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Development of a neural network model for dissolved oxygen in seawater

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Present paper consists the results from a study conducted to test the adequacy of artificial neural networks in modelling of dissolved oxygen (DO) in seawater. The input variables for ANN DO models are selected by statistical analysis. The ranking of important inputs and their mode of action on the output DO are obtained based on the expert's opinion. The calibrated neural network models predict the DO concentration with satisfactory accuracy, producing high correlations between measured and predicted values (R2>0.8, MAE<1.25 mg/L for training and overfitting test) at specified location and time in the selected domain where there are training stations. It is shown that one can forecast the next week's DO level from antecedent measurements with an acceptable confidence.

Introducion

In recent years, Artificial Neural Network (ANN) methods have become increasingly popular for prediction and forecasting in a number of disciplines, including water resources and environmental science. Although the concept of artificial neurons was first introduced in 1943[1], research into the application of ANNs has blossomed since the introduction of the backpropagation training algorithm for feedforward ANNs in 1986[2]. ANN may thus be considered as a fairly new tool in the field of prediction and forecasting. Though a variety of linear and nonlinear modelling techniques[3] could be applied, neural networks with active neurons, is believed to be a more appropriate prediction algorithm for noisy and short time-series. ANNs are able to find and identify complex patterns in datasets that may not be well described by a set of known processes or simple mathematical formulae. Neural network training methods generally fall into the categories of supervised (Multilayer perceptron, Radial basis function and Recurrent backpropagation method), unsupervised (Kohonen and Hopfield method) and various hybrid approaches (combines the best features of two different methods). Due to the correlation and interactions between the water quality variables, it is interesting to investigate the underlying mechanism governing the data and therefore prove the predictability of these variables. The identification of such models is particularly useful for ecologists and environmentalists to predict in advance the pollution levels in the sea water and therefore instruct all the necessary countermeasures.

Measures of Dissolved Oxygen (DO) refer to the amount of oxygen contained in water, and define the living conditions for oxygen-requiring (aerobic) aquatic organisms. Oxygen has limited solubility in water, usually ranging from 6 to 14 mg/L[4]. DO concentrations reflect an equilibrium between oxygen-producing processes (e.g. photosynthesis) and oxygen-consuming processes (e.g. aerobic respiration, nitrification, and chemical oxidation) and the rate of atmospheric exchange. DO concentration in water column is influenced by many factors such as temperature, salinity, oxygen depletion, sources of oxygen and other water quality parameters or variables; therefore, it is important to develop predictive/forecasting DO models for the management of water quality.

Many modelling studies have been carried out to compute DO concentration in streams[5] rivers[6], lakes[7], and estuaries[8]. However, these water quality models are often complex in nature and data demanding. Alternative modelling techniques such as ANN, fuzzy logic, and genetic algorithms have been successfully used in the past decade. Most of these applications are focused on modelling of water quality variables in fresh water bodies[9-11] and there have been limited number of studies for coastal waters[12-14].

This paper presents the ANN models developed to forecast DO based on weekly measured water quality data at three points of an estuary (Fig. 1). The choice of input variables for the neural network modelling is based on a statistical correlation analysis of the field data, a priori knowledge of causal variables in conjunction with the inspections of time series plots, the prediction accuracy of water quality variables and the domain knowledge[15]. The input variables for ANN DO models are selected by statistical analysis. The ranking of important inputs and their mode of action on the output DO are obtained based on the correlation analysis, relevance to the output variable and knowledge of the field characteristics. The purpose of this study is to determine the extent to which the DO concentration in Singapore seawater can be forecasted using continuous weekly measurements of selected water quality variables, such as temperature, salinity, pH, secchi depth (SD), Chlorophyll-a (Chl-a) and DO.

