行政院國家科學委員會專題研究計畫 成果報告

水庫營養源濃度預測與監控之最佳策略研究(第 2 年) 研究成果報告(完整版)

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行政院國家科學委員會補助專題研究計畫 ■成果報告 □期中進度報告

水庫營養源濃度預測與監控之最佳策略研究

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中 華 民 國 99 年 10 月 15 日

CONCENTS

中文摘要

本研究計畫之主要目的為以遺傳進化程式(GE)建立北臺灣翡翠水庫之每月水質預測模式, GE 具有 發掘重要輸入變數之能力, 並且將其自動組成數學方程式, 本計劃中 GE 模式以十五個輸入變數來決 定最適合之非線性方程式, 可預測水庫中之總磷(TP)濃度, 結果經過 GE 程序搜尋出三個顯著的輸入因 子: 包括兩項 TP 來源 (上游兩個支流 TP)與最大月降雨量, 因為 GE 模式可有效的模擬水庫水質之動 態過程, 接下來則利用巨觀遺傳演算法(MGA)為最佳化模式結合此 GE 預測模式, 藉以控制從集水區 而來的營養源, 發現可有效的維持水庫中 TP 濃度。

關鍵詞: 遺傳進化程式(GE), 水質預測模式, 遺傳演算法(GA), 總磷(TP)

Abstract

The objective of this study is to establish a monthly water quality predicting model using a grammatical evolution (GE) programming system for Feitsui Reservoir in Northern Taiwan. Grammatical evolution (GE) has an ability to find out significant input variables and combine them to form mathematical equations automatically. In this study, GE model was fed with fifteen input variables to determine a reasonable nonlinear mathematical equation for predicting the total phosphorous (TP) concentration in reservoir. Three significant input variables, including two TP sources and maximum rainfall were chosen through GE process. Because the obtained GE model can effectively simulate the dynamics of reservoir water quality, a Macro-Genetic Algorithm (MGA) was then used as an optimization model mixed with this GE predicting model to control the nutrient loads from the watershed and maintain the in-reservoir TP concentration efficiently.

Keywords: grammatical evolution (GE), water quality predicting model, genetic algorithm (GA), total phosphorous (TP)

1. Introduction

Taiwan is located in a transition zone between the tropical and subtropical climates and is characterized by high temperature and ample rainfall. In the present time, the reservoirs provide about 70% of drinking water for a population of nearly 23 millions and industrial water use in Taiwan. According to Kao et al. (2006), various types of anthropogenic disturbance are affecting Taiwan watersheds. Nutrient loads from excessive watershed development continue to increase, resulting in accelerated eutrophication in many reservoirs (Kuo et al., 2007). Therefore, we developed a nutrient model to simulate the behavior of nutrient loads in an important reservoir located in Northern Taiwan. In this study, the model is based on data from nutrient loads of a main creek and two tributaries to forecast the total phosphorous (TP) concentration in Feitsui Reservoir.

Evolutionary computation techniques are based on a powerful principle of evolution i.e. survival of the fittest. They are considered to be very efficient optimization methods. Among these methods, genetic algorithm (GA) is one of the most popular search algorithms. But there are some kinds of difficulties of GA related to the fixed-length encoding and premature convergence. Indeed; researchers have successfully used evolutionary algorithms for automatically generating programs or equations among the inputs and outputs. The lately developed grammatical evolution (GE) technique is a biologically plausible approach that performs the evolutionary processes on simple variable-length binary strings. This new data structure is flexible and it allows researchers to exploit benefits of genetic algorithms. Chen et al. (2008) applied it to improve the remote monitoring on water quality in a subtropical reservoir with satellite imagery successfully.

