Determination of optimal coagulant dosing rate using an artificial neural network

Dae-Sung Joo, Dong-Jin Choi and Heekyung Park

ABSTRACT

Determining coagulant dosing rates currently depends on Jar-test results and the experience of the operators in many cases. The nature of these practices makes it difficult to cope quickly with the rapid fluctuation of raw water quality, mainly because it takes a relatively long time to obtain Jar-test results. For promptly predicting required coagulant doses in response to water quality changes, a number of researchers have attempted to use the multi-variable regression (MVR) approach. However, the prediction capability of the MVR approach has not been satisfactory. An artificial neural network (ANN) is an excellent estimator of the nonlinear relationship between the accumulated input and output numerical data. Using this characteristic of the ANN, this study has attempted to predict the optimal coagulant dosing rate accurately and quickly. To train the ANN and deduce the MVR equation, a set of 142 units of data chosen from the 2-year operation of a water treatment plant was used. Another set of 72 units of data, not used in training, was also used to check the prediction capability of the trained ANN and MVR equation. Root-mean-square normalized error (RMSE) was used as a quantitative indicator of prediction capability. For the training data set and the raw data set, the RMSEs of the MVR equation were, respectively, 0.0143 and 0.0193 while those of the ANN were 0.0058 and 0.0092, respectively. These results indicate that the ANN reduced the prediction error for the training data by about 59%, and for the raw data by about 52%. Thus, our study demonstrates that the prediction capability of the ANN for raw data is enhanced by twice that of MVR. As the advancement of on-line monitoring techniques enables the ANN to update the weights periodically, its prediction capability can be also continuously enhanced.

Key words | artificial neural network, multi-variable regression, optimal coagulant dosing rate

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INTRODUCTION

Typical coagulation practices at the water treatment plant consist of pre-rapid-mix addition of the coagulant, mixing, flocculation and sedimentation. Enhanced coagulation is required by most water systems treating surface water in order to facilitate the removal of chemical floc from suspension through gravity settling, and consequently to reduce the operating load in the following processes including sand filtering. However it is also typical that the coagulation process has a short reaction time and its reaction mechanism is very complex. Chemical reactions of coagulants in water are thus presented in the form of hypothetical equations which approximate what happens in water (Hammer 1986). Because of this characteristic, the type of coagulant is selected by considering the plant process scheme and raw water quality, and dosages of coagulants are continuously controlled to meet time-varying changes of raw water quality. Until now Jar tests have been widely used to determine optimum dosages of coagulants. The nature of this practice makes it difficult to cope quickly with the rapid fluctuation of raw water quality, mainly because it takes a relatively long time to obtain Jar-test results.

To overcome such shortcomings, current research to determine the optimal coagulant dosages according to

real-time on-line monitoring results of raw water and settled water quality is conducted in two directions. One is the feedback control approach which attempts to regulate coagulant dosages for the zeta-potential of the effluent of the rapid mixer to follow the set-point of the zeta-potential. Bean *et al.* (1964) suggested a desirable range for the zeta-potential for the removal of turbidity and colour-producing material. Hannah *et al.* (1967) evaluated the treated water quality according to coagulant dosages and compared the relationship between the treated water quality and the zeta-potential. Neuman (1981) showed that stable treated water quality can be obtained by adding the coagulant dosages determined by the zeta-potential. After proving that streaming current is theoretically proportional to the zeta-potential, Dentel & Kingery (1989) were able to reduce the cost of coagulants using a streaming current detector (SCD) which is relatively easy to use. Hubele (1992) developed a simple control algorithm which adjusts the coagulant dosage until the set point of the SCD is obtained. A constant SCD response was observed for the optimum coagulant dosage for different conditions of raw water quality. Even though the SCD is generally adapted as a continuous monitoring method to determine the required coagulant dosages, Dentel (1995) pointed out that the output of the SCD sometimes exhibits a contradictory result for the coagulation activation.

The other direction of research is the feed-forward control approach. Coagulant dosages are associated with water quality parameters such as turbidity, alkalinity, water temperature and pH. The relationship between raw water quality and coagulant dosages is established by statistical analysis using the accumulated operating data determined by a Jar-test in the water treatment plant. Nakamura (1974) and Kim & Kim (1993) set up relational equations between the raw water quality parameters and coagulant dosage through multi-variable regression. These equations can be used to determine the coagulant dosage quickly according to the time-varying quality of the influent.

