STUDY ON SPECTRAL FEATURES OF SOIL ORGANIC MATTER

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KEY WORDS: Soil Organic Matter (SOM); Spectral Features, Stepwise Regression Analysis

ABSTRACT:

The study on soil spectral reflectance features is the physical basis for soil remote sensing. Soil organic matter content influences the soil spectral reflectance dramatically. This paper studied the spectral curves between 400nm~2500nm of 174 soil samples which were collected in Hengshan county and Yixing county. Fourteen types of transformation were applied to the soil reflectance R to remove the noise and linearize the correlation between reflectance (independent variable) and soil organic matter (SOM) content (dependent variable). Then, methods such as derivative spectrum technology, stepwise regression analysis, were applied to study the relationship between these soil spectral features and soil organic matter content. It shows that order 1derivative of the logarithm of reflectance (O1DLA) is the most sensitive to SOM among the various transform types of reflectance in consideration. The regression model whose coefficient of determination reaches 0.885 is built. It predicted the soil organic matter content with higher effect.
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1. INTRODUCTION

The research of earth resources and environment by remote sensing method is directly or indirectly related to soil optical characters because soil is one kind of the most exposed earth backgrounds. Therefore, the study on reflective characteristic of soil spectra is the physical base of soil remote sensing. The appearance of High Spectral Resolution Imaging Spectrometer provides a new technique for this study. Researchers can fully take the advantage of the Imaging Spectrometer, Spectra-Image conformity, to reconstruct spectra from images and compare them to spectra data collected on the ground, and then to perform synthetically analysis. It supports not only on band selection and design of sensors, but also on interpretation and analysis of remote sensing image data. Soil organic matter is an ingredient of soil solid-phase matter and serves as a reserve for many essential nutrients which called “nutrient bank for plant”, and its loss is closely linked with the decline of soil productivity. The content and composition of soil organic matter have strong effects on soil reflectance. The color of the soil is usually closely related to its organic matter content, with darker soils being higher in organic matter, which indicates the relationship between soil organic matter content and its visible light reflectance. Although there are a lot of inversion methods used to get the organic matter content from soil reflectance [1]-[9], all of these methods subject to certain limitation to some extent, and display biggish error when applying in different soil categories. To date, there is no versatile model which is fit for all over the world and the waveband selection for different study area is also diverse. This paper intended to analyze the relationship between soil reflectance data and organic matter content from 174 soil samples, accordingly extracting organic matter content information from reflectance data, evaluating the application potential of hyperspectral remote sensing technique in monitoring soil organic matter content in the visible and near infrared spectrum, detecting spectral characteristics sensitive to organic matter content and establishing corresponding inversion model for soil organic matter content prediction.

2. DATA AND METHODS

2.1 SAMPLING DESIGN

174 soil samples are collected from topsoil (about 5cm), including 43 soil samples collected from Yixing sample plot and 132 soil samples collected from Hengshan sample plot. There are two typical kinds of geomorphy in Hengshan County: Loess Plateau and Maowusu Desert, and its main soil types are loessal soil, sand soil, aeolian sandy soil and so on. Its soil is relative infertile and contains low content soil organic matter; Yixing county is located at Tai Lake bank, its soil is comparative fertile, the main soil types include yellow-brown soil, limestone soil, brown-red soil, paddy soil and so on, containing higher content soil organic matter. The selection of these two areas can make sure that there are comparative large range of organic matter values (0.124% ~ 4.86%). The soil samples were collected from planar areas containing bare soil, and the selection of sampling areas considered various land-use types and soil types. 4 or 5 typical survey stations were selected in each sampling area, and then one soil sample was selected in each survey station with 5 times spectral measurements before each soil sampling. Spectral measurements used ASD FieldSpec FR field spectrometer, and used a fiber optic probe with 3 degree field-of-view to vertically observe objectives. The wavelength coverage of ASD FieldSpec FR Spectrometer is from 350 nm-2500 nm, including 3 nm spectral resolution between 350 nm-1000 nm, 10 nm spectral resolution between 1000 nm-2500 nm[10]。During observation, the surveyors should take the fiber optic probe in their hands and face to light source (the sun) direction, and the probe must be vertical with measuring objectives. A 75cm×75cm white reflection plate was used for obtaining absolute reflectance. While measuring, radiance but not reflectance was directly detected. Firstly, the radiance of white plates was measured for 5 times, and then the radiance of soil objectives was also measured for 5 times. The illumination conditions between objectives and reference white plates must be consistent as much as possible, and then the average values were calculated. The ratio between averaged soil radiance and radiance of white plates is the soil reflectance. This kind of measurement method can eliminate the effects of some random noises compared with direct measurement of soil reflectance.

