PREDICTION RESULTS OF DIFFERENT MODELLING METHODS IN SOIL NUTRIENT CONCENTRATIONS BASED ON SPECTRAL TECHNOLOGY **

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Spectroscopy has been applied in monitoring soil nutrient concentrations. Two types of soil samples, sandy loam and silty loam, were selected as the research objects. The UV-visible-near infrared reflectance spectroscopy data and total carbon (TC), total nitrogen (TN), total phosphorus (TP), total potassium (TK), available nitrogen (AN), available phosphorus (AP), available potassium (FK), and slowly available potassium (SK) concentrations were measured. We compared the prediction results within and between two different types of soil with regard to the soil nutrient concentrations using four modelling methods, which were principal component regression (PCR), partial least squares regression (PLSR), least squares support vector machine (LS-SVM), and back propagation neural network (BPNN) models. In the prediction results within a given type of soil, LS-SVM and PLSR had better stability. In the prediction results of different types of soil, BPNN and LS-SVM had a high accuracy in most soil nutrient concentrations. By comparing different modelling methods, this study provides a basis for the subsequent selection of suitable models based on spectral technology to establish various soil nutrient models.

Keywords: *UV-visible-near infrared reflectance spectroscopy, soil nutrient, least squares support vector machines, back propagation neural network, modelling methods.*

ПРОГНОЗИРОВАНИЕ СОДЕРЖАНИЯ ПИТАТЕЛЬНЫХ ВЕЩЕСТВ В ПОЧВЕ МЕТОДАМИ МОДЕЛИРОВАНИЯ НА ОСНОВЕ СПЕКТРАЛЬНОЙ ТЕХНОЛОГИИ

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Спектроскопия применена для мониторинга концентрации питательных веществ в почве. В качестве объектов исследования выбраны два типа образцов почвы: супеси и илистый суглинок. Данные спектроскопии отражения в УФ-видимой и ближней ИК областях сопоставлены с результатами измерений концентраций общего углерода, общего азота, общего фосфора, общего калия, доступного азота, доступного фосфора, доступного калия и медленно доступного калия. Проведено сравнение результатов прогнозирования концентраций питательных веществ в почве внутри и между двумя типами почвы с использованием четырех методов моделирования: регрессии основного

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компонента (PCR), регрессии частичных наименьших квадратов (PLSR), метод опорных векторов с использованием наименьших квадратов (LS-SVM), а также модели нейронной сети обратного распространения (BPNN). Методы LS-SVM и PLSR имели лучшую стабильность результатов прогнозирования для данных типов почвы, методы BPNN и LS-SVM — высокую точность определения концентраций большинства питательных веществ в почве. Сравнение методов моделирования обеспечивает основу для последующего выбора подходящих методов моделирования на основе спектральной технологии и создания различных моделей оценки питательных веществ в почве.

Ключевые слова: *УФ-видимая и ближняя инфракрасная отражательная спектроскопия, питательные вещества почвы, метод опорных векторов с использованием наименьших квадратов, нейронная сеть обратного распространения, методы моделирования.*

Introduction. Soil is one of the important components in the Earth's natural environment, and it is the basis of human existence [1]. Carbon, nitrogen, phosphorus, potassium and other nutrients in soil are important factors that affect plant growth [2]. It is of great significance to obtain the soil nutrient concentrations, such as carbon, nitrogen, phosphorus, and potassium, in order to master the information and spatial distribution of nutrients [3]. Further, it is beneficial to the ecological construction of the region. Therefore, it is helpful to improve crop yield, ensure food safety, and avoid environmental pollution by obtaining, in real-time, the dynamic change of soil nutrient concentrations [4].

Measuring soil carbon, nitrogen, phosphorus, potassium, and other nutrients by traditional chemical analysis methods is time consuming, has a high cost, and requires professional analysis and testing. This method is only suitable for laboratory small-scale measurements and cannot truly achieve large-scale, rapid, real-time measurement of soil nutrients. Spectral technology is a rapid, real-time, non-destructive analysis method, widely used to analyze soil, food, tobacco, petroleum, and other substances in other fields [5–9]. Based on the advantages of spectral technology, researchers have carried studies on the rapid measurement of soil nutrient concentrations and have demonstrated positive results [10–12].

