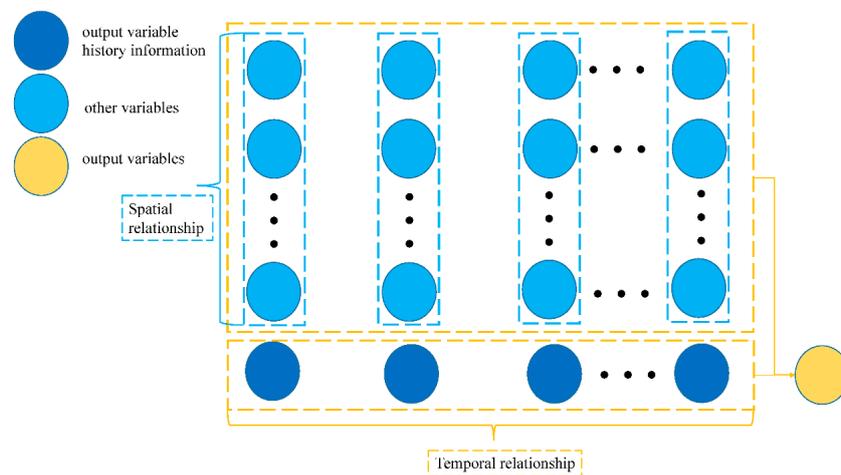


Figure 11. Temporal and spatial relationship in Multivariate-Input-Itself-Other (multi)-Output.

Table 5. Five different output strategies.

Category	Type	Relationship	Description
Univariate-Input-Itself-Output (Category 0)	Univariate	Temporal relationship	The output(s) at a specific point are learned from its own historical information
Univariate-Input-Other(one)-Output (Category 1)	Univariate	Temporal relationship	The output(s) at a specific point are learned the historical information from other variables (one)
Multivariate- Input-Other (multi)-Output (Category 2)	Multivariate	Temporal relationship	The output(s) at a specific point are learned the historical information from other variables (more than one)
Multivariate-Input-Itself -Other-Output (Category 3)	Multivariate	Temporal relationship	The output(s) at a specific point are learned the historical information from both its own and other variables
Multivariate-Input-Itself-Other (multi)-Output (Category 4)	Multivariate	Temporal relationship and spatial relationship	The output(s) at a specific point are learned the historical information from both its own and other variables (more than one)

5.3. Input Selection

There are two main approaches to select the most significant predictors of ANN models which are model-free and model-based methods (see Table 6) [166]. The biggest difference between the two methods is that the former does not consider model performance, while the latter does. In the majority of the studies, many researchers utilized ad-hoc [27] methods to select the inputs, whether in model-free or model-based methods. Some researchers used cross-correlation and analytical approaches to explore the linear and non-linear relationship between input(s) and output(s). Other input selection methods are summarized in Table 6.

Table 6. Model-free and model-based methods in input selection.

Categories	Methods	Comments
model-free	ad-hoc analytic other	Based on domain knowledge or casual way The linear and non-linear relationship between input and output IGRA, Garson method
model-based	ad-hoc stepwise sensitivity analysis global optimization	e.g., trial-and-error Constructive and pruning methods e.g., MCS e.g., GA

5.4. Data Dividing

Data dividing is an important step in the modeling process (see Table 7). The training set is used for data samples of model fitting [95]. The validation set, which can adjust the model’s hyperparameters, is a set of samples set apart during model training. Finally, the testing set is to check the model’s generalization ability [139] and its error is utilized to compare different model’s predictive performance. Not all data needs to be divided into three sets, because regularization [55] is an approach that can divide the datasets into two sets—namely training and validation sets—and has the advantage of providing more data points for the model training and stopping the models from over-fitting [167]. Data dividing methods can be categorized into supervised and unsupervised methods [31]. There are

no uniform rules for how to divide the training set, the validation set, and the test set which also applies to the division of training sets and test sets. Most researchers divided the data either by domain knowledge or in any arbitrary manner. In the majority of the reviewed papers, the data set was divided into the training and testing two parts (see the ninth column in Appendix A). The division range of the training set is from 50% to 98% [16], and the test set varies from 2% to 50% [105]

Table 7. Supervised and unsupervised methods in data dividing.

Categories	Methods	Comments
supervised	trial-and-error	Taking the statistical properties of each subset into consideration
	temporal partitioning	Dividing the data into diel, diurnal, and nocturnal
	M-test	The number of the data points was obtained through the winGamma software
unsupervised	ad-hoc	Based on domain knowledge or a casual way
	random	Divide the data randomly
	cross-validation	e.g., K-fold cross-validation, leave-one-out cross-validation
	stratified method	e.g., SOM

5.5. Data Preprocessing

It should be noted that data preprocessing is carried out after the data dividing. Normalization, missing values imputation and data correct are three primary preprocessing methods in the field of water quality modeling (see Table 8). Most reviewed papers took the normalization step, although they did not give clear details about normalization. As [31] pointed out, this step requires matching the range of the predictors to the transfer function in the hidden layer. Range scaling [132] and standardization [113] are two popular categories in normalization. There are three main scopes, namely [0, 1], [-1, 1] and [0.1, 0.9], under range scaling. Although missing data often occurs in transmission, only a few investigated papers dealt with this phenomenon. The majority of researchers deleted the missing data directly. This is not a recommended practice, as the obtained data are precious and limited. As a whole, researchers pay less attention to data imputation, correct, and identification of abnormal data. Table 4 presented some data preprocessing techniques.

Table 8. The data preprocessing approaches.

Categories	Methods	Comments
Normalization	No details	Built-in functions in platforms
	Range scaling	The scale of each feature is in the same range
	Standardization	A new variable with zero mean and unit standard deviation
Missing data imputation	Only mentioned	Not recommend
	Deletion	Not recommend
	Linear interpolation	The slope of the assumed line to calculate the data increment
	Improved mean value method	Solve the breakpoint phenomenon of mean value method and linear interpolation method
	Missing-refilling scheme	Dividing of ID and SD and using Temporal exponentially moving average to fill the missing data
Data correct	Gap-filling	Temporal partitioning as gap-filling in order to get continuous records
	Filling in the predicted values of the model	The missing values of predictors at time T0 are obtained by prediction values of the model at time T0 by other predictors
Data abnormal	Smoothing method	The moving average filtering can attenuate high-frequency signals
	Mean value method	Need to be corrected as a median of k data before and after
	The fixed threshold method	Setting the upper and lower threshold ranges (discard)

5.6. Model Structure Determination

Until recently, a general method for determining the optimal model structure remains unknown [31]. Therefore, different approaches have been adopted to determine the ANN model structure to avoid the initial difficulty in model building step as much as possible. There are three mainstream

methods—namely ad-hoc, stepwise trial-and-error, and global methods—for the determination of an optimal model structure [31] (see Table 9). The neural network structure defines the functional form of the input–output relationship [59]. The model structure determination, an essential step in the model development, refers to the number of layers, the number of nodes in each layer and the way they connect [30], aiming to strike a balance between network complexity and generalization ability [27]. The model structure determination and model training process are often conducted together. For example, when the trial-and-error method is implemented, the weights of the MLPs are optimized at the same time. Categories and comments on the ANN methods in the model structure determination are given in Table 9. M, N, and O are the number of neurons of the hidden layer, input layer, and output layer. A is a constant from 1 to 10. Sqrt is a mathematical function [83] used to calculate the square root of a non-negative real number. Nearly half of the investigated papers did not provide details on the methods used to determine the ANNs structure. When using fixed network structures such as GRNNs, this step is not necessary to carry out, although its proportion is relatively small compared with papers that did not mention this step (see the last two lines in Table 9). In 73 of the 90 times which provide details of the methods, ad-hoc approaches were utilized to determine the structure of model. That is to say, most studies still rely on trial-and-error approach to determine the model structure. This also reveals that researchers have not been very innovative in the methodology of model structure determination. Seven empirical formulas can help to determine the structure of the model to a certain extent in the investigated articles. Table 9 also presents the various global approaches and their improvements in the reviewed articles.