2.2 Measurement of soil organic matter content

This study used volumetry assay to measure organic matter content of soil samples. The method is described as follows:

under the heating conditions, excessive potassium dichromate and sulphuric acid standard solution was used to oxidize soil organic matter, and then ferrous salts (ferrous sulfate or ferrous ammonium sulfate) standard solution was used to titrate in the presence of appropriate redox indicator. The organic carbons content can be calculated from the amount of potassium dichromate consumed by organic matter oxidization, consequently the soil organic matter content can be worked out.

2.3 Pretreatment of spectral data

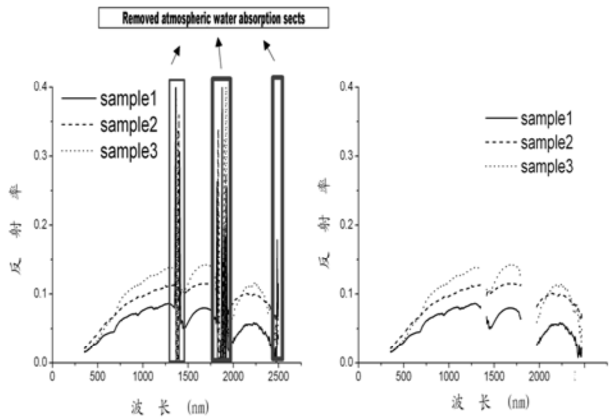
2.3.1 Smoothing spectral curves

Because of the different response to energy among spectrometer bands, the spectral curve always has some noises. In order to obtain a smooth change, it is necessary to smooth waveform to remove a small amount of noise included in signals. The practice has showed that, if noises have high frequency and low magnitude, the smooth methods could reduce noises to some extent. The smooth methods in common use include Moving Average, Static Average, and Fourier Series Approximation and so on. In this study, the 9-Point Weight Moving Average was used to smooth spectral curves and eliminate noises. The spectral curves give sequences of N survey points ($\{R_i, i = 1,2,3\cdots, N\}$) (for spectral data of ASD FieldSpec FR Spectrometer, the spectral resolution between 350 nm-1000 nm is 3 nm, the spectral resolution between 1000 nm-2500 nm is 10 nm , and the spectrometer re-samples the data as 1 nm). Here, the value of point i is weighted average of its anterior 4 points and posterior 4 points. That is, the new value of point i, R_i', is replaced by weighted average of 9 points including point i, which is called smooth value.

$$
\begin{aligned}
R_i' &= 0.04R_{i-4} + 0.08R_{i-3} + 0.12R_{i-2} + 0.16R_{i-1} + 0.20R_i \\
&\quad + 0.16R_{i+1} + 0.12R_{i+2} + 0.08R_{i+3} + 0.04R_{i+4}
\end{aligned} \tag{1}
$$

2.3.2 Removing atmospheric water absorption bands

In order to make sure that the ground findings can be finally applied in the OMIS or Hyperion imaging spectrometer data, the disposal and analysis of spectral curve in this paper directly aim at field soil spectral data instead of indoor laboratory data. Three sects of wavebands with serious water absorption peaks were removed through concrete data analysis and reference of conclusions from relative literatures [11] [12]. The removed three sects of wavebands including: (1)1350-1416 nm； (2)1796-1970 nm； (3)2470-2500 nm. The eliminated water-absorption peaks wavebands and spectral curves after elimination are shown in figure 1, the spectral curves after elimination are divided into three sections:



2.4 Analytical methods

In addition to direct analysis of soil reflectance, we also perform 14 transforms of soil reflectance to find spectral indicators sensitive to soil organic matter (SOM) content. The purpose of the analysis was to relate SOM content to spectral properties. Fourteen types of transformation were applied to the soil reflectance R (Table 1).