2. Grammatical Evolution

Grammatical evolution (GE) is an evolutionary automatic programming type system that combines a variable length binary string genome and Backus-Naur Form (BNF) grammar to evolve interesting structures. Variable length binary string genomes are used with each codon representing an integer value where codons are consecutive groups of 8 bits. The integer values are used in a mapping function to select an appropriate production rule from the BNF definition; the numbers generated always represent one of the rules that can be used at that time (Elseth and Baumgardner, 1995). The details of this procedure are described as the following:

2.1 Backus-Naur form

BNF is a notation for expressing the grammar of a language in the form of production rules (Naur, 1963). BNF grammars consist of so called terminals representing the items that can appear in the language, e.g., +, -, etc., and nonterminals, which can be expanded into one or more terminals and nonterminals. A grammar can be represented by the tuple {N, T, P, S}, in which N is the set of nonterminals, T the set of terminals, P is a set of production rules that maps the elements of N to T, and S is a start symbol that is a member of N. When there are a number of productions that can be applied to one particular N, the choices are delimited with the '|' symbol.

Below is a BNF example, where $N = \{ \exp r, op, pre \text{ } op \}$ $T = \{Sin, Cos, Log, +, -, *, /, Variable X, Constant 1.0\}$ $S = \langle expr \rangle$

And P can be represented as:

2.2 Mapping Process

The genotype is used to map the start symbol onto terminals by reading codons of 8 bits to generate a corresponding integer value from which an appropriate production rule is selected by using the following mapping function:

Rule = (codon integer value) MOD (number of rules for the current nonterminal).......(1)

Considering the following rule, i.e., given the nonterminal op, there are four production rules to select from:

If we assume the codon being read produces the integer 6, then

6 MOD 4 = 2

would select <op> as rule 2: /. Each time a production rule has to be selected to map from a nonterminal, another codon is read. In this way, the system traverses the genome.

For example, considering the individual in Table 1, there are fourteen 8-bit binary codons in one string. The decoding process is described as follows:

- (1) First, concentrating on the start symbol <expr>, four possible productions to be chosen are distinguished. To make this choice, we read the first codon from the chromosome "11001000" and use it to generate a number "200". Because the standard decode of the binary 11001000 equals to 200. This number will then be used to decide which production rule to use according to Eq. (1) in BNF. Thus, we have 200 MOD 4 = 0, meaning we must take the zeroth production, rule (0), so that $\langle \text{expr} \rangle$ is now replace with \langle expr $>$ \langle op $>$ \langle expr $>$.
- (2) Continuing with the first $\langle \text{expr} \rangle$, i.e., always starting from the leftmost nonterminal, a similar choice must be made by reading the next codon value 160 and again using the given formula we get 160 MOD $4 =$ 0, i.e., rule 0. The leftmost $\langle \text{expr} \rangle$ will now be replaced with $\langle \text{expr} \rangle \langle \text{opp} \rangle \langle \text{expr} \rangle$ to give

<expr>>>>>><expr>>expr>>expr>.

(3) Again, we have the same choice for the first <expr> by reading the next codon value 206, the result being the application of rule 2 to give

<pre-op>(<expr>)<op><expr><op><expr>.

(4) Now, the leftmost \langle pre-op \rangle will be determined by the codon value 96 that gives us rule 0, which is \langle pre-op $>$ becomes Sin. We have the following:

> **. . .**

Sin(<expr>>>>>><expr>><expr>>>>><expr>

(14) The mapping continues until eventually we are left with the following expression: $Sin(X)*Cos(X)+1.0$

Notice that if there had been any extra codons, they would have been simply ignored during the genotype-to-phenotype mapping process. It is possible for individuals to run out of codons and in this case, we wrap the individual and reuse the codons. This technique of wrapping the individual draws inspiration from the gene-overlapping phenomenon, which has been observed in many organisms (Elseth and Baumgardner, 1995). It is possible that an incomplete mapping could occur even after several wrapping events and in this case, the individual in question is given the lowest possible fitness value.

Because there is a problem that only integers can be presented by using the binary coding scheme mentioned above, we revised it as a real-coded representation. The real numbers which imply that, each chromosome is a real-valued vector, as opposed to binary-coded GA, where chromosomes are 0-1 vectors. It is very useful and efficient to generate the real-number constants and coefficients shown in these output equations. When a codon is decoded as a constant, the value of real-coded genome can be generated directly. Whereas mapping a codon to the BNF rule, just need to round it off as a non-negative integer within the range between 0~255 then choose one corresponding BNF rule.