Materials and Methods

Study area and water quality data

The data used in this study are adopted from Singapore seawater quality survey conducted by Chuah[16] between December 1996 and June 1997 at the mouth of the East Johor Strait (Fig. 1) with the goal to investigate a potential for "red tide" occurrence, an outbreak of harmful algal bloom. The measurements during each sampling were taken systematically at similar tidal variation (spring/neap; low/high tide). The Johor Strait lies between mainland Malaysia to the north and Singapore to the south. During flood tide, the tidal current transports water via the Kuala Johor into the East Johor Strait; during ebb tide, the tidal current reverses its direction of flow. Due to the flow constriction, the surface and near-bottom tidal currents in Kuala Johor are stronger than those in the East Johor Strait. In the both areas ebb flows are stronger than flood flows, and surface currents are stronger than near-bottom ones[17-18]. Temperature and salinity variations in the East Johor Strait show daily and seasonal patterns, as well as affected by precipitation. The dominant forces in the East Johor Strait are similar to those of the Singapore Strait, both being affected by a semi-diurnal tide. Increased phytoplankton densities, higher temperatures, and lower salinity values are observed during low tide which might be due to freshwater flow from rivers. Out of selected four sites (Fig. 1), Station 3 is relatively shallow, lying within Serangoon Harbour, while Station 1 is located in deeper water off Changi Jetty. Station 2 might reflect the transition between Station 3 in the Johor Strait and Station 1 in offshore. During ebb tide, Serangoon Harbour receives the higher volume of water flowing eastward out of the East Johor Strait[17-18].

Fig. 1—Map showing geographical location of present study survey area with 4 field monitoring Stations in Singapore (1. Paku, 2. Malang Papan, 2alt. Sajahat and 3. Squance) and the major rivers in the East Johor Strait.

Seawater samples collected weekly from surface were analyzed[16] for the estimation of Chl-a, water temperature, salinity, pH, SD, DO and nutrients, such as ammonium (NH_4^+), nitrite (NO_2^-), nitrate (NO_3^-), total nitrogen (TN), phosphate (PO_4^-) and total phosphorus (TP). Other water quality variables are "derived, including nitrate nitrogen (NO_2+NO_3)", dissolved inorganic nitrogen (DIN=NH_4^++NO_2^- "+NO_3)", organic nitrogen (ON=TN-DIN) and organic phosphorous (OP=TP-PO_4^-). The range of measured water quality variables are given in Table 1. Measurements of nutrient concentrations (TN and TP), algal biomass (Chl-a/algal biovolume), and secchi disk transparency are essential parameters to manage and monitor coastal zone eutrophication[19].

Artificial neural network

The ANN is a mathematical structure designed to mimic the information processing functions of a network of neurons in the brain[20, 21]. ANNs are highly parallel systems that process information through many interconnected units that respond to inputs through modifiable weights, thresholds, and mathematical transfer functions. Each unit processes the pattern of activity it receives from other units, and then broadcasts its response to still other units.

Table 1—Water quality variables range in the model domain, measured during January 1997 to May 1997 in East Johor Strait

Parameters	unit	Min	Max	Mean	SD
Temperature	°C	27.6	31.8	29.4	1.10
Salinity	ppt	19.0	31.0	27.6	2.58
pH		7.50	8.70	8.26	0.27
SD	m	0.70	3.20	1.35	0.42
DO	mg/L	4.31	14.4	7.55	2.08
NH_4	mg/L	0.34	0.73	0.54	0.09
NO_2+NO_2	mg/L	0.06	0.20	0.11	0.02
DIN	mg/L	0.44	0.86	0.65	0.10
TN	mg/L	1.97	5.77	3.22	0.92
ON	mg/L	1.30	5.11	2.57	0.88
PO_4	mg/L	0.01	0.08	0.03	0.02
TP	mg/L	0.02	0.12	0.06	0.02
OP	mg/L	0.01	0.07	0.03	0.01
Chl-a	mg/m^3	0.85	71.7	11.6	13.8

