

Artificial neural network modeling for predicting the quality of water in the Sabak Bernam River

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ABSTRACT

Water quality prediction is aided by environmental monitoring, ecological sustainability, and aquaculture. Traditional prediction approaches capture the nonlinearity and non-stationarity of water quality well. Due to their rapid progress, artificial neural networks (ANNs) have become a hotspot in water quality prediction in recent years. ANNs are utilised in this study to predict water quality using soft computing techniques. The feedforward network and the standard back-propagation method of Levenberg-Marquardt and scaled conjugate gradient learning algorithm were employed in this research. One hidden layer has been recommended for the modelling, with the number of hidden neurons set at 3, 24, and 49. For this analysis, six different testing percentages were used, and the output data can be categorised as '0' for clean water and '1' for polluted water. From the results, it can be shown that the most optimised model was from the model of trainlm with a testing percentage of 18% and with 3 number of neurons. This most optimised model obtains an accuracy of 91.7%, the best validation performance of 0.073346 with 24 epochs, and having a receiver operating characteristic (ROC) curve that is closer to the true positive rate compared to other samples.

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1. INTRODUCTION

Fresh water consumption has increased in many parts of the world due to population growth and socioeconomic development. The world's population will require 64 billion cubic metres of freshwater per year by 2050, when it is estimated to reach 7.2 billion people and grow at a rate of 77 million people per year. Nonetheless, developing countries will be responsible for 90% of the projected three billion people by 2050, the majority of whom will live in water-scarce locations. Based on a 2% annual growth rate, domestic and industrial water demand in Malaysia alone is expected to rise by more than 20% in the next 50 years [1]. Malaysia is a fast-developing country on its way to achieving the 2020 objective. The development, on the other hand, has a severe environmental impact, particularly on water quality. Rapid urbanisation, which results from the development of residential, commercial, and industrial sites, as well as infrastructure and other facilities, are the main causes of river pollution [2]–[4]. Poor water quality management can be disastrous to human civilization, as it can lead to disease outbreaks. Most countries have built water quality management frameworks to ensure water quality because of the detrimental consequences to human health if water quality is not properly managed. With the expansion of water quality management in 1985, the creation of water quality criteria and benchmarks based on the water quality index began [5]. Poor water quality can also be a concern because when a problem arises, resources must be redirected to improve water delivery infrastructure.

To address water quality issues, water quality modeling has been developed using current computing and artificial intelligence (AI) techniques. Artificial neural networks (ANNs) have aided in the monitoring of water quality systems by detecting changes in water quality. Feed-forward neural networks, for example, have been employed in a variety of applications. ANN models require parameter values in order to design predictions. ANNs offer several advantages, including the ability to learn, manage highly complex nonlinear systems, and work in parallel [4]. By skipping complicated procedures and utilizing a step function as the activation function (ϕ), which creates the output value, the single-layer neural network can be generated rapidly [6].

The chemical, physical, and biological qualities of water are referred to as "water quality". Thus, in order to define water quality, several physical, biological, and chemical parameter elements that have a significant impact on it must be recognized [7]. These parameters feature a body of water to indicate its suitability for a certain value, such as potability, ecosystem status, agriculture, industry, or recreation [8]. Having access to high-quality water is essential in our daily life. Water quality is important not only for drinking but also for agriculture, industry, human life, and the ecosystem [9]. Furthermore, water is the most crucial aspect in human well-being and economic progress. Individuals, as well as all living creatures, horticulture, and industrialization, require water [10]. The quantity and quality of water for sustaining livelihoods, human well-being, and socio-economic development cannot be secured without intentional efforts to solve water resources management challenges [11]. Water quality monitoring at the moment is primarily based on manual sampling detection and underwater sensor networking. In addition, a typical water quality test includes three main steps: water sampling, sample testing, and investigative analysis [12]. However, manual sample and detection has been shown to be ineffective since it is unable to monitor dynamically at a fixed time and fixed point, and it is costly in terms of personnel demand [13], [14].