Description	Formula
Reciprocal of R	$1/R$
Reciprocal of $\lg R$	$1/\lg R$
First derivative of R	R'
First derivative of $\lg R$	$(\lg R)'$
First derivative of $\sqrt{R}$	$\sqrt{R}'$
Second derivative of $1/R$	$(1/R)''$
Second derivative of $1/\lg R$	$(1/\lg R)''$
Logarithm of R	$\lg R$
Square root of R	$\sqrt{R}$
First derivative of $1/R$	$(1/R)'$
First derivative of $1/\lg R$	$(1/\lg R)'$
Second derivative of R	R''
Second derivative of $\lg R$	$(\lg R)''$
Second derivative of $\sqrt{R}$	$\sqrt{R}''$

Table 1 Fourteen transformation types of reflectance

Transforming reflectance is in consideration of two respects. On one hand, it is a need for removing the noise, for instance, first derivative of R reduces the impacts of linear or linear-like background noise on target spectra; Log(R) weakens multiplication noise caused by the change of illumination condition. On the other hand, the relationship between reflectance (independent variable) and SOM content (dependent variable) was not linear correlation. Reflectance transformation actually linearizes the correlation between reflectance and soil physical-chemical properties.

After logarithmic transformation, the spectral data not only tend to enhance spectral differences of visible light (the original value of visible spectra is low as a whole), but also intend to reduce multiplicative factor effects induced by changes in illumination conditions. Differential spectra will help to limit the effects of low frequency noises on objective spectra. In the study, not only the reflectance differentiate was calculated, but also the first order and second order differentiate of four transforms of reflectance (reciprocal, logarithm, logarithmic reciprocal and square root) were calculated. And statistical analytical technique was used to evaluate and compare their sensitivity as indicators of SOM.Figure.1 Removal of Water Absorption Sects

2.4.1 Derivative spectroscopy technique

Among the developed methods of spectrometry, derivative spectroscopy technique has a promising application in remote sensing data processing. Differential (difference) values with different orders can help people to quickly determine the wavelength location of spectral curve inflection point and extremum reflectance. Cloutis's study showed that the sensitivity to noise of spectra data decreased by low-order differential processing. Therefore it is comparatively effective in practical application [13]. Spectral difference is practically used as a limited approximation of differentiate. The calculative formula is as follows:

$$R'(\lambda_i) = [R(\lambda_i) - R(\lambda_{i-1})] / 2\Delta\lambda \quad \ldots\ldots\ldots(2)$$

$$R''(\lambda_i) = [R'(\lambda_i) - R'(\lambda_{i-1})] / 2\Delta\lambda = [R(\lambda_{i+1}) - 2R(\lambda_i) + R(\lambda_{i-1})] / \Delta\lambda^2 \quad \ldots\ldots\ldots(3)$$

In above formula, λ_i represent wavelength of each band; $R'(\lambda_i)$ and $R''(\lambda_i)$ represent first order and second order differential spectra for wavelength λ_i, respectively; $\Delta\lambda$ is interval between wavelength λ_{i-1} and λ_i. With the increase of $\Delta\lambda$, the spectral differential curve inclined to becoming smoother, leading possibly to elimination of many subtle spectral characteristics (as shown in figure 2). In this study, $\Delta\lambda$ =10 nm is selected。

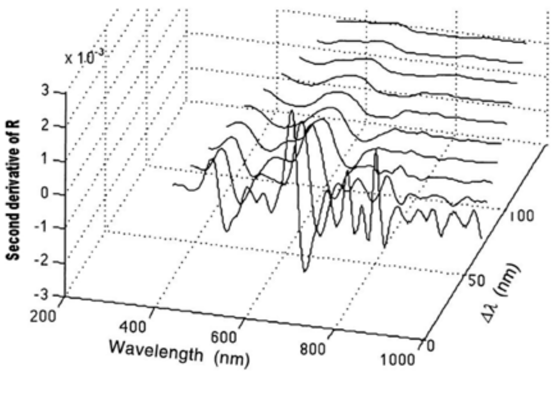


Figure.2 Order 2 Derivative of Albedo with Different Band Interval

2.4.2 Correlation analysis

The SOM contents of 174 soil samples measured by volumetry assay method and soil reflectance as well as its 14 types of transform were conducted single correlation analysis in each waveband (formula 4):

$$r_i = \frac{Cov(R,OM)}{\sqrt{D(R)}\sqrt{D(OM)}} = \frac{\sum_{n=1}^{N}(R_{ni} - \overline{R_i})(OM_n - \overline{OM})}{\sqrt{\sum_{n=1}^{N}(R_{ni} - \overline{R_i})^2 \sum_{n=1}^{N}(OM_n - \overline{OM})^2}} \quad \ldots\ldots\ldots\ldots(4)$$