A process-based model requires a lot of input data and model parameters (often unknown) such as initial boundary conditions of state variables, kinetic coefficients and hydrodynamic forcing. Unlike a process based model[22], it is not necessary to know exactly how those variables interact, the nature of the physical, chemical and biological processes that cause those patterns, or any mathematical representation of those processes before applying an ANN. However, the physics-based models may provide a better understanding of the system's behaviour and provide a better methodology for extrapolating to environmental conditions that are not manifested in the historical data[23]. As a result, ANN models can be developed more quickly and with less expense than typical process-based models. Though or since ANNs contain no internal “knowledge” of the processes behind the data patterns, they are less able to provide additional insight into those processes[24]. ANN’s are useful tools for finding and predicting patterns in water quality data. The most commonly used type of ANN, the feed forward network termed as the multilayer perception was used in this study (Fig. 2). Back propagation training algorithms are often too slow for practical problems. There exist faster and efficient algorithms such as heuristic technique (variable learning rate back propagation, resilient back propagation) and numerical optimization techniques (conjugate gradient, quasi-Newton, Levenberg-Marquardt). The most commonly used type of ANN, the feed forward network termed as the multilayer perception (MLP), is used in this study. The performance of this method was found to be good for the present problem.

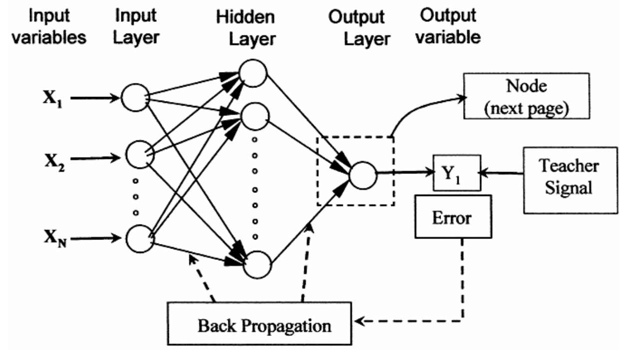

Fig. 2—Typical structure of artificial neural network.

In MLP network, the artificial neurons, or processing units, are arranged in a layered configuration containing an input layer, usually one “hidden” layer, and an output layer. Units in the input layer (x_i) introduce normalized or filtered values of each input into the network. Units in the hidden and output layers are connected to all of the units in the preceding layer. Each node ‘j’ receives incoming signals from every node ‘i’ in the previous layer. Each connection carries a weighting factor (W_{ji}). The effective incoming signal (I_j) to node ‘j’ is the weighted sum of all the incoming signals. The weighted sum of all inputs to a processing unit is calculated [Eq. (1)] and compared to a threshold value. The effective incoming signal, I_j, is passed through an activation function (sometimes called a transfer function) to produce the output signal (y_j) of the node ‘j’ that is sent to the processing units in the next layer. In this study, the linear function [$y_j = f(I_j)$] is used in the output layer and the sigmoid non-linear function is used in the hidden layers [Eq. (2)]. To determine the set of weights, a corrective repetitive process called ‘learning’ or ‘training’ is performed. This training forms the interconnections between neurons, and is accomplished using known inputs and outputs (training sets or patterns). The weight of these interconnections is adjusted using an error convergence technique so as to produce a desired output for a given input. Optimization routines can be used to determine the ideal number of units in the hidden layer and the nature of their transfer functions. ANN’s “learn” by example as long as the input dataset contains a wide range of the types of patterns that the ANN will be asked to predict and the model uses them successfully to predict the output using those patterns. The training method used is a standard back-propagation proposed by Reference 2. Data of field monitoring Stations 1 & 3 are used for model calibration while data from Stations 2 & 2-alt are used for model validation.

