Multi-task convolution neural network regression prediction model based on vis-NIR spectroscopy

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Abstract. Aiming at the limitation of the current time-consuming and low-efficiency of regression prediction model based on visible and near infrared (vis-NIR) spectroscopy, this paper uses multi-task convolutional neural network model to predict various attributes such as soil total carbon, total nitrogen and alkali nitrogen. Considering the influence of the soil itself and the uncertain factors in the measurement process on the prediction results, the near-infrared soil spectral data is subjected to multi-scatter correction pre-processing, and the model is input and trained to optimize various parameters in the network. The experimental results verify that compared with the single attribute model, multi-task learning optimizes all output variables, maintains the correlation between data, improves learning efficiency and reduces training parameters and training time. The network model also achieves excellent evaluation criteria.

1. Introduction

Soil is the most important means of production in agricultural production. The timely and accurate information of soil nutrient content can guide agricultural production scientifically. However, due to the large cost of soil samples collection, predicting soil nutrient content has become a hot topic in current soil research. In recent years, vis-NIR spectroscopy has been widely applied in the quantitative analysis and detection of soil nutrients for its rapid detection, non-destructive, non-polluting, pretreatment and real-time detection [1,2]. With the development of machine learning, many new spectral model regression prediction algorithms have been put forward and applied [3,4]. But for the various nutrients contained in the soil, it is necessary to establish a corresponding network model to predict a nutrient content, which is inevitably time-consuming and inefficient. Therefore, the study establishes a soil nutrient spectral prediction model with higher efficiency, robustness and accuracy, and explores the goal of predicting multiple soil nutrient content of the same model. It is of great significance to speed up the development of China's agricultural informatization, raise the level of agricultural scientific management and develop our agricultural economy.

In this paper, multiple scattering correction method is applied to soil spectral data preprocessing to eliminate the interference factors in the soil itself or in the process of measurement to improve the accuracy of the prediction model. And construct a convolutional neural network regression model to...
achieve multi-task learning, and the concentration of total carbon, total nitrogen and alkali nitrogen in the soil was predicted in a single model.

The structure of the article is as follows. The second part introduces the current researcher's work on soil nutrient prediction. The third part elaborates the multi-scattering correction preprocessing method involved in the experiment and the processing process of building multi-task convolutional neural network regression model. The fourth part introduces the experimental data used in this paper and the model prediction evaluation results, and finally summarizes this article.

2. Related work

In 2003, Waktola first used artificial neural network to estimate soil organic matter from vis-NIR data [5]. Prior to this, Chang's principal component regression (PCR) and McCarty's partial least squares regression (PLSR) were the most commonly used techniques for spectral calibration and prediction [6,7]. In 2005, Viscarra et al. compiled a complete table linking soil spectra with soil properties, which listed various soil properties measured by vis-NIR spectra [8]. Based on this, various deep learning methods and traditional regression methods have been used to predict various soil nutrients.

Due to the low learning efficiency and long training time of single attribute prediction model, the effect of multi-task model has been widely studied recently. In 2017, Ruder mentioned in his article that multi-task model can reduce the risk of overfitting while improving the efficiency of model training [9]. In 2019, Padarian et al. converted the original spectral data into two-dimensional spectrographs to predict a variety of soil characteristics. Compared with ordinary single-attribute prediction, the experiment verified that multi-task learning could improve prediction accuracy [10]. In this paper, based on the original data, a multitask convolutional neural network model was built to predict the concentration of soil total carbon, total nitrogen and alkalized nitrogen. While improving the learning efficiency of the model, the training time and training parameters are reduced.

3. Theory

3.1. Multiple scattering correction algorithm

Multiple scattering correction (MSC) is one of the commonly used algorithms for spectral data preprocessing. MSC can effectively eliminate spectral differences caused by different scattering levels, thus enhancing the correlation between spectra and data [11]. In addition, it can effectively eliminate the baseline shift and deviation caused by scattering between samples, and improve the signal-to-noise ratio of the original absorbance spectrum. For the vis-NIR soil spectroscopy dataset, this paper uses the multi-scattering correction algorithm to preprocess the spectral data to minimize the interference factors and improve the accuracy of the prediction model.