Table 9. Three main model structure determination methods.

Categories	Methods	Comments	Typical Examples	
Ad-hoc	Empirical formula and trial-and-error approach	Rule 1: M is less than N minus 1	[123]	
		Rule 2: one range of M is equal to the sqrt of N plus O and finally plus A		
		Rule 3: the other range of M is equal to log base 2 logarithm of N		
		Rule 4: M is equal to 5 multiplied by sqrt of N		[102]
		Rule 5: M is equal to half of the sum of N and O plus square root of the number of training patterns		[102]
		Rule 6: M is equal to sqrt of N plus one and finally plus A		[33]
		Rule 7: M is equal to sqrt of N multiplied by O		[99]
	Trial-and-error	Purely on a trial-and-error approach	[105]	
Stepwise trial-and-error	Stepwise trial-and-error	With each modification of the trial, a structure that is neither too complex nor too simple is building	[99]	
Global methods	GA	Searching the solution space through simulated natural evolution	[166]	
	u GA	Introducing creep mutation in a small population	[140]	
	IGA	Selecting excellent individuals effectively to avoid the situation of discarding by GA	[152]	
	PSO	Excitation function does not need to be differentiable and derivable	[143]	
	IPSO	The convergence rate and accuracy of the solution are improved	[148]	
	ABC IABC	More precise than PSO and GA Updating formulas just like the PSO algorithm	[4] [4]	
Others	Not mentioned	Not recommend	[40]	
	Not required	Fixed structures such as GRNNs	[25]	

5.7. Model Training

There are two main training methods, namely deterministic and stochastic methods [31] (see Table 10). Deterministic methods look for a single parameter vector while the stochastic methods search for the distribution of the model parameters with the purpose of minimizing the model error [27]. In a more detailed division, local methods (L) that often work on gradient information and global optimization approaches are two kinds of deterministic methods. Gradient methods can be further sub-divided into first-order methods or second-order methods. Deterministic methods based on gradient information have been widely used in model training algorithm. The Levenberg–Marquardt algorithm, a second-order method, was most widely used in deterministic methods. The Levenberg–Marquardt method combines the advantages of BP and Newton algorithm, and its training speed is obviously faster than BP and momentum algorithm [81]. However, it has the disadvantage of being incompatible with regular terms, and requires a lot of memory when datasets are large. Sixty-two of the papers did not provide details about the model training algorithm. Seven categories of local methods (see line 1 to line 7 in Table 10) are summarized. Relatively speaking, there were few works on network training using Bayesian [27] and the Adam optimization methods [57].

Table 10. The deterministic and stochastic methods in model training.

Categories	Methods	Comments
Deterministic	BP algorithm(L)	Computing the direction of gradient descent
	Newton's methods(L)	The computing tasks are implemented by Hessian matrix
	Conjugate gradient method(L)	The search direction is carried along the conjugate direction and does not need to use Hessian matrix
	Levenberg–Marquardt method(L)	A method, combination of BP and Newton algorithm, use Jacobian matrix to do the computing tasks
	The Quasi-Newton method(L)	It is applied to the situation of that Jacobian matrix or Hessian matrix is difficult or even impossible to compute
	BFGS	A Quasi-Newton method implemented by the built-in function in R
	TRAINLM	A gradient descent with momentum and Levenberg–Marquardt backpropagation
	Global optimization	See Table 9
Stochastic methods	Bayesian methods	Prediction limits can be obtained
	Adam optimization method	It implemented a reverse gradient update with the value obtained by Mini batch data
Emerging methods	Online learning algorithm	Quickly adjust the model in real time

6. Discussion

6.1. Data Are the Foundation

Data selection strategy: Data collection is a costly and time-consuming process. This is mainly due to the expensive equipment, limited experimental time, and conditions. The ANN model is a data-driven model, so obtaining enough data is the basis of modeling. The need to collect as much data as possible has been put forward in the existing literature. To address this need, researchers need to consider two factors. One is whether the historical information of the output variable can be collected. The second is what strategy researchers need to choose when the historical information of output variables are difficult to measure. If researchers can collect historical observations of target variables, they can process the data and model it. If target variables cannot be obtained, researchers can collect variables such as water quality and meteorology data associated with output variables. Part of the literatures collect target variables by means of obtaining open-source data. This approach has benefited from a number of government data collection programs. However, research to obtain open-source

water quality data is rather limited. Therefore, researchers are encouraged to open up their own data resources in the future to make contributions to themselves, others, and society.

Data volume demand: According to the results of the existing literature review, there is no systematic research to investigate how to determine the optimal number of samples required for each type of ANN model. In general, RNN requires more data than feedforward artificial neural networks. In addition, GRNN in feedforward artificial neural networks can handle small sample problems. When researchers use the RNN method to make water quality predictions, they need about a thousand pieces of data. When the researchers utilized the feedforward artificial neural networks method to make the prediction, about 500 pieces of data are needed. When researchers used the GRNN method to make predictions, they need about 100 pieces of data. When researchers want to make long-term forecasts of water quality data that are periodic after a year, at least one year of data needs to be collected. This also applies when researchers want to include four seasons in the model validation and testing phase.

6.2. Data Processing Is Key

Data imbalance problem: Both the peak and the extreme value occupy a relatively small proportion of the distribution. Only a handful of researchers currently consider data imbalances. In order to obtain higher prediction accuracy and reduce the error of the peak, some new prediction approaches, such as wavelet analysis method, can be used for reference. Besides, modelers in the future can develop a form of extreme value loss for detecting the future occurrence of extreme values (Ding et al., 2019) and apply it to the water quality prediction.

Input selection problem: The quality of data sets has been affected by many factors. These factors include but are not limited to temporal resolution (e.g., monthly vs. hourly), number of predictors, or noise in the data. Therefore, it is very important to select the appropriate input and preprocess the data. This review found that the vast majority of researchers chose inputs based on their domain knowledge or in any arbitrary manner. Such input selection methods have some limitations because they neither analyze the relationship between input and output, nor consider the performance of the model. Some studies use cross-correlation to explore the relationship between inputs and outputs. It is a linear approach, which is contrary to the premise of using a nonlinear neural network model. Researchers can use nonlinear analysis methods such as mutual information to select inputs.

Output strategies problem: A variety of output strategies were adopted in the reviewed papers—the quantity of which is 18—because researchers hope to select the most suitable through comparison to illustrate the relationship between input(s) and output(s), which is good practice. Multivariate-Input-Other (multi)-Output is the most popular output strategy which represents the case where the output(s) at a specific point is learned the historical information from other variables (more than one). Few studies have considered the spatial relationship between exogenous variables. This may be due to the fact that external variables do not influence the outcome of the forecast most of the time. However, researchers must be aware that exogenous variables can have a significant impact on predictions at some point. For example, the effect of water circulation on dissolved oxygen. A recent research used the mechanism of attention to simultaneously explore the relationship between temporal and spatical, and applied it to DO prediction. Researchers can use this method for reference to further explore the spatial relationship of other water quality variables.

