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Support Vector Regression Model of Chlorophyll-*a* during Spring Algal Bloom in Xiangxi Bay of Three Gorges Reservoir, China

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ABSTRACT

To study the relationship between chlorophyll-*a* and environmental variables during spring algal bloom in Xiangxi Bay of Three Gorges Reservoir, the support vector regression (SVR) model was established. In surveys, 11 stations have been investigated and 264 samples were collected weekly from March 4 to May 13 in 2007 and February 16 to May 10 in 2008. The parameters in SVR model were optimized by leave one out cross validation. The squared correlation coefficient R^2 and the cross validated squared correlation coefficient Q^2 of the optimal SVR model are 0.8202 and 0.7301, respectively. Compared with stepwise multiple linear regression and back propagation artificial neural network models using external validation, the SVR model has been shown to perform well for regression with the predictive squared correlation coefficient R^2_{pred} value of 0.7842 for the test set.

Keywords: Support Vector Regression; Chlorophyll-*a*; Algal Bloom; Three Gorges Reservoir

1. Introduction

The eutrophication of reservoirs and lakes has been a major water quality problem for decades, causing turbid water with high algal biomass [1-3]. This trend is expected to increase by high levels of nutrient input as a result of human activities such as sewage and storm overflows, runoff of commercial fertilizer, and so on [4]. In water research and management, chlorophyll-*a* is the fundamental index of phytoplankton abundance and a good indicator of algal bloom (a rapid increase in the biomass of phytoplankton) [5-7]. The concentration of chlorophyll-*a* in aquatic system depends on a number of variables including nutrients, light, temperature, physicochemical properties of the water mass [8] as well as interactions between these physical, chemical and biological compartments of the system. There are many study methods to the relationship between chlorophyll-*a* and environmental factors such as stepwise multiple linear regression (MLR) analysis [9-12] and artificial neural network (ANN) [13,14]. But the algal bloom is the multivariate interaction and nonlinear process. Many times, linear based methods such as MLR are not able to represent satisfactorily the correlation between chlorophyll-*a* and respective environmental variables, because these methods do not account for non-linearity. ANN can in principle model nonlinear relations but often difficult to train or even yield unstable models and another drawback is the fact that ANN does not lead to one global or unique solution due to differences in their initial weight set.

Support vector regression (SVR), originally proposed and developed by Vladimir Vapnikn [15,16], is a nonlinear machine learning technique and has many theoretical advantages in the field of chemometrics. These advantages stem from the specific formulation of a (convex) objective function with constraints which is solved using Lagrange Multipliers and has the characteristics that: 1) a global optimal solution exists which will be found, 2) the result is a general solution avoiding overtraining, 3) the solution is sparse and only a limited set of training points contribute to this solution, and 4) nonlinear solutions can be calculated efficiently due to the usage of inner products [17]. So the aim of this present paper is to construct the relationship model between chlorophyll-*a* and environmental factors during spring algal bloom in Xiangxi Bay of Three Gorges Reservoir using support

vector regression method.

2. Materials and Methods

2.1. Area Description

The Three-Gorge Dam (TGD) in China is the world's largest dam, measuring 2335 m long and 185 m high, and the reservoir created by it has an area of 1080 km^2 in 2009 [18]. The Xiangxi River, which lies 38 km upstream from the Dam, is the largest tributary in the Hubei portion of Three-Gorge Reservoir (TGR). This river is 94 km long with a watershed of 3099 km^2 (between 110˚25' and 111˚06′E long., 30˚57′ and 31˚34′N lat.) [19]. With impoundment of TGR, the downriver stretch of Xiangxi River was inundated and Xiangxi Bay was formed. Then the water flow velocity has dropped from the original 0.43 - 0.92 m/s [20] to 0.0020 - 0.0041 m/s [21]. So when water temperature increased in spring, there were algal blooms with prolonged retention time and high nutrient concentrations in Xiangxi Bay.

