EVALUATING THE ACCURACY OF THE REGULARIZED AND TENSION SPLINE INTERPOLATION METHODS TO ESTIMATE AND MAP THE CONCENTRATION OF NITRATE ON THE SURFACE WATER OF PULAU TUBA, LANGKAWI, KEDAH

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Abstract

This study aims to evaluate the efficiency of the regularized and tension spline interpolation methods to predict and map nitrate concentration on the surface water of Pulau Tuba, Langkawi. Kedah. Sampling activities were carried out using the Niskin Water Sampler and immediately brought into the lab to determine the nitrate level using an Ultraviolet Visible spectrophotometer and the cadmium reduction method. The geolocations of sampling points were recorded using the Geographic Positioning System (GPS). The training set (50%) and the testing set (50%) were chosen randomly based on 20 sampling points. Two types of spline interpolation methods were compared: the regularized and tension spline interpolation methods. Evaluation of prediction of models was carried out using the correlation analyses, linear regression analysis and error analyses when comparing the actual and prediction values. Determination of the map accuracy was carried out after inserting map elements. The study found that the tension spline method had a better prediction of nitrate concentration. The accuracy of the map was found to be at 90%. The study's outcome can be used as guidelines by concerned parties to monitor, manage, and develop strategic policies for the sustainable development of the coastal water of Pulau Tuba, Langkawi, Kedah.

Keywords: Interpolation, Nitrate, Regularized, Spline, Tension

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Introduction

Marine water pollution, especially in the mangrove ecosystem, poses threats, especially by human activity (Deng et al., 2021). Such pollution that affects the ecosystem, whether locally or globally, could be organic wastes, polymer wastes, or even nutrient pollution (Ferronato & Torretta, 2019). Nutrients in water such as phosphate, nitrate, ammonia, and chlorophyll are needed at normal levels to support life in water (Kamaruddin et al., 2022). Excessive levels of these water parameters may accelerate the rate of eutrophication (Yang et al., 2008). Eutrophication phenomena may disrupt the ecological role and marine biodiversity (Ehrnsten et al., 2020). One of the sources of eutrophication in the estuarine and coastal ecosystem is the increment of nitrate concentration.

Irrigation water containing nitrate into the water is the common culprit of nutrient pollution that leaches into the soil and the water supply from numerous sources ((McIsaac, 2020). A high concentration of nitrate may harm a person's health systems (Keller et al., 2017), especially in the respiratory and reproductive systems, kidney, spleen, and thyroid (Balazs et al., 2011). Nitrate in the river and coastal water can also evoke and accelerate the eutrophication process (Suteja & Purwiyanto, 2018). Due to this concern, strategic and cost-time effective measures should be taken. One of the strategies for the early detection of the extreme level of nitrate pollution is through spatial interpolation techniques.

Spatial interpolation methods used mathematical statistics to predict or estimate unknown data of an area using known data (Bezyk et al., 2021). Before using the technique, the known value must be collected and processed efficiently. Some interpolators, such as the Inverse Distance Weighting (IDW) interpolation method, is very popular and simple but does not provide standard prediction error (Njeban, 2018). Kamaruddin et al., (2021a) for instance, used the IDW interpolation method to map the water pH at the coastal water of Pulau Tuba, Langkawi. Kriging is the most popular geostatistical method that considers the autocorrelation characteristic of the data (Ogryzek et al., 2020). Another deterministic interpolator used for environmental studies is spline interpolation methods (Kamaruddin et al., 2020a). Previous studies have highlighted that many academicians and researchers have used the spline interpolation method to map the surface water temperature at Pulau Tuba, Langkawi. Kamaruddin et al., (2018) used the spline interpolation method to map the surface water temperature at Pulau Tuba, Langkawi. Kamaruddin et al., (2018) used the spline interpolation method to map the surface water temperature at Pulau Tuba, Langkawi. Kamaruddin et al., (2018) used the spline interpolation method to map the surface salinity over the coastal water of Sungai Merbok, Kedah. In addition, Kamaruddin et al., (2019) used the spline interpolation technique to map the surface water salinity over the coastal water of Pulau Tuba, Langkawi.