An artificial neural network (ANN) is an excellent estimator of the nonlinear relationship between the accumulated input and output numerical data. An ANN is well suited for processing noisy, incomplete or inconsistent data. Also, once trained, an ANN can calculate results from a given input very quickly, so it has the potential to be used online in a control system. Using these properties of the ANN, this study has attempted to predict the optimal coagulant dosage with accuracy and in a short time.

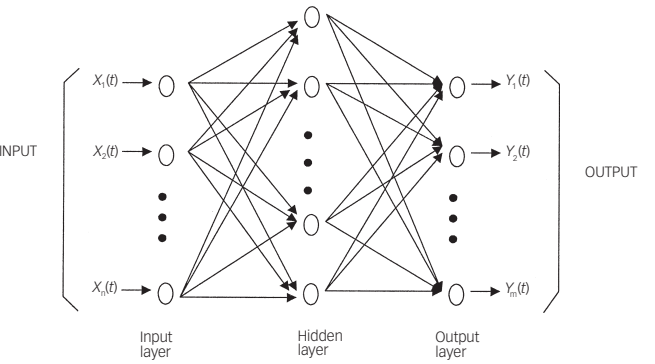

Figure 1 | Structure of an artificial neural network.

THE ARTIFICIAL NEURAL NETWORK

The structure of an ANN

An artificial neural network (ANN) is a network formed by interlinked unit elements called artificial neurons. Many researchers have developed various types of neural network models for different purposes. In this study, a model called the back-propagation neural network (BPNN) or multilayer perceptron is used for relational identification. The BPNN consists of an input layer, hidden layers, and an output layer as shown in Figure 1. The input and output relationship of a neural network can be nonlinear as well as linear, and its characteristics are determined by the weights assigned to the connections between nodes in two adjacent layers. Changing these weights will change the input/output behaviour of the network.

An artificial neuron, which is a unit element of an ANN, is an apparatus to generate one output, y, from n inputs x (x_1, x_2, . . . , x_n). To accomplish this function, the artificial neuron has a variable weighting vector,

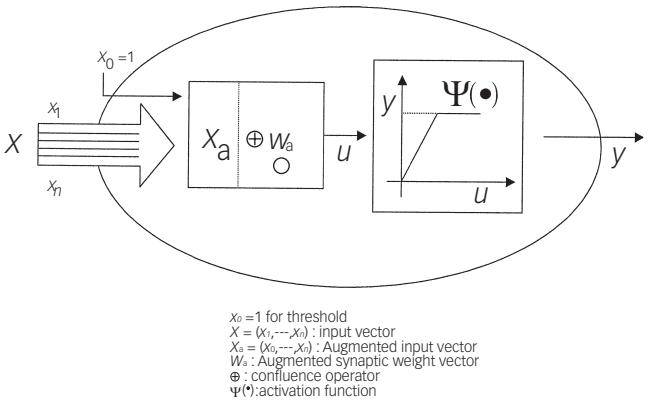

Figure 2 | Structure of an artificial neuron.

$w = (w_0, w_1, \ldots, w_n)$, a confluence operator, and an activation function as shown in Figure 2.

Operating principle of an ANN

The relationship between input and output in an ANN can be represented as Equation (1).

$$y(t) = N_3\left[N_2\left\{N_1\left(x(t)\right)\right\}\right] = \Psi^3\left[w_a^3(t) \oplus \Psi^2\left\{w_a^2(t) \oplus \Psi^1\left(w_a^1(t) \oplus x_a(t)\right)\right\}\right] \quad (1)$$

N_1, N_2, N_3: Numerical calculation step
$x(t)$: Input vector
$x_a(t)$: Augmented input vector
$w_a(t)$: Augmented weight vector
$\oplus$: Confluence operator
$\Psi(\bullet)$: Activation function

The operation of an ANN is composed of two steps, the learning phase and the computational phase.

Learning phase

The learning phase of a neural network with appropriate data containing information regarding cause and effect relationships is at the heart of the proposed method for relational identification. In the supervised learning method in which the desired output (y_d) is given, the output value ($o(t)$) obtained through the ANN for each input vector (x) is compared with the desired output and then the weighting vector (w) is tuned to minimize the difference (E) expressed as Equation (2),

$$E = \sum (o(t) - y_d) \; . \quad (2)$$

The error back-propagation algorithm based on gradient descent direction as a learning method allows us to find a set of weights by successive improvement from an arbitrary set of starting weights. For improved learning efficiency, the quasi-Newton method is used. The quasi-Newton method is regarded as the most efficient algorithm in the unconstrained optimization. It is explained in detail in Bien (1997) and Lapedes & Farber (1988).

