

Artificial neural network and mathematical approach for estimation of surface water quality parameters (case study: California, USA)

Esmail Salami Shahid^a, Marjan Salari^b, Mohammad Rastegar^{c,*}, Solmaz Nikbakht Sheibani^a, Majid Ehteshami^d

^aDepartment of Civil and Environmental Engineering, Shiraz University, Shiraz, Iran

^bDepartment of Civil and Environmental Engineering, Sirjan University of Technology, Kerman, Iran

^cDepartment of Power and Control, Shiraz University, Shiraz, Iran, email: Mohammadrastegar@shirazu.ac.ir

^dDepartment of Civil and Environmental Engineering, K.N. Toosi University of Technology, Tehran, Iran

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ABSTRACT

Determination of salinity, dissolved oxygen (DO), DO percentage, and chlorophyll content of water as four major surface water quality parameters is necessary for environmental and practical purposes. The presented study uses mathematical methods in combination with an artificial neural network (ANN) to represent models that use electrical conductivity (EC), temperature (T), and pH values as their inputs to estimate salinity, DO, DO percentage, and chlorophyll content. 3,473 sets of data are obtained from Doughty Cut above Grant Line Canal, California, USA—water quality monitoring station from 6/20/2006 to 8/7/2018. Two mathematical models are used for the estimation of salinity. One just uses EC as the input, while the other one uses both EC and T variables. Accuracy rates of 98.6% and 99.1% are achieved from these mathematical models, respectively. In addition, four feed-forward back propagation ANN models are used to estimate the four mentioned parameters. All these models use EC, T , pH values as their inputs. The accuracy rates are obtained equal to 99.2%, 94.1%, 93.5%, and 75.9% in these ANN models. Most of the presented models have high and promising accuracies, although in the case of chlorophyll model, the accuracy is low.

Keywords: Salinity; Dissolved oxygen; Chlorophyll; Artificial neural network; Modeling

1. Introduction

Water scarcity in the world is turning into a more serious challenge every year. During the last century, the growth rate of water consumption was twice the rate of population increase, and the complexity of managing natural resources generally increases as the human population grows [1–8]. In addition to being the major sources of water, river systems are used as the principal disposal pathways for industrial, agricultural, and domestic effluents. As demand for water increases and water quality deteriorates, there is a requirement for some effective decision-making techniques

that can be applied to solve water quality management problems [4]. In this regard, water quality models can be useful tools for simulating and predicting pollutant transport [5,6], which can contribute to saving the cost of labors and materials for a large number of chemical experiments [7].

In order to estimate and model the quality of water, one should use parameters that can be measured easily and accurately at low cost. Temperature (T), pH, and electrical conductivity (EC) is the easiest parameters that could be measured in real-time with very simple and cheap equipment [1–3].

* Corresponding author.

EC is the ability of current conduction [9] and is measured by an electronic probe, which applies an electric voltage between two electrodes [10,11]. Pure liquid water has a very low electrical conductivity. The presence of charged particles in the water increases its conductivity. In general, as the concentration of total dissolved solids (TDS) in the water increases, its conductance also increases [10,11], and thus, EC is a proper indicator for salinity in water [10,11] and soil environment [12]. In the following, surface water quality parameters are described, and associated works are reviewed. Then, the proposed algorithm for modeling these parameters and the main contributions of this paper are presented.

Estimating the value of salinity and DO value with measurement equipment is tricky, and the determination of chlorophyll amount needs complicated processes and sophisticated equipment.

The goal of this study is to present models for estimating salinity, DO, DO percentage, and chlorophyll values based on EC, pH, and T values, and the contributions of this study are:

- This study presented models that use three measurable parameters, that is, EC, pH, and T , to estimate four important water quality parameters, with high accuracy and low cost.
- Mathematical models and ANN-based approaches are used to estimate salinity, DO, DO percentage, and chlorophyll values based on EC, pH, and T values.
- Proposed models are achieved based on real daily data from 2006 to 2018 which is a very wide timespan and makes models reliable in any environmental conditions.
- Models are proposed for estimating DO percentage and chlorophyll content based on EC, pH, and T .
- Proposed modeling methods can be developed for other water sources.

The main objective of this study was to introduce an artificial neural network (ANN) and mathematical approach for estimation of surface water quality parameters of salinity, dissolved oxygen, dissolved oxygen percentage, and chlorophyll.

