Spectral Features of Soil Organic Matter

HE Ting  WANG Jing  LIN Zongjian  CHENG Ye

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 400 nm−2500 nm of 174 soil samples which were collected in Hengshan county and Yixing county. Fourteen types of transformations were applied to the soil reflectance $R$ to remove the noise and to linearize the correlation between reflectance (independent variable) and soil organic matter (SOM) content (dependent variable). Then, the methods such as derivative spectrum technology and stepwise regression analysis, were applied to study the relationship between these soil spectral features and soil organic matter content. It shows that order 1 derivative 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.

Keywords  soil organic matter (SOM); spectral features; stepwise regression analysis

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Introduction

The research of the earth’s resources and environment by remote sensing method is directly or indirectly related to soil optical characteristics, because soil is a kind of the most exposed earth backgrounds. Therefore, the study on the reflective characteristic of soil spectra is the physical basis of soil remote sensing. The introduction of the high spectral resolution imaging spectrometer provides a new technique for this study. Researchers can fully take advantage of the imaging spectrometer and spectra-image conformity to reconstruct spectra from images and to compare them to spectra data collected on the ground, then to perform synthetic analysis. It supports not only band selection and design of sensors, but also 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 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 are subject to certain limitations to some extent, and display biggish error when applied in different soil categories. To date, there is no versatile model which fits all over...
the world, and the waveband selection for different study areas 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.

1 Data and methods

1.1 Sampling design

We collected 174 soil samples from topsoil (about 5cm thick), including 43 soil samples collected from Yixing sample plot and 132 soil samples collected from Hengshan sample plot. There are two typical kinds of geomorphology 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 relatively infertile and contains low contents of soil organic matter. Yixing County is located at the Tai Lake bank, its soil is comparatively 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 is a comparatively 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. Four or five typical survey stations were selected in each sample area, 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 degrees field-of-view to vertically-observed objectives. The wavelength coverage of ASD FieldSpec FR Spectrometer is from 350 nm~2 500 nm, including 3 nm spectral resolution between 350 nm~1 000 nm, 10 nm spectral resolution between 1 000 nm~2 500 nm\(^{[10]}\). During observation, the surveyors should take the fiber-optic probe in their hands and face the light source (the sun) direction, and the probe must be vertical with measuring objectives. A 75 cm×75 cm white reflection plate was used for obtaining absolute reflectance. While measuring, radiance but not reflectance was directly detected. First, the radiance of white plates was measured 5 times, then the radiance of soil objectives was also measured 5 times. The illumination conditions between objectives and reference white plates must be consistent as much as possible, 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.

1.2 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 ferrous salts (ferrous sulfate or ferrous ammonium sulfate) standard solution was used to titrate in the presence of appropriate redox indicator. The organic carbon 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.

1.3 Pretreatment of spectral data

1.3.1 Smoothing spectral curves

Because of the different responses to energy among spectrometer bands, the spectral curve always has some noises. In order to obtain a smooth change, it is necessary to smooth the 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 can 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 (\(\{R_i, i = 1,2,3\ldots,N\}\))
(for spectral data of ASD FieldSpec FR spectrometer, the spectral resolution between 350 nm ~ 1 000 nm is 3 nm, the spectral resolution between 1 000 nm ~ 2 500 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.

\[
R'_i = 0.04R_{i-4} + 0.08R_{i-3} + 0.12R_{i-2} + 0.16R_{i-1} + 0.20R_i + 0.16R_{i+1} + 0.12R_{i+2} + 0.08R_{i+3} + 0.04R_{i+4}
\]

(1)

1.3.2 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 three removed sects of wavebands include: (1) 1 350~1 416 nm; (2) 1 796~1 