Water Quality Retrieval and Performance Analysis Using Landsat Thermatic Mapper Imagery Based on LS-SVM

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***Abstract*—Because of the limited number of monitoring points on the ground, the accuracy of traditional monitoring methods using remote sensing was lower. This paper proposed to use the Least Squares Support Vector Machine (LS-SVM) theory to improve the accuracy of water quality retrieval, which is suitable for the small-sample fitting. The Radial Basic Function (RBF) was chosen as the kernel function of the retrieval model, and the grid searching and *k*-cross validation were used to choose and optimize the parameters. This paper made use of the LS-SVM model and some traditional retrieval models to retrieve concentration of suspended matter. Comparing the results of experiment, it showed that the proposed method had good performance and at the same time, the complexity is lower and the speed of the modeling was rapid.**

***Index Terms*— LS-SVM, water retrieval, grid searching, remote sensing**

I. Introduction

The use of remote sensing for water quality monitoring is an uncertain problem [1]. How to establish an appropriate model for the retrieval of the water quality parameters is a difficult problem, when it referred to either different water regions or different water characteristic.

There are three mainly conventional methods for water quality monitoring which are empirical method, semi-empirical method and analysis method [3]. In fact, these methods are based on the estimation of linear regression model to complete the water quality retrieval. However, because of the complex chemical reaction and mutual influence of various pollutants in the water, the monitoring of the eutrophication in lake water should be a non-linear prediction problem. Thus, using linear regression to estimate the water quality parameters could not get the accurate retrieval results.

BP neural network method is a nonlinear approximation algorithm, which is based on the empirical quality retrieval field. However, BP neural network has minimization rule. It was applied widely in the water some disadvantages.

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Firstly, BP algorithm has the over fitting phenomenon, so the generalization ability of the system decreased. Secondly, it depends on the quantity of the samples, namely, BP algorithm requires a large number of learning samples. Because the number of points for water quality monitoring was often limited, it leaded to the lack of the training samples. So the results of the retrieval by the BP algorithm were poorly accreted. Finally, BP algorithm is easy to fall into the local minimum; the hidden number is hard to determine and the training speed is slower. All these factors of BP neural network method affected the accuracy of retrieved result.

Compared with BP neural network, the SVM have a more solid theoretical foundation and a sound theoretical system. SVM algorithm can be transformed into a quadratic optimization problem, and it also can avoid the local optimal point and achieve the global optimal point. Besides these, the SVM has fewer parameters than those in neural network, and at the same time it applies a new approach for the machine learning with little samples.

However there were also some problems for the SVM algorithm. For example, the selection of parameters was a vexing problem because of the absence of theoretical guidance. The SVM uses quadratic programming to solve the support vector. The solving of quadratic programming will involve the calculation of m-matrix, which was a matrix with m order. When the number of samples m is too large, the solving and computing of the matrix will cost a lot of memory and computing time of the machine. Another drawback of the SVM is that the optimum kernel transfer function and its corresponding parameters for respective data sets are difficult to set. And whenever the emergence of new data sets, they need to re-determine the function and its parameters. It reduces the generalization ability. Use searching loop within the possible value range will help to solve the problem at some extent, but it requires large enough data sets to complete a reliable cross-examination. So the complexity of algorithm is increasing.

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LS-SVM is a reformulation of the standard SVM [13]. LS-SVM uses the least-squares linear system instead of the quadratic programming method to estimating the function. So it has good generalization ability. According to the limited sample points of water monitoring, and the requirement of good generalization ability, the LS-SVM algorithm and theory was proposed to retrieve the water quality of Tai Lake. This method provides a new retrieval method for the water quality monitoring of the Tai Lake and gets good performance.

II. THE MODEL OF LS-SVM

In 1995, Vapnik developed a novel algorithm called support vector machine (SVM), which is a learning machine based on statistical learning theory. SVM implements the principle of structural risk minimization for seeking to minimize an upper bound of the generalization error rather than minimize the training error. SVM has been applied to solve regression problems by the introduction an alternative loss function, which referred to support vector regression (SVR).