2.2. Sampling and Analysis

Water samples were collected at 11 stations (X0 - X10) in Xiangxi River (**Figure 1**). Samplings were performed weekly from March 4 to May 13, 2007 and February 16 to May 10, 2008. Water samples were collected at 0.5 m depth from surface in the middle of the river using a 5-L Niskin sampler (Hydrobios-Kiel). Water temperature (WT), dissolved oxygen (DO), pH, turbidity (Turb) were recorded in situ using multi-parameter water quality analyzer (Hydrolab DS5). Total phosphates (TP), phosphate (PO_4), total nitrogen (TN), ammonium nitrogen (NH_4), nitrate (NO_3), silicate (SiO_4) were determined in the laboratory using State Environmental Protection Administration (SEPA) standard methods [22]. For chlorophyll-*a* (Chl-*a*) analysis, samples filtered through Whatman GF/F filters were extracted with cold 90% acetone and estimated by spectrophotometer [23].

2.3. Support Vector Regression

In support vector regression, the basic idea is to map the data X into a higher dimensional feature space F via a nonlinear mapping Φ and then to do linear regression in this space [16,17]. Therefore, regression approximation addresses the problem of estimating a function based on a given data set $G=\{(\boldsymbol{x}_i,d_i)\}_{i=1}^{l}$ ($\boldsymbol{x}_i$ is input vector, d_i is the desired value). SVR approximates the function in the following form:

$$y=\sum_{i=1}^{l} w_i\Phi_i(x)+b \tag{1}$$

where $\{\Phi_i(x)\}_{i=1}^{l}$ is the set of mappings of input features,

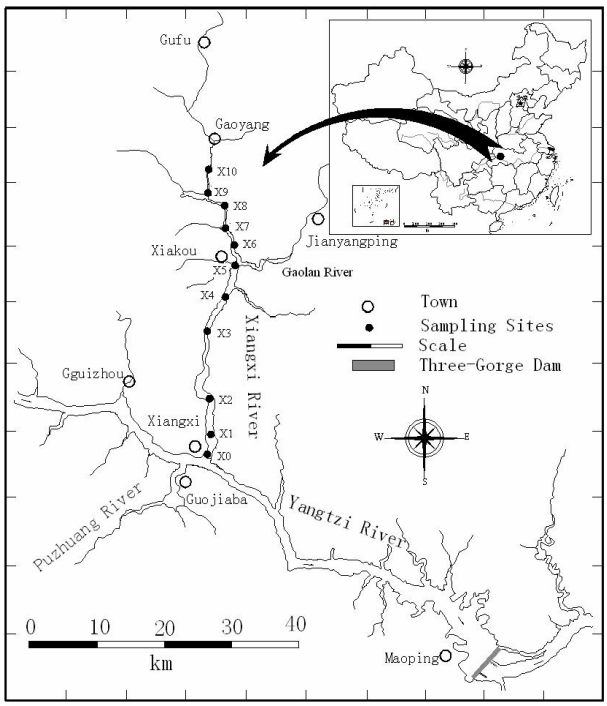

Figure 1. Sampling stations in Xiangxi Bay.

$\{w_i\}_{i=1}^{l}$ and b are coefficients. They are estimated by minimizing the regularized risk function $R(C)$:

$$R(C)=C\frac{1}{N}\sum_{i=1}^{l}L_\varepsilon(d_i,y_i)+\frac{1}{2}\|w\|^2 \tag{2}$$

where

$$L_\varepsilon(d,y)=\begin{cases}|d-y|-\varepsilon & \text{for } |d-y|\geq\varepsilon\\ 0 & \text{otherwise}\end{cases} \tag{3}$$

and ε is a prescribed parameter in the insensitive loss function.