Fig. 1 shows a combination of GE and GA, called GEGA, to generate the optimal relationship among inputs and outputs automatically. First, a GE was employed to transfer the real-coded string through BNF grammars to mathematical function. The data from several bands of remotely sensed imagery were used in the GE as inputs to predict the water quality in the reservoir. Further, a GA was incorporated with this GE to optimize the objective value of those functions. In other words, the GA was used to determine the most proper relationship among the input and output data pairs.

2.3 Fitness Function

The correlation coefficient (CC) between predicted and actual values is adopted as the fitness function of GE. Through several experiments, it is observed that this fitness function can accelerate the speed of search procedure compared with using the root mean squared error (RMSE) directly. It is able to achieve both "high linear correlation" and "small RMSE"simultaneous in most cases, so we chose the former as the objective function. This study therefore employed single linear regression analysis to decrease the RMSE of estimation (Yeh et al., 2010).

^y ⁼^α ⁺ ^β [⋅] *^f* ………………………………………………………………….(2)

where

 $f =$ output value of data predicted by the GE;

 $y =$ actual output value of data in the dataset; α *and* β = the intercept and slope, respectively.

3. The Case Study

3.1 Feitsui Reservoir

Feitsui Reservoir at $25^{0}27$ ' N and $121^{0}33$ ' E is the most important reservoir of Northern Taiwan, supplying drinking water for more than five million people in the Taipei City. The main dam is located at the downstream of Peishih Creek, a tributary of Hsintien Creek (Fig. 2). The reservoir construction started in mid-1979 and completed in 1987 with an initial storage of 406×10^6 m³. It has a surface area of 10.24 km² (at EL.170m), and its catchments area is 30 times the total reservoir area. With about 20 km in length, the mainstream is of meandering morphology. The effective storage capacity near the dam was 359 million $m³$, 39.68 m and 113.5 m for the mean depth and maximum depth, respectively. The average bed slope is 0.3%. The main landscape in the reservoir watersheds is terrace and hardwood montane. Most banks of this reservoir are the previous agricultural farms, primarily tea farms, which were flooded after the reservoir operation. The average annual precipitation is around 2,500 mm or more. The main geological substrates are interstratified with sandstone and shale formed after the Oligocene. The primary soils are Entisol and Inceptisol according to Soil Taxonomy. Agricultural activities are surrounded the catchment area, while there are no industrial activities over the catchments, and accordingly the reservoir is isolated from any industrial pollution sources. The atmospheric influx and domestic sewage as well as agricultural fertilizers would be the primary sources for most anthropogenic chemicals. Feitsui reservoir is one of the most extensively monitored reservoirs in Taiwan. Although water quality in Feitsui Reservoir is among the best in Taiwan, the reservoir still receives much attention because of significant watershed nutrient loads. The nutrient loads are mainly from non-point agricultural and tourist activities. Under the Carlson trophic state index, water quality of the reservoir is listed as mesotrophic most of the time and eutrophic for only a few months in recent years.