In coastal locations, water quality indicators such as conductivity or electrical conductivity (EC) and total dissolved solids (TDS) are frequently used. Total dissolved solids (TDS) refers to the inorganic salts and small amounts of organic matter in solution in water. The most common elements are calcium, magnesium, sodium, and potassium cations, as well as carbonate, hydrogen carbonate, chloride, sulphate, and nitrate anions [15], whereas electrical conductivity (EC) refers to the water's ability to carry electrical current. TDS and EC can be found in natural and man-made environments, such as geological conditions and the ocean, as well as household, industrial waste and agriculture. Dissolved ion concentrations, ionic strength, and temperature measurements are used to establish its capabilities. Salt concentration is also described as water quality indicators for conductivity (EC) and total dissolved solids (TDS). According to the United States environmental protection agency (US EPA), the maximum pollutant level of TDS is 500 parts per million (ppm), while according to the world health organization (WHO), the maximum contaminant level is 1,000 parts per million (ppm) [16]. This indicates that TDS should be kept between 500 and 1,000 mg/L for health reasons, and EC should not exceed 1,500 $\mu\text{S}/\text{cm}$ [17].

ANNs have been the focus of many scientific domains, including ecology, analytical chemistry, and water quality. The ANN, also known as a neural network, was created to simulate the operation of a human brain. There are various types of ANN depending on the function used, but for this project, the type of ANN used was the Levenberg Marquardt (LM) algorithm and scaled conjugate gradient (SCG) feedforward backpropagation. The training algorithm that was used to calibrate the model parameters is very important for the network to approximate complex non-linear input-output relationships. Based on previous studies, the Levenberg Marquardt algorithm and scaled conjugate gradient were used as the training algorithms because they could achieve high accuracy in modelling parameters. The accuracy that has been achieved by previous researchers for LM is 95.9%, whereas for SCG is 90%. In addition to that, another learning algorithm that gives high accuracy is the support vector machine (SVM) at a level of 87.10% [18]–[20]. Thus, in this research, the objective was to prove that ANN can achieve the highest accuracy for predicting the level of water pollution. Based on the literature review, this research focused on developing a classifying system that could identify the condition of tap and drain water which is best done using LM and SCG learning algorithms for the analysis section, the classification inference between measured data from clean and polluted water is based on statistical analysis methods. The intensity of the network can be detected based on the group behaviour of the connected neurons, and the output is determined by assessing its output by examining its input.

This network's main benefit is that it learns how to assess and detect input patterns [21]. While the hidden layer, or link between neurons, is for illustrating the system's complexity [22]. In engineering, neural networks serve two important functions, which are pattern classifiers and also as nonlinear adaptive filters [23]. Based on the research done by E. Salami, the input arcs from other hidden nodes or input nodes are connected to each node, which is included in this research. In ANN, the process of developing the system models is done in the hidden layer via a system of weighted 'connections'. At the end of the process, the output layer will represent the network results [24], [25].

2. METHOD

In this paper, a statistical analysis-based approach using reliable total dissolved solid (TDS) and conductivity (EC) of water was proposed to develop a classifying system that could identify the condition of drain and tap water quality by using the Levenberg-Marquardt algorithm and scale conjugate gradient algorithm. Figure 1 shows one of the neural networks used in this project, which consists of two inputs, a single hidden layer that contains three number of neurons, and one output. The data collected for this project was taken by using a total dissolved solid (TDS) Sensor to detect the value of TDS and an EC sensor to detect the value of the electrical conductivity of the water and the block diagram that was used in this research to evaluate the samples based on the parameters is shown in Figure 2. The flowchart of the entire system process is shown in Figure 3, and each part of the flowchart will be discussed in detail throughout this section.