1.1. Salinity

Salinity is one of the most important properties of drink and agricultural water and aquatic habitats, and many researchers worked on the effect of salinity on water quality for drinking, agricultural, industrial, and environmental purposes [13–17]. Salinity also affects the melting point of ice (or freezing point of water) [16].

EC and TDS are indicators of salinity. Many researchers believe that the salinity of water has a direct correlation with EC and TDS [2,9,18–21]. Eq. (1) is a proper estimation for evaluating the value of TDS (or salinity value) [2,18,19,21].

$$\text{TDS or Salinity (mg/L)} = \alpha \times \text{EC } (\mu\text{S/cm}) \quad (1)$$

TDS meters estimate TDS value based on this equation but α is not a constant value. Rusydi estimated α to be

0.5–0.75 for evaluating TDS in different waters [19], and Thirumalini and Joseph [19] consider α to be 0.55–0.7 as a true assumption for estimating the TDS value [18]. Salami et al. calculated $\alpha = 0.5$ as the best approximation for estimation of the salinity value of San Joaquin River basin (California, USA) [2]. According to the effect of temperature on the ion movements in solution, we could have different EC readings in constant TDS (s) in different temperatures [9].

1.2. Dissolved oxygen and DO percentage

Dissolved oxygen (DO) is an essential component that determines the water quality and trophodynamics of an aquatic system [22–27]. DO dynamics are complex in nature and are affected by many physical, chemical, and biological processes. The important factors that affect DO dynamics in an aquatic environment are temperature, atmosphere-water surface exchange, photosynthesis, respiration, and mineralization [22–24].

A fluctuation of DO near its saturation indicates relatively healthy waters [22]. The value of DO for saturation depends on temperature and DO percentage is an indicator of the step of DO saturation [22,25]:

$$\text{DO percentage (\%)} = \frac{\text{DO (mg/L)}}{\text{DO}_{\text{sat}} \text{ (mg/L)}} \times 100 \quad (2)$$

There are several methods for DO determination, which vary from chemical laboratory tests (Winkler titration method) to measurements by means of instruments equipped with sensors sensitive to DO concentration in a sample [26]. Accurate DO measurement with sensors is not an easy task because it is influenced by numerous uncertainty sources [25]. Therefore, using models for estimating DO (and DO percentage) could be very useful [27–29].

1.3. Chlorophyll

Chlorophyll is a key biochemical component in the molecular apparatus that is responsible for photosynthesis, the critical process in which the energy from sunlight is used to produce life-sustaining oxygen. As a representative index of eutrophication, the concentration of chlorophyll has always been a key indicator monitored by environmental managers [30–36]. Phytoplankton as chlorophyll-containing organisms is the first step of production in most marine processes and food chains [33]. Utilities that use surface water supplies should measure planktonic algal chlorophyll as a raw water quality parameter on a routine basis [36]. The higher ranges, encountered in chlorophyll, and other nutrient content, indicate changes in water quality and a resultant eutrophication process in water bodies [31]. Many other researchers tried to monitor the amount of chlorophyll (chlorophyll-a) in water reservoirs as an indicator of nourishing of water bodies [31–35] and some researchers worked on the factors that could affect the chlorophyll concentration, such as the speed of wind blowing [37] and salinity stress [38]. There are various techniques to measure chlorophyll, including spectrophotometry, high-performance liquid chromatography (HPLC), and fluorometry [39].

1.4. ANN modeling

ANNs have seen an explosion of interest over the last two decades, and have been successfully applied in all fields of chemistry and particularly in analytical chemistry. Inspired from biological systems and originated from the perceptron, that is, a program unit that learns concepts, ANNs are capable of gradual learning over time and modeling extremely complex functions [1–3,39–41]. ANN eliminates the limitations of the classical approaches by extracting the desired information from the input data. Applying ANN to a system needs sufficient input and output data instead of a mathematical equation, and it is a good alternative to conventional empirical modeling based on polynomial and linear regressions [1–3,42]. ANNs have been found to be very efficient in solving nonlinear problems including those in real world [43].

Many researchers use ANN for modeling water quality parameters such as salinity, DO, and chlorophyll [1–3,28–30,44–49], and many others use the ANN method for modeling hydrological phenomenon like flood forecasting [48] and treatment processes such as predicting Pb adsorption [47]. Flowchart of the proposed methodology for estimation of surface water quality parameters shows that in Fig. 1.