This study highlights two problems. The first problem is the lack of knowledge on the accuracy of the spline interpolation method to estimate the distribution of nitrate on the surface water of Pulau Tuba, Langkawi, Kedah. The second problem is the unknown spatial distribution of nitrate on the surface water of Pulau Tuba, Langkawi, Kedah. Both problems are significantly essential to be addressed as high accuracy of estimation is required to reduce the error of prediction. A high level of nitrate in water may increase the potential of eutrophication processes in the euphotic zones ranging between <50m to about 200m, contributing to a significant loss in social-economic sectors and marine life biodiversity.

This study aims to evaluate the accuracy of the spline interpolation method to estimate and map the concentration of nitrate to explain the spatial pattern of this water parameter on the surface water of Pulau Tuba, Langkawi, Kedah. To achieve the aim of the study, several specific objectives are developed, which are (1) to determine the correlation between the actual and predicted concentration of nitrate using regularized and tension spline methods; (2) to examine the differences in the actual value of nitrate can be explained by the differences in the estimated value predicted by both methods; (3) to investigate the error between the actual and predicted value of nitrate predicted by both methods (4) to choose the best model based on the comparison of the error of prediction between the regularized and tension spline interpolation method and (5) to determine the accuracy of the map developed using spline interpolation method.

The significant contributions of this study are (1) providing the fundamental knowledge on the accuracy of spline interpolation method to predict the concentration of nitrate in the study area; (2) developing spatial models that can be used by concerned parties to monitor the area for potential eutrophication phenomena and marine pollution events; (3) as guidelines for concerned parties to construct acts and policies for sustainable development for this area and (4) fulfilling nation mission on the achieving the sustainable development Goal 14 - Life Below Water based on the 17 sustainable development goals established by the United Nations in 2015.

Methods

The study area is the coastal water of Pulau Tuba, Langkawi, Kedah located next to Pulau Dayang Bunting, Langkawi. Both islands are in the southeast of the main island of Pulau Langkawi, Kedah. The human activities expected in this area are agricultural, tourism, transportation, and residential areas near the coastal areas. Natural environments such as the mangrove ecosystem flourished in both islands' strait and interior regions (Kamaruddin et al., 2020b). Abundances of marine fauna such as monitor lizards, eagles and crustaceans inhabit the mangrove areas and can be easily noticed during the daytime.

Sampling activities were done during high tide at noon using a small boat. The Niskin water sampler was lowered at 1 meter below the surface to collect the samples. Samples were collected, strained, and kept in the dark bottles. These bottles were then placed carefully in the cool box and stored at 6-degree

Celsius by covering them with crushed ice purchased from the local shop. The geolocations of each sampling point were recorded using the Global Positioning System (GPS). For laboratory analyses, the samples were immediately transferred to the marine technology laboratories at the Universiti Teknologi MARA Cawangan Perlis, Kampus Arau. The Ultraviolet-Visible spectrophotometer was used to determine the nitrate concentration in the samples. Data are triplicated to avoid bias of readings. Data was carefully examined and recorded using excel spreadsheets. The method for determining nitrate was based on the Cadmium Reduction Method at 543-nanometer wavelength using the Standard Section 4500 -Nitrate (APHA., 1999).

Development and validation of spatial models were carried out using ArcGIS software. In this study, two types of splined interpolations methods were applied. The regularized spline method produced estimated smoothness data, while the tension spline method produced a coarser data distribution. The general and specific mathematical functions of spline are shown below (Kamaruddin et al., 2021b):

A. Splines Equation

$$S(x,y) = T(x,y) + \sum_{j=1}^{N} \lambda j R(r_j)$$
(1)

Where:

 $J = 1,2, \dots, N$ N = Number of points $\lambda j = \text{Coefficients found by the solution of a system of linear equations.}$ $r_j = \text{Distance from the point } (x, y) \text{ to the } j^{\text{th}} \text{ point.}$

B. Tension Spline Method

$$T(x, y) = a_1$$
(2)

Where:

 a_1 = coefficients found by the solution of a system of linear equations.

And

$$R(r) = \frac{1}{2\pi\varphi^2} \left[\ln\left(\frac{r\varphi}{2}\right) + c + K_{\circ}(r\varphi) \right]$$
(3)

Where:

 φ^2 = Weight parameter K_{\circ} = Modified Bessel function C = constant equal to 0.0577215

C. Regularized Spline Method

$$T(x, y) = a_1 + a_2 x + a_3 y$$
(4)

Where:

 a_1 = coefficients found by the solution of a system of linear equations.