3.2 TP Data Set

All the nutrient loads in Feitsui Reservoir were considered the summation of three sources of the main flow Peishih Creek and two tributaries, Diyu Creek and Kingkwa Creek in this case study (Fig. 2). The monthly monitoring data records of 1996–2005 were obtained from the Feitsui Reservoir Administration Bureau and the Research Center for Environmental Change, Academia Sinica. The first 6-year records were used for model training (calibration) and the following 4-year records for model testing (verification) The input variables includes the phosphorus loads (which indicates the main inflow Peishih Creek, the tributaries Diyu Creek, and Kingkwa Creek), two meteorological variables (including average and maximum rainfall inthe watershed), and two hydrological variables (including inflow and outflow). These seven input variables are chosen as the main factors to predict the TP in reservoir. Study done by Kuo et al. (2006) used similar data sets in reservoir water quality prediction. However, the TP concentrations in Feitsui Reservoir become increasingly high in recent years. Under such circumstance, by employing only the seven input variables early mentioned cannot achieve a satisfied accuracy of prediction in this study. Therefore, total fifteen input variables contain seven input variables described above at time step t and the other seven input variables: their values one step ahead (time step t-1), as well as one input variable: the TP in reservoir at time step t-1. This system identification problem may be viewed as a searching for a proper function (and its parameters) which maps fifteen input values onto an output value (average TP in reservoir at time step t). Table 2 presents the statistical parameters of the data set used in this study in order to prescreen the data characteristics. In the Table 2, the x_{mean} , S_x , C_y , x_{max} and x_{min}

denote the data mean, standard deviation, variation coefficient, maximum and minimum, respectively.

3.3 Models Performances Evaluation

The root mean square errors (RMSE) and mean absolute errors (MAE) denoted below are used as the comparison criteria to evaluate the models performances in these applications.

RMSE =
$$
\sqrt{\frac{1}{N} \sum_{i=1}^{N} (Y_i \text{observed - } Y_i \text{predicted})^2}
$$
(3)
MAE = $\frac{1}{N} \sum_{i=1}^{N} |Y_i \text{observed - } Y_i \text{predicted}|$ (4)

where N is the number of data, Y_i is the TP concentration for the time step i.

3.4 Results

The function library types in BNF include several general mathematical operators such as {+, -, *, /, LN, EXP, POWER}. The IGE model was carried out for three times (runs). Results of these three mathematical formulas are listed as follows:

 $Y_1 = 19.5 + 0.00000011*(X_1 - X_{12} + 199.94) * (181.81 * X_1 * X_2) \dots (5)$

Where

 X_1 is the TP concentration (μg/L) of tributary Diyu Creek at time step t.

 X_3 is the TP concentration (μg/L) of main inflow Peishih Creek at time step t.

 X_{12} is the maximum rainfall (mm) in the watershed at time step t-1.

Y is the average TP concentration $(\mu g/L)$ in the reservoir at time step t

Only three input variables, square of X_1 , X_3 and X_{12} , were chosen automatically from the total fifteen input variables by GE to form the equation shown as Eq. (5). From the statistical results, the RMSE value found is equals to 9.96 at the training. The scatter plots was shown in Fig. 3.

3.5 Optimization of the Water Quality Control

3.5.1 MacroGA (MGA)

A macro genetic algorithm (MGA) was adopted to optimize the control of nutrient loads of phosphorus from the watershed. A flow diagram of this combined method is shown in Fig. 4. In this study, the IGE model is used to forecast average TP in reservoir. Then, the MGA is used as a search strategy to quantify the phosphorus reduction rates of the inflows so that the trophic state can be improved to reach different lower levels representing by the Scenarios 1 and 2. The proposed approach has the advantage of coupling the nonlinear function generator of the IGE with the global solution exploration of the MGA.

The genetic algorithm (GA) is an iterative procedure, which includes a population of individuals that are candidate solutions to specific domain. During each generation, the individuals in the current population are related to their effective evaluations, and a new population of candidate solutions is formed by specific genetic operators like reproduction, crossover, and mutation. These steps are repeated until the convergence criterion is satisfied or a predetermined number of generations are achieved. According to a couple of our previous works, real-coded GAs has advantages over binary coded GAs (Chang and Chen, 1998; Chen, 2003a; Chang et al., 2005). Hence, in this study, we only considered real-coded GAs. Blend crossover (BLX- α) uniformly picks values that lie between two points contain the two parents, but may extend equally on either side determined by a user specified GA-parameter $α$ (Chen and Chang, 2007).