$$I_j = \sum_{i=1}^{q} x_i W_{ji} \quad \ldots (1)$$

$$y_j = f\left(I_j\right) = \frac{1}{1+e^{(-I_j)}} \quad \ldots (2)$$

Choice of network variables

In this paper, water quality variables such as temperature, salinity, pH, SD, Chl-a and DO concentrations are thought to be sufficient for DO forecasting. Using Neuroshell[24], ANN models are developed to forecast DO dynamics at Stations 2 & 2-alt using the water quality observations from Stations 1 & 3. The factors influencing DO concentration such as temperature, salinity, DO, pH, SD and Chl-a are considered as input variables. The DO concentration at week 't' is the output for ANN prediction and DO at 't+1' is the output for forecast model. The time lags of selected input variables of the ANN are t, t-1, and t-2. DO values at time lag t, t-1 and t-2 at Stations 1 and 3 are considered as input variables. The selection of appropriate model inputs is extremely important for ANN[25]. The choice of input variables is generally based on a priori knowledge of causal variables in conjunction with inspections of time series plots, and statistical analysis of potential inputs and outputs. A stepwise approach can also be used in which the separate networks are trained for each input variable. The network performing best DO forecast is then retained and the effect of adding each of the remaining inputs in turn is assessed. This process is repeated for combination of input variables, until the addition of extra variables does not result in a significant improvement in model performance[26]. A stepwise approach was then used to select the optimal ANN networks and its corresponding input variables to forecast (1 week ahead) or predict (present week t) DO.

Two ANN architectures such as Multi-Layer Back-Propagation (MLBP) and General Regression Neural Networks (GRNN) are selected for this study. The MLBP ANN architecture consisted of two hidden layers having logistic activation function. The GRNN was first introduced by Specht[27]. Unlike feed-forward neural networks, GRNN requires neither time-consuming trials nor over-training conditions. Furthermore, GRNN does not require initial setting of learning parameters; instead, a smoothing factor or bandwidth of all the parameters is calculated. Neural networks are intended to analyse data in a similar way to the way that the biological neural networks do. Instance-based learning techniques work essentially by keeping typical attribute examples for each class. One of the techniques that has a potential to resolve the issue of non-transparency in machine learning is instance-based learning (IBL). In this, the prediction is made on the basis of combining historical example (instances) that are in some way close to the new vector of inputs[28]. IBL techniques work essentially by keeping typical attribute examples for each class. The GRNN predicts continuous outputs. GRNN nodes require two main functions (i) to calculate the difference between all pairs of input pattern vectors, and (ii) to estimate the probability density function of the input variables. The architecture of GRNN works by measuring how far a given sample pattern is from patterns in the training set in N_i-dimensional space, where N_i is the number of inputs in the problem. The output that is predicted by the network is a proportional amount of all of the outputs in the training set. A typical GRNN architecture consists of a three-layer network where there must be one hidden neuron for each training pattern. There are no training parameters such as learning rate and momentum as in Back-Propagation (BP), but there is a smoothing factor that is applied after the network is trained. The number of hidden layers and nodes in the hidden layers are determined by trial and error.

In the present study, the water quality data (5 months, total of 32 numbers) from Stations 1 and 3 are divided into two sets. The first set with 80% records was used as training set; the second test with 20% records was used as overfitting test set. The data (11 numbers) for the Station 2 and data (5 numbers) for the Station 2alt, which have never seen before by trained ANN, were used as the validation set. MLBP ANNs with two hidden layers and 2–16 hidden nodes, learning rate = 0.1 and momentum term = 0.1 are successively trained based on the calibration data set. For GRNN modelling, genetic breeding size of 100 and genetic adaptive calibration are used. The learning process was controlled by the method of internal validation (about 20% of calibration data was held back and used to test the error at the end of each epoch)[29]. The weights are updated at the end of each epoch. The number of epochs with the smallest error of the internal validation indicates the weights to be selected. The ANN having the best performance when applied to the validation set was selected. In present DO forecast/prediction, it has been found that GRNN performed much better than MLBP.