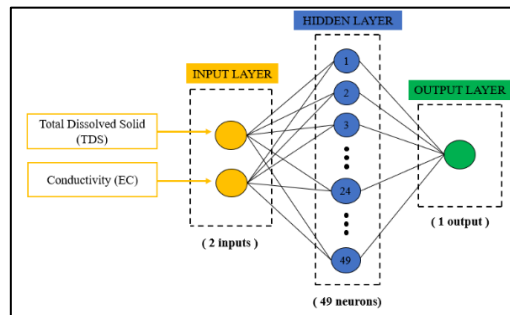


Figure 1. ANN structure that is used for this project

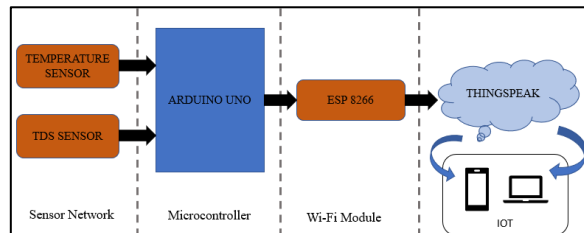


Figure 2. Block diagram of the water quality monitoring (WQM) classification

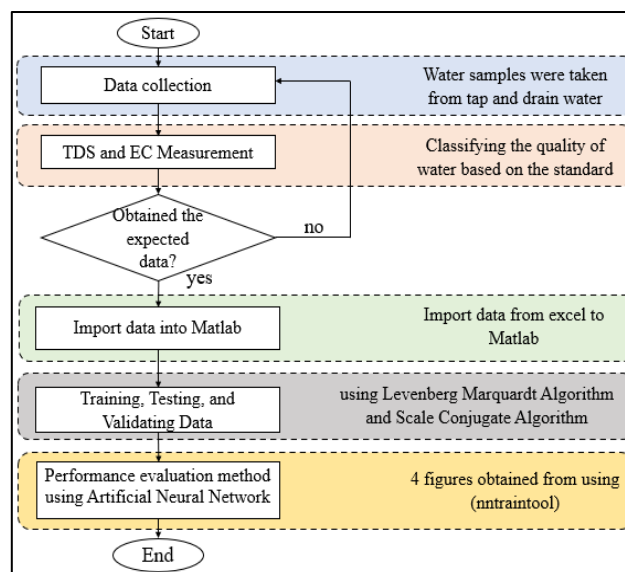


Figure 3. Flowchart of overall process

2.1. Data collection and sample preparation

A total of 200 data were collected from the Sungai Besar River in Sabak Bernam, Selangor, Malaysia. The selection of this river is based on the factor of high-water consumption for agricultural activities such as palm oil, rubber tree plantations and paddy fields. At the beginning of the data collection process, 100 samples of tap water were taken as clean water whereas 100 samples of drain water from the river were taken as polluted water. The water sample was collected from December to January 2021. The water was collected directly from the drain using water quality measurement device. The water was stored in a container that was guaranteed to be contaminant-free. To perform the test, a minimum of 50 mL of water was collected from the tap and drain. The sample containers were placed in a box that was kept in a wet location to control the water temperature.

2.2. Measurement of TDS and EC

The formula as in (1) was used to calculate the EC value from the TDS value. The EC reading from the experiment in milli Siemens/centimeter (mS/cm) is multiplied by 1000 and divided by two to get an approximate TDS value for water. While for the EC value, the TDS (in parts per million (ppm)) value is multiplied by two and divided by 1000 as in (2).

$$\text{TDS (ppm)} = \text{EC} \times 1000 / 2 \tag{1}$$

$$\text{EC (mS/cm)} = \text{TDS} \times 2 / 1000 \tag{2}$$

2.3. Training, testing and validating using trainlm and trainscg

The terms "trainlm" (Levenberg Marquardt) and "trainscg" (scale conjugate gradient) refer to two different types of training models that were used to analyse and evaluate the performance of ANN. The model was put to the test using 200 testing samples. The testing percentage was tested from a range of 15% to 20%. The number of neurons was increased until 49 in a step size of 2, with only the initial, middle and last number of neurons being considered. The name of the model was selected as "type of learning algorithm_testing percentage_number of neurons" for example "trainlm_16_3". This showed that the tests were carried out for every 3, 24, and 49 neurons. The percentages employed in each model are shown in Table 1. The neural network was trained with 200 samples. Its performance was evaluated using the confusion matrix's parameters consisted of specificity, sensitivity, and accuracy.

Table 1. The training, testing, and validating percentage
Total no. of samples: 200

Training	Testing	Vallidating	Ratio of samples
70%	15%	15%	1:140 141:170 171:200
70%	16%	14%	1:140 141:172 173:200
70%	17%	13%	1:140 141:174 175:200
70%	18%	12%	1:140 141:176 177:200
70%	19%	11%	1:140 141:178 179:200
70%	20%	10%	1:140 141:180 181:200

2.4. Performance evaluation method using ANN

Following the testing of the samples, the MATLAB outcome included four figures: neural network training (NNtraintool), plot performance, receiver operating characteristic (ROC), and confusion matrix research. The number of neurons that was used to test the sample was displayed in the hidden layer portion. Examples of the generated figure from ANN are illustrated in Figure 4 where Figure 4(a) shows the network architecture based on the hidden layer with 49 number of neurons and the output is either '1' for polluted or '0' for clean water. Meanwhile, Figure 4(b) illustrates the plot performance for the training, validation, and test performance of the training record.