And,

$$R(r) = \frac{1}{2\pi} \left\{ \frac{r^2}{4} \left[\ln\left(\frac{r}{2\pi}\right) + c - 1 \right] + \tau^2 \left[K_{\circ}\left(\frac{r}{\tau}\right) + c + \ln\left(\frac{r}{2\pi}\right) \right] \right\}$$
(5)

Where:

r = Distance between the point and the sample τ^2 = Weight parameter K_{\circ} = Modified Bessel function

The data were divided randomly into two sets: training and testing sets. Both groups had the same number of sampling points. Spatial analyst tools were used for the development of the model. The weightage was set at 0.1 while the number of points was fixed at 10. Interpolation and extraction tools were used to map and collect the predicted values. The estimated data was validated using a series of statistical analyses. Correlation, Regression and Error analyses were used to compare the actual and predicted values. For the error analysis, the Mean Absolute Error (MAE), Mean Absolute Percentage Error (MAPE), Mean Squared Error (MSE) and Root Mean Squared Error (RMSE) were reported to assist the validation processed. When comparing the best method (between the regularized and tension spline interpolation method), the study evaluates the RMSE data to choose the best spline interpolation and the study area.

Statistical analyses were carried out using Statistical Package for the Social Sciences (SPSS) software version 21.0. The Pearson product-moment correlation analysis, the linear regression analysis and paired sample T-Test were set at the alpha before 0.05 (95%, Confidence level). The error analyses (MAE, MAPE, MSE, and RMSE) were carried out using Excel Spreadsheets.

Transformation of the map was carried out later by inserting several map elements for better presentation, communication, and visualization to the reader. An accuracy assessment was carried out later to determine the accuracy of the map to predict the concentration of nitrate in surface water. The formulae below show the calculation for overall map accuracy (%).

$$Overall Accuracy (OA) = \frac{Number of Correct Occurrences}{Total Occurrences} \times 100\%$$
(6)

Result and Discussion

20 sampling points were randomly distributed along the Strait of Pulau Tuba-Pulau Dayang Bunting to collect samples. 50% of the samples were randomly chosen to develop the spatial model (training set), and the leftover (testing set) was used for validation purposes. Figure 1 shows the location of each sampling point.



Figure 1. The map shows the location of the study area and sampling points established over the coastal water of Pulau Tuba, Langkawi, Kedah

Next, the training set was uploaded into the ArcMap software to develop the model. Table 1 shows the estimated data predicted by both methods. Overall, the regularized spline interpolation method predicted more overestimation value, while the tension spline interpolation produced more underestimation value of the concentration of nitrate. For estimation made by the regularized spline interpolation method, overestimation of the nitrate concentration can be observed at the sampling points 4,10, 14 and 18, while underestimation can be detected at the sampling point of 2, 6, 8, 12, 16, and 20. On the other hand, for prediction made by the tension spline interpolation method, underestimation value can be observed at the sampling point of 2,4, 6, 8, 12, 16, and 20, whereas overestimation of the concentration of nitrate can be detected at the sampling point of 10, 14 and 18. Figure 2 shows the raw raster image produced by both methods.

Sampling point	Actual value (mg/L)	Regularized method (mg/L)	Tension method (mg/L)
2	0.572400	0.503669	0.530085
4	0.646400	0.684337	0.641564
6	0.568500	0.529984	0.547033
8	0.611400	0.599246	0.594064
10	0.564600	0.776905	0.708308
12	0.572400	0.474706	0.513391
14	0.447600	0.614427	0.583742
16	0.806300	0.729576	0.727382
18	0.455400	0.493372	0.502239

Table 1. Prediction of the concentration of nitrate estimated using the regularized and tension spline interpolation method



Figure 2. Raster images produced by the Regularized spline interpolation method (Left) and Tension spline interpolation method (Right)

Next, the frequency analyses are carried out to describe the data characteristics in the form of mean, median, variance etc. Table 2 shows the frequency analysis carried out for both sets. The study found that the regularised interpolation method's mean prediction is higher than the mean actual value of nitrate concentration. In contrast, the mean prediction estimated by the tension interpolation method is lower than the mean actual value of nitrate concentration.