Error terms: model selections

To assess the performance of the ANN during the validation phase and therefore to identify the best model, several measures of accuracy are applied, as there is not a unique and more suitable performance evaluation test[30]. The performance indicator Nash-Sutcliffe coefficient of efficiency (R^2)[31] is employed to see how far the model is able to explain the total variance of the data. The Nash–Sutcliffe coefficient of efficiency [Eq. (3)] (R^2) value of 1 indicates a perfect fit, while increasingly negative values indicate poorer fit[32]. In addition, it is advisable to quantify the error in the same units than the variables. These error terms are representative of the size of a "typical" error and easier to understand. These measures or absolute error measures included the square root of the mean square error (RMSE) [Eq. (4)], the mean square error (MSE) [Eq. (4)] and the mean absolute error (MAE) [Eq. (5)]. RMSE/MSE, MAE, R^2 and correlation coefficient (r) [Eq. (6)] are given below.

$$R^2=1-\left(\frac{F}{F_0}\right);\ F=\sum\left(Q_{obs}-Q_{pred}\right)^2;$$

$$F_0=\sum\left(Q_{obs}-Q_{meanobs}\right)^2 \qquad \dots (3)$$

$$RMSE=\sqrt{\frac{1}{N}\sum\left(Q_{obs}-Q_{pred}\right)^2}=MSE^{1/2} \qquad \dots (4)$$

$$MAE=\frac{1}{N}\sum\left|Q_{obs}-Q_{pred}\right| \qquad \dots (5)$$

$$r=\frac{N\sum xy-\left(\sum x\right)\left(\sum y\right)}{\sqrt{N\left(\sum x^2\right)-\left(\sum x\right)^2}\sqrt{N\left(\sum y^2\right)-\left(\sum y\right)^2}} \qquad \dots (6)$$

where Q_{obs} is the observed concentration at the time step t, Q_{pred} the estimated concentration at the same time step t and N is the total number of observations of the data set.

Results and Discussions.

Two models are built to forecast (model-1/model-2) the value of the DO at required time lag. The input variables of both forecast and prediction ANN models are the concentrations of Temperature, Salinity, DO, pH, SD and Chl-a at time t, t-Δt, and t-2Δt, at fixed locations (Stations 1 and 3), longitude (x) and latitude (y) of respective location. The subtitle t-Δt indicates the time lag of Δ week prior of the time t. The value of Δ could be selected depending on period of available data and required forecast period. Fig. 3 shows the temporal variation of DO, SD, pH, Temperature and Salinity at field monitoring stations in Singapore in the East Johor Strait. ANN forecast

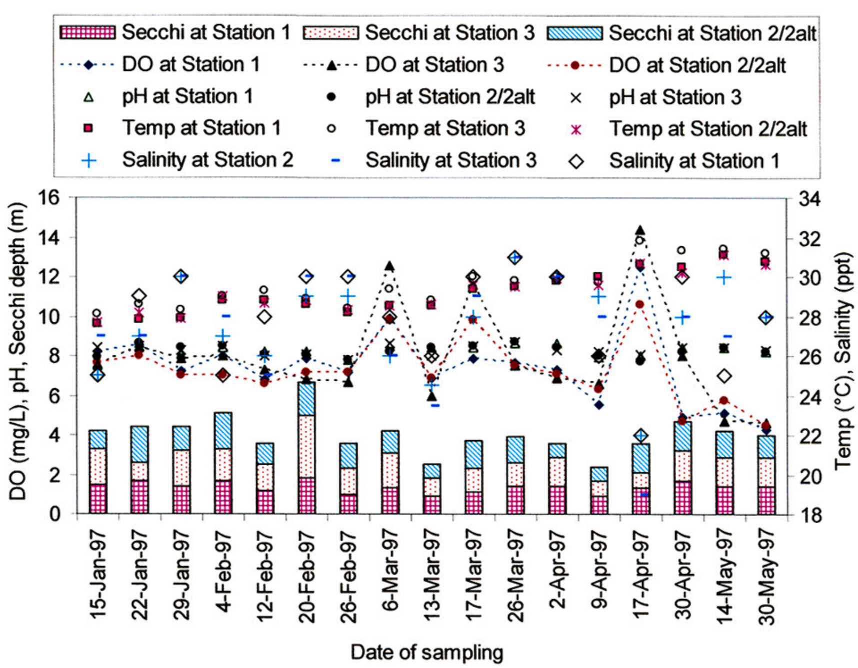

Fig. 3—Temporal variation of DO, Secchi depth (SD), pH, Temperature (Temp) and Salinity at four field monitoring Stations in the East Johor Strait, Singapore.

models are named as model-1a and model-1b and that of prediction as model-2a and model-2b with GRNN and MLBP architectures, respectively. Among the selected two ANN architectures, the developed DO ANN model with GRNN architecture simulated the DO concentrations of the Singapore seawater more accurately when compared to that with MLBP architecture. The performance indicators for best DO forecast ANN models are shown in Table 2.