Figure 1 shows the original data spectrum and the spectrum obtained after multi-scatter correction. It can be seen that the near-infrared scattering correction spectrum of all samples has a relatively
uniform baseline standard, and the baseline shift and nonlinear offset between the spectral data are well controlled. The spectral data obtained after scattering correction can more accurately reflect the change of vis-NIR spectral characteristics with soil concentration.

3.2. Multitask convolutional neural network

As a nonlinear model, convolutional neural network has excellent model representation ability because its unique convolution and pooling structure can extract essential features from complex input information. In this paper, a multi-task convolutional neural network regression model was built to predict soil total carbon, total nitrogen and alkali-hydrolyzed nitrogen concentrations.

Figure 2. Multitask convolutional network architecture.

Figure 2 shows the multi-task convolution neural network regression model proposed in this paper. The "public layer" represents Shared by all prediction attributes. Each branch, that is, each predicted soil property, corresponds to a fully connected layer with different neurons.

After the original spectral data is preprocessed by MSC, it enters the hidden layer as the input of the model to form a more abstract deep representation. After the Shared convolutional layer and pooling layer, it extracts and learns the internal features of the spectral data, and at the same time obtains a more effective and detailed local abstract feature mapping. In the two convolution layers, 256 convolution kernels and 64 convolution kernels with a size of 5 were used respectively, and the sampling scale was set as 5×5 to reduce overfitting and improve fault tolerance of the model. Finally, multilayer full connection layer is used for feature refinement and information integration. Three different values of soil nutrients correspond to different number of neurons. After several experiments, the number of neurons used to predict the soil carbon value in the fully connected layer is: 64, 64, 8. The number of fully connected neurons for soil total nitrogen was 64, 32, 8 and the number of fully connected neurons for soil alkaline nitrogen was set to 128, 64, 8.
4. Experiment

In this experiment, the data set was selected as vis-NIR spectroscopy data, 270 soil samples were sampled from multiple areas, and spectral information was collected through laboratory methods, among which the detected content was the concentration value of soil total nitrogen (TN), total carbon (TC) and alkali-hydrolyzed nitrogen (AN). The physical and chemical values of soil TN and TC were determined by carbon nitrogen analyzer, and the physical and chemical values of soil AN were determined by alkali-hydrolysis diffusion method. The basic data set information is shown in table 1. Moreover, each sample contains 750 dimensional data, and all samples are divided into training and test sets in a 7:3 ratio.

| Soil nutrients | Minimum | Maximum | Mean  | Standard deviation |
|----------------|---------|---------|-------|--------------------|
| TC             | 1.6     | 30.9    | 11.9  | 6.9                |
| TN             | 0.29    | 3.41    | 1.22  | 0.61               |
| AN             | 11.0    | 479.0   | 107.9 | 75.7               |

4.1. Model prediction results

This experiment builds a prediction model of multitask convolutional network based on the Keras deep learning framework based on Python.

![Figure 3. Trend of loss function in model training.](image)

The mean square error (MSE) is adopted as the loss function of the neural network model, and its change in the training process of 100 rounds is shown in figure 3. It can be seen that the loss values of three soil attributes in the network gradually converge with the increase of the number of iterations, and the curve drops smoothly on the macro level, indicating that the learning state is good and no overfitting state appears.

![Figure 4. (a) Prediction results of TC by model. (b) Prediction results of TN by model. (c) Prediction results of AN by model.](image)
Figure 4 scatter diagram of the predicted values of soil TC, TN and AN by the multi-task model and the measured values by the laboratory method respectively. It can be seen that the scatter points of the three soil attributes are evenly distributed on both sides of the regression line, and the predicted values are positively correlated with the actual values. It is proved that the vis-NIR spectroscopy is effective in predicting soil total carbon, total nitrogen and alkali-hydrolyzed nitrogen concentrations.