In Equation (2), $\left[C(1/N)\sum L_\varepsilon(d_i,y_i)\right]$ is the so-called empirical error (risk) measured by ε-insensitive loss function $L_\varepsilon(d,y)$, which indicates that it does not penalize errors below ε. The second term, $\left[(1/2)\|w\|^2\right]$, is used as a measurement of function flatness. C is a regularized constant determining the tradeoff between the training error and the model flatness. Introduction of slack variables ξ leads Equation (4) to the following constrained function Max:

$$\max R(w,\xi^*)=\frac{1}{2}\|w\|^2+C^*\sum_{i=1}^{l}(\xi_i+\xi_i^*) \tag{4}$$

s.t. $w\Phi(x_i)+b-d_i\leq\varepsilon+\xi_i$, $d_i-w\Phi(x_i)-b_i\leq\varepsilon+\xi_i^*$, $\xi_i,\xi_i^*\geq 0$.

The minimization of Equation (1) is a standard prob-

lem in optimization theory and it can be derived that the weight vector $\boldsymbol{w}$ equals the linear combination of the training data:

$$\boldsymbol{w} = \sum_{i=1}^{l} \left(\alpha_i - \alpha_i^* \right) x_i \tag{5}$$

In this formula, α_i and α_i^* are Lagrange multipliers. Thus, decision function becomes the following form:

$$f(x) = \sum_{i=1}^{l} \left(\alpha_i - \alpha_i^* \right) K(\boldsymbol{x}_i, x) + b \tag{6}$$

where $K(x_i, x)$ is the kernel function and the value is equal to the inner product of two vectors $\boldsymbol{x}_i$ and $\boldsymbol{x}_j$ in the feature space $\Phi(x)$. That is, $K(\boldsymbol{x}_i, x_j) = \Phi(\boldsymbol{x}_i)\Phi(x_j)$. The most used kernel functions include radial basis function (RBF) kernel, polynomial kernel and linear kernel. For the SVR calculations, a Matlab toolbox was used, developed by Gunn [24].

3. Results and Discussion

3.1. Selection of the Environmental Factors

Statistic summary of chlorophyll-*a* and environmental factors during the observation period in Xiangxi Bay of Three Gorges Reservoir are presented in **Tables 1** and **2**. There is a clear spatial and temporal variation in chlorophyll-*a* across Xiangxi Bay. The concentration of chlorophyll-*a* ranged from 0.1280 to 160.2060 mg/m^3 in the spring of 2007 and from 1.9380 to 335.7360 mg/m^3 in the spring of 2008 with mean values of 11.4910 mg/m^3 and 31.8219 mg/m^3, respectively. Mean concentration of chlorophyll-*a* for each station ranged from 3.6723 to 23.7129 mg/m^3 in the spring of 2007 and from 17.5191 to 63.6717 mg/m^3 in the spring of 2008. The spring algal bloom in 2008 is serious than that in 2007.

The environmental variables were selected using stepwise multiple linear regression method. In the stepwise MLR method, all variables were assessed and evaluated to determine important factors. As the stepping process was terminated, the model with seven important environmental factors was obtained as follows:

$$\begin{aligned} Chl-a = {} & 157.4835 + 3.5579\mathrm{DO} \\ & + 18.8673\mathrm{pH} + 0.2443\mathrm{Turb} \\ & - 80.1043\mathrm{PO_4} + 39.8839\mathrm{NH_4} \\ & - 11.3617\mathrm{NO_3} - 4.0525\mathrm{SiO_4} \end{aligned} \tag{7}$$

($R^2 = 0.4131$, $R^2_{adj} = 0.3970$, $S = 30.6541$, $F = 25.7431$, $Q^2 = 0.3526$, $P = 0.0001$, $n = 264$)

The statistical quality of the regression equation was examined using parameters such as the squared correlation coefficient (R^2), the squared adjusted correlation coefficient (R^2_{adj}), the standard error (S), the Fisher ratio at the 95% confidence level (F), and the cross validated squared correlation coefficient obtained based on Leave One Out (LOO) method (Q^2). The stepwise MLR analysis shows that the environmental variables (DO, pH, Turb, PO_4, NH_4, NO_3, SiO_4) are more important to the chlorophyll-*a* concentration of spring algal bloom in Xiangxi Bay. But Equation (7) only predicted 35.26% of the variance and explained 39.70% of the variance of chlorophyll-*a*. So the MLR model is not satisfactory.