The aim of SVR is to generate a regression function by applying a set of high dimensional functions [13]. The regression function is formulated as follows:

$$f(x) = \omega \cdot \phi(x) + b \tag{1}$$

Where $\phi(x)$ is the feature of the inputs, and ω and b are coefficients. The coefficients are estimated by the following regularized risk function

$$P(x) = C\frac{1}{N}\sum_{i=1}^{N} L_g + \frac{1}{2}\|\omega\|^2 \tag{2}$$

Where

$$L_g = |y - f(x,\omega)|_{\varepsilon} = \begin{cases} 0 & |y-f(x,\omega)| >= \varepsilon \\ |y-f(x,\omega)|_{\varepsilon} & \text{otherwise} \end{cases} \tag{3}$$

C and ε are prescribed parameters, L_g is the ε-insensitive loss function, $\frac{1}{2}\|\omega\|^2$ is used as a measure of the flatness of the function.

By the structural risk minimization principle, the generalization accuracy is optimized over the empirical error and the flatness of the regression function which is guaranteed on a small ω. Therefore, the objective of SVR is to include training patterns inside a ε-insensitive tube while keeping the norm $\|\omega\|^2$ as small as possible. An optimization problem can be formulated as the following soft margin problem:

$$\min \phi(\omega) = \frac{1}{2}\|\omega\|^2 + C\sum_{i=1}^{l}(\xi_i + \xi_i^*)$$
$$s.t. \begin{cases} y_i - \omega x_i - b \le \varepsilon + \xi_i \\ \omega x_i + b - y_i \le \varepsilon + \xi_i^* \end{cases} \tag{4}$$
$$\xi_i, \xi_i^* \ge 0,\ C > 0,\ i = 1, 2, \cdots, l$$

Where C, ε and ξ_i (ξ_i^*) are a trade-off cost between the empirical error and the flatness, the size of the ε-tube, and slack variables, respectively. By adding Lagrange multiplies α and α^*, the quadratic programming problems can be optimized as a dual problem. SVR can estimate a nonlinear function by employing a kernel function $K(x_i, x_j)$. The regression function can be written as:

$$f(x) = \sum_{i=1}^{l}(\alpha_i - \alpha_i^*) \cdot K(x_i, x) + b \tag{5}$$

The kernel function $K(x_i, x_j)$ is used to construct a nonlinear decision hyper-surface on the SVR input space. However, equation (5) is subjected to the restriction of the in equation and needed to make a solution to the restriction of the in equation and needed to make a solution of complex quadratic planning.

The LS-SVM uses the square of deviance cost function instead of ε-insensitive loss function, so the restriction of the inequality is transformed into the restriction of the equation. The LS-SVM has good generalization ability, because it avoids solving a difficult quadratic planning as SVM.

Therefore, compared with the SVM, LS-SVM algorithm greatly reduces the complexity of the algorithm, making the training speed very fast, so the retrieval precision is increased.

For the training sample sets $D = (x_k, y_k)$, $x_k \in R^n$, $y_k \in R^{n_h}$, $k = 1, 2, ...N$ .Where, x_k is the input data, y_k is the output data. According to the theorem Mercer, the kernel function $K(\cdot,\cdot)$ and the mapping function $\varphi(\cdot)$ allow:

$$K(x_k, y_k) = \varphi(x_i)^T \varphi(x_j) \tag{6}$$

LS-SVM is solved in the original space, so the following optimization problem is obtained:

$$\min J(\omega, b, \xi) = \frac{1}{2}\omega^T\omega + \frac{1}{2}\gamma\sum_{k=1}^{N}\xi_k^2$$
$$s.t. y_k = \omega^T\varphi(x_k) + b + \xi_k\ (k = 1, 2...N) \tag{7}$$

Where γ is an adjustable regularization parameter, γ is the compromise between the training error and model complexity, so that the desired function has good generalization ability. The value of γ is greater, the regression error of the model is smaller [4].The variable ω reflects the complexity of the function, which is a linear combination of non-linear mapping function $\varphi(\cdot)$.