Typical DO forecast model (model-1) results are shown in Fig. 4. Fig. 4a shows the DO forecast accuracy of ANN for training, overfitting test, and two independent validation sets. The DO forecast ANN model (model-1a) performance was good, with mean absolute errors less than 0.9 mg/L. The performance accuracy of the DO forecast model for "unseen" validation set at Stations 2 and 2alt was shown in scatter plots (Fig. 4b) and Table 2. The trained model-1 can be applied to estimate the DO concentration in Singapore seawater at any location and time when the real value cannot be obtained in the domain of interest (circled area in Fig. 1). The developed forecast model can be used to estimate interpolated data between two consecutives samples at same Station and to simulate different water quality scenarios for extreme ranges of input/output parameters at any location and time.

Table 2—Performance indicators for DO forecast and precast ANN model

Architecture	GRNN			
	R^2	MSE	MAE	r
Prediction DO(t) (Model-2a)				
Training	0.99	0.06	0.16	0.99
Overfitting test	0.81	1.53	0.87	0.96
Validation at 2-alt	0.70	1.52	0.99	0.98
Validation at 2	0.83	0.23	0.41	0.92
Forecast DO(t+1) (Model-1a)				
Training	0.98	0.10	0.21	0.99
Overfitting test	0.95	0.36	0.47	0.98
Validation at 2-alt	0.83	1.05	0.85	0.98
Validation at 2	0.78	0.30	0.45	0.91
Architecture	**MLBP**			
	R^2	MSE	MAE	r
Prediction DO(t) (Model-2b)				
Training	0.98	0.12	0.28	0.99
Overfitting test	0.90	0.79	0.76	0.97
Validation at 2-alt	0.56	2.23	1.21	0.96
Validation at 2	0.79	0.29	0.44	0.93
Forecast DO(t+1) (Model-1b)				
Training	0.97	0.15	0.31	0.99
Overfitting test	0.95	0.37	0.52	0.98
Validation at 2-alt	0.68	1.98	1.17	0.97
Validation at 2	0.60	0.54	0.49	0.93

Temporal DO variation and scatter plots of measured and predicted DO concentration in East Johor Strait at monitoring Stations 1 & 3 for training and overfitting test, Stations 2 & 2-alt for validation for model-2a are shown in Fig. 5a-b. The ANN DO prediction model with selected input variables for training and overfitting test more accurately simulates the range of DO values at Stations 2 and 2alt. Depending on the water quality sensitivity and variation of the DO prediction from that observed, the predictability of the developed ANN model is accurate enough to take the important decision or data usage.

The developed ANN model of DO was successful in simulating the patterns of measured DO concentrations that result from seasonal temperature variations, periodic blooms of phytoplankton, and discharges of oxygen-consuming substances from the pollution source. Oxygen solubility decreases with increasing temperature and vice versa with salinity. However, oxygen in seawater is not conservative because it is biologically active. In tropical environment where there are more chances for occurrences of phytoplankton blooms, DO concentration fluctuates and supersaturates. It was evident that the algal biomass undergoes short term variations throughout a given year, and the dissolved oxygen exhibits corresponding fluctuations. Pearson correlation for