Table 1. Statistic summary of chlorophyll-*a* (mg/m^3) during the observation period in Xiangxi Bay.

	2007				2008			
	Mean	Std.	Minimum	Maximum	Mean	Std.	Minimum	Maximum
All data	11.4910	23.6217	0.1280	160.2060	31.8219	47.1616	1.9380	335.7360
X0	3.6723	4.0436	0.4380	12.5890	23.3225	25.9015	2.0130	87.4200
X1	23.7129	38.9107	1.0150	132.3120	27.0729	31.6546	1.9380	92.4000
X2	21.5977	46.4572	0.6750	160.2060	28.6073	36.6705	2.1450	104.7980
X3	16.2165	29.6656	0.3670	98.7500	32.3891	64.4767	2.0160	240.5200
X4	5.6552	9.7656	0.1280	32.9670	17.5191	15.8523	3.6720	58.1500
X5	9.9516	24.1192	0.6100	82.2310	18.6323	14.0088	4.2240	43.0580
X6	11.7786	22.1321	0.1450	66.3000	24.0688	24.1290	3.9640	92.4390
X7	5.3327	5.8171	0.1630	17.1290	26.1929	35.8963	4.1150	142.1160
X8	10.7885	12.8801	0.3330	38.4300	40.7369	61.4108	6.3610	235.8210
X9	9.0060	10.2170	0.1670	33.9000	63.6717	85.9708	5.9240	335.7360
X10	8.6895	13.7744	1.1330	43.6580	47.8277	59.8171	5.2400	208.8600

Table 2. Statistic summary of environmental factors during the observation period in Xiangxi Bay.

	2007				2008			
	Mean	Std.	Minimum	Maximum	Mean	Std.	Minimum	Maximum
WT (℃)	16.0786	3.0021	11.1390	21.0700	14.6379	3.8563	9.3430	23.4960
DO (mg/L)	11.0207	3.6202	1.5860	21.4950	8.6148	2.3404	4.7190	19.5430
PH	8.2857	0.5235	6.7360	9.1780	8.7269	0.5044	7.7860	9.9110
Turb (NTU)	8.2411	12.5880	0.2000	89.5500	13.8815	27.3549	2.6140	210.1430
TP (mg/L)	0.1838	0.1020	0.0290	0.5100	0.7507	1.5386	0.0133	6.9316
PO_4 (mg/L)	0.1450	0.0939	0.0020	0.4200	0.1324	0.0949	0.0064	0.6639
TN (mg/L)	1.1259	0.4022	0.3170	2.4670	1.7713	0.9359	0.1791	6.3797
NH_4 (mg/L)	0.3368	0.1639	0.0600	0.8980	0.5327	0.2665	0.0042	2.0908
NO_3 (mg/L)	0.7392	0.3839	0.0410	1.5130	0.7382	0.5547	0.0050	3.0321
SiO_4 (mg/L)	3.6650	1.0079	0.9190	5.8810	4.3640	3.3591	0.0590	21.8886

3.2. Selection of the SVR Model Parameters

The resulting environmental factors in Equation (7) decided by stepwise MLR were used for SVR model. The performance of SVR model is related to variables as well as the combination of parameters used in the model. So some parameters in SVR (the type of kernel function, the regularization parameter C and ε-insensitive loss function) ought to be optimized. In this work, Q^2 was used as a measurement of generalization in leave one out cross validation (LOOCV) of SVR. **Figures 2-4** illustrated Q^2 versus ε and C with different kernel functions [RBF with a width of σ = 0.10, polynomial, linear] respectively. It is found that optimal SVR model with Q^2 = 0.7301 is available when the kernel function is polynomial with ε = 0.03 and C = 150. **Figure 5** shows the calculated values of optimal SVR model versus observed values for chlorophyll-*a* (R^2 = 0.8202). It can be concluded that the predicted results are in good agreement with the observation ones.