Forecasting length problem: At present, the research mainly focuses on the short-term prediction, and the research on the long-term prediction is relatively limited. The reason for this phenomenon is that with the increase in the prediction length, the uncertainty factors also increase, which leads to the accumulation of errors and thus reduces the accuracy of the prediction. Researchers can adopt appropriate strategies to solve such problems in forecating field, such as Recursive, DirRec, and Multiple Output Strategies [168].

Data dividing problem: At present, researchers tend to use ad-hoc method to divide the training set data into 70% to 90% of the total data. The most common percentage of the training, validation,

and testing is 60%, 20%, 20%, and 50%, 25%, 25%. Such methods based on the expertise of researchers or divide data in arbitrary ways has certain universality. However, this approach has not promoted the development of data partitioning methods. It is always difficult to determine the number of K for common K-fold cross-validation, as the results may have a considerable bias [169]. Therefore, leave-one-out cross-validation, the most extreme form of K-fold cross-validation, should be encouraged for use because it has been shown to provide a good estimation of the model's true generalization capabilities in the case of fewer training data or more model parameters despite the limited usage.

Data preprocessing problem: Most studies use the normalization method for pre-processing data, but it does not disclose specific details. This is probably due to the use of built-in functions to deal with normalization in many platforms. However, this basic information should be clearly defined, because different scaling ranges have different effects on the final result of the model. In the face of missing data, researchers will simply delete it. This approach is not worth advocating because data is precious. Researchers can adopt appropriate populating strategies to deal with missing data. Some imputation methods besides linear interpolation—such as the improved mean value method that can solve the breakpoint phenomenon of linear interpolation, and designing filling schemes such as missing–refilling schemes or gap–filling to obtain continuous records—are worthy of exploring. The restricted condition of the model forecasting methods using prediction values to fill the missing values is that the data are appropriately and normally distributed. Therefore, it is uncertain whether the above method can be applied to other prediction tasks that do not meet the above conditions. Existing literature has shown that the identification of error and abnormal data is a difficult task because they are difficult to define in water quality prediction. How to deal with such data still needs further exploration by researchers.

6.3. Model Is the Core

Model structure determination problem: Most researchers use a trial-and-error method to determine the ANN structure, which does not fundamentally promote the further development of the model. This review summarizes some empirical formulas to determine the number of neurons in the hidden layer that future researchers can apply to their studies. This review does not reveal the science behind these formulas or the conditions under which they apply. To some extent, the use of these empirical formulas contributes to the determination of the model structure, because researchers build on previous studies rather than stay at the level of trial-and-error with no rules to find. Global methods can obtain topology and network weights, which have been developed to some extent in recent years. Compared with the trial-and-error method, the global method has a sound theoretical basis. Researchers can further study and improve global methods.

Activation function determination problem: Most of the time, researchers choose S-shaped functions because they create a random nonlinear mapping between the input and output. The essential reason is that the S-type transfer function is differentiable, continuous, and monotonically increasing in its domain. Purelin is used more frequently in the output layer than other functions because its output can be arbitrary rather than limited to a small range compared to the sigmoid function.

Model training problem: The reason for developing so many subclasses of training algorithms is that researchers want to use the appropriate matrix (e.g., Hessian matrix, Jacobian matrix) to accomplish the computing tasks easily. The Quasi-Newton method is suited for the situation that the matrix (whether Hessian or Jacobian) is difficult or even impossible to compute. In water quality prediction, the deterministic methods are more mature than the stochastic methods. One possible reason is that the former only looks for a single parameter vector, while the latter looks for the model parameter distribution, so the latter parameter is more uncertain. The online learning algorithm has the characteristics of real-time and rapid adjustment model which is suitable for prediction tasks. However, its application in water quality prediction is still very limited. Therefore, the algorithm is worthy of further study.

Model structure selection problem: Many researchers utilized MLP architectures in ANN to complete prediction tasks between 2008–2019. This result is as same as the conclusion of the review between 1999 to 2007, which may be due to the fact that the MLPs architecture has the advantage of being easy to use, and they can approximate any relationship between input(s) and output(s) through the typical three layers [81]. Global methods (see Table 9), obtaining topology structure and network weights, are drawing the attention of researchers—in contrast to the previous review [27]. It must be noted that the GA, PSO, and ABC methods are typical examples of evolution-related methods. In general, evolutionary methods are combined with ANNs to meet different constraints.

Much effort has been made regarding the data-intensive methods, while the model-intensive and technique-intensive approaches were implemented relatively infrequently. Wavelet analyses were widely used in data-intensive methods, while the decomposing approaches were used less. This may be because wavelet analysis has the ability to extract the trends, discontinuities, and breakdown points of the original data. Furthermore, it is also able to process signals by compressing or denoising.

In recent years, CNN, as a new feedforward neural network method, has been used in water quality prediction. However, its application is rather limited. Researchers can further expand CNN's reach. RNN has good memory ability, so it can make full use of historical information and lay a solid foundation for realizing long-term prediction of water quality. Hybrid Models should be further developed because they are not a substitute for traditional technologies, but a combination of their strengths. Researchers can refer to the ensemble approaches, transfer learning technology, and evidence theory in the literature to improve the prediction accuracy and generalization ability, and accommodate uncertainty.

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Appendix A

Table A1. Details of the reviewed papers.

Categories	Authors (Year)	Locations	Water Quality Variables	Meteorological Factors	Other Factors	Output Strategy	Dataset	Time Step	Data Dividing	Methods	Prediction Lengths
Feedforward	[75]	WWTP(Turkey)	BOD; SS, TN, TP	NA	Q	Category 2	364 samples (1 year)	daily	Train: 67%, test:33%	ANN, MLR	NA
Feedforward	[76]	Mamasin dam reservoir (Turkey)	DO, EC; SS, TN, WT	RF	AODD	Category 2	No details	No details	No details	ANN(MLP)	NA
Feedforward	[40]	Singapore coastal waters (Singapore)	S, DO, Chl-a;; WT	NA	NA	Category 3	32 samples (5 months)	No details	No details	ANN(MLP), GRNN	1
Feedforward	[19]	Feitsui Reservoir (China)	Chl-a;	NA	Bands	Category 2	No details	No details	Train: 75%, test:25%	ANN(MLP)	NA
Feedforward	[90]	Pyeongchang river (Korea)	DO, TOC; WT	NA	Q	Category 3	No details (3 months)	5 minutes	No details	ANN, MNN, ANFIS	12,24
Feedforward	[170]	Feitsui Reservoir (China)	Chl-a;	NA	Bands	Category 2	No details (7 years)	No details	Train:57%, validate: 29%, test: 14%	ANN(MLP)	NA
Feedforward	[91]	Melen River (Turkey)	BOD; COD, WT, DO, Chl-a, NH ₃ -N, NO ₃ , NO ₂	NA	F, Ns	Category 2	No details (over 6 years)	monthly	Train:60%, validate: 20%, test: 20%	ANN(MLP)	NA
Feedforward	[92]	Moshui River (China)	COD, NH ₃ -N;;	NA	mineral oil;;	Category 0	No details (5 years)	No details	Train:80%, test: 20%	BPNN	NA
Feedforward	[93]	Doce River (Brazil)	WT, pH, EC, TN	NA	other ions	Category 2	232samples (3 years)	No details	Train:50%, validate: 25%, test: 25%	ANN	NA
Feedforward	[94]	NA (China)	pH, DO;; WT, S, NH ₃ -N, NO ₂	NA	NA	Category 3	500 samples	No details	Train:80%, test: 20%	BPNN	NA
Feedforward	[95]	Gomti river (India)	DO, BOD; pH, TA, TH, TS, COD, NH ₃ -N, NO ₃ , P	RF	NA	Category 2	500 samples (10 years)	monthly	Train:60%, validate: 20%, test: 20%	ANN	NA

Table A1. Cont.