2. Methods and materials

2.1. Data

Data used in this study is obtained from the surface water quality monitoring station from the department of water resources of California, USA site (www.water.ca.gov). Monitoring station profile is: Code: B9532500.

Address: Doughty Cut above Grant Line Canal – Water quality monitoring station.

Coordinates: latitude: 37.8147169 and longitude: -121.4252089.

Elevation: 0 m. Fig. 2 shows the map of the proposed doughty cut above the Grant Line Canal.

Data include the daily mean value of quality parameters of EC (μS/cm), pH, T (°C), salinity (mg/L), DO (mg/L), DO percentage (%), and chlorophyll (μg/L). These data are available from 6/20/2006 to 8/7/2018, so the number of existed data is 4,433 rows. However, there were some missing data for each parameter, and after filtering the data; 3,473 rows of data remain. One row of data is removed from each year (randomly) and not participating in the modeling process. After modeling, these 13 rows of data are used for testing (Table 3), so 3,460 rows of data are used for the modeling process, which is presented in Figs. 2–8.

2.2. Mathematical modeling

Because of the direct correlation between salinity and EC, it is possible to develop simple equations like Eq. (1). The first model is based on this equation and α value is estimated by the average ratio between EC and salinity:

$$\alpha = \frac{1}{3,460} \times \sum_{i=1}^{3,460} \frac{\text{Salinity}}{\text{EC}} \tag{1}$$

Second model is counted for the effect of temperature on the EC value (in constant salinity) and is expressed as a first-degree polynomial with EC and T variables:

$$\text{Salinity} = c_1 + c_2 \times \text{EC} + c_3 \times T \tag{4}$$

Best combination of constant coefficients c_1 , c_2 , and c_3 can be determined by the curve fitting tool of MATLAB software.

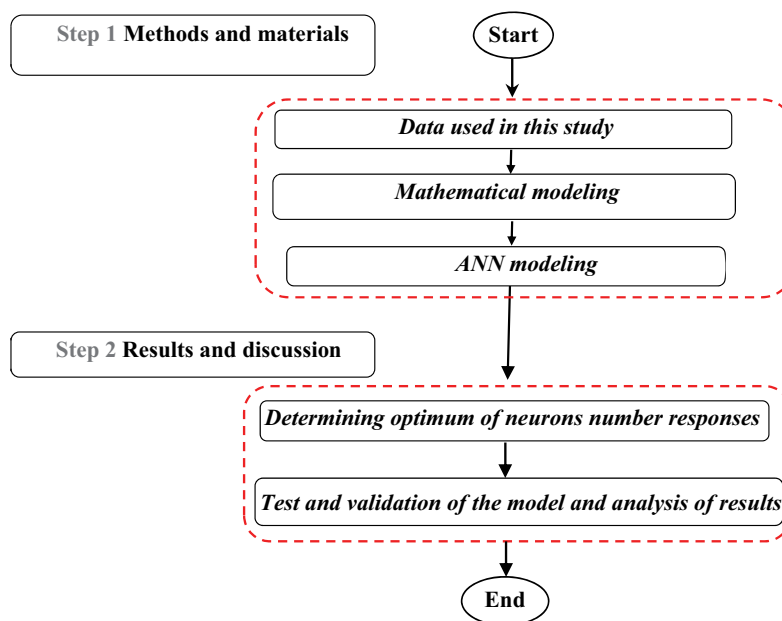


Fig. 1. Flowchart of the proposed methodology for estimation of surface water quality parameters.