Computation phase

In the learning phase, the cause and effect relationships are stored within the weighting vectors of the proposed back-propagation neural network. In the computation phase, the trained network is tested with data which were not presented in the training data set. This step is actually a test of the performance capability of the network.

METHODS

Data for learning and verification

As learning data for the ANN, two years' operating data of a water treatment plant were used. This plant has a capacity of 250,000 m^3/d and its raw water comes from a reservoir where the water quality undergoes seasonal changes. The learning data included one operational factor (coagulant injection rate), and four raw water quality parameters such as temperature, pH, turbidity and alkalinity. The coagulant dosages were determined through Jar-tests and the coagulant injection rate was calculated from the determined dosages. The temperature range was from 4 to 30°C. The hydrogen ion concentration (pH) varied from 6.9 to 7.9. The alkalinity as $CaCO_3$ ranged from 26 to 37 mg/l. The turbidity had a very wide range of

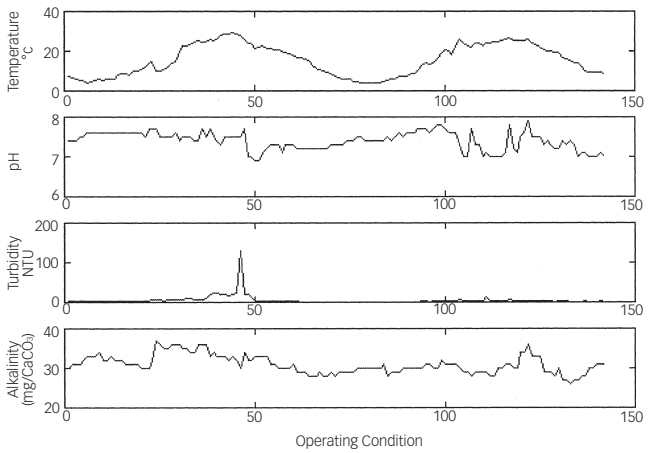

Figure 3 | The water quality parameter changes of the learning data.

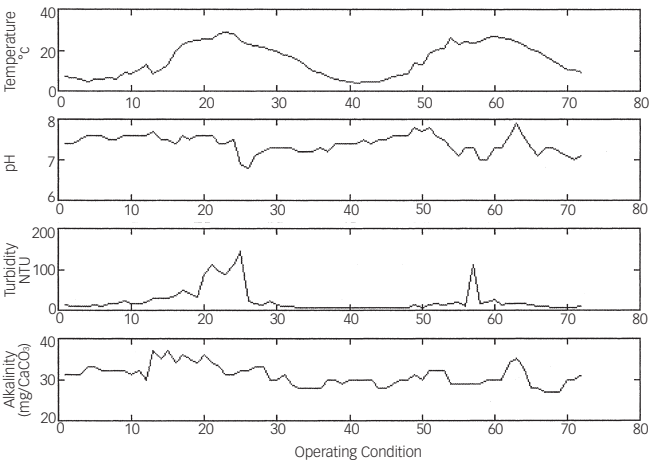

Figure 4 | The water quality parameter changes of the computation phase.

1 to 130 NTU. Over a year the turbidity usually varied within a range of 1 to 10 NTU, except during rainy days when its fluctuation was very drastic. In particular, July and August were the most difficult operation periods for the plant operator to cope with the rapid change of turbidity.

From the historical 2-year data, 142 units of learning data were selected to represent the seasonal changes of temperature and drastic fluctuation of turbidity on rainy days (Figure 3). Another set of 72 units of data was used to verify the prediction capability of the developed ANN (Figure 4).

Multi-variable regression (MVR)

To confirm the enhancement of the prediction capability of the ANN, a multi-variable regression (MVR) was conducted using the same historical data. The statistical program used for the MVR was MINITAB (Devore 1991).

Artificial neural network (ANN)

The ANN used in this study is composed of three layers (one input layer, one hidden layer, one output layer). The number of artificial neurons in each layer is 5-10-1. The ANN was trained with learning data. The data not used in the training were then used to verify the performance of the trained ANN. The simulation was carried out by an ANN program coded in 'C' language at a workstation.