The optimal SVR model was compared with stepwise MLR and back propagation artificial neural network (BPANN). The parameters of BPANN model with three layers used were as follows: the number of hidden nodes was seven; the transformation function was sigmoid; the learning rate and momentum of each epoch were set to 0.30 and 0.20 respectively. External validation was used to compare the predictive capacity of models. The data set was randomly classified into training set (80% data) and test set (20% data) and the predictive R^2 (R^2_{pred}) values were calculated according to the following equation:

$$R^2_{pred} = 1 - \frac{\sum\left(Y_{pred\,(\mathrm{Test})} - Y_{(\mathrm{Test})}\right)^2}{\sum\left(Y_{(\mathrm{Test})} - \overline{Y}_{\mathrm{training}}\right)^2} \quad (8)$$

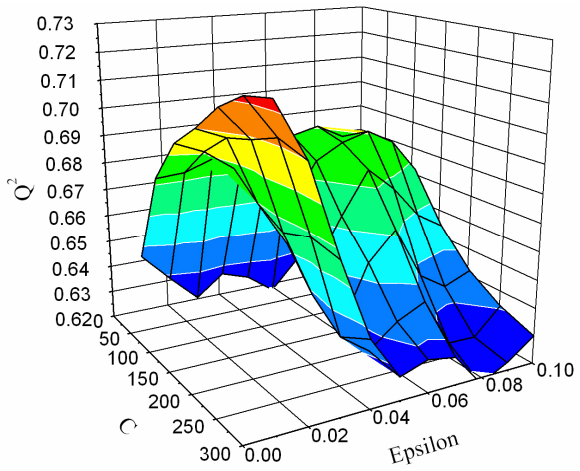

Figure 2. Q^2 versus ε and C with RBF kernel function (σ = 0.10).

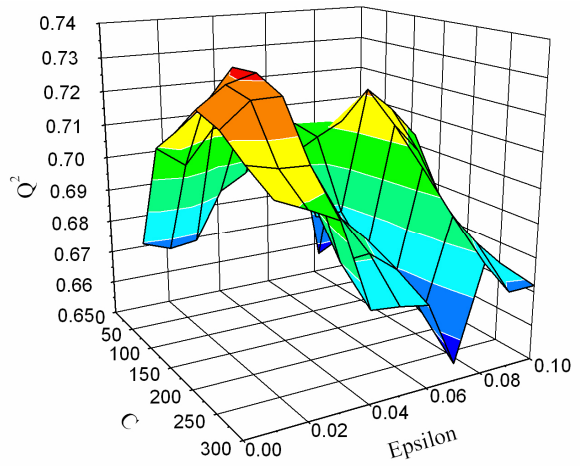

Figure 3. Q^2 versus ε and C with polynomial kernel function.