LS-SVM defines a different loss function compared with the standard SVM, and it transfers the restriction of the inequality into the restriction of the equation. By adding Lagrange function:

$$L(\omega, b, \xi, a) = J(\omega, b, \xi) - \sum_{k=1}^{N} a_k[\omega^T\varphi(x_k) + b + \xi_k - y_k] \tag{8}$$

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Lagrange multipliers $a_k \in R$, the optimal a, b can be obtained through the KKT conditions:

$$\frac{\partial_L}{\partial_\omega} = 0 , \frac{\partial_L}{\partial_b} = 0 , \frac{\partial_L}{\partial_\xi} = 0 , \frac{\partial_L}{\partial_a} = 0 \tag{9}$$

Further by calculating, the following equations will be obtained:

$$\begin{cases} \omega = \sum_{k=1}^{N} a_k \varphi(x_k) \\ \sum_{k=1}^{N} a_k = 0 \\ a_k = \gamma \xi_k \\ \omega^T \varphi(x_k) + b + \xi_k - y_k = 0 \end{cases} \tag{10}$$

The matrix equation (11) will be given by the equation 8and equation (10), by eliminating the variables ω and ξ:

$$\begin{bmatrix} 0 & \Theta^T \\ \Theta & K + \gamma^{-1} I_n \end{bmatrix} \begin{bmatrix} b \\ a \end{bmatrix} = \begin{bmatrix} 0 \\ y \end{bmatrix} \tag{11}$$

Where $y = [y_1, \cdots, y_n]^T$, $\Theta = [1, \cdots, l]$, $a = [a_1, \cdots, a_N]^T$ and

$$K_{i,j} = \varphi(x_i)^T \varphi(x_j) \quad (i, j = 1, \cdots, N) \tag{12}$$

The values a, b will be obtained by solving the equation (11). So the following equation shows LS-SVM model function that is used for water quality monitoring.

$$f(x) = \sum_{i=1}^{N} a_i K(x, x_i) + b \tag{13}$$

The selection and construction of kernel functions is a key issue which greatly influences the performance of LS-SVM, and provides an important approach to expand LS-SVM from linear field to nonlinear field. The kernel functions of LS-SVM are Mercer functions which meet Mercer condition. In the application of the kernel function, there are different forms. At present, there are several commonly used kernel functions [5]:

1) Linear kernel:

$$K(x, x_i) = x^T x_i \tag{14}$$

2) Q-order polynomial kernel function:

$$K(x_i, x_j) = (\gamma x_i^T x_j + r)^q, \gamma > 0 \tag{15}$$

3) RBF function:

$$K(x_i, x_j) = \exp(-\frac{\left\| x_i - x_j \right\|^2}{\sigma^2}) \tag{16}$$

4) Sigmoid kernel function:

$$K(x_i, x_j) = \tanh(\gamma x_i^T x_j + r) \tag{17}$$

The above kernel functions possess their respective traits, and have different effects on LS-SVM performance. Among these kernel functions, RBF kernel function is a local kernel function with a stronger learning ability [17], and it can achieve a good balance between the computing time and the effectiveness of the prediction. So the RBF function was accepted by this paper.

III. STRCTURE OF THE WATER QUALITY RETRIEVAL

For a long time, quantitative retrieval of the inland water quality has been the difficulty for water research using remote sensing. The lack of an effective means of monitoring and evaluation system make the existing measurement data can not be well analyzed and mined [1].In this paper, LS-SVM model was applied to the field of water quality monitoring. The process of the retrieval model based on LS-SVM was shown in Fig.1.

The association information between the remote sensing and ground-monitoring were used to build the information processing model, which was fused by the ground survey data and remote sensed data. The model can provide good generalization ability and reduce the complexity of the system. As the Fig.1 shows, the sensing data, which is corresponding to the ground monitoring points on the remote sensing image and the ground survey data, were composed to the training sets, the input vector is sensing data, and the target vector is the ground survey data. The pre-prepared training sets was used to train LS-SVM, and then the required retrieval region on the remote sensing image will be input into the trained LS-SVM pixel-by-pixel to retrieve. Finally, the water quality retrieval results of the part of or the entire water field will be obtained.

IV. THE EXPERIMENT AND ANALYSIS

Tai Lake was as an example accepted by this study. The original information included Landsat5 TM remote sensing image data and the synchronous ground survey data on May 4, 1997. As is shown in the Fig. 2, there were 12 monitoring points were set up, the measured data were acquired from these monitoring points. The locations of the monitoring points were marked by the five-pointed star in the Fig.2.

In this paper, the experimental platform was Matlab 7.1, the concentration of the suspended matter of Tai Lake was retrieved on this platform. The LS-SVM lab contains Matlab/C implementation for a number of LS-SVM algorithms related to classification, regression and time-series prediction. The LS-SVM lab is calculated specifically for SVM, which is an open-source code package. It provides a large number of interfaces for classification and regression. Because there is no LS-SVM lab code package in the Matlab toolbox, so the code should be added into the Matlab toolbox.