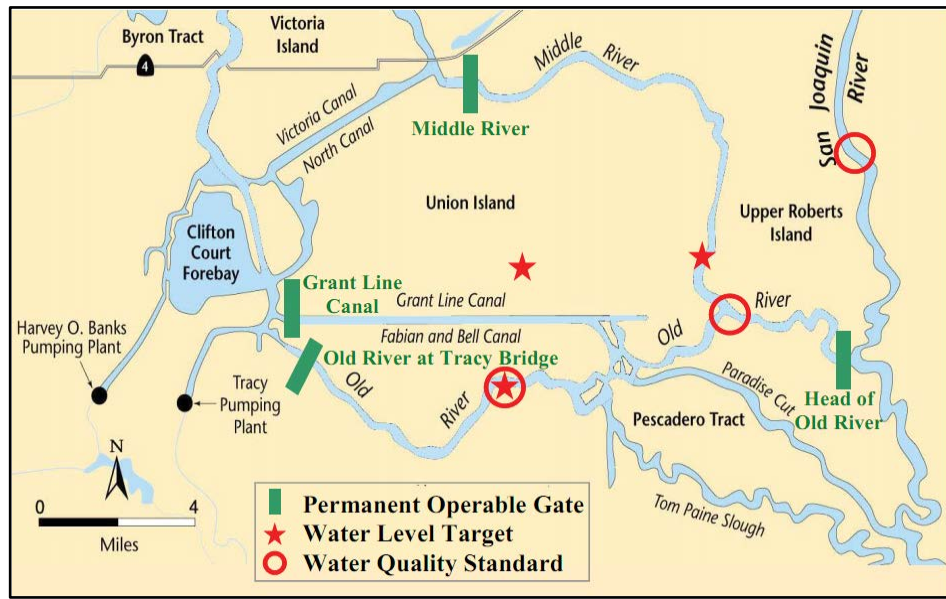


Fig. 2. Map of proposed doughty cut above Grant Line Canal [48].

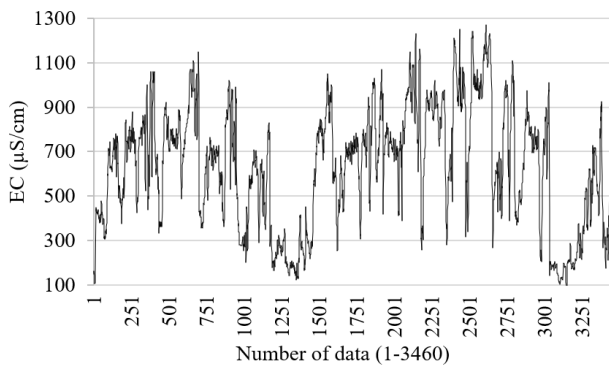


Fig. 2. EC data.

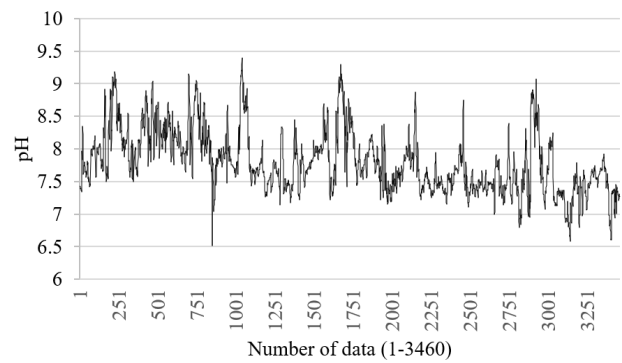


Fig. 4. pH data.

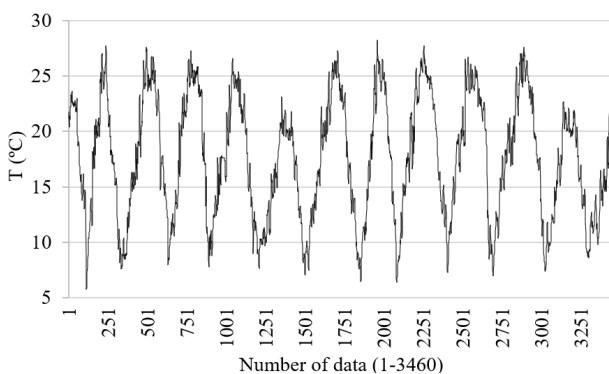


Fig. 3. Temperature data.

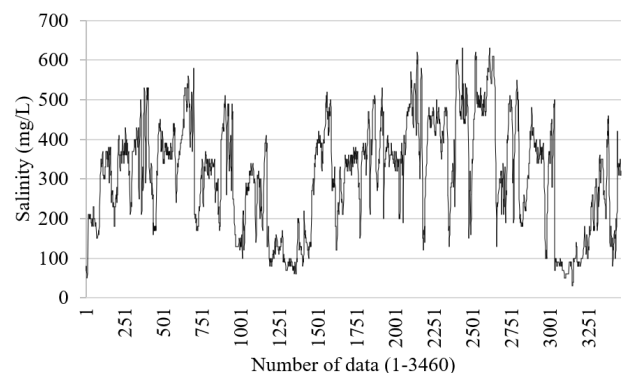


Fig. 5. Salinity data.

To achieve a more accurate model to estimate salinity and to estimate the other three parameters, DO, DO percentage, and chlorophyll, which does not have a simple linear relationship with EC, pH, and T, the ANN modeling approach is employed.