Statistics	Actual	Predicted	Predicted
	Observation	Regularized	Tension
Mean	0.575500	0.583609	0.575429
Std. Error of Mean	0.032463	0.036956	0.030939
Median	0.570450	0.564615	0.565388
Std. Deviation	0.102656	0.116864	0.097836
Variance	0.011000	0.014000	0.010000
Skewness	1.103000	0.441000	0.086000
Std. Error of Skewness	0.687000	0.687000	0.687000
Kurtosis	2.261000	-1.100000	-0.225000
Std. Error of Kurtosis	1.334000	1.334000	1.334000
Range	0.358700	0.347034	0.320899
Minimum	0.447600	0.429871	0.406483
Maximum	0.806300	0.776905	0.727382
Sum	5.755000	5.836093	5.754291

 Table 2. Frequency table describing the data distribution for the actual observation and predicted data estimated using regularized and tension spline methods (six decimal places).

A paired-samples t-test was conducted to compare nitrate concentration in actual values and predicted values estimated using regularized interpolation method condition. There was no statistically significant difference in the scores actual value (M = 0.57550000, SD = 0.102655822) and predicted value estimated using regularized spline method (M = 0.58360930, SD = 0.116863691) condition; t (9) = -0.239, p = 0.816. Similarly, A paired-samples t-test was conducted to compare the nitrate concentration in actual value and predicted value estimated using tension interpolation method condition. There was

no statistically significant difference in the scores actual value (M = 0.57550000, SD = 0.102655822) and predicted value estimated using regularized spline method (M = 0.57542910, SD = 0.097836259) condition; t (9) = -0.003, p = 0.998. These results suggest that the nitrate concentrations in the actual values are related to the predicted values. Specifically, the results suggest that when there is an increased value in the actual observation, the predicted value estimated by both methods will increase. Table 3 shows the results for paired samples tests for Pair 1 (actual vs predicted value produced by regularized spline interpolation method) and Pair 2 (actual vs predicted value produced by tension spline interpolation method).

Table 3. Paired samples tests indicated no statistically significant difference between the actual and predicted values for both methods.

				Paired I	Differences				
						95% Coi Interva Diffei	nfidence l of the rence		
		Mean	Std. Deviati on	Std. Error Mean	Lower	Upper	t	df	Sig. (2- tailed)
Pair	Actual –	-	.107152	.033884	-	.068542	239	9	.816
1	Predicted	.0081	4	5	.084761	9			
	Regularized	093			5				
Pair	Actual –	.0000	.084578	.026746	-	.060574	.003	9	.998
2	Predicted	709	5	1	.060432	7			
	Tension				9				

A Pearson product-moment correlation coefficient was computed to assess the relationship between the actual value and predicted value estimated using both methods. Table 4 shows the correlation between the actual and predicted values. Overall, estimation of nitrate concentration by using both methods produced a strong and positive correlation. Correlation between the actual and expected value of nitrate estimated using the regularized spline interpolation method indicates a statistically insignificant difference between the two variables, r = 0.530, n = 10, p = 0.058. On the other hand, the Correlation between the actual and predicted value of nitrate estimated using the tension spline interpolation method indicates a statistically significant difference between the two variables, r = 0.645, n = 10, p = 0.022. Specifically, the results showed that an increased value of the actual concentration of nitrate correlated with the increased value of the predicted concentration of nitrate for both methods.

Table 4. Only the correlation between the actual and predicted values of nitrate estimated using the tension spline method produced statistically significant results (p<.05).

	Nitrate	Regularized method	Tension method
Pearson Correlation	1	.530	.645
Sig. (1-tailed)		.058	.022
Sum of Squares and	.095	.057	.058
Cross-products			
Covariance	.011	.006	.006
Ν	10	10	10

A simple linear regression analysis was used to predict the relationship between the observed and predicted values of nitrate concentrations based on the regularized and tension spline methods at a 95% confidence level. The prediction value of nitrate estimated by the regularized spline method did not explain significant variance in the observed value of nitrate, F (1,8) = 3.123, p =0.115, R² = 0.281, R² adjusted = 0.191. On the other hand, the prediction value of nitrate estimated by the tension spline method did explain significant variance in the observed value of nitrate, F (1,8) = 5.700, p = 0.044, R² = 0.416, R² adjusted = 0.343. Table 5 shows the result of the F test for both methods.