In this paper, the LS-SVMlab1.5 code package was added into the Matlab toolbox, which used the interface provided by LS-SVM to realize the regression function.

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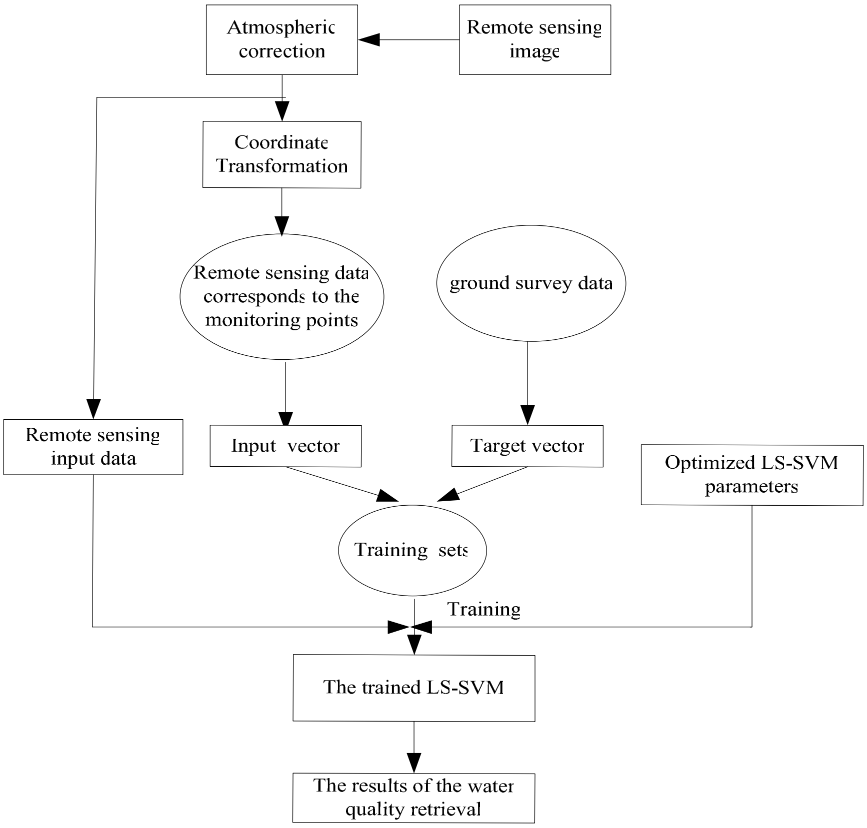

Figure 1.The structure of water quality retrieval model based on LS-SVM

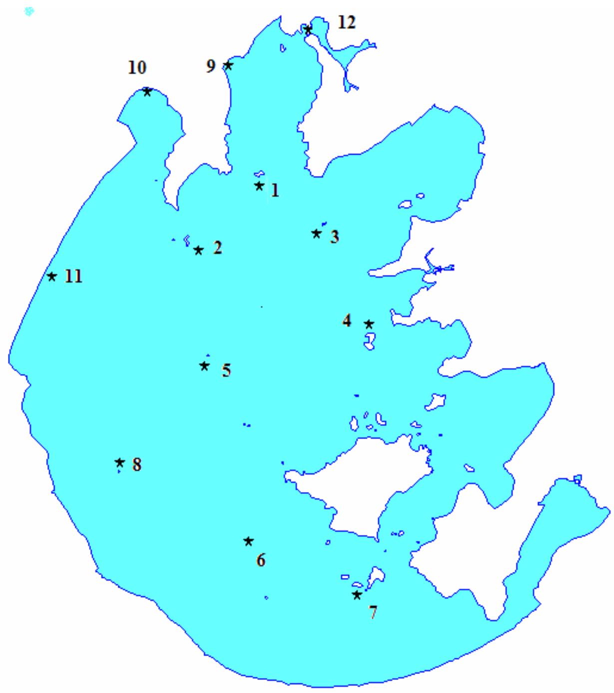

Figure 2. The ground-monitoring points of the Tai Lake

A. The Selection Parameters of the LS-SVM

The kernel function and its parameters γ and σ^2 of the LS-SVM have great effect to the performance of the algorithm [4], and there is no simple way to determine the parameters. In this paper, the grid-searching and cross-validation were used to select the parameters of the LS-SVM automatically. At the same time, the RBF function was used to only determine two parameters γ and σ^2, so the search space of parameters was reduced to two-dimensional from tree-dimensional of the SVM, and the speed of modeling was accelerated.