In standard GA, the selection operator chooses individuals with a probability proportional to their relative fitness, but this can lead to "premature convergence". Therefore, a macro-evolutionary algorithm (MA) is presented as a selection scheme to improve the capability of searching global optimum solutions in GA, which is called MGA. Unlike population-level evolution, which is employed in standard evolutionary algorithms; MGA is evolution at the higher level. The model exploits the presence of links between "species" that represent candidate solutions to the optimization problem (Chen, 2003 b). In addition, MGA has many advantages when compared with GA using a traditional selection operator. First, MGA can reach higher fitness values than traditional GAs for equal population sizes. Second, the probability of success in reaching a good fitness value in a typical run is higher in MGA than in GA. Finally, the time needed to reach the optimum using the same population size is lower in MGA (Marin and Sole, 1999). This method has been applied successfully to water resources optimization problems that can be formulated in terms of an optimization function even if the function is highly multimodal or highly multidimensional (Chen et al., 2007), .

3.5.2 Objective Function

The objective function of optimization model can be written as:

∑ ⁺ ² 3 ² Minimize ^μ¹ ^μ ……………………………………………………….(7)

subject to:

The in-reservoir TP concentration achieves the expected water quality which is considered as two scenarios: the first scenario is set to be 20 (μg/L) and the second scenario is set to be 30 (μg/L).

Here u_1 is the phosphorus reduction rate of the tributary Diyu Creek; and u_3 is the phosphorus reduction rate of the main flow Peishih Creek. The range of the two phosphorus reduction rates is set to the same interval 0–1. Applying real-coded GA to the optimization problems, chromosomes may be generated that fail to meet constraints. Therefore, each generated chromosome must be checked against such constraints.

The optimum values of the phosphorus reduction rate of the two sources, u_1 and u_3 , obtained by using the MGA for scenario 1 to control Feitsui Reservoir water quality are presented in Fig.5. The average phosphorus reduction rate (u_1) of scenario 1 (TP in reservoir under 20 (μ g/L) is 0.024(2.4%) for the tributary Diyu Creek; and average $u_3=0.298$ (29.8%) for the main flow Peishih Creek. It indicates that the reduction rate of main flow is larger than that of the tributary at most time periods. In the scenario 2, the optimum values of u_1 and u_3 are also presented in Fig.5. Based on the calculation, the average u_1 and u_3 are equals to 0.016 (1.6%) and 0.022 (2.2%), respectively. The result shows that these two reduction rates are close to each other for scenario 2 (TP in reservoir under 30 (μg/L). Fig. 6 reveals the TP concentration in Feitsui Reservoir through reducing the phosphorus loads from the watershed for scenarios 1 and 2, respectively. In addition, the average reduction rate of TP in reservoir equals 81% for scenario 1; while it reaches 95% for scenario 2.

4. Summary and Conclusions

This paper provides a grammatical evolution (GE) method combining with macro-evolutionary genetic algorithm (MGA) to potentially predict and control the total phosphorous (TP) concentration of a reservoir in Taiwan. Statistically, the result shows that the GE is not as simple as basic formula; but it provides an appropriate model to simulate TP concentration. From the results of GE, three input variables were found available. These three inputs include the TP concentration of tributary Diyu Creek at time step t (X_1) , the TP concentration of main inflow Peishih Creek at time step t (X_3) and the maximum rainfall in the watershed at time step t-1 (X_{12}) , to predict the TP concentration in reservoir at time step t (Y) .

It is seen from the results that the MGA is able to identify control schemes that reduce the in-reservoir TP concentration and water quality in the reservoir can be expected to achieve a lower level. For scenario 1, if the watershed loads are reduced by average 16%, the TP in reservoir will stay below 20 $(\mu g/L)$. In the scenario 2, if the watershed loads are reduced by average 1.9%, the TP in reservoir can be under 30 (μg/L). Finally, it is concluded that the mixture of GE with MGA has a potential ability to optimally control nutrient loads from the watershed.