Categories	Authors (Year)	Locations	Water Quality Variables	Meteorological Factors	Other Factors	Output Strategy	Dataset	Time Step	Data Dividing	Methods	Prediction Lengths
Feedforward	[96]	Pyeongchang River (Korea)	TOC;;	Precip	Q;;	Category 3	No details (7 years)	No details	No details	ANN	NA
Feedforward	[97]	Groundwater (China)	NO ₂ , COD;;	NA	other 7 variables	Category 3	97 samples	No details	Train:56%, test: 44%	ANN	NA
Feedforward	[98]	Omerli Lake (Turkey)	DO; BOD, NH ₃ -N, NO ₃ , NO ₂ , P	NA	NA	Category 2	No details (17 years)	No details	No details	ANN, MLR, NLR	NA
Feedforward	[99]	Changle River (China)	DO, TN, TP;; WT	RF	F, FTT	Category 3	No details (18months)	monthly	No details	BPNN	NA
Feedforward	[105]	Sangamon River (USA)	NO ₃ ;;	AT, Precip	Q	Category 3	No details (6 years)	weekly	Train:50%, test: 50%	ANN	1
Feedforward	[106]	Surface water (Turkey)	Chl-a;	NA	other 12 variables	Category 2	110 samples	No details	Train:67%, test: 33%	ANN(MLP)	NA
Feedforward	[107]	Gru'za reservoir (Serbia)	DO; pH, WT, CL, TP, NO ₂ , NH ₃ -N, EC	NA	Fe, Mn	Category 2	180samples (3 years)	No details	Train:84%, test: 16%	ANN	NA
Feedforward	[108]	The tank (China)	DO;; pH, S, WT	AT	NA	Category 3	No details (22 months)	1 minute	Train:57%, validate: 29%, test: 14%	ANN	30
Feedforward	[109]	Groundwater (India)	S; EC	NA	WL, T, Pumping, Rainp	Category 2	No details (7 years)	No details	Train:29%, test: 71%	ANN	NA
Feedforward	[110]	WWTP(China)	BOD; COD, SS, pH, NH ₃ -N	NA	Oil	Category 2	No details	No details	Train:50%, test: 50%	RBFNN	5
Feedforward	[10]	Groundwater (Iran)	NO ₃ ; pH, EC, TDS, TH	NA	Mg, Cl, Na, K, HCO ₃ , SO ₄ , Ca, ICs	Category 2	818samples (nearly 17days)	30 minutes	Train:70%, test: 30%	ANN, Linear regression (LR)	NA
Feedforward	[77]	Wells (Palestine)	NO ₃ ;	NA	Q, other five variables	Category 2	975samples (16 years)	No details	No details	MLP, RBF, GRNN	NA
Feedforward	[112]	Upstream and downstream (USA)	DO; pH, WT, EC	NA	Q	Category 2	2063, 4765 samples (18 years)	daily	Train:50%, validate:25%, test: 25%	RBFNN, ANN(MLP), MLR,	NA
Feedforward	[50]	WWTP (Korea)	DO;; NH ₃ -N	NA	NA	Category 3	1900 samples	No details	Train:45%, validate:5%, test: 50%	MNN	NA

Table A1. Cont.

Categories	Authors (Year)	Locations	Water Quality Variables	Meteorological Factors	Other Factors	Output Strategy	Dataset	Time Step	Data Dividing	Methods	Prediction Lengths
Feedforward	[79]	Eastern Black Sea Basin (Turkey)	SS; Tur	NA	NA	Category 1	144 samples (1 year)	fortnightly	Train:75%, validate:8%, test: 17%	ANN(MLP)	NA
Feedforward	[113]	Kinta River (Malaysia)	DO, BOD, NH ₃ -N, pH, COD, Tur;;	NA	NA	Category 2	255 samples (7 months)	No details	Train:80%, validate:10%, test: 10%	ANN(MLP)	NA
Feedforward	[78]	Power station (New Zealand)	WT;	AT, AP, WD, WS	other 8 variables	Category 2	45,594 samples (2 years)	10 minutes	Train:70%, test: 30%	ANN(MLP)	12
Feedforward	[114]	Yuan-Yang Lake (China)	WT;	SR, AP, RH, AT, WS, WD	ST	Category 2	No details (2 months)	10 minutes	Train:70%, validate & test: 30%	ANN(MLP)	1
Feedforward	[22]	Experimental system (UK)	BOD, NH ₃ -N, NO ₃ , P; DO, WT, pH, EC, TSS, Tur	NA	RP	Category 2	195samples (4 years)	No details	Train: 62%, test: 38%	ANN	NA
Feedforward	[11]	Lake Fuxian (China)	DO, TP, SD, Chl-a;; TN, WT, pH	NA	Month;	Category 2 and Category 3	No details	No details	No details	ANN	NA
Feedforward	[115]	Doiraj River (Iran)	SS;	RF	Q	Category 1 and Category 2	more than 3000 samples (11 years)	daily	No details	ANN, Support vector regression (SVR) ANN, Multiple nonlinear regression (MNLN)	1
Feedforward	[116]	Lake Abant (Turkey)	DO, Chl-a; WT, EC	NA	MDHM	Category 2	6674 samples (86 days)	15 minutes	Train:60%, validate:15%, test: 25%	ANN(MLP), RBFNN, LR	NA
Feedforward	[37]	Johor River, Sayong River (Malaysia)	TDS, EC, Tur;	NA	NA	Category 1	No details (5 years)	No details	The test set is approximately 10–40 % of the size of the training data set	ANN(MLP), RBFNN, LR	NA
Feedforward	[158]	Mine water (India)	BOD, COD; WT, pH, DO, TSS	NA	other	Category 2	73 samples	No details	Train:79%, test: 21%	ANN	NA

Table A1. Cont.