The search scope of the two parameters γ and σ^2 should be firstly determined when the parameters is searched by the grid-searching method. In this paper, after the repeated experiment, the search scope of γ was $[2^{-2}, 2^{-1} \cdots 2^{10}]$, and σ^2 was $[2^{-2}, 2^{-1} \cdots 2^{5}]$, so a two-dimensional network was constituted in the coordinate system. For each γ and σ^2 group, the cross-validation evaluation algorithm can be used, γ and σ^2 as a set of parameters would be searched, whose algorithm performance was the best. A small scope search area was chosen to search the two parameters, which were set at the center of the area, consequently a set of optimal parameters was searched.

The algorithm of the cross-validation evaluation was to divide the 1 samples randomly into k-disjoint subsets, namely, k-cross $S_1, S_2 \cdots S_n$.The size of each fold was approximately equal, a total of k times training and testing process was conducted. For $i = 1, 2 \cdots k$ was iterated k times, for example, the approach of the first i iteration is to select S_i as the testing set, the rest of the training set, after the decision function was solved by the

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algorithm, the testing set can be tested, the MSE of the testing would be get. After k times iterations, value of the average was taken as the evaluation criteria of the algorithm. This method was called k -cross validation evaluation [6]. The MSE used the parameter of the cross validation evaluation:

$$MSE = \sum_{i=1}^{k} MSE_i = \frac{k}{n} \sum_{k=1}^{n} e_k^2 \tag{18}$$

Where $e_k = y_i - \hat{y}_i$, y_i was the true value of the sample, $\hat{y}_i$ was the predictive value of the sample.

In the process of conducting cross-training, the value of k was usually taken 5 [2], but in this paper, $k = 4$. Every time, one of the three sets of the nine monitoring points as the training sample, the rest of the three data as the testing sample. After the final trials, the value of $\gamma = 100$ and $\sigma^2 = 0.5$.

B. The Implication of the Water Quality Retrieval

The ground survey and remote sensing data was fused by this paper, LS-SVM model was built to complete the retrieval of the concentration of suspended matter. The ground survey data is the concentration of suspended matter value, which is also the output of the model, was measured in Tai Lake. After the atmospheric correction, the remote sensing data was used by this model.

By analyzing the reflection spectra of the Tai Lake water, the reflectance values in the vicinity of 580nm and 810nm of the concentration of suspended matter is more sensitive than others [8]. TM1-TM4 are just within the scope of this spectrum. The reflectivity of 12 monitoring points and the corresponding ground survey data of the concentration of suspended matter were listed in the Table I. The content of the Table I is the data for training. From the Table I, it can be seen that ρ_1 is the reflectivity of the TM1, so are the others.

The process of training, used the LS-SVM model, took advantage of the interface of trainlssvm() , which was encapsulated in the LS-SVM lab. The interface input the training data of the Table I and the two optimal parameters into LS-SVM to train, a new model will be produced to predict the results, as a result the interface of simlssvm() will be called. A new file will be produced, in which the values of the concentration of the suspended matter is. After the process of the retrieval, the MSE is 9.969027×10^{-6}, this means that the MSE is very small. According to the drawing function plotlssvm() , the fitting chat about Fig.3 can intuitively show the fitting effect. From the Fig.3 we can see that apart from the retrieval value of the eighth monitoring point is slightly lower than the measured value and the second point is higher than the measured value, the rest of the points are close to measured values.

According to the established water quality retrieval model and the experiments, the retrieval concentration of suspended matter map is shown in the Fig.4. From the Fig. 4 it can be seen that in the central and south-east of the Tai Lake the concentration of the suspended matter was high. In the southeastern area where was the active exchange of the lake water and the area where other rivers go into the lake, the suspended matter was also high. The Fig.4 also told that, the pollution of the lake bank district was high too. These places were regions that the eutrophication was serious, this was due to human activities such as the sewage discharge, and paddock breeding would accelerate the development of the eutrophication. In western and eastern areas of cardiac side, the concentration of the suspended matter is lower, eutrophication was not very serious, and other area was between in the two areas.

C. Comparison of Other Model Results

LS-SVM model was also compared with other three traditional models in this paper.