Prediction capability performance index

A root-mean-square normalized error (RMSE) was used as a performance index to compare the prediction capability of the MVR equation and the ANN. RMSE is known to be descriptive when comparing the prediction capability between predictors (Zurada 1992), see Equation (3).

$$\mathrm{RMSE} = \frac{1}{N}\sqrt{\sum_{i=1}^{N}(o_p - o_d)^2} \tag{3}$$

Where: N is the number of data, o_p is the predicted value, o_d is the real operating value.

RESULTS AND DISCUSSION

Multi-variable regression (MVR)

The relation between the coagulant dosing rate and the raw water quality parameters can be expressed statistically as Equation (4):

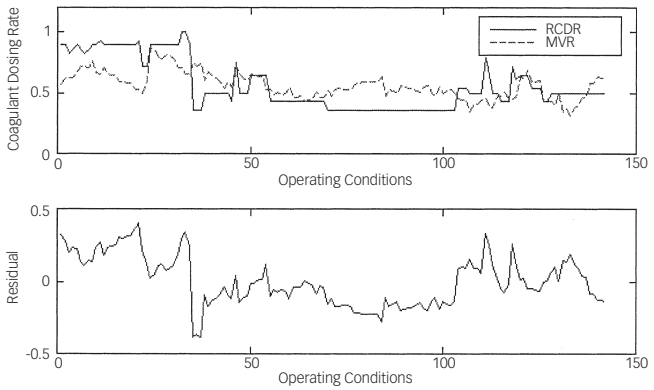

Figure 5 | Comparison of predicted (MR) and real injection rate (RCDR) (top) and the residual (bottom) of multi-variable regression for data used in regression.

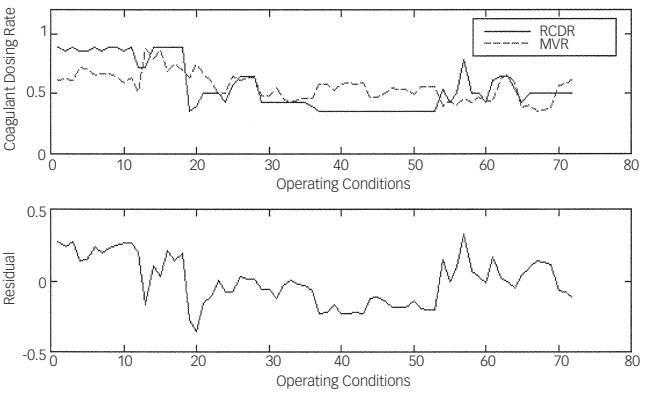

Figure 6 | Comparison of predicted (MVR) and real injection rate (RCDR) (top) and the residual (bottom) of multi-variable regression for data not used in regression.

$$\text{Coagulant dosing rate} = -0.242 - 0.00708*\text{temperature} - 0.0824*\text{pH} + 0.00237*\text{turbidity} + 0.0488*\text{alkalinity} \quad (4)$$

The equation shows that turbidity and alkalinity have a positive effect of increasing the coagulant dosing rate, and temperature and pH have a negative effect of decreasing the coagulant dosing rate. Figure 5 (top) represents the comparison of the real coagulant dosing rate and the predicted value. Figure 5 (bottom) shows the residual which is equivalent to the real coagulant dosing rate minus the predicted value. The RMSE calculated from the real coagulant dosing rate and the predicted value of MVR is 0.0143.

Figure 6 (top) shows the prediction results of MVR for the data not used in deriving the regression equation. The calculated RMSE is 0.0193 which is close to 0.0143. There is little difference in the RMSE for the data not used in deriving the regression equation.

Artificial neural network (ANN)

The self-organization and learning capability of the ANN are utilized to eliminate the need for explicitly extracting cause and effect relationships. These relationships are just distributed within the connection strengths of the neural networks so the relationships are not obvious or externally available to the researcher.