ANO Mode	VA el	Sum of Squares	df	Mean Square	F	Sig.
1	Regression	.027	1	.027	3.123	.115
	Residual	.068	8	.009		
	Total	.095	9			
2	Regression	.039	1	.039	5.700	.044
	Residual	.055	8	.007		
	Total	.095	9			

Table 5. ANOVA table showing the results of the F test for a prediction r	made by the regularized spline
interpolation method (model 1) and tension spline interpolation	method (method 2)

For the regularized spline method, the regression coefficient (B = 0.465) indicated an increase in the predicted value of nitrate corresponded to an increase in the observed value of 0.465. The simple linear regression equation was reported as observed value = 0.304 + 0.465 (predicted value). On the other hand, for the tension spline method, the regression coefficient (B = 0.677) indicated that an increase in the predicted value of nitrate corresponded to an increase in the observed value of 0.677. The simple linear regression equation was reported as observed value = 0.186 + 0.677 (predicted value). Table 6 shows the result of the coefficient and t-statistics for both methods.

Table 6. The coefficients and t-statistics after the regression analysis was carried out between the actual and predicted value of nitrate for regularized (Model 1) and tension (Model 2) methods.

Model	Unstandar	dized Coefficients	Standardized Coefficients		
	В	Std. Error	Beta	t	Sig.
1 (Constant)	0.304	0.156		1.942	0.088
Predicted Regularized Nitrate	0.465	0.263	0.530	1.767	0.115
2 (Constant)	0.186	0.165		1.126	0.293
Predicted Tension Nitrate	0.677	0.283	0.645	2.387	0.044
a. Dependent Variable: Observed 1	Nitrate				

In the error analysis, the prediction made by the tension spline interpolation method produced less error of prediction compared to the estimation made by the regularized spline. Table 7 shows the tabulated data calculated for the MAE, MAPE, MSE and RMSE. Absolute error is used to avoid mutual cancellation of the positive and negative errors (Chen et al., 2017). Data inserted in the absolute error has only non-negative values. This mathematical function facilitates the aggregation of point distances over the data set. However, the absolute error does not determine the skewness of the data. Chai & Draxler (2014) stated that applying absolute value would give difficulties in gradient calculations. On the other hand, a square error has the same concept as absolute error; however, if the model consists of large or minor errors, the impact will be extreme due to squared errors.

Table 7. Error analyses were carried out to identify the prediction error made by both methods.

Statistics	Regularized spline interpolation	Tension spline interpolation
	method	method
MAE	0.0828989 (0.08)	0.0654087 (0.07)
MAPE (%)	15.21463059 (15.21)	12.13007152 (12.13)
MSE	0.01039922485 (0.01)	0.00643817225 (0.00)
RMSE	0.10197658971 (0.10)	0.08023822191 (0.08)
() rounded to 2 decimal places		

Later, the decision to choose the best interpolation method was carried out. The study found that the tension spline interpolation method produced less prediction error. The root means square of prediction shows the value of 0.08. Next, the transformation of spatial prediction using the tension spline interpolation method to a map by inserting map elements such as title, legend, north arrow, nest line, scale, and supplementary information. The legend was set at (< 0.4 mg/L, 0.4-0.6 mg/L and > 0.6 mg/L) in mg/L unit. Figure 3 shows the map of nitrate produced.



Figure 3. The developed map of the concentration of nitrate on the surface water of Pulau Tuba, Langkawi, Kedah.

The map produced shows that the middle part of the strait of Pulau Tuba, Langkawi, Kedah had an increased nitrate concentration in the range of more than 0.60 mg/L. This region is full of human activities where boating, agriculture activities (aquaculture) and residential areas can be found. Human activities have a great potential for incrementing the concentration of nitrate. On the other hand, the inner part of the strait shows the reduction of nitrate concentration as mangrove trees flourished along the coastal area. Some studies have suggested that mangrove soils had limited nitrate concentration (Nedwell, 1975; Fernandes & Loka Bharathi, 2010; Molnar et al., 2013). The denitrification rate is relatively low in mangrove soils (Bauza et al., 2002). The lower part of the island has the lowest concentration of nitrate concentration on the surface water. The findings suggest that anthropogenic activities potentially cause a high concentration of nitrate. Thus, the study had opened the opportunities to investigate and determine nitrate's point and non-point pollution for future research.