Categories	Authors (Year)	Locations	Water Quality Variables	Meteorological Factors	Other Factors	Output Strategy	Dataset	Time Step	Data Dividing	Methods	Prediction Lengths
Feedforward	[160]	Heihe River (China)	DO; pH, NO ₃ , NH ₃ -N, EC, TA, TH	NA	Cl, Ca	Category 2	164 samples (over 6 years)	monthly	Train:60%, validate:20%, test: 20%	ANN(MLP)	NA
Feedforward	[117]	Danube River (Serbia)	DO; WT, pH, NO ₃ , EC		Na, CL, SO ₄ , HCO ₃ , other 11 variables	Category 2	1512 samples (9 years)	No details	Train:70%, validate:20%, test: 10%	GRNN	NA
Feedforward	[80]	Stream Harsit (Turkey)	SS; Tur	NA	TCC, TIC	Category 1 and Category 2	132 samples (11months)	No details	No details	ANN(MLP)	NA
Feedforward	[118]	Feitsui Reservoir (China)	DO; WT, pH, EC, Tur, SS, TH, TA, NH ₃ -N	NA	NA	Category 2	400 samples (20 years)	No details	No details	BPNN, ANFIS, MLR	NA
Feedforward	[163]	Stream (USA)	WT;	AT	Form attributes, forested land cover	Category 2	982 (6 months)	daily	Train:90%, validate & test: 10%	ANN(MLP)	NA
Feedforward	[49]	The Bahr Hadus drain (Egypt)	DO, TDS;;	NA	NA	Category 0	No details	monthly	Train:80%, test: 20%	CCNN, BPNN	NA
Feedforward	[161]	Karoon River (Iran)	DO, COD, BOD; EC, pH, Tur, NO ₃ , NO ₂ , P	NA	Ca, Mg, Na	Category 2	200 samples (17 years)	monthly	Train:80%, test: 20%	ANN(MLP), RBFNN, ANFIS	NA
Feedforward	[121]	Manawatu River (New Zealand)	NO ₃ ;	NA	EMS (Energy, Mean, Skewness)	Category 1	144 samples	weekly	Train: 70%, test: 30%	RBFNN	NA
Feedforward	[119]	WWTP (China)	BOD; DO, pH, SS	NA	F, TNs	Category 2	360 samples	daily	Train: 83%, test: 17%	HELM, Bayesian approach, ELM	NA
Feedforward	[35]	Nalón river (Spain)	Tur; NH ₃ -N, EC, DO, pH, WT	NA	NA	Category 2	No details (1 year)	15 minutes	Train: 90%, test: 10%	ANN(MLP)	NA
Feedforward	[128]	Groundwater (Turkey)	pH, TDS, TH	NA	SAR, SO ₄ ; CL	Category 2	124 samples (1 year)	monthly	Train: 84.1%, test: 15.9%	ANN	NA

Table A1. Cont.

Categories	Authors (Year)	Locations	Water Quality Variables	Meteorological Factors	Other Factors	Output Strategy	Dataset	Time Step	Data Dividing	Methods	Prediction Lengths
Feedforward	[89]	Johor River (Malaysia)	DO; WT, pH, NO ₃ , NH ₃ -N	NA	NA	Category 2	No details (10 year)	monthly	Train:60%, validate: 25%, test: 15%	ANN(MLP), ANFIS	NA
Feedforward	[129]	The Taipei Water Source Domain (China)	Tur;	RF	NA	Category 2	No details (1 year)	No details	No details	BPNN	NA
Feedforward	[130]	Mashhad plain (Iran)	EC;	NA	CL; Lon, Lat	Category 2 and Category 3	122 samples	No details	Train:65%, validate: 20%, test: 15%	ANN(MLP), ANFIS, geostatistical models	NA
Feedforward	[122]	Tai Po River (China)	DO; pH, EC, WT, NH ₃ -N, TP, NO ₂ , NO ₃	NA	CL	Category 2	252 samples (21 years)	No details	Train:85%, test: 15%	ANN, ANFIS, MLR	NA
Feedforward	[137]	Ireland Rivers (Ireland)	DO, BOD, Alk, TH;; WT, pH, EC	NA	DOP (dissolved oxygen percentage), CL;;	Category 2	3001 samples (No details)	No details	No details	ANN	NA
Feedforward	[42]	Twostatistical databases (European countries)	BOD; DO	NA	other 20 variables	Category 2	159 samples (9 years)	No details	Train:88%, test: 12%	GRNN, MLR	NA
Feedforward	[81]	Maroon River (Iran)	WT, Tur, pH, EC, TDS, TH;	NA	HCO ₃ , SO ₄ , CL, Na, K, Mg, Ca	Category 2	No details (20 years)	monthly	Train:60%, validate: 15%, test: 35%	ANN(MLP), RBFNN	NA
Feedforward	[36]	River Zayanderud (Iran)	TSS; pH, TH	NA	Na, Mg, CO ₃ ²⁻ , HCO ₃ , CL, Ca	Category 2	1320 samples (10 years)	monthly	No details	RBFNN, TDNN	NA
Feedforward	[9]	Ardabil plain (Iran)	EC, TDS;	RF	RO, WL	Category 2	No details (17 years)	6 months	Train:71%, test: 29%	ANN, MLR	1
Feedforward	[25]	Danube River (Serbia)	BOD; WT, DO, pH, NH ₃ -N, COD, EC, NO ₃ , TH, TP	NA	other 8 variables	Category 2	more than 32,000 samples (years)	No details	Train:72%, validate: 18%, test: 10%	GRNN	NA

Table A1. Cont.

Categories	Authors (Year)	Locations	Water Quality Variables	Meteorological Factors	Other Factors	Output Strategy	Dataset	Time Step	Data Dividing	Methods	Prediction Lengths
Feedforward	[82]	Hydrometric stations (USA)	SS;;	NA	Q	Category 0 and Category 3	No details (8 years)	daily	Train and test:80%, validate:20%	ANN(MLP), SVR, MLR	1
Feedforward	[138]	Surma River (Angladesh)	BOD, COD;;	NA	NA	Category 0 and Category 3	No details (3 years)	No details	Train:70%, validate: 15%, test: 15%	RBFNN, MLP	NA
Feedforward	[85]	Groundwater (Palestine)	S; EC, TDS, NO ₃	NA	Mg, Ca, Na	Category 2	No details (11 years)	No details	Train: more than 50%, test: less than 50%	ANN(MLP), SVM	NA
Feedforward	[24]	River Danube (Hungary)	DO; pH, WT, EC	NA	RO	Category 2	More than 151 samples (6 years)	monthly	No details	GRNN, ANN(MLP), RBFNN, MLR	NA
Feedforward	[60]	Langat River and Klang River (Malaysia)	DO, BOD, COD, SS, pH, NH ₃ -N;	NA	NA	Category 2	No details (10 years)	monthly	Train:80%, validate: 20%	RBFNN	NA
Feedforward	[47]	Eight United States Geological Survey stations (USA)	DO; WT, EC, Tur, pH	NA	YMDH	Category 2	35,064 samples (4 years)	hourly	Train:70%, test: 30%	ELM, ANN(MLP)	1, 12, 24, 48, 72, 168
Feedforward	[162]	Rivers (China)	DO; WT, pH, BOD, NH ₃ -N, TN, TP	NA	other variables	Category 2	969 samples	No details	Train and validate: 80%, test: 20%	BPNN, SVM, MLR	NA
Feedforward	[86]	Syrenie Stawy Ponds (Poland)	DO, BOD, COD, TN, TP, TA	NA	CL; other ions	Category 2	No details (19 months)	monthly	Train:60%, validate: 20%, test: 20%	ANN(MLP)	NA
Feedforward	[83]	Delaware River (USA)	DO; pH, EC, WT	NA	Q	Category 1 and Category 2	2063 samples (6 years)	daily	Train:75%, test: 25%	ANN(MLP), RBFNN, SVM	NA
Feedforward	[84]	Zayandeh-rood River (Iran)	NO ₃ ; EC, pH, TH	NA	Na, K, Ca, Mg, SO ₄ , CL, bicarbonate	Category 2	No details	No details	Train:50%, validate: 30%, test: 20%	ANN(MLP)	NA

Table A1. Cont.