TABLE I.
THE DATE OF TRAINING

Monitoring Points	Measured concentration	ρ_1	ρ_2	ρ_3	ρ_4
1	46.0	0.029	0.039	0.052	0.037
2	107.0	0.040	0.052	0.065	0.053
3	14.0	0.038	0.047	0.041	0.037
4	18.0	0.038	0.047	0.047	0.048
5	41.0	0.036	0.049	0.054	0.053
6	35.0	0.038	0.049	0.058	0.045
7	15.0	0.039	0.051	0.050	0.043
8	15.0	0.039	0.051	0.065	0.056
9	22.0	0.020	0.021	0.027	0.045
10	16.0	0.019	0.021	0.032	0.054
11	41.0	0.037	0.049	0.055	0.069
12	25.0	0.015	0.015	0.017	0.048

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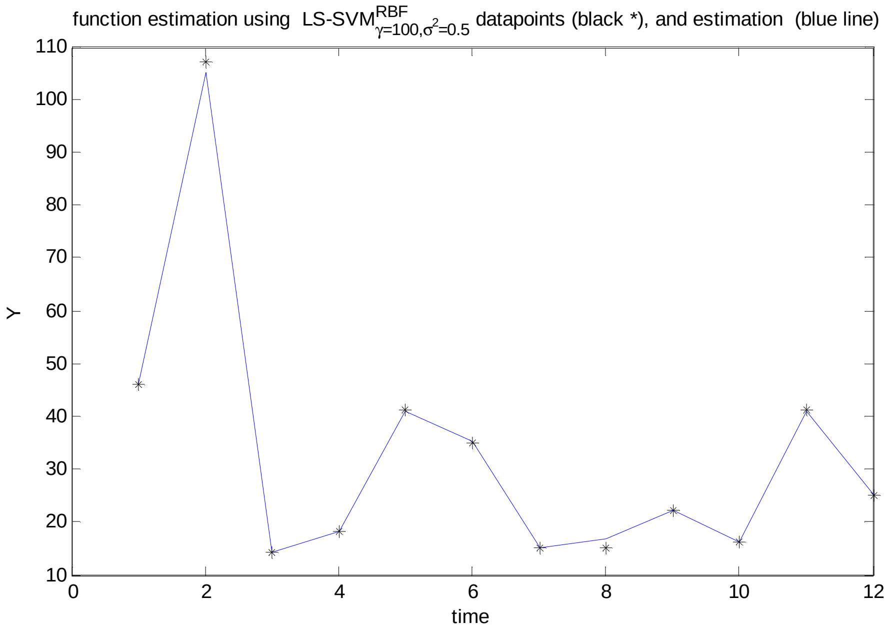