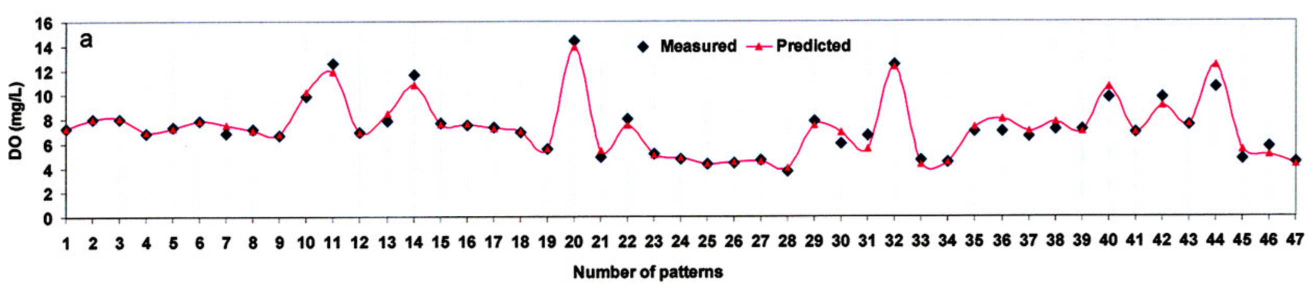

Fig. 4a—Model-1a results: Forecast of DO concentration (mg/L) in a week ahead in Singapore seawater.

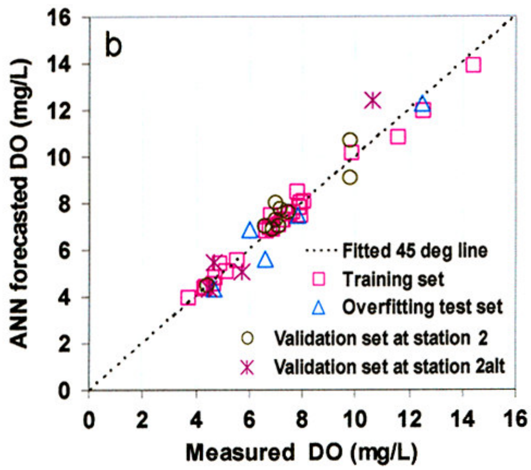

Fig. 4b—Scatter diagram of observed and forecasted DO at Stations 1 & 3 for training & overfitting test, and 2 & 2-alt for validation.

measured Chl-a is positive with measured DO (R^2=0.624, P=0.007). The model-1a forecasted the DO concentrations with good accuracy, producing a MAE of 0.21, 0.47, 0.85 and 0.45 mg/L at four field measurement stations for training, overfitting test and two validation sets. The model-2a simulated the DO concentrations with good accuracy, producing a MAE of 0.16, 0.87, 0.99, and 0.41 mg/L at four field measurement stations for training, overfitting test and two validation sets. The trained model-1 and model-2 can be applied to forecast (a week ahead) and predict (at present week t) DO concentration of the Singapore seawater at specified location and time between the field survey period of January 1997 and June 1997 in the domain of interest (circled area in Figure 1). The DO level which should not fall below 4 mg/L for seawater[33] is an important variable in the eutrophication processes. Thus, the model result helps for the quick management of seawater quality.

The autocorrelation of predicted DO showed a significant correlation at 95% confidence level interval up to adjacent stations at the same time lag. DO is highly correlated to temperature and salinity than all other factors related to DO variability. The general findings are that ANN modelling with only DO as input or DO together with salinity and temperature at measurement stations can be correlated to DO at a nearby gauge where sensitivities between the water quality variables vary greatly with changing tidal and ambient conditions. The results show that GRNN not only has a higher degree of forecasting accuracy but also performs statistically better than MLBP for DO forecast. Accuracy of the developed