Using spectral technology to obtain soil nutrient concentrations, we build a model of the spectra and concentration values of known soil nutrients, mainly through chemometrics. Common modelling methods are principal component regression (PCR), partial least squares regression (PLSR), least squares support vector machine (LS-SVM), back propagation neural network (BPNN), etc. [13–16]. Through various modelling algorithms, useful information is extracted from the spectrum in order to predict the nutrient concentrations of unknown soil.

Based on current spectral techniques, partial least squares regression is often used to model and predict the concentrations of a soil nutrient within a given soil type [17, 18], but it was not clear how the modelling method affected the prediction results. The modelling prediction analyses of different types of soil nutrient concentrations through different modelling method were rarely reported. In this paper, we adopt four modelling methods (PCR, PLSR, LS-SVM, BPNN), which are popular at present, to model and predict the nutrient concentrations within and between two different types of soil and small modelling of soil samples. The nutrient concentrations included the total nitrogen (TC), total phosphorus (TP), total potassium (TK), available nitrogen (AN), available phosphorus (AP), available potassium (FK), and slowly available potassium (SK). Then the prediction results of different modelling methods on soil nutrient concentrations were compared.

Materials and methods. Soil from the Qingdao Fushan Mountain foothills, Qingdao Zaoshan Mountain farmland, and Qingdao Licun River were collected, and each sample plot had 60 soil samples. The soil of Qingdao Fushan Mountain foothills and Qingdao Zaoshan Mountain farmland were sandy loam, and the soil of Qingdao Licun River were silty loam. The soil samples were dried and sifted (0.45 mm), and two soil samples were removed because of man-made anomalies. In total, there were 60 soil samples from the Qingdao Fushan Mountain foothills and 58 soil samples from the Qingdao Zaoshan Mountain farmland, resulting in 118 sandy loam soil samples. The final number of Qingdao Licun River soil samples, which were also the silt loam soil samples, was 60, bringing the total number of different soil samples to 178.

Visible near-infrared spectroscopy acquisition. An Ocean Optical QE65000 spectrometer was used to acquire spectral data, the spectral sampling interval was 1 nm, the integration time was 600 ms, and the spectral region ranged from 200–1100 nm, which was used in UV-visible-near infrared spectroscopy. To eliminate the influence of noise, the reflectance spectra of the anterior and posterior segments of the soil samples were removed, and their 226–975 nm reflectance spectra data were preserved.

Nutrient concentration acquisition. Five to ten grams of soil was taken from the soil samples, and the soil nutrient concentrations were determined by chemical analysis. The TC of the soil was determined by the

carbon-nitrogen analyzer; TN of the soil was determined by the elemental analyzer; AN of the soil was determined by the sodium hydroxide indirect diffusion method; TP of the soil was determined by alkali dissolving-molybdenum antimony resistance spectrophotometry; AP of the soil was measured by the sodium carbonate leaching-molybdenum antimony resistance colorimetric method; TK of the soil was determined by atomic absorption spectrophotometry; FK of the soil was determined by neutral ammonium acetate-atomic absorption spectrophotometry; and SK of the soil was determined by atomic absorption spectrophotometry. The soil nutrient concentrations in the three regions are shown in Fig. 1.