As part of nitrogen, nitrates can be found in many terrestrial or aquatic ecosystems (Vitousek et al., 1997). Nitrates are essential for the growth of many vegetation species (Yao et al., 2011); however, a high concentration of nitrate may increase the rate of water pollution (Yu et al., 2020). Combining effects with potassium, chlorophyll, ammonia, nitrites and organic pollutant, severe eutrophication cases can be experienced (Liu et al., 2010). Furthermore, changes in nitrate level can also disrupt

ecology (Zhao et al., 2021), primary production (Henley et al., 2020) and biodiversity (Cano-Rocabayera et al., 2019), especially in an area where there is aquatic life sensitive to drastic changes of nitrate level (Bashir et al., 2020). Furthermore, excessive nitrate levels may directly or indirectly affect the oxygen level in the water (Alam et al., 2020), as eutrophication causes a dramatic increase of plants or microscopic animals such as phytoplankton to take up oxygen levels (Wagner & Erickson, 2017). Loss of dissolved oxygen in water can contribute to hypoxia conditions (Elshout et al., 2013), which could directly affect the social-economic and ecology, especially in the estuarine ecosystem (Kamaruddin et al., 2021a).

Finally, the accuracy of the map was investigated. Table 8 shows the accuracy assessment carried out for the map. The symbol (/) represents correct occurrences, while symbol (x) represents the incorrect occurrences. The study found that the accuracy of the map was calculated at 90%. The reasons for the incorrect occurrences are due to overestimation and underestimation of the concentration of nitrate predicted by the tension spline interpolation method. The study shows that the overestimation of nitrate level was found in sampling points 10.

Sampling points	Actual value (mg/L)	Prediction using tension spline method (mg/L)	Correct occurrences		
2	0.4-0.6	0.4-0.6	/		
4	>0.6	>0.6	/		
6	0.4-0.6	0.4-0.6	/		
8	>0.6	>0.6	/		
10	0.4-0.6	>0.6	Х		
12	0.4-0.6	0.4-0.6	/		
14	0.4-0.6	0.4-0.6	/		
16	>0.6	>0.6	/		
18	0.4-0.6	0.4-0.6	/		
20	0.4-0.6	0.4-0.6	/		
Overall accuracy = (9/10) *100% = 90%					

Table 8. Accuracy assessment	of the developed map wa	as calculated at 90%
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Conclusion

Overall, the concentration of nitrate in the surface water of Pulau Tuba, Langkawi is normal and under 1 mg/L. Revisiting the aim of this study, the prediction made by the tension spline interpolation method produced a better estimation of the concentration of nitrate than the regularized spline interpolation method. There is a positive and stronger correlation between the actual and predicted value when incorporating the tension spline interpolation method. In the regression analyses, the prediction value of nitrate estimated by the tension spline method did explain significant variance in the observed nitrate value. All the error analyses calculated low prediction errors using the tension spline interpolation method to evaluate forecast accuracy. Transformation of the spatial model to map was done successfully, and the map's accuracy was high.

This study has outlined several contributions. One of the contributions is determining and evaluating the accuracy of the spline interpolation methods for water quality study. Secondly, the study has produced a map that monitors and predicts potential hot spots for eutrophication events and nitrate pollution. Thirdly, concerned parties can use the map to sustainably develop this area without harming the ecological importance, such as the mangrove ecosystem. Fourthly, the study also evokes the awareness and knowledge of the importance of the marine ecosystem to the social-economic development and significant ecological role. Stakeholders, for instance, may outline influential acts and policies to realise the sustainable development Goal 14 - Life Below Water based on the 17 sustainable

development goals established by the United Nations in 2015. Lastly, the study also investigates and examines the current concentration of nitrate in the surface water of Pulau Tuba, Langkawi, Kedah. The study wishes to acknowledge several recommendations for the subsequent research relating to the topic discussed here. There should be a comparison of the nitrate level during variations of seasons and months to observe the spatial-temporal pattern of nitrate. The addition of more sampling points should be encouraged; however, a pilot study can be made to study the optimum number of sampling points required to produce an effective and efficient prediction of the concentration of nitrate.

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