In the above formula, r_i is single correlation coefficient between soil organic matter content OM and spectral reflectance or its transforms (all denote as R), i is the serial number of waveband, R_{ni} is the spectral reflectance (or its transforms) value at the ith waveband of the nth soil sample, $\overline{R_i}$ is the mean value of spectral reflectance (or its transforms) of the N soil samples at waveband i, OM_n is the SOM content of the nth soil sample, $\overline{OM}$ is the actual measured mean for SOM content of N soil samples, N equal to 174, total number of soil samples.

2.4.3 Stepwise regression

According to single correlation analytical results, several optimal wavebands with comparatively high correlation coefficients in each transforms were selected for stepwise regression analysis, and then used to compose predictive equation. The total 174 samples were randomly divided into two groups, one was used for establishing regression predictive model (called modeling sample collection, total is 134, possessing 77% of total number), another group was used for testing established regression model (called testing sample collection, total is 40, possessing 23% of total number).

Stepwise regression analysis is a typical mathematic method used for selecting regression variable in multiple linear regression models. Its basic idea is described as follows: regression variables are selected one by one, and the selective qualification is their sum of partial regression square is remarkable; the selected variables are performed significance test one by one after selection of each new variable, and the non-significant variables are removed. Repeat the process of selection, test and elimination until there is no variable can be selected or eliminated. When using stepwise regression analysis to determine waveband combination related to organic matter, the input variables are organic matter content measured and the value of spectral reflectance or its transforms at the optimal wavebands with comparatively high correlation coefficients in single correlation analysis. The output result are a series of multiple linear equations containing different wave bands and corresponding validation coefficient R^2 (formula 5), and the SOM content is calculated by multivariate regression model finally. The validation coefficient R^2 is also called multiple correlation coefficient or fitting degree of curve, which is a good measurement for regression effectiveness. When regression effectiveness is rather bad, R^2 equal to 0 approximately, which manifests the fitting value $\hat{Y}_i$ is irrelevant to the observed value Y_i at all.

$$R^2 = \frac{\sum_{i=1}^{n}(\hat{Y}_i - \overline{Y})^2}{\sum_{i=1}^{n}(Y_i - \overline{Y})^2} = \frac{[\sum_{i=1}^{n}(Y_i - \overline{Y})(\hat{Y}_i - \overline{\hat{Y}_i})]^2}{\sum_{i=1}^{n}(\hat{Y}_i - \overline{\hat{Y}})^2 \cdot \sum_{i=1}^{n}(Y_i - \overline{Y})^2} = r_{Y\hat{Y}}^2$$
………(5)

However, the value of validation coefficient R^2 is increased along with the increasing amount of independent variable n (or sample capacity). Therefore, to reflect as accurately as possible the fitting degree of model and eliminate the effects of independent variable amount and sample size on validation coefficient, the adjusted validation coefficient (Adjusted R Square) is introduced. Its formula is:

$$AdjustedR^2 = 1 - \frac{\sum_{i=1}^{n}(Y_i - \hat{Y}_i)^2 / (n-k-1)}{\sum_{i=1}^{n}(Y_i - \overline{Y})^2 / (n-1)} \quad \text{…………(6)}$$

In the formula, k is the amount of independent variables (number of selected wavebands), n is the amount of observe objectives (number of samples). When the amount of independent variables is more than 1, the value of adjusted R2 is less than validation coefficient R2. As shown in the formulas, the larger n is, the greater difference between R2 and adjusted R2.