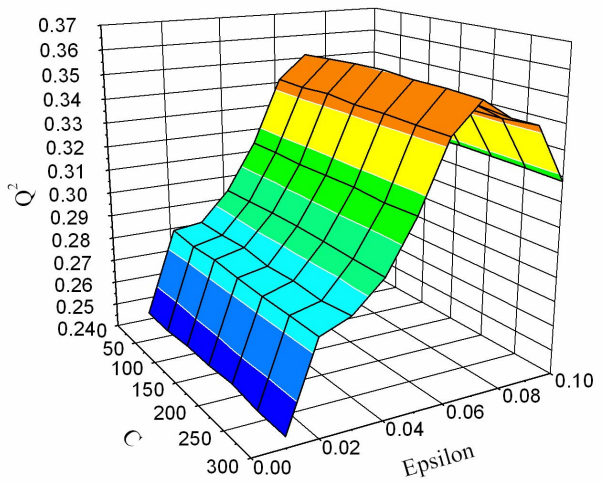

Figure 4. Q^2 **versus** ε **and** C **with linear kernel function.**

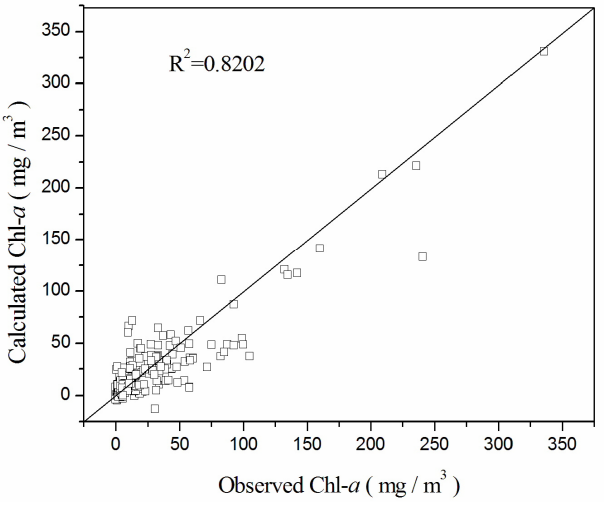

Figure 5. Observed values versus calculated values for chlorophyll-*a* using optimal SVR model.

where $Y_{pred\,(\mathrm{Test})}$ and $Y_{(\mathrm{Test})}$ represent the predicted and observed chlorophyll-*a* values of the test set, respectively. $\overline{Y}_{\mathrm{training}}$ is the mean chlorophyll-*a* value of the training set.

The R^2_{pred} values of MLR, BPANN and SVR models were 0.4127, 0.7644 and 0.7842 respectively. **Figure 6** shows the predicted values of optimal SVR model versus observed values for chlorophyll-*a*. Based on the above results. The SVR method has been shown to perform well for regression and be a useful and powerful technique to construct the chlorophyll-*a* model during spring algal bloom.

4. Conclusion

The support vector regression model of chlorophyll-*a* during spring algal bloom in Xiangxi Bay of Three Gorges Reservoir was established. Using stepwise MLR method, the important environmental variables (DO, pH, Turb, PO_4, NH_4, NO_3 and SiO_4) were selected. The parameters in SVR such as the type of kernel function, the regularization parameter C and ε -insensitive loss function were optimized by leave one out cross validation. R^2 and Q^2 of the optimal SVR model are 0.8202 and 0.7301, respectively. Compared with MLR and BPANN models, the SVR model has been shown to perform well for regression with the R^2_{pred} value of 0.7842 for the test set.

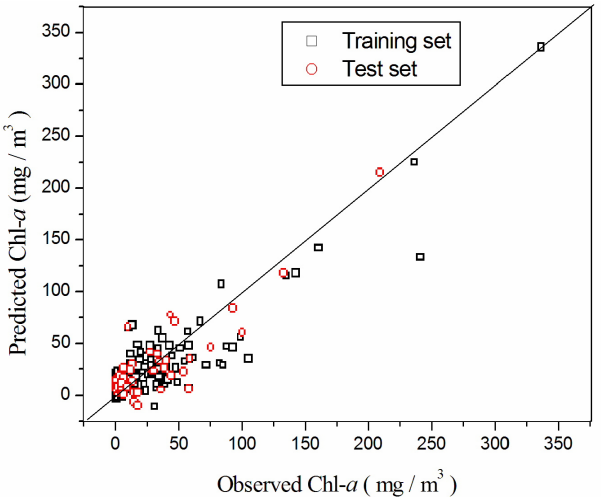

Figure 6. Observed values versus predicted values for chlorophyll-*a* using optimal SVR model.

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