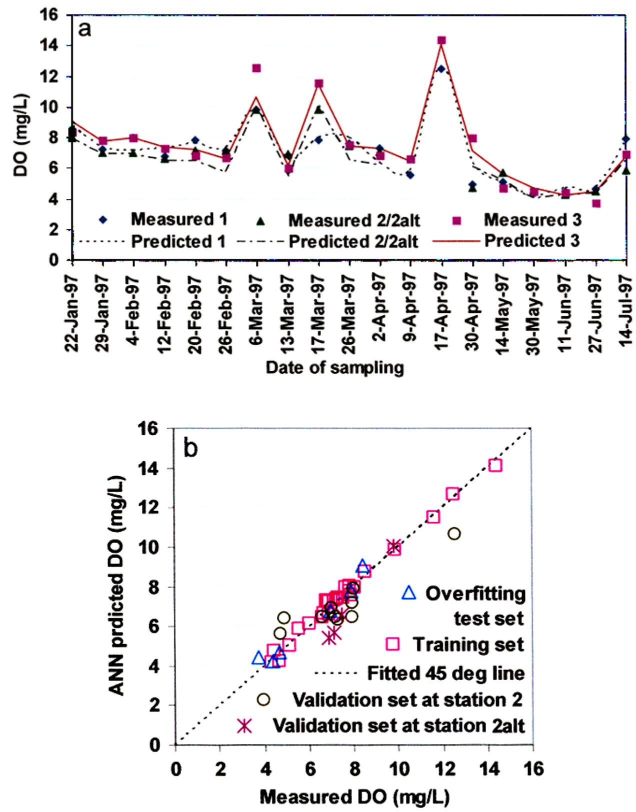

Fig. 5—Model-2a results: a. Temporal variation and b. scatter plots of measured and predicted concentration of DO (mg/L) at monitoring Stations in East Johor Strait at Stations 1 & 3 for training & overfitting test, and 2 & 2-alt for validation.

models should be compared using n-fold cross-validation as the available data is limited. On a smaller sample of data, these methods can be used to evaluate how well a model generalises without the need to set aside some instances purely for testing. The procedure of n-fold cross validation approach can be summarized as follows: (1) divide the data into 'n' subsets of equal size; (2) train ANN 'n' times, each time leaving out one of the subsets for test from the training set; (3) predict DO of unseen validation data set based on the averaged predicted DO values resulting from the 'n' number of trained ANN models. In this study, only 2 out of the 4 available stations (for neural network training) were used to demonstrate the ANN application in the dynamic water quality prediction. Even though, the available data size is relatively small, sufficiently good results were obtained for the water quality prediction of unseen validation dataset at location away from the training dataset station. Should more data be available, the proposed approach should provide better prediction. It is also clear that much more observation data are needed to further verify the applicability of the conclusions. Once the concept is accepted (i.e. validations are sufficiently accurate), field monitoring stations can be (spatially) more optimally selected which will result in reduction of monitoring cost. The trained ANN may then be used in parallel to complement physics-based model and for the field monitoring expeditions in the region.

Conclusion

Artificial neural network models are developed to simulate weekly DO concentrations in the East Johor Strait of Singapore seawater with respect to time and space. The DO at that site is affected by its solubility as well as biological processes. The effects of these biological processes are hypothesized to be constrained by a small set of physical factors, such as water temperature, salinity, and DO itself at the domain of interest. ANN models are successful in predicting patterns in the DO data on weekly and they can be applied on hourly, daily, monthly and seasonal time scales. ANN model performance is good, with MSE less than 1.55 mg/L for GRNN and 2.25 mg/L for MLBP. Good accuracy level of DO estimates (ranging R^2 from 0.7 to 1) by GRNN model has been obtained at "any" location and time in the domain where training stations exist. It is demonstrated that DO in the seawater can be forecasted with an acceptable accuracy. With largely still unknown factors of water quality variation and limited data size, a relatively good correlation was observed between the measured and predicted DO values. The ANN model has tremendous potential as a forecasting tool. The ANN forecasting capability was tested and found to be better and faster than those from a process-based model with minimal input requirements. However, ANN and process-based models have different purposes. The process-based model is useful for providing insight into identifying important processes and management strategies. Refinements may include the prediction of DO by including various other physical, chemical and meteorological parameters as model input. The results showed that the neural network models are more accurate at simulating the dissolved oxygen of very complex seawater.

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