The accuracy of predictive equation is evaluated by the total root-mean-square error ($RMSE$) (formula 7).

$$RMSE = \sqrt{\frac{1}{n-k-1}\sum_{i=1}^{n}(Y_i - \hat{Y}_i)^2} \quad \text{…………(7)}$$

In the formula, Y_i and $\hat{Y}_i$ represent measured value and predictive value, n is the amount of soil samples, k is the amount of selected wavebands.

After establishment of the equation, variance analysis was also used to test the regression equation. The hypothesis of test was that the global regression coefficients are 0 or not 0, and it was the significance test for the whole regression equation.

3 ANALYSIS AND RESULTS

3.1 Correlation analytic results

The SOM contents of 174 soil samples were measured by volumetry assay, the minimal value is 0.12% and the maximal value is 4.86%, and the mean value is 1.18%. The mean square deviation was 1.12. The correlation coefficient between measured SOM content and smoothed spectral reflectance at the range of 350nm-2500nm was calculated according to formula 4.

The results indicated that, the transforms, except the logarithmic reciprocal of reflectance, all increased correlation of soil organic matter content to some extent. Among them, the most significant was the first order differential transforms for reflectance logarithm. The maximal correlation coefficient between original reflectance before transforming and SOM content was 0.72 (at 2137 nm wavelength), while correlation coefficient between first order differential transforms of reflectance logarithm and SOM content at 2187 nm was 0.89, the maximum of all correlation coefficients (Figure 3). This also indicated that some subtle information obscured in original spectral data was amplified and made clear after differential transformation.

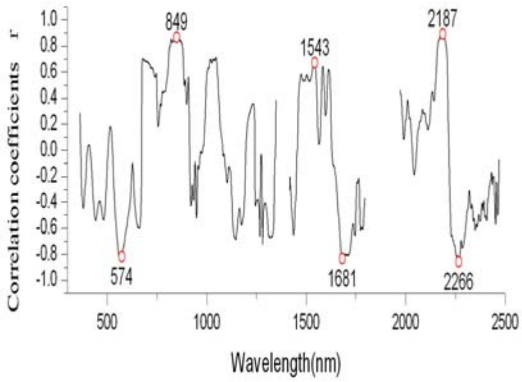


Figure. 3 Correlation Coefficients between (lg*R*)′ and SOM Content

The analytic results also manifested that, SOM content was negative correlated with spectral reflectance but positive correlated with the reciprocal of reflectance, and the change trend of absolute values of both correlation coefficients was basically consistent. The changes of correlation coefficients between differential transforms (both first and second order) and SOM displayed no rule, different from the mild changes in correlation coefficients of logarithmic and reciprocal transforms. Its value oscillates between 1 and -1.

3.2 Stepwise regression results

Stepwise regression analysis methods commonly used to identify the wavebands sensitive to a certain chemical constituent, and to demonstrate these wavebands has a good correlation with the concentration of a certain chemical constituent. Accordingly, we can use these determined locations of the wavelength (band values) to estimate the concentration of a certain chemical composition. However, there are two aspects of deficiency: firstly, there exists overfitting phenomenon in establishment of regression model. This phenomenon mainly appears while the sample size is less than the amount of wavebands. Then spectral reflectance values may not correlated with certain chemical composition while its noise pattern may be related to certain chemical composition. This kind of risk is increasing along with increase of the number of wavebands. Secondly, the deficiency is highly correlation among wavebands. An important hypothesis of stepwise regression method is that some input variables in multiple regression analysis have no significant impact on output. If this assumption is valid, it is easy to simplify the model, retaining only those items with statistical significance. But, in fact, multiple interactions exist among input variables, and input variables are not only related to outputs, but also relevant to one another. Under this condition, an input variable of model possibly shields the effects of the other variables on results. In short, stepwise regression, as a fixed processing, has risks for users to a certain extent, because regressive results are closely related to the initial model as well as the selective strategy for variables.

Considering the shortcomings of stepwise regression analysis, this study firstly used single-correlation analysis, then selected the wavebands with high correlation and long intervals (weakly relevant to one another) as regressive input variables. Thus, on one hand, under the premise of remaining sensitive wavebands, the amount of input wavebands was reduced and overfitting phenomenon was avoided; on the other hand, the selection of input wavebands were not entirely based on the magnitude of correlation coefficients but selecting 1 extremum (or 2 extremum for differential transforms with positive and negative correlation coefficients) from each sect of data which divided into three sections after elimination of water-absorption peaks. The longer the intervals among selected wavebands are, the weaker the correlation among them. Accordingly, high correlation among selected variables (wavebands) was effectively preventing by this way.