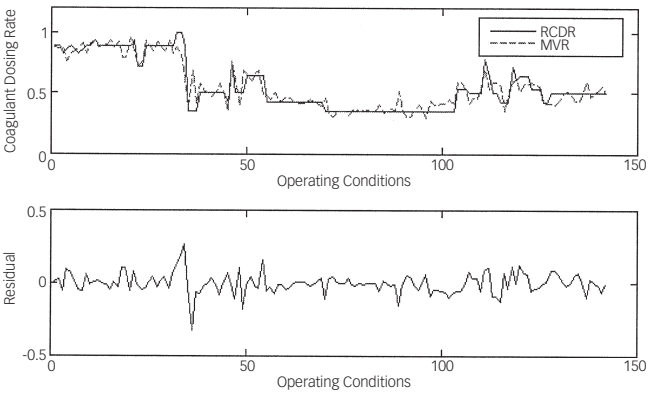

Figure 7 | Comparison of predicted (ANN) and real injection rate (RCDR) (top) and the residual (bottom) of the ANN for data used in the ANN training.

The comparison result of the ANN for the real coagulant dosing rate and the predicted value of the ANN is shown in Figure 7 (top). Figure 7 (bottom) represents the residual of the real coagulant dosing rate and the predicted value of the ANN. The RMSE calculated from the real coagulant dosing rate and the predicted value of ANN is 0.0058.

Figure 8 (top) shows the prediction of the ANN for the data not used in ANN learning, Figure 8 (bottom) shows the residual. The RMSE calculated is 0.0092. The RMSEs for the four cases are summarized in Table 1.

As shown in Figures 5–8 and Table 1, the ANN has a better prediction capability from the viewpoint of RMSE value and residual range. When comparing the RMSE

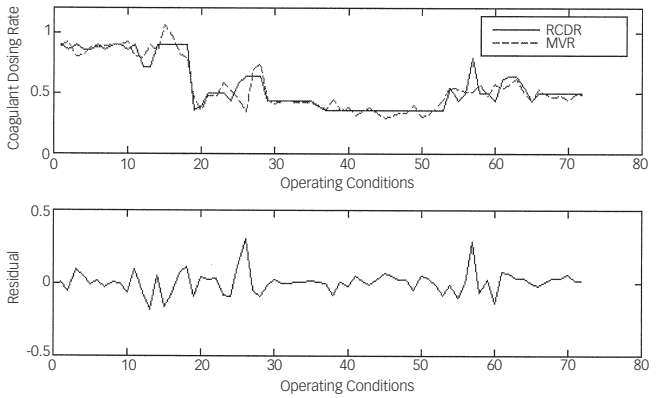

Figure 8 | Comparison of predicted (ANN) and real injection rate (RCDR) (top) and the residual (bottom) of the ANN for data not used in the ANN training.

Table 1 | RMSE and residual of each prediction model.

Prediction model	RMSE	Residual range
MVR (for the training data)	0.0143	(0.399, – 0.388)
MVR (for the data not used in training)	0.0193	(0.328, – 0.358)
ANN (for the training data)	0.0058	(0.268, – 0.326)
ANN (for the data not used in training)	0.0092	(0.302, – 0.188)

values, the ANN reduces the RMSE by 59% for the learning data and by 52% for the data not used in learning. The prediction capability of the ANN is better than the MVR even during the period when there was a drastic change in the coagulant dosing rate. This suggests that ANN can be an alternative predictor for coagulant dosage when the feed-forward control algorithm is applied to cope with the raw water quality and operating condition changes.

CONCLUSION

Enhanced coagulation and sedimentation determine the overall efficiency of the water treatment process by reducing the load on the downstream processes, including sand filtering. Removal of turbidity by coagulation depends on the type of colloids in suspension, the temperature, pH, the type and dosage of coagulants and aids, and the degree and time of mixing provided for chemical dispersion and floc formation. As a means of responding to the rapid change of raw water quality, the feed-forward control method is most often used. The method can determine the necessary coagulant dosage from continuously measured influent water quality data using the techniques of MVR and ANN. The prediction capability of MVR and ANN are compared using example sets of data in this study. The results show that ANN has a better prediction capability when measured in terms of RMSE value and residual range. The prediction capability of ANN is shown to be better than MVR even during the period of a drastic change in the coagulant dosing rate. Therefore, this study concludes that ANN can be used for predicting optimum coagulant dosage when the feed-forward control algorithm is applied to cope with the raw water quality and operating condition changes. However, since ANN cannot reveal the direct mechanistic relationship between water quality parameters and required coagulant dosages, the training data must be prepared correctly in advance to derive a reliable ANN prediction. Further research is necessary for improving the precision of the training data.

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