2.3. ANN modeling

An ANN consists of a number of layers and each layer contains a number of neurons, which are matrices whose sizes depend on the number of input and output parameters

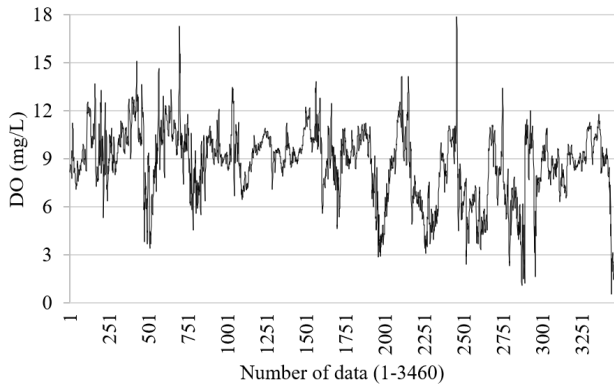


Fig. 6. DO data.

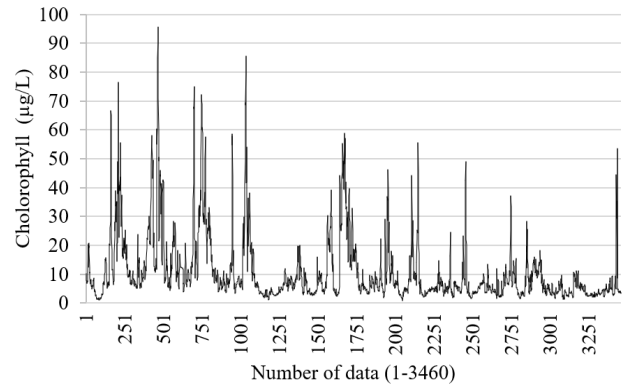


Fig. 8. Chlorophyll content data.

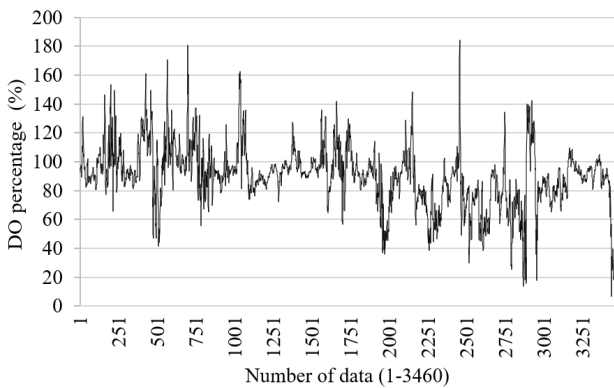


Fig. 7. DO percentage data.

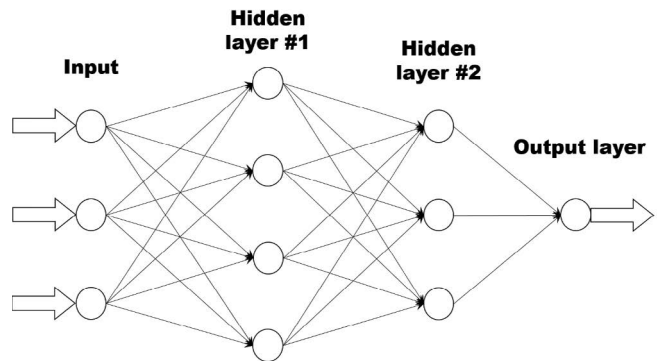


Fig. 9. Feed-forward ANN with two hidden layers.

[1–3,43,44,50–58]. Fig. 8 shows a three-layer feed-forward back-propagation network. In this study, the networks have three inputs (EC, pH, and *T*). Therefore, the first layer, which is not considered as a design layer, has three neurons, each of which has 1 column and 3,460 rows. Each model has a target (for example salinity); so, the output layer consists of one neuron, as presented in Fig. 9.

$$p = \begin{bmatrix} p_1 \\ p_2 \\ \cdot \\ \cdot \\ \cdot \\ p_{3,460} \end{bmatrix}, w = \begin{bmatrix} w_1 \\ w_2 \\ \cdot \\ \cdot \\ \cdot \\ w_{3,460} \end{bmatrix}, b = \begin{bmatrix} b_1 \\ b_2 \\ \cdot \\ \cdot \\ \cdot \\ b_{3,460} \end{bmatrix}, a = \begin{bmatrix} a_1 \\ a_2 \\ \cdot \\ \cdot \\ \cdot \\ a_{3,460} \end{bmatrix} \quad (5)$$