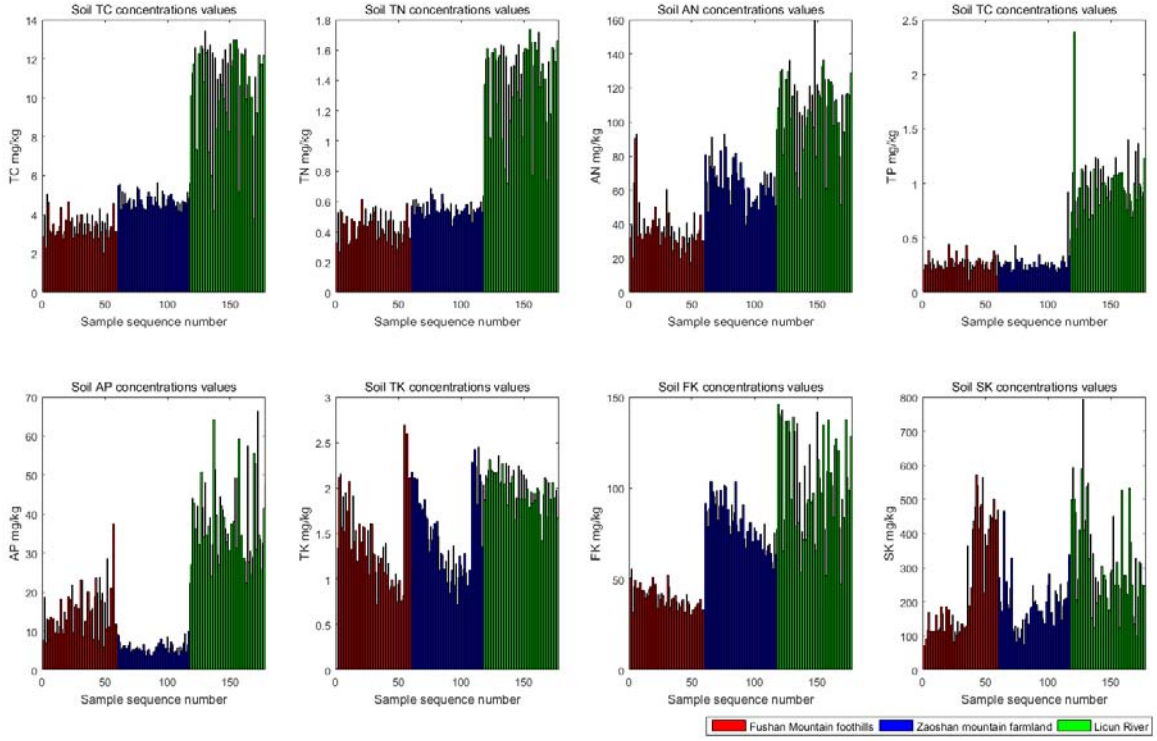

Fig. 1. Soil nutrient concentrations in three regions.

Modelling method. *Principal component regression* (PCR) is based on the orthogonal relations of principal components, and the regression model is established using the principal component to create a prediction for unknown samples [15, 19]. The modelling method can preserve the useful information in the spectrum and avoid the fitting phenomenon.

Partial least square regression. When using multiple independent variables for regression modelling, the partial least-squares regression (PLSR) method recombines information in an independent variable system. PLSR can effectively extract the comprehensive variables, which are the strongest explanatory variables for the system's dependent variable and have the greatest generalization of the information in the independent variable system. PLSR is able to determine the latent variables by a dimension reduction operation and can achieve the purpose of eliminating useless information. Based on the known spectral data and the chemical value data, the correlation model is established by partial least squares regression to achieve the prediction of unknown samples [14, 20]. This method is one of the most commonly used chemometrics modelling methods at present.

PCR and PLSR both first extract the components from the set of independent variables and then conduct multiple regressions on the extracted components. However, there are essential differences between the idea and method of extracting the components. The idea behind PCR extraction is that a few principal components are derived from the independent variables so that they retain the original variable information as completely as possible and are not related to each other. In the whole process of extracting the components, there is no connection with the dependent variables, which are completely independent of the dependent variables, and the process of extracting the components is relatively simple. The idea behind PLSR is that it finds a low-dimensional space of so-called latent variables, which are projections of independent and dependent variables into matrices that have maximum covariance. The process is much more complicated than PCR.