4.2 Model evaluation

This paper studies the performance of the model from two aspects of regression fit and prediction accuracy. The evaluation indexes used are: root mean square error determination coefficient ($R^2$), corrected root mean square error (RMSEC), prediction root mean square error (RMSEP) and prediction relative analysis error (RPD). The closer $R^2$ is to 1, indicating that the higher the fit, the better the model prediction effect. Error is an important index to measure the degree of data dispersion. The smaller the value, the more stable the model and the better the prediction effect. For relative analysis errors, an RPD value of more than 2.5 is an excellent model for high performance prediction.

Table 2. Soil nutrient prediction results of multitasking model.

| Soil nutrients | Model evaluation parameters |  |  |  |
|----------------|-----------------------------|---|---|---|
|                | $R^2_C$ | RMSEC | $R^2_P$ | RMSEP | RPD |
| TC             | 0.913   | 0.837  | 0.898   | 0.771  | 3.136 |
| TN             | 0.890   | 0.154  | 0.862   | 0.166  | 2.693 |
| AN             | 0.899   | 11.556 | 0.859   | 16.673 | 2.635 |

Table 2 shows the comparison of the evaluation parameters of three soil nutrients predicted by the multi-task convolutional neural network model. Where $R^2_C$ and RMSEC are the evaluation parameters of the training set, and $R^2_P$, RMSEP and RPD are the evaluation parameters of the test set. It can be seen that multi-task learning using convolutional neural networks can achieve better prediction results. Among them, compared with TN and AN, the concentration model of TC has the highest evaluation quality and the most accurate prediction result.

Table 3. Comparison of pretreatment effects.

| Soil nutrients | The original spectrum | Corrected spectrum |  |  |
|----------------|-----------------------|--------------------|---|---|
|                | $R^2_P$ | RPD | $R^2_P$ | RPD |
| TC             | 0.817   | 2.338  | 0.898   | 3.136 |
| TN             | 0.759   | 2.041  | 0.862   | 2.693 |
| AN             | 0.771   | 2.089  | 0.859   | 2.635 |

Table 3 shows the model evaluation comparison parameters of the test set after the original spectral data and the spectral data of the multivariate scatter corrected input into the multitasking network model. It can be seen that after the raw data is preprocessed, the model training ability is improved and the prediction accuracy is more accurate.

In addition, from the training time and training parameters of the model, this paper compares the multi-task network to achieve soil multi-attribute prediction and network single attribute prediction. From Table 4, it can be seen that the training parameters of the multi-task network are 24,233,299 lower than the three types. The sum of the training parameters of the attribute prediction network is 24,564,307, and the training time 11323.855s is also much smaller than the time sum of the three attribute predictions of 28801.41s, which overcomes the limitation of the long time and low efficiency of the single attribute prediction model.
Table 4. Single attribute model versus multi-task model

| Performance       | Single attribute prediction | Multitask prediction |
|-------------------|----------------------------|----------------------|
|                   | TC | TN | AN |                      |                      |
| Training time     | 9672.716s | 9156.195s | 9972.499s | 11323.855s |
| Training parameters | 6,183,185 | 6,180,849 | 12,200,273 | 24,233,299 |

5. Conclusion
The multitasking learning model has always been a hot and difficult point in regression prediction. To solve this problem, this paper based on vis-NIR spectroscopy data to construct multi-task convolution depth neural network to predict soil total carbon, total nitrogen and alkali nitrogen three different concentration values. The spectral data was pre-processed using a multivariate scatter correction technique prior to inputting the model to more accurately reflect the near-infrared spectral characteristics of the sample as a function of soil concentration. The experimental results show that the corrected spectral data is more accurate than the original data.

Multi-task learning was performed using soil vis-NIR spectroscopy as input, and the predicted soil component content was used as an output to achieve a target for accurately predicting soil composition by measuring near-infrared spectra of soil samples. Multi-task model prediction greatly improves learning efficiency and reduces training parameters and training time compared to single-attribute prediction. The experiment proves the feasibility and accuracy of using multi-task convolutional neural network in soil component content prediction.

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