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Table1.Example of each codon converted into corresponding BNF grammar

	Variables	Diyu Creek	Kingkwa Creek	Peishih Creek	Average rainfall	Maximum rainfall	Inflow	Outflow	TP
Statistical parameters			$(X1, X8_{t-1})$ $(X2, X9_{t-1})$ $(X3, X10_{t-1})$ $(X4, X11_{t-1})$ $(X5, X12_{t-1})$					$(X6_r, X13_{r-1})$ $(X7_r, X14_{r-1})$ $(Y_r, X15_{r-1})$	
Units		CMSD	CMSD	CMSD	mm	mm	CMSD	CMSD	$\mu g/L$
x_{mean}	\boldsymbol{t}	31.78	36.83	35.92	11.05	89.37	1000.51	1013.26	23.13
	$t-1$	31.85	36.88	36.06	11.09	89.84	1005.18	1017.00	23.04
S_{x}	\boldsymbol{t}	22.39	36.32	30.33	9.62	86.03	906.43	1037.20	12.82
	$t-1$	22.47	36.47	30.42	9.65	86.24	908.81	1040.77	12.84
$C_{\rm v}(S_{\rm x}/x_{\rm mean})$	\boldsymbol{t}	0.7	0.99	0.84	0.87	0.96	0.91	1.02	0.55
	$t-1$	0.71	0.99	0.84	0.87	0.96	0.90	1.02	0.56
x_{max}	t $t-1$	100	255	120.72	70.54	468.8	6937.24	7287.83	98.57
x_{\min}	\boldsymbol{t} $t-1$	4.9	6.25	6.2	1.18	8.9	98.86	161.65	5.26

Table 2. The statistical parameters of data set

Fig. 1. The flowchart of GE combined with GA

Fig. 2. Location of Feitsui Reservoir and its watershed

Fig. 3The scatter plots of GE

Fig. 4. Flowchart of GE predictor combined with MGA optimizer

Fig. 5. u1 and u3 for scenarios 1 and 2

Fig. 6. The in-reservoir total phosphorus (TP) concentration before and after reduction of phosphorus loads from the watershed (Scenarios 1 and 2)

國科會補助專題研究計畫項下出席國際學術會議心得報告

日期: 99年09月19日

一、參加會議經過

本人於 8/13 日當天早上由台灣出發到達北京,在經由火車前往天津,於下午到達研討會會場,完 成報到手續,並與主辦單位初步交流;第二天上午前往會場參加開幕儀式,並於下午聽取專題演講; 第三天本人於上午 08:10~10:00 進行論文發表,期間亦聽取其他與會人士之報告,與其他發表者進行學 術交流彼此交換意見;第四天參加研討會單位安排參觀天津市行程;由於飛機時間問題需至 8/18 才能 回國,於是第五天到北京參觀;第六天早上至機場回台灣。

二、與會心得

第三次參加國際性的研討會,皆於會議中發表相關文章,本次研討會會將發表者所報告文章收入 於 EI 期刊研討會中,所以本人覺得這可以刺激投稿者發表之意願,其他則與國內的大型研討會差不多, 會議期間聽取了一些有關電腦計算機與人工智慧方面的研究,對這領域有了更深的瞭解。

三、考察參觀活動(無是項活動者省略)

會議單位有安排行程可參觀天津市,有前往天津港及租界處參觀,由於天津亦在建設中,所以覺 得市區滿凌亂的。另亦有安排前往長城之八達嶺與居庸關等段,參觀歷史古蹟。

四、建議

希望國內也可以跟相關 SCI 或是 EI 等級的期刊合作辦研討會,一來增加文章的深度,亦可提高投 稿的意願。

五、攜回資料名稱及內容

研討會論文集光碟片一片及其紀念品。

六、其他

無

97 年度專題研究計畫研究成果彙整表

國科會補助專題研究計畫成果報告自評表

請就研究內容與原計畫相符程度、達成預期目標情況、研究成果之學術或應用價 值(簡要敘述成果所代表之意義、價值、影響或進一步發展之可能性)、是否適 合在學術期刊發表或申請專利、主要發現或其他有關價值等,作一綜合評估。