Least squares support vector machines. Differing from the principal component regression and partial least squares regression methods, the least squares support vector machine (LS-SVM) is a nonlinear modelling method. The training process for least squares support vector machines is to follow the principle of structural risk minimization, set the optimal combination of the parameters σ^2 and γ, train known spectral data and chemical values, and establish the relevant models [13, 21]. Here σ^2 and γ are the penalty parameter and kernel function parameter, respectively, of the support vector machine. This modelling method is more suitable for small sample learning. In this paper, $\sigma^2 = 0.01$ and $\gamma = 100$.

Back propagation neural network (BPNN) is also one of the nonlinear modelling methods, which is a multilayer feed forward neural network based on the error back propagation algorithm. The operation process for a back propagation neural network is mainly divided into two parts: the first is the forward calculation process, where the information is selected from the samples, and the information is taken from the input layer through the hidden layer to calculate the output value of each unit; the second is the error reversal process, in which the error is calculated from the output layer, and the error of each element of the hidden layer is calculated layer by layer and used to modify the previous layer's weight value [16, 22]. In this paper, the number of iterations is 100.

According to the Kennard–Stone algorithm, the calibration set and the test set for soil samples within and between two different types of soil were divided into proportions of 2:1, respectively. The soil nutrient concentrations models of TC, TN, AN, TP, AP, TK, FK, and SK are established by the PLS, PCR, LS-SVM, and BPNN modelling methods, and the results of the soil nutrient concentration tests are predicted.

Evaluation standard. In this paper, the model evaluation standards were the determination coefficient of calibration set (R_c^2), the determination coefficient of test set (R_p^2), the predicted root mean square error (RMSEP), and the residual predictive deviation (RPD) [23, 24]. RPD is defined as the standard deviation of the observed values divided by the RMSEP. The RDP takes both the prediction error and the variation of the observed values into account, providing a metric of model validity that is more objective than the RMSEP and more easily comparable across model validation studies. The closer the determination coefficient was to 1, the better the prediction ability of the model was. The smaller the predicted root mean square error was, the more stable the model was, and the better the predicted effects were. The greater the RPD, the better the model's predictive capacity was. When the residual predictive deviation is greater than 2, the model can be regarded as a good model and can be used for quantitative prediction.

Results and discussion. To ensure the consistency of the prediction in soil nutrient concentrations of the four modelling methods for both within and between two different types of soil, the original spectra without pre-treatment were used to predict each soil's nutrient concentration.

Comparison of four modelling methods for predicting the nutrients concentrations within a soil type. Prediction results of nutrients concentrations in sandy loam. In the PCR and PLSR modelling methods, the number of main components for PCR and the number of latent structures for PLSR were the same, and were 6, 6, 5, 2, 3, 4, 6, and 6 for TC, TP, TK, AN, AP, FK, and SK, respectively. The prediction results of the four modelling methods for the nutrient concentration of sandy loam were estimated by R_c^2, R_p^2, RMSEP, and RPD.

The general prediction for the concentration of nutrients in sandy loam was consistent in all four modelling methods. The model for the FK concentrations gave a better result, as R_c^2 and R_p^2 were both above 0.7 and 0.8 respectively, and the RPD values were above 2. The prediction results for the TC and TN concentrations were general, the RPD values were between 1.5 and 2, and the prediction presented the possibility of quantitative analysis. The prediction results for the AN, AP, and SK concentrations were poor, as the RPD values were below 1.5. The prediction results for the TP and TK concentrations were very poor, and the RPD values were below 1.

In the prediction results for the FK concentrations, R_c^2 and R_p^2 of the two nonlinear modelling methods, LS-SVM and BPNN, were both higher than 0.9. The prediction results of the nonlinear modelling methods were higher than those of the linear modelling methods, PLSR and PCR, and the prediction results of PCR were the worst. In the prediction results for the SK concentrations, the results were similar to those for FK, and the prediction results of the PLSR, LS-SVM and BPNN models were obviously better than PCR. In the prediction results for TC, AN, AP, and TK, BPNN had the worst prediction results. Compared with other two modelling algorithms, the prediction results of LS-SVM and PLSR were better, and the PCR predictive effects were the second best. In the prediction results for the TN and TP concentrations, the results of the four modelling methods were basically consistent.