Figure 3. Fitting chart of the water quality retrieval

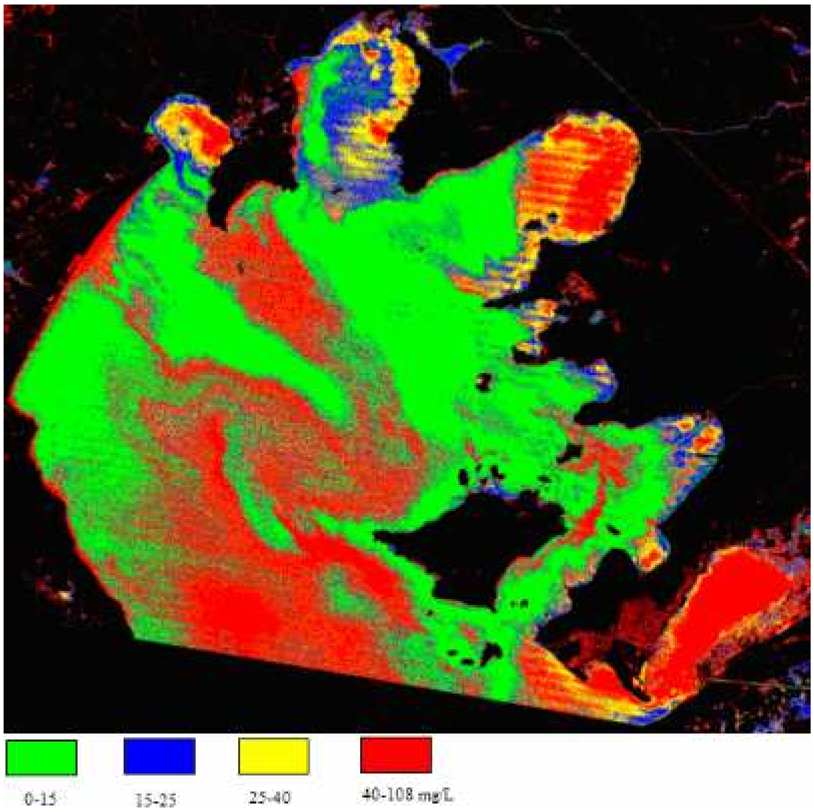

Figure 4. Retrieval of the suspended solids concentration map

1) Linear Model

According to the results of the reflection spectrum of Tai Lake, the reflectance values of TM2 and TM4 were as independent variables, and at the same time, the concentration of suspended matter was as the dependent variable. So after the regression analysis, the regression equation can be obtained:

$$SS = 689.18 \times \rho_2 \tag{19}$$

$$SS = 1485.84 \times \rho_4 + 22.95 \tag{20}$$

This study found that when the concentration is less than 60mg/L, equation (19) can give a high retrieval precision, when more than 60mg/L, the result of estimate

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is not satisfactory because of the lack of samples. However, the equation (20) can give high results, when the concentration is greater than 60mg/L.

2) BP Neural Network Model

BP neural network can not only satisfy the accuracy requirements, but also improve the learning efficiency [12]. Therefore, the three layer structure of the BP neural network was chosen by this paper, namely, input layer, hidden layer, output layer.

The design method of neural network model is as follows. The measured concentration of the suspended matter of nine monitoring points were selected arbitrary from the twelve points to compose the training samples, the remaining concentration values of the three monitoring points were as the validation sample. According to this division, there are 220 kinds of division method ($C_{12}^3 = 220$).

In this paper, the number of the input neurons is expressed by *m*, hidden neurons were p , output neurons were n , and so the neural network structure can be expressed as $m \to p \to n$. The trained data, which consists of five parts, are shown in Table I, so $m = 5, n = 1$ in this paper. In order to make neural network has good generalization performance, without making the structure overly complex, this paper used $3, 4$ and 5 respectively as the numbers of the hidden layer neurons, by comparing their own performance of neural networks, the optimal neural network structure was found. In the process of the experiment, which used the software of Matlab, the 220 different samples were input into the BP neural network, if the average training error and the average validation error were both the smallest, the correlation coefficient was the largest, then the network was the optimal neural network structure. After comparing the number of hidden layer neurons of different neural networks, this paper chose $p = 3$. Thus, the structure of the BP neural network had been established, the connection weights and thresholds of every layer had been also determined.

The initial value and the threshold value of the BP neural network were determined by the rand() function, which generates uniformly distributed random matrix in the Matlab toolbox, the control error was 0.001. Hidden layer neurons used tansing() hyperbolic activation function; the output layer neurons used linear activation function purelin() .

3) SVR Model

From the perspective of the loss function, currently, SVR focused on studying the linear ε -insensitive loss function [2]. Based on this, the loss function used in the SVR is also the linear ε -insensitive loss function in this paper.

In the algorithm of the ε -SVR, the σ^2 , which is the parameter of the kernel function, the penalty coefficient C and the width of the insensitive loss function ε are the three most critical parameters. It makes the performance of SVR model depends on the interaction of all parameters, the individual optimization of each parameter is very difficult to make optimal regression model [5].The greater C , the higher the level of data fitting, but the generalization ability will be reduced. For this reason, this paper selected $C = 500$, $\varepsilon = 0.25$ and $\sigma^2 = 128$, with these values, the precision of the retrieval was more accurate than other combination methods.

In the LIBSVM library, the SVR was built, Matlab software package has not LIBSVM toolbox, so in the process of the experiment, the LIBSVM library should be added into the Matlab toolbox. After that, the Matlab software can apply the function of the training and predicting. The classification and regression functions were encapsulated in the LIBSVM. The interface svm-train() of the LIBSVM was called to train the training data, and in the same way, the svm-predict() interface of the LIBSVM can be called to predict the trained data. The last, the concentration of the suspended matter retrieval values will be output into the file called $output\_file$.