In general, as the number of training epochs increases, the error reduces, but it may gradually climb on the validation data set as the network begins to overfit the training data. In ANN, an epoch is one cycle of the complete training dataset. It normally takes several epochs to train a neural network. It is well known that an epoch can cause an iteration to fail [26]. A confusion matrix is a machine learning concept that stores data about a classification system's actual and expected classifications. A confusion matrix has two dimensions, one for the actual class of the item and the other for the anticipated class of the classifier [27]. The key portion of analysing the neural network's performance is based on the test confusion matrix, which will then be compared to the specificity, sensitivity, and accuracy values.

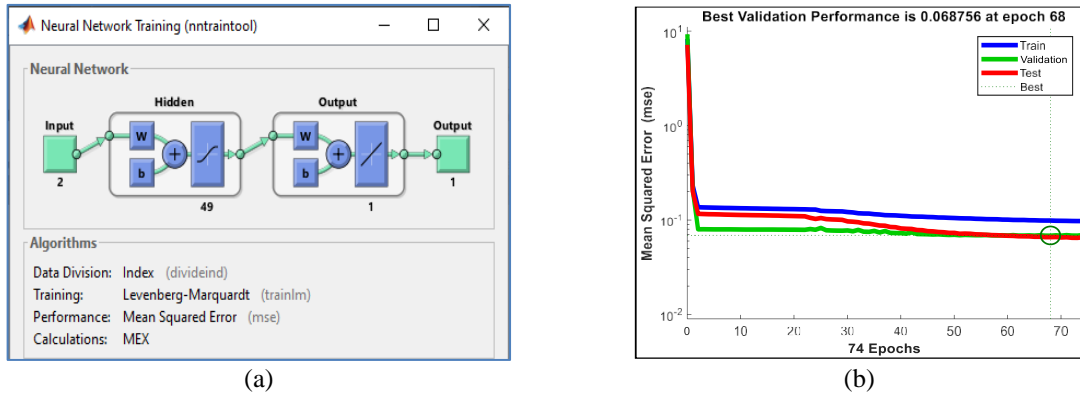


Figure 4. Examples of generated figures from ANN where in (a) the schematic diagram of ANN architecture and (b) graph of plot performance for mean square error

There are four measurements in the confusion matrix: true positive (TP): both the standard and the predicted outcome are positive. true negative (TN): both the standard and the predicted value are negative. false positive (FP) occurs when the standard is negative, but the predicted value is positive. false negative (FN): the standard is positive, while the predicted outcome is negative as shown in Figure 5. A variety of overall performance were developed based on the confusion matrix.

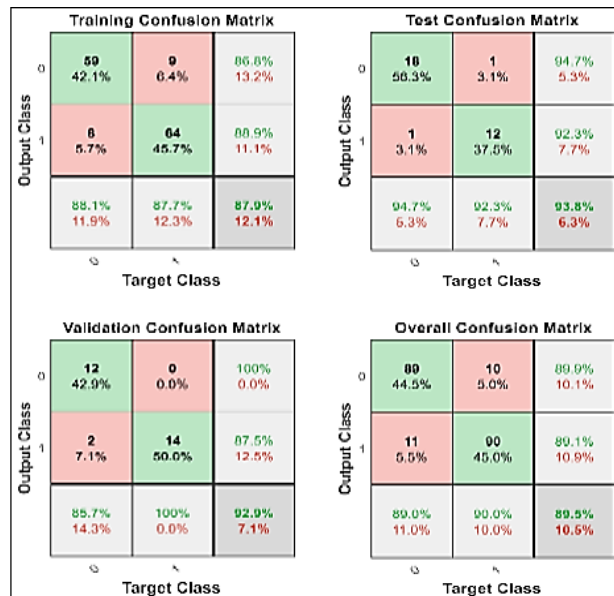


Figure 5. Confusion matrix for training, testing validation, and overall

3. RESULTS AND DISCUSSION

In this research, mean square error (MSE), epoch, specificity, sensitivity, and accuracy for each testing percentage and number of neurons will be evaluated and discussed. Table 2 shows the values that had been obtained from the mean square error vs epoch validation graph. The best validation performance is where the validation performance and the number of epochs is low. Thus, the best validation performance is when the testing percentage is at 19% with 0.058764 of mean square error (MSE) and at 1 epoch. Meanwhile, for Table 3, the best validation performance was when the testing percentage is at 20% with 0.048046 of mean square error (MSE) and at 1 epoch.