Prediction results of nutrients concentrations in silty loam. In the PCR and PLSR modelling methods, the number of main components for PCR and the number of latent structures for PLSR are the same; they are

5, 6, 2, 6, 6, 4, 2, and 5 for TC, TP, TK, AN, AP, FK, and SK, respectively. The prediction results of PCR, PLSR and LS-SVM for the nutrient concentrations of sandy loam were basically consistent. TN and TC gave better prediction results, and the RPD values were ≈2; R_c^2 and R_p^2 were above 0.8; TP, AP, TK, FK, and SK gave poor predictive effects, and these models could not be used for quantitative analysis. The prediction results of LS-SVM were obviously superior to the other three modelling methods for the AN concentrations, with R_c^2 and R_p^2 values that were both higher than 0.85, and an RPD value that was nearly 1.9. The prediction results of BPNN for each nutrient concentration were sometimes superior to the other three modelling algorithms and sometimes the worst. The PLSR and LS-SVM modelling methods were more stable, and the prediction results were better than PCR.

Comparison of four modelling methods for predicting the nutrients concentrations of different types of soil. The sandy loam and silty loam samples were analyzed together, that is, as different types of soil samples. The predictive results of the four modelling methods for the nutrient concentrations of different soil types are shown in the Table 1. In the PCR and PLSR modelling methods, the number of main components for PCR and the number of latent structures for PLSR are the same, and they are 9, 9, 8, 6, 14, 5, 7, and 1 for TC, TP, TK, AN, AP, FK, and SK, respectively.

Table 1 shows that the modelling results for different modelling methods were some what different between the two different types of soil. Similar to the results when analyzing within a given type of soil, the overall trend of the nutrient concentrations was basically consistent. In the prediction results for the TN and TC concentrations, other than the PCR algorithm, all algorithms could be used as an effective model to predict unknown soil samples, and the prediction results of the two non-linear modelling methods, BPNN and LS-SVM, were better than the two linear modelling methods, PCR and PLSR. In the prediction results for the AN, TP, FK and SK concentrations, the nonlinear modelling methods, BPNN and LS-SVM, had higher accuracy than the linear modelling methods, PCR and PLSR. The BPNN and LS-SVM models could be regarded as good quantitative models. The models of the SK concentrations based on the PCR and PLSR algorithm could not be used for quantitative analysis, and the prediction results were improved by the BPNN and LS-SVM algorithms. In the prediction results for the AP and TK concentrations, the four modelling methods had the same effects on different types of soil.

From Table 1, when calibrated by the LS-SVM method for all indicators, the correlation coefficient in the calibration set was equal to 1, and in the test samples for TK and SK had values of 0.22 and 0.52, respectively. This ratio showed that, most likely, the constructed models were very refined. The test samples could not be predicted by this model.

TABLE 1. Four Modelling Methods for the Prediction Results of Nutrient Concentrations in Different Types of Soil