The results of the retrieval of the concentration of the suspended matter were listed in the Table II, which was computed by four models. The sum of square error (SSE) reflects the retrieval precision between the output vector and the objective vector. In order to more accurately describe the retrieval precision of the monitoring points, the square related coefficient (SRC) was introduced. From the Table II, it can be seen that, based on the LS-SVM model, the SRC, which is between the measured values and the retrieval values, is the largest and the SSE is the smallest. So from the monitoring points itself, the concentration of retrieval based on LS- SVM model shows the highest accuracy, so the retrieval result is the best.

The Fig.5 shows the monitoring curves of the concentration of the suspended matter with four models. From the Fig.5, it can be seen that the result of the SVR is better than BP neural network method. BP neural network result is not satisfactory due to a small number of samples and the selection of the model is based on the experiential [12]. Although the retrieval result of the SVR can also achieve a good result and is not much different to the LS-SVM , but the LS-SVM, which has been used RBF function, only to determine γ and σ^2 parameters, so the search space of the parameters reduced to two-dimensional from three-dimensional of the standard SVM. The complexity of the algorithm was greatly reduced. At the same time, the speed of the system modeling was greatly accelerated.

V. CONCLUSION

Referred to analysis of relationship between the remote sensing data and the ground survey data of Tai lake, this paper established the water quality monitoring model based on LS-SVM theory and algorithm.

The concentration of the suspended matter in Tai lake

TABLE II.
THE COMPARED RETRIEVAL RESULTS BETWEEN THE THREE MODEL (MG/L)

Monitoring points	Measured concentration	Leaner Model	LS-SVM Model	SVM Model	BP Neural Network Model
1	46.0	26.88	45.9968	46.0	45.9
2	107.0	101.70	107.997	106.3	101.8
3	14.0	32.39	13.9974	14.8	15.1
4	18.0	32.39	18.0034	17.8	18.1
5	41.0	33.77	40.9966	41.3	44.8
6	35.0	33.77	35.0029	35.4	35.9
7	15.0	35.15	15.0029	14.8	14.9
8	15.0	35.15	14.8045	15.3	15.7
9	22.0	14.47	22.0033	24.9	22.0
10	16.0	14.47	16.0029	16.9	15.5
11	41.0	33.77	40.9969	44.9	41.2
12	25.0	10.34	24.9969	21.0	25.0
Sum of Square Error (SSE)		1991.925	43.56	44.78	62.43
Square Related Coefficient (SRC)		0.766	0.99985	0.998	0.996

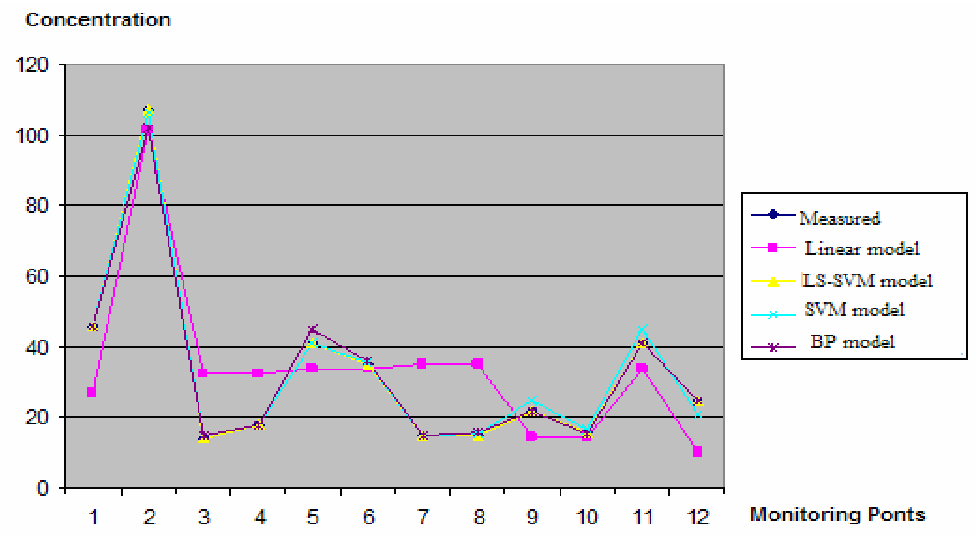

Figure 5. The monitoring curve of the suspended matter concentration

was monitored by the proposed method and other traditional methods. The results indicated that, the proposed modeling method was simple, the adjustments of the parameters were convenient and the speed of the learning was fast. The non-linear retrieve system, which was established by the LS-SVM method, can give a high precision, so it was able to satisfy the demand of the water quality monitoring.

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