Table 2 shows the regression equations used for prediction of SOM from various transforms of reflectance. And all equations were performed F-value test with significance level 0.001. As shown in table 2, among all transforms, the first order differentiate of logarithm of reflectance ($(\lg R)'$) has the strongest ability to predict SOM content, and the validation coefficient of its regression equation consisting of three wavebands is 0.89, the maximum among all regression equations. The effect of SOM content predictions from different regression equations are as shown in figure 4, 5, 6, 7.

Transforms	Regression Equations	R^2	Adjusted R^2	*RMSE*
$X = R$	$Y = 1.990 - 20.949X_{2137} + 22.318X_{1501}$	0.684	0.679	0.608
$X = \sqrt{R}$	$Y = 2.386 - 24.938X_{2137} + 24.689X_{1499}$	0.802	0.799	0.480
$X = 1/R$	$Y = 0.053 + 0.307X_{2277}$	0.789	0.787	0.486
$X = \lg R$	$Y = 1.029 - 12.359X_{2149} + 10.878X_{1504}$	0.851	0.849	0.417
$X = (1/R)'$	$Y = 0.581 - 362.003X_{863} + 64.680X_{1145}$	0.840	0.837	0.432
$X = (1/R)''$	$Y = 0.626 + 1308.365X_{2222} + 2027.007X_{1740} - 135.885X_{672}$	0.706	0.699	0.586
$X = (\lg R)'$	$Y = 1.772 + 1004.071X_{2187} + 2893.272X_{849} - 1682.915X_{1681}$	0.888	0.885	0.360
$X = (\lg R)''$	$Y = 2.451 + 21952.91X_{587} - 47995.4X_{905} - 4577.994X_{2219} + 13138.89X_{1726}$	0.839	0.833	0.431
$X = \sqrt{R}'$	$Y = 1.971 + 1399.130X_{2180} + 4260.033X_{846} - 2459.097X_{1685}$	0.861	0.858	0.403
$X = \sqrt{R}''$	$Y = 2.661 + 38552.87X_{587} - 40731.4X_{905} + 33733.12X_{1725} - 6072.362X_{2199}$	0.842	0.837	0.432
$X = R'$	$Y = 1.891 + 5024.556X_{845} - 941.121X_{2037} + 576.462X_{2180} + 615.901X_{1521}$	0.789	0.782	0.500
$X = R''$	$Y = 2.305 + 13830.69X_{587} + 52867.66X_{1725} - 35305.5X_{529}$	0.754	0.748	0.537

Table 2 Regression analytical result between different reflectance transforms and SOM Content

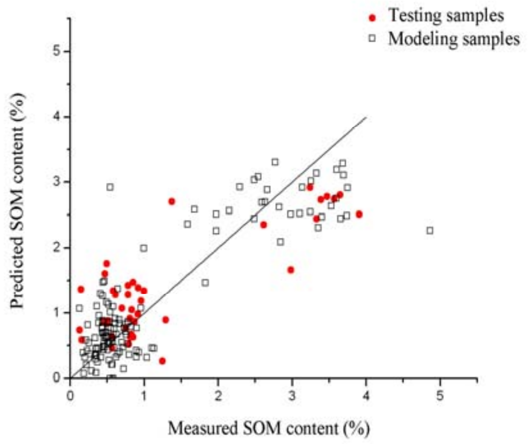


Figure. 4 Comparison between measured value and predicted with reflectance

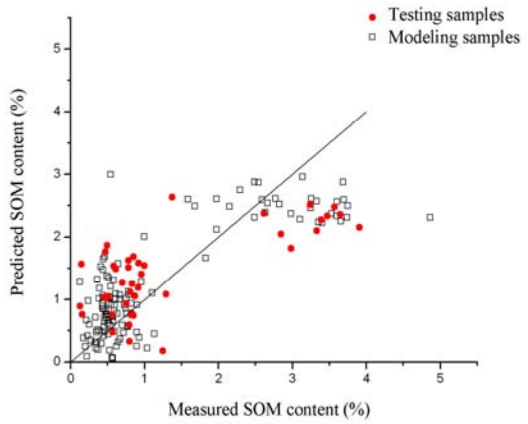


Figure 5 Comparison between measured value and predicted with square root of reflectance