Categories	Authors (Year)	Locations	Water Quality Variables	Meteorological Factors	Other Factors	Output Strategy	Dataset	Time Step	Data Dividing	Methods	Prediction Lengths
Feedforward	[59]	Saint John River (Canada)	TSS, COD, BOD, DO, Tur;	NA	NA	Category 2	39 samples (3 days)	No details	Train:60%, validate: 20%, test: 20%	BPNN, SVM	NA
Feedforward	[164]	Karkheh River (Iran)	BOD; TDS, EC	NA	CL, Na, SO ₄ , Mg, SAR, Ca	Category 2	13,800 samples (5 years)	No details	No details	ANN	NA
Feedforward	[159]	Xuxi River (China)	COD; WT, DO, TN, TP, NH ₃ -N, SD, SS DO; pH, WT, EC, BOD, COD, SS, P, NO ₃ , TA, TH	NA	NA	Category 2	110 samples (8 hours)	No details	No details	MLP	NA
Feedforward	[102]	Danube River (Serbia)	EC, BOD, COD, SS, P, NO ₃ , TA, TH	NA	five metal ions	Category 2	No details (6 years; 7 years)	monthly or fortnightly	Train:72%, validate: 18%, test: 10%	BPNN	NA
Feedforward	[131]	Sufi Chai river (Iran)	TDS;	NA	Q, Other 4 variables	Category 2	144 samples (12 years)	monthly	Train:66%, validate: 17%, test: 17%	ANN(MLP)	NA
Feedforward	[127]	River Tisza (Hungary)	DO; WT, EC, pH	NA	RO	Category 2	More than 1300 samples (6 years)	No details	Train:67%, test: 33%	RBFNN, GRNN, MLR	12
Feedforward	[171]	Karoon River (Iran)	TH; EC, TDS, pH	NA	SAR; HCO ₃ , CL, SO ₄ , Ca, Mg, Na, K, TAC	Category 2	No details (49 years)	No details	No details	ANN(MLP), RBFNN	NA
Feedforward	[32]	Yamuna River (India)	DO;; BOD, COD, pH, WT, NH ₃ -N	NA	Q	Category 3	No details (4 years)	monthly	Train:75%, test: 25%	BPNN, SVM, ANFIS, ARIMA	NA
Feedforward	[88]	Lakes (USA)	Chl-a; TP, TN, Tur	NA	SD	Category 2	1087 samples (6 years)	No details	Train:75%, test: 25%	MLP, ANFIS, ANN, ANFIS,	NA
Feedforward	[139]	Karoun River (Iran)	BOD, COD; EC, Tur, pH	NA	six mental ions	Category 2	200 samples (16 years)	No details	No details	Least Squares SVM(LSSVM)	NA

Table A1. Cont.

Categories	Authors (Year)	Locations	Water Quality Variables	Meteorological Factors	Other Factors	Output Strategy	Dataset	Time Step	Data Dividing	Methods	Prediction Lengths
Feedforward	[133]	Lakes (USA)	TN, TP; pH, EC, Tur	NA	NA	Category 2	1217 samples	No details	Train:55%, validate: 22%, test: 23%	ANN, LR	NA
Feedforward	[48]	Three rivers (USA)	WT;	AT	Q, DOY	Category 2	No details (8 years)	No details	No details	ELM, ANN(MLP), MLR	NA
Feedforward	[63]	St. Johns River (USA)	DO; NH ₃ -N, TDS, pH, WT	NA	CL	Category 2	232 samples (12 years)	half a month	Train:75%, test: 25%	CCNN, DWT, VMD-MLP, MLP	NA
Recurrent	[111]	Talkheh Rud River (Iran)	TDS;	NA	Q	Category 1	No details (13 years)	No details	Train:69%, validate & test: 31%	Elman, ANN(MLP)	1
Recurrent	[3]	Hyriopsis Cumingii ponds (China)	DO;; pH, WT	SR, WS, AT	NA	Category 3	816 samples (34 days)	No details	Train and validate:80%, test: 20%	Elman	NA
Recurrent	[41]	Danube River (Serbia)	DO; WT, pH, EC	NA	Q	Category 2	61 samples	monthly or semi-monthly	Train: 85%, test: 15%	Elman, GRNN, BPNN, MLR	NA
Recurrent	[167]	Chou-Shui River (China)	pH, Alk	NA	As;; Ca	Category 3	No details (8 years)	No details	No details	Systematical dynamic-neural modeling (SDM), BPNN, NARX	NA
Recurrent	[55]	Yenicaga Lake (Turkey)	DO; WT, EC, pH	NA	WL, DOY, hour	Category 2	13,744 samples (573 days)	15 minutes	Train:60%, validate: 15%, test: 25%	TLRN, RNN, TDNN	NA
Recurrent	[12]	Dahan River (China)	TP;; EC, SS, pH, DO, BOD, COD, WT, NH ₃ -N	NA	Coli	Category 3	280 samples (11 years)	monthly	Train:75%, test: 25%	NARX, BPNN, MLR	1

Table A1. Cont.

Categories	Authors (Year)	Locations	Water Quality Variables	Meteorological Factors	Other Factors	Output Strategy	Dataset	Time Step	Data Dividing	Methods	Prediction Lengths
Recurrent	[6]	Taihu Lake (China)	DO, TP;;	NA	NA	Category 0	657 samples (7 years)	monthly	Train:90%, test: 10%	LSTM, BPNN, OS-ELM	NA
Recurrent	[38]	WWTP(China)	BOD, TP;; COD, TSS, pH, DO, WT	NA	ORP	Category 2 and Category 3	5000 samples	No details	Train:45%, validate: 15%, test: 40%	RESN	NA
Recurrent	[66]	Mariculturebase (China)	WT, pH; EC, S, Chl-a, Tur, DO	NA	NA	Category 2	710 samples (21 days)	5 minutes	Train:86%, test: 14%	LSTM, RNN	>32
Recurrent	[67]	Marine aquaculture base (China)	pH, WT;;	NA	NA	Category 0	710 samples	No details	Train:86%, test: 14%	SRU	NA
Recurrent	[53]	Geum River basin (Korea)	BOD, COD, SS;	AT, WS	WL, Q	Category 2	No details (10 years)	daily	Train:70%, test: 30%	RNN, LSTM	1
Recurrent	[165]	Lakes (USA)	WT;;	NA	NA	Category 0	1520 samples	No details	Train:65%, test: 35%	LSTM	NA
Recurrent	[153]	Reservoir (China)	Chl-a;; WT, pH, EC, DO, Tur	NA	ORP	Category 0 and Category 2	1440 samples (5 days)	5 minutes	No details	TL-FNN, RNN, LSTM	NA
Recurrent	[134]	Two gauged stations (USA)	SS;;	NA	Q	Category 1	10,060 samples (30 years)	daily	Train: 70–90%, test: 30–10%	WANN	NA
Recurrent	[135]	Agricultural catchment (France)	NO ₃ , SS;	RF	Q	Category 1 and Category 2	26,355 samples (1 year)	daily	Train: 66.67%, test: 33.33%	SOM-MLP, MLP	NA
Recurrent	[140]	Four streams (USA)	WT;	SR, AT	NA	Category 2	No details (4 years)	10 minutes	Train:50%, validate: 25%, test: 25%	GA-ANN, BPNN, RBFNN	NA
Hybrid	[141]	Chaohu Lake (China)	TP, TN, Chl-a;	NA	Bands	Category 2	18,368 (TN),1050(TP) samples (more than 3 years)	No details	Train:86%, test: 14%	GA-BP, BPNN, RBFNN	NA
Hybrid	[142]	Two stations (USA)	SS;;	NA	Q	Category 1 and Category 3	730 samples (2 years)	daily	Train:50%, test: 50%	ANN-differential evolution	NA

Table A1. Cont.