Based on Table 4, there were three models that gave the best accuracy compared to other models. Firstly, even though the model with a testing percentage of 16% and 49 neurons obtained the highest accuracy in the confusion matrix, it was not selected as the best model. This is because, the high number of neurons

would affect the complexity of the system compared to the other two models with samples that had lower number of neurons. So, in order to compare the models, other parameters should be considered as well. The parameters were testing percentage, number of neurons, accuracy, validation performance, epoch, and ROC. Table 4 shows that model trainlm with 18% testing percentage, an accuracy of 91.7%, validation performance of 0.073346 with 24 epochs and only 3 number of neurons was the most optimised model compared to others. In addition, the curve of ROC from the model shows a better approach to the true positive rate compared to the other models. It shows that the LM learning algorithm can achieve high accuracy in modelling parameters. This can be seen based on the consistent value of accuracy as shown in Table 5.

Table 2. Best validation performance and epoch for mean square error in trainlm

	Testing %	Neuron	Best validation performance	Epoch
(a)	15	49	0.070041	44
(b)	16	49	0.068756	68
(c)	17	3	0.081770	2
(d)	18	3	0.073346	24
(e)	19	3	0.058764	1
(f)	20	3	0.062318	3

Table 3. Best validation performance and epoch for mean square error in trainscg

	Testing %	Neuron	Best validation performance	Epoch
(a)	15	3	0.074121	14
(b)	16	3	0.071393	2
(c)	17	3	0.081021	2
(d)	18	3	0.086117	6
(e)	19	3	0.059714	3
(f)	20	3	0.048046	1

Table 4. Comparison between samples

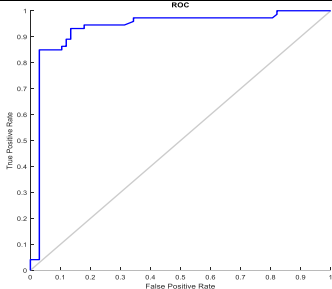
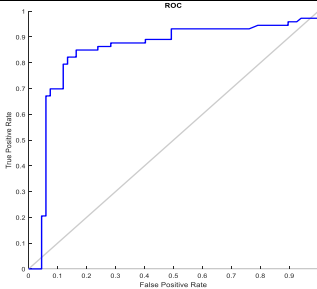
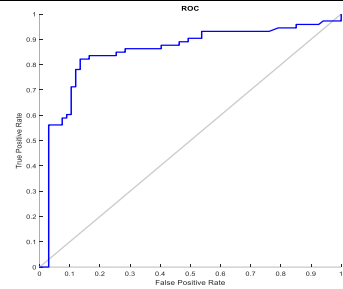
Model	Trainlm_16_3	Trainlm_18_3	Trainscg_18_3
Testing	16%	18%	18%
Neuron	49	3	3
Accuracy	93.8%	91.7%	88.9%
MSE	0.068756	0.073346	0.086117
Epoch	68	24	6
ROC			

Table 5. Comparison between models in previous studies

Algorithm	Accuracy
Levenberg-Marquardt	95.9%
Scaled conjugate gradient	90%
Support vector machine	87.10%
Trainlm_16_3	93.8%
Trainlm_18_3	91.7%
Trainscg_18_3	88.9%

4. CONCLUSION

This research was undertaken to predict the river water quality using the soft computing techniques of ANN that used standard back-propagation method that are Levenberg-Marquardt algorithm and scaled conjugate gradient as the learning technique. In this paper, a comparison between the two learning algorithms has been proven to achieve the objective which was to classify the quality of water in the Sabak Bernam river most effectively. Both models used one hidden layer for modelling, and the number of hidden neurons was set at 3, 24, and 49. In addition to that, six different testing percentages were used for this analysis, which were (15%, 16%, 17%, 18%, 19%, and 20%). From the obtained results, it can be shown that the best model was from the model of

trainlm at a testing percentage of 18% with 3 number of neurons and an accuracy of 91.7%. The best validation performance of this model was 0.073346 with 24 epochs and having a ROC curve that was closer to true positive rate compared to other samples. It is concluded that the main objectives of this work were successfully achieved, which was to find the most optimised model based on the Levenberg-Marquardt algorithm and the scaled conjugate gradient learning algorithm. This system can be expanded in the future by considering integrating it with internet of things (IoT) capabilities, making it fully automated and implementing the sensing activity on other sensors. In addition, the classification process will be the main essence of this research, which aims to find the most optimised model with the highest performance at the highest achievable accuracy.

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