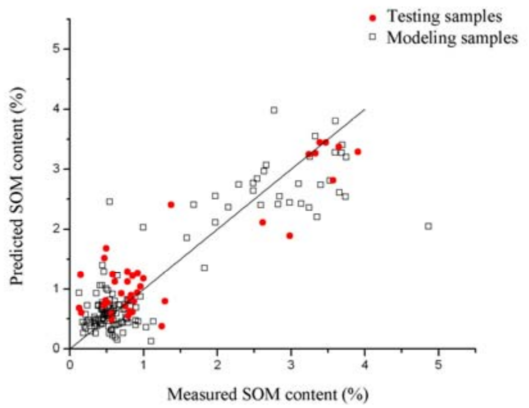


Figure. 6 Comparison between measured value and predicted with logarithm of reflectance

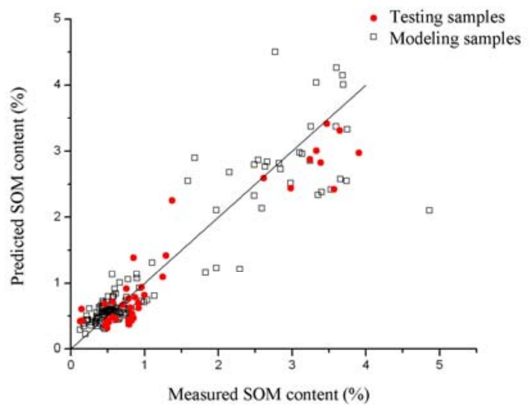


Figure. 7 Comparison between measured value and predicted with order 1 derivative of the logarithm of reflectance

4 CONCLUSIONS

(1) In the studied 350-2500 nm wavelength range, absorption peak of SOM does not exist. But in the range of wavelength, spectral reflectance is negative correlated with SOM content, and the highest correlation is near 675 nm. The results are consistent with previous study [14], considering that SOM is negative correlated with reflectance in the whole range of visible light. This study further extends the conclusion to infrared bands.

(2) The reciprocal of reflectance logarithmic $1/\lg R$ was inefficient for detecting SOM content. It can not increase the correlation between spectral indicator and SOM content, but decreased their correlation. All the other transforms, such as reciprocal, logarithm, square root and differentiate, improve sensitivity to SOM content to different extent. The transform type of $(\lg R)'$ is the most significant among them. The logarithmic transform of reflectance reduces effects of multiplicative factors induced by changes of illumination conditions. But it is insufficient to only perform logarithmic transform, it also need differential treatment to obtain better effect. Spectral differential technique can partially eliminate atmospheric effect; especially the first order differential treatment can remove effects of partially linear or approximately linear background and noise spectra on objective spectra.

(3) Overall, before performing differential transform, the detect ability of SOM content at visible light wavebands is stronger than infrared bands, and the most sensitive band is near 675 nm; while after spectral differential transform, infrared bands becomes more sensitive, and the correlation coefficient between (lg*R*)´ and SOM content is as high as 0.89 at 2187 nm position, the maximum among congeneric correlation coefficients.

(4) The optimal model for predicting SOM content is the regression equation composed with (lg*R*)´ value at 849 nm, 1681 nm and 2187 nm wavebands as independent variables:

$$Y = 1.772 + 1004.071 X_{2187} + 2893.272 X_{849} - 1682.915 X_{1681}$$

In the equation $X = (\lg R)'$, Y is SOM content (%). The *Adjusted* R^2=0.885 and *RMSE*=0.36. It is the best one among all models. Although the model is distinct from the predictive model for SOM content established by Krishnan [3], and the selected wavebands are also totally different, but they are in essence selecting differential transforms for the logarithm of reflectance as variables. It was obvious that this transform type is extremely sensitive to SOM content. Both our soil samples collected from Yixing and Hengshan County in China and Krishnan's soil samples collected from Illinois in America are all proved this point.

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