Categories	Authors (Year)	Locations	Water Quality Variables	Meteorological Factors	Other Factors	Output Strategy	Dataset	Time Step	Data Dividing	Methods	Prediction Lengths
Hybrid	[71]	Büyükdere river (Turkey)	WT, DO, B ₅	NA	NA	Category 0	108 samples (9 years)	monthly	Train:67%, test: 33%	ARIMA-ANN, ANN, ARIMA	NA
Hybrid	[143]	Karkheh reservoir (Iran)	water quality variables	NA	NA	Category 2	No details (6 months)	No details	No details	PSO-ANN	NA
Hybrid	[1]	WWTP(China)	DO; COD, BOD, SS	NA	other two variables	Category 3	No details	daily	No details	SOM-RBFNN, ANN(MLP)	NA
Hybrid	[144]	Bangkok canals (Thailand)	DO; WT, pH, BOD, COD, SS, NH ₃ -N, TP, NO ₂ , NO ₃ , Chl-a; WT, pH,	NA	total coliform, hydrogen sulfide	Category 3	13,846 samples (5 years)	monthly	Train: 70%, test: 30%	FCM-MLP, MLP	1
Hybrid	[56]	Lake Baiyangdian (China)	DO, SD, TP, TN, NH ₃ -N, BOD, COD	Precip, Evap	WL, LV, Sth	Category 2	No details (10 years)	monthly	No details	WANN, ANN, ARIMA	NA
Hybrid	[64]	Songhua River (China)	DO, NH ₃ -N;	NA	NA	Category 0	No details (7 years)	monthly	Train:71%, test: 29%	BWNN, ANN, WANN, ARIMA	1
Hybrid	[136]	Gazacoastal aquifer (Palestine)	NO ₃ ; EC, TDS, NO ₃ ,		CL, SO ₄ , Ca, Mg, Na	Category 2	No details (10 year)	No details	No details	K-means-ANN	NA
Hybrid	[43]	WWTP (Turkey)	COD; SS, pH, WT	NA	Q	Category 2	265 samples (3 years)	daily	Train:50%, validate:25%, test: 25%	k-means-MLP, Arima-RBF, ANN(MLP), MLR, RBFNN, GRNN, ANFIS	NA
Hybrid	[70]	Yangtze River (China)	DO, NH ₃ -N;	NA	NA	Category 0	480 samples (9 years)	weekly	Train:67%, validate & test: 33%	ARIMA-RBFNN	1
Hybrid	[120]	Taihu Lake (China)	DO, EC, pH, NH ₃ -N, TN, COD, TP, BOD, COD;	NA	VP, petroleum, other 11 variables	Category 2	2680 samples	No details	Train:75%, test: 25%	PCA-GA-BPNN	NA

Table A1. Cont.

Categories	Authors (Year)	Locations	Water Quality Variables	Meteorological Factors	Other Factors	Output Strategy	Dataset	Time Step	Data Dividing	Methods	Prediction Lengths
Hybrid	[62]	Gauging station (Iran)	DO, WT, S;; Tur, Chl-a	NA	NA	Category 0 and Category 2 and Category 3	650, 540 samples	daily, hourly	Train:70%, validate: 15%, test: 15%	WANN, ANN	1, 2, 3
Hybrid	[172]	Two gauging stations (USA)	SS;;	NA	Q	Category 0 and Category 3	1974 samples (8 years)	daily	Train:75%, test: 25%	WANN	NA
Hybrid	[173]	River Yamuna (India)	COD;;	NA	NA	Category 0	120 samples (10 years)	monthly	Train:92.5%, test: 7.5%	ANN, ANFIS, WANFIS, MLP, ANFIS, WNN,	9
Hybrid	[100]	Two catchments (Poland)	WT;	AT	Q, declination of the Sun	Category 2	No details (10 years)	daily	No details	Product-Unit ANNs (PUNN), ensemble aggregation approach	1, 3, 5
Hybrid	[7]	South San Francisco bay (USA)	Chl-a;;	NA	NA	Category 0	No details (20 years)	monthly	Train:60%, validate: 20%, test: 20%	WANN, MLR, GA-SVR	1
Hybrid	[72]	Asi River (Turkey)	EC;;	NA	Q	Category 0 and Category 3	274 samples (23 years)	No details	Train:75%, test: 25%	WANN, ANN	NA
Hybrid	[146]	Klamath River (USA)	DO;; pH, WT, EC, SD	NA	NA	Category 0 and Category 2	No details	monthly	Train:80%, validate: 10%, test: 10%	WANN, ANN, MLR	NA
Hybrid	[147]	Prawn culture ponds (China)	WT;	NA	NA	Category 0	1152 samples (8 days)	10 minutes	Train:87.5%, test: 12.5%	EMD-BPNN, BPNN	1
Hybrid	[44]	WWTP(China)	BOD; COD, SS, DO, pH	NA	NA	Category 2	598 samples (19 months)	daily	No details	Chaos Theory-PCA-ANN	NA

Table A1. Cont.

Categories	Authors (Year)	Locations	Water Quality Variables	Meteorological Factors	Other Factors	Output Strategy	Dataset	Time Step	Data Dividing	Methods	Prediction Lengths
Hybrid	[174]	Charlotte harbor marine waters	TN;	NA	NA	Category 0	No details (13 years)	monthly	Train:70%, validate: 15%, test: 15%	WANN, wavelet-gene expression programming (WGEP), TDNN, GEP, MLR	1
Hybrid	[73]	Groundwater (Iran)	EC, Tur, pH, NO ₂ , NO ₃	NA	Cu	Category 2	No details (8 years)	No details	Train:80%, test: 20%	PCA-ANN	NA
Hybrid	[17]	Downstream (China)	WT, DO, pH, EC, TN, TP, Tur, Chl-a;	NA	NA	Category 0	No details (13 months)	daily	Train:80%, validate: 10%, test: 10%	Ensemble-ANN	1
Hybrid	[104]	Karaj River (Iran)	NO ₃ ;	NA	CL; Q	Category 0 and Category 1 and Category 3	No details	monthly	Train:80%, validate: 10%, test: 10%	WANN, ANN, MLR	NA
Hybrid	[148]	Crab ponds (China)	DO;; WT	SR, WS, AT, AH	NA	Category 3	700 samples (22 days)	20 minutes	Train:71%, test: 29%	RBFNN-IPSO-LSSVM, BPNN	3
Hybrid	[149]	Guanting reservoirs (China)	DO, COD, NH ₃ -N;;	NA	NA	Category 0	No details (18 weeks)	weekly	No details	Kalman-BPNN	2
Hybrid	[101]	Toutle River (USA)	SS;;	NA	Q	Category 0 and Category 3	2000 samples (8 years)	daily	No details	A least-square ensemble models-WANN	NA
Hybrid	[69]	WWTP (China)	DO; pH	NA	NA	Category 2	50 samples	No details	Train:70%, test: 30%	FNN-WNN	NA
Hybrid	[52]	Clackamas River (USA)	DO;; WT	NA	Q	Category 3	1623 samples (6 years)	daily	Train:78%, test: 22%	WANN, WMLR, ANN(MLP), MLR	1, 31

Table A1. Cont.