Matrices “*w*” and “*b*,” presented in Eq. 5, are called weight and bias matrices, respectively. Each neuron in hidden layers has an operator that is displayed in Fig. 10 and is presented by Eqs. (6) and (7). Output of each neuron (matrix “*a*” in Eq. (5)) will be as input (matrix “*p*” in Eq. (5)) to the next hidden layer. The number of hidden layers and the number of neurons in each layer should be designed (by try and error). However, the number of neurons depends on the number of input data, and the number of

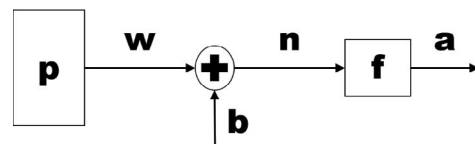


Fig. 10. Simple neuron.

layers depends on the complexity of the modeling problem. There is no specific definition for optimized ANN and usually, the accuracy of the model evaluates the quality of the model, but the smaller the network, the higher the speed of calculations will be [2,41,43,51].

$$n = w \cdot p + b \quad (6)$$

$$a = f(w \cdot p + b) \quad (7)$$

The “*f*” function is called transfer function. In this study, $\text{tansig}(x)$ is used for the transfer function of all networks. It returns the output of neuron to numbers between –1 and 1. This transfer function is shown in Fig. 11.

In output layer, that is, the last layer, the network compares the estimations (results of network) with the target data (for example real salinity data) and produces the difference value “*e*” (matrix). The network adjusts the training

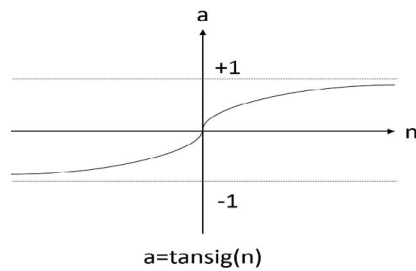


Fig. 11. Tansig(x) transformer function that transforms “n” value to a value between –1 and 1.

parameter (μ value) according to the training function and “e”, and goes to the next step. In this study, Levenberg–Marquardt (trainlm) training algorithm is deployed for training of the network that could be represented by Eqs. (8)–(10):

$$H = J^T \cdot J \quad (8)$$

$$g = J^T \cdot e \quad (9)$$

$$p_{k+1} = p_k - [H + \mu \cdot I]^{-1} \cdot g \quad (10)$$

Matrix “J” is the Jacobin matrix that contains the first derivatives of the network errors (“e” matrix) with respect to the weights and biases (“w” and “b” matrices) through a standard back-propagation method [42]. The process is repeated until reaching the goal of training (minimum of “e”) or maximum number of fails. Fails happen when a training step has errors greater than (or equals to) previous step and (in this study) the performance function is the mean of squared (MSE) error value:

$$e_k = [e_1, e_2, \dots, e_{3,460}]^T \quad (11)$$

$$MSE_k = \frac{1}{3,460} \times \sum_{i=1}^{3,460} e_i \quad (12)$$

$$MSE_{k+1} \geq MSE_k \Rightarrow \text{Fail} \quad (13)$$

where e_k and MSE_k are error matrix and MSE of k th training step, respectively.

Table 1
Optimal results for ANN and training parameters

Network type	Feed-forward back propagation	μ_0	0.001
Training function	Trainlm	μ decrease	0.1
Performance function	MSE	μ increase	10
Transfer function	Tansig(x)	maximum μ	1E+10
Maximum fail	6	Minimum of g	1E-10

The training parameters of ANNs and the computations and networks training accomplished by NN tool of MATLAB software are shown in Table 1.

To show the precision of models, the mean absolute error (MAE) would be the benchmark that could compare with mean value of data (M).

$$MAE = \frac{1}{3,460} \times \sum_{i=1}^{3,460} |R_i - y_i| \quad (14)$$

$$M = \frac{1}{3,460} \times \sum_{i=1}^{3,460} R_i \quad (15)$$

$$\text{Accuracy rate} = \left(1 - \frac{MAE}{M}\right) \times 100 \quad (16)$$

where R_i is the real target (salinity, DO, DO percentage, and chlorophyll) data and y_i is the model output.