Evaluation standard	Modeling methods	TC	TN	AN	TP	AP	TK	FK	SK
R_c^2	PCR	0.78	0.80	0.72	0.79	0.79	0.26	0.67	0.01
	PLSR	0.95	0.96	0.89	0.89	0.99	0.33	0.82	0.01
	LS-SVM	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00
	BPNN	0.98	0.98	0.96	0.90	0.71	0.84	0.88	0.80
R_p^2	PCR	0.86	0.87	0.75	0.63	0.83	0.29	0.68	0.02
	PLSR	0.92	0.94	0.81	0.70	0.77	0.34	0.76	0.01
	LS-SVM	0.96	0.97	0.86	0.72	0.84	0.22	0.82	0.52
	BPNN	0.96	0.97	0.85	0.77	0.77	0.45	0.78	0.41
RMSEP	PCR	1.48	0.20	17.29	0.26	6.00	0.41	17.80	139.98
	PLSR	1.02	0.13	14.76	0.23	7.52	0.39	15.42	139.89
	LS-SVM	0.73	0.09	12.42	0.22	6.07	0.43	13.20	96.21
	BPNN	0.72	0.08	14.02	0.19	7.30	0.36	14.75	106.56
RPD	PCR	2.47	2.52	1.94	1.64	2.47	1.19	1.77	0.99
	PLSR	3.58	3.93	2.27	1.82	1.97	1.23	2.04	0.99
	LS-SVM	5.04	5.59	2.70	1.92	2.44	1.14	2.38	1.44
	BPNN	5.06	5.97	2.39	2.07	2.03	1.34	2.13	1.30

The prediction results of the PCR algorithm were the lowest in the soil nutrient concentrations models. One of the reasons might be that when useless information was eliminated, some useful information was eliminated at the same time. The other reason is that PCR algorithm does not have any connection with the nutrient concentration values during the modelling process and cannot have the same ability to explain the nutrient concentrations value as the PLSR model. Because of this, the modelling information was incomplete and the prediction results were not good. The PLSR algorithm was the most common modelling method used [25]. It was a simple linear algorithm, which had advantages in the case of large differences in sample concentrations values. However, in the actual measurement modelling, not all models conformed to the linear condition, and we could not build a good model using the PLSR algorithm. Compared with the other three algorithms, the LS-SVM algorithm gave better predictive results and had some advantages in small sample modelling [26]. Modelling by a nonlinear method could maximize the outline of the trend of the modelling samples. Due to the randomness of the BPNN algorithm, including the selection of the number of hidden network nodes, the network parameters, and so on [27], the same spectrum and the same soil nutrient concentrations values using the BPNN algorithm would produce different prediction results. The BPNN algorithm some excellent models within and between two different types of soil, but there were some models using the BPNN algorithm with very bad prediction results. To minimize the randomness, we needed to build several models more frequently and measure the average value. However, it would increase the modelling time and affect the running speed. In this paper, averaging of the results of multiple BPNN models was not used, which is probably the reason why the method sometimes produced good prediction results and sometimes bad results. How to decrease the modelling time as much as possible while ensuring the stability of the BPNN algorithm was a problem that needed to be solved.

When using multiple samples of different soil types, the prediction results were better, and the overall trend showed that the four modelling methods were consistent. This is because the values for the different types of soil nutrient concentrations varied widely. In the prediction results for small modelling samples [28], most of them still conform to the rule, and the higher the number of modelling samples, the better the prediction results. The higher the number of modelling samples that could accurately describe the model for the soil nutrient concentrations, the better the prediction results for unknown samples. Further, the nonlinear modelling methods had some advantages in the prediction of sets with small modelling samples.

Conclusion. Two different types of soil samples, sandy loam and silty loam, were selected as research objects. We determined the visible near-infrared reflectance spectra of soil and total nitrogen, total phosphorus, total potassium, available nitrogen, available phosphorus, available potassium, and slowly available potassium concentrations of soil. Principal component regression, partial least squares regression, least squares support vector machine, and back propagation neural network were four modelling methods that were compared to predict the soil nutrient concentrations both within and between two different types of soil. In the prediction results for nutrient concentrations within a given type of soil, the four modelling methods showed a general trend in their results for both sandy loam and silty loam. The LS-SVM and PLSR algorithms had better stability when predicting the results. In the prediction results of nutrient concentrations in the different types of soil, the results from different modelling methods varied. The nonlinear modelling methods, the BPNN and LS-SVM algorithms, had high accuracy for most soil nutrient concentrations. The prediction results of the four modelling methods became more accurate with higher numbers of modelling samples. By comparing different modelling methods, this study provides a basis for the subsequent selection of suitable models based on spectral technology to establish various soil nutrient models.

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