Categories	Authors (Year)	Locations	Water Quality Variables	Meteorological Factors	Other Factors	Output Strategy	Dataset	Time Step	Data Dividing	Methods	Prediction Lengths
Hybrid	[123]	Representative lakes (China)	Chl-a; WT, pH;; NH ₃ -N, TN, TP, DO, BOD	NA	other 17 variables	Category 3	No details (3 years)	No details	Train:80%, test: 20%	GA-BP	NA
Hybrid	[16]	Miyun reservoir (China)	DO, COD, NH ₃ -N;	NA	NA	Category 0	5000 samples (2 years)	weekly	Train:98%, test: 2%	PSO-WNN, WNN, BPNN, SVM	NA
Hybrid	[126]	Aji-Chay River (Iran)	EC;;	NA	NA	Category 0	315 samples (26 years)	monthly	Train:90%, test: 10%	WA-ELM, ANFIS	1, 2, 3
Hybrid	[4]	Yangtze River (China)	DO, COD _{Mn} , BOD;;	NA	NA	Category 3	65 samples (2 months)	daily	Train:50%, validate: 16%, test: 34%	IABC-BPNN, BPNN	NA
Hybrid	[33]	WWTP(China)	COD; COD, SS, pH, NH ₃ -N	NA	NA	Category 2	250 samples	No details	No details	WANN, ANN(MLP)	NA
Hybrid	[175]	The Stream Veszprémi-Séd (Hungary)	pH, EC, DO, Tur;;	NA	NA	Category 2	No details (7 years)	yearly	No details	DE-ANN	NA
Hybrid	[54]	Shrimp pond (China)	DO; WT, NH ₃ -N, pH	AT, AH, AP, WS	NA	Category 2	2880 samples (20 days)	10 minutes	Train:75%, test: 25%	SAE-LSTM, SAE-BPNN, LSTM, BPNN	18, 36, 72
Hybrid	[124]	Four basins (Iran)	TDS; EC	NA	Na, CL	Category 2	No details (20 years)	No details	Train:80%, test: 20%	WANN, GEP, WANFIS	NA
Hybrid	[125]	Blue River (USA)	pH, DO, Tur; WT	NA	Q	Category 0 and Category 3	No details (4 years)	daily	Train:80%, test: 20%	WANN, WGEP	1
Hybrid	[157]	Chattahoochee River (USA)	pH;;	NA	Q	Category 3	730 samples (2 years)	daily	Train:75%, test: 20%	WANN, ANN, WMLR, MLR	1, 2, 3
Hybrid	[176]	Morava River Basin (Serbia)	WT, EC; SS, DO	NA	other ions	Category 2	No details (10 years)	15 days	No details	PCA-ANN	NA
Hybrid	[151]	Tai Lake, Victoria Bay (China)	DO;; WT, pH, NO ₂ , TP	Precip	NA	Category 3	No details (7 years)	No details	Train:80%, test: 20%	IGRA-LSTM, BPNN, ARIMA	NA

Table A1. Cont.

Categories	Authors (Year)	Locations	Water Quality Variables	Meteorological Factors	Other Factors	Output Strategy	Dataset	Time Step	Data Dividing	Methods	Prediction Lengths
Hybrid	[46]	WWTP (Saudi Arabia)	C, DO, SS, pH	NA	CL;;	Category 3	774 samples	No details	No details	PCA-ELM	NA
Hybrid	[5]	Prespa Lake (Greece)	DO, Chl-a;;	NA	NA	Category 0	363 samples (11 months)	daily	Train:70%, validate: 15%, test: 15%	CEEMDAN-VMD-ELM)	NA
Hybrid	[87]	The Warta River (Poland)	WT;;	AT	NA	Category 3	No details (22 to 27 years)	daily	Train:4/9, validate: 2/9, test: 1/3	WANN(MLP), MLP	1
Hybrid	[152]	Ashi River (China)	DO, NH ₃ -N, Tur;;	NA	NA	Category 0	846 samples (4 hours)	more than 4 months	Train:70%, test: 30%	IGA-BPNN	1
Hybrid	[15]	Qiantang River (China)	pH, TP, DO;;	NA	NA	Category 0	1448 samples	No details	Train:70%, test: 30%	DS-RNN, RNN, BPNN, SVR	NA
Hybrid	[132]	The Johor river (Malaysia)	NH ₃ -N, SS, pH; Tur, WT,	NA	COD _{Mn} , Mg, Na	Category 2	No details (1 year)	No details	No details	WANFIS, MLP, RBFNN, ANFIS	NA
Hybrid	[103]	Hilo Bay (the Pacific Ocean)	Chl-a, S;;	NA	NA	Category 0	No details (5 years)	daily	No details	Bates–Granger (BG)-least square based ensemble (LSE)-WANN	1, 3, 5
Hybrid	[154]	WWTP (China)	COD, TP, pH, TN; DO, NH ₃ -N, BOD, TH	NA	CL, oil-related quality indicators	Category 2	23,268 samples (4 years)	hourly	Train:80%, test: 20%	PSO-LSTM	1
Hybrid	[68]	Beihai Lake (China)	pH, Chl-a, DO, BOD, EC;	NA	HA;;	Category 3	No details (5 days)	30 minutes	Train:70%, test: 30%	PSO-GA-BPNN	12
Hybrid	[26]	River (China)	COD;;	NA	NA	Category 0	460 samples (14 months)	12 hours	Train:95%, test: 5%	LSTM-RNN	1

Table A1. Cont.

Categories	Authors (Year)	Locations	Water Quality Variables	Meteorological Factors	Other Factors	Output Strategy	Dataset	Time Step	Data Dividing	Methods	Prediction Lengths
Hybrid	[45]	Zhejiang Institute of Freshwater Fisheries (China)	DO; WT	AT, AH, WS, WD, SR, AP	SM, ST	Category 4	5006 samples (1 year)	10 minutes	Train:80%, test: 20%	attention-RNN	6, 12, 48, 144, 288
Hybrid	[39]	Taihu Lake (China)	pH; DO, COD, NH ₃ -N	NA	NA	Category 2	28 samples (6 months)	Weekly	Train:75%, test: 25%	grey theory-GRNN, BPNN, RBFNN	1
Emerging	[58]	Wastewater factory (China)	TP; WT, TSS, pH, NH ₃ -N, NO ₃ , DO	NA	other 3 variables	Category 2	1000 samples (4 months)	No details	Train:80%, test: 20%	SODBN	NA
Emerging	[57]	Recirculating Aquaculture Systems (China)	DO;; EC, pH, WT	NA	NA	Category 3	4500 samples (13 months)	10 minutes	Train:67%, validate: 11%, test: 22%	CNN, BPNN	18

The contents before the “;” symbol were the output variables; The contents before the “;;” symbol were output and predictors; NA represents blank content.

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