3. Results

Two mathematical models are developed for estimating salinity (Eqs. (17) and (18)), and four ANN models are designed for estimating salinity (model 1), DO (model 2), DO percentage (model 3), and chlorophyll (model 4). These models can be run by MATLAB software, and the user can import the number of desired input data sets consisting of EC, T , and pH values. Each model estimates the associated target parameter (Table 2).

$$\text{Salinity} \left(\frac{\text{mg}}{\text{L}} \right) = 0.48 \times \text{EC} (\mu\text{S/cm}) \quad (17)$$

$$\text{Salinity} \left(\frac{\text{mg}}{\text{L}} \right) = -3.37 + 0.5 \times \text{EC} \left(\frac{\mu\text{S}}{\text{cm}} \right) - 0.25 \times T (^\circ\text{C}) \quad (18)$$

As mentioned in methods and materials section, 13 rows of data sets have been removed from modeling process for testing the models and verifying the capability of these models to estimate the targets with new inputs. One data set is randomly chosen from each year from different months, so that all possible environmental seasonal conditions are covered. These data are presented in Table 3. Figs. 12–15 show comparison between models results and real data (the purpose of deleting these 13 rows is to test the model, and at the end, the obtained model was tested with these 13 rows of selected data).

Table 2
Models' properties

	Model	Number of hidden layers	Neurons in layer1	Neurons in layer2	Mean value of data	MAE	Accuracy rate
Salinity (mg/L)	Eq. (17)	–	–	–	309.84	4.45	98.6%
Salinity (mg/L)	Eq. (18)	–	–	–	309.84	2.80	99.1%
Salinity (mg/L)	Model 1	1	10	–	309.84	2.56	99.2%
DO (mg/L)	Model 2	2	25	16	8.7	0.51	94.1%
DO percentage (%)	Model 3	2	25	16	90	5.84	93.5%
Chlorophyll (µg/L)	Model 4	2	28	22	10.86	2.62	75.9%

Table 3
13 sets of data removed from modeling process in order to test model's precision

Date	EC (µS/cm)	T (°C)	pH	Salinity (mg/L)	DO (mg/L)	DO% (%)	Chlorophyll (µg/L)
12/27/2006	595	9.3	7.94	290	11.21	97.83	5.04
1/21/2007	616	7.4	7.95	300	11.93	99.47	6.80
2/15/2008	899	10.9	8.15	450	11.83	107.28	11.81
3/29/2009	1,020	17.5	9.05	510	14.96	156.81	61.70
4/19/2010	366	18.1	7.96	180	8.91	94.35	5.69
5/23/2011	199	17.0	7.42	90	9.44	97.77	6.70
6/6/2012	562	20.0	8.30	270	9.60	105.90	20.91
7/3/2013	769	28.8	7.36	370	2.89	37.63	16.00
8/17/2014	1,000	25.8	7.45	490	5.21	64.21	5.09
9/11/2015	1,180	24.0	7.48	580	5.50	65.58	5.62
10/16/2016	629	19.6	7.58	310	6.67	72.95	5.97
11/25/2017	525	15.1	7.60	260	8.82	87.84	3.24
1/19/2018	730	12.2	7.57	360	9.55	89.18	2.91

As Figs. 12–15 show the trend of changes in real data related to parameters (salinity (mg/L), DO (mg/L), DO%, (%), and chlorophyll (g/L). It has a very close correlation with the obtained neural network models, which indicates that the mathematical methods in combination with ANN the ability to predict changes in qualitative parameters.

4. Conclusions

In this research, application of ANN and mathematical approach was investigated for estimation of surface water quality parameters, that is, salinity, DO, DO percentage, and chlorophyll content in Grant Line Canal, California, USA. Proposed models reduced the cost and time needed for measurement process, which can make the real-time monitoring possible. The presented study used mathematical methods in combination with ANN to represent models that use electrical conductivity (EC), temperature (T), and pH values as their inputs to estimate salinity, DO, DO percentage, and chlorophyll content. 3,473 sets of data have been obtained from Doughty Cut above Grant Line Canal, California, USA – water quality monitoring station from 6/20/2006 to 8/7/2018. The following conclusions can be drawn based on the presented analysis:

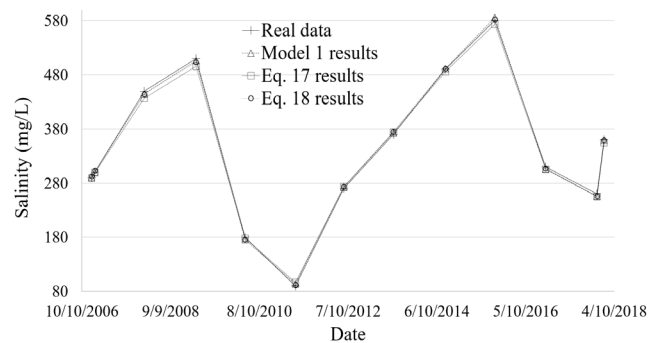


Fig. 12. Comparison between salinity real data and models estimation.

- Conventional methods like polynomial optimization could be deployed for modeling parameters like salinity that have linear correlation with EC and T, but for parameters that do not have such linear relations with input parameters and depend on several input parameters, ANN-based approaches can be used to model nonlinear and complex multi parameter correlations.
- Lower accuracy of model 4 implies that the chlorophyll content of surface water depends on other parameters

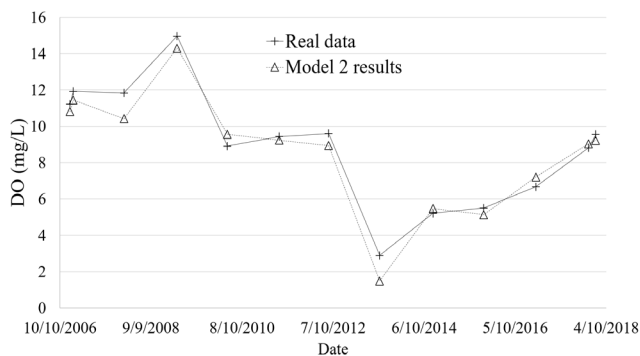


Fig. 13. Comparison between DO real data and model estimation.

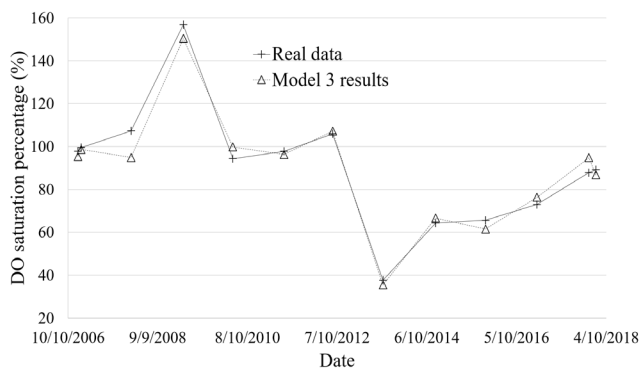


Fig. 14. Comparison between DO percentage real data and model estimation.

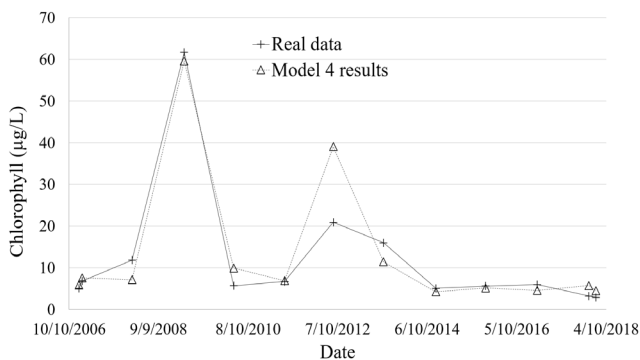


Fig. 15. Comparison between chlorophyll content real data and model estimation.

(beside EC, T , and pH) such as wind blowing nutrient content, turbidity, and light irradiation.

- One just uses EC as the input, while the other one uses both EC and T variables. Accuracy rates of 98.6% and 99.1% are achieved from these mathematical models, respectively. In addition, four feed-forward back propagation ANN models are used to estimate four mentioned parameters. All these models use EC, T , pH values as their inputs. The accuracy rates are obtained equal to 99.2%, 94.1%, 93.5%, and 75.9% in these ANN models. Most of presented models have high and promising

accuracies, although in the case of chlorophyll model, the accuracy is low.

- ANN is a reliable tool for estimating quality parameters of water bodies, which can be developed for other water resources and other quality parameters.

Comparison of the results of this study with those of previously conducted [1–3] indicates that the efficiency of estimation of surface water quality parameters was improved by utilizing application of ANN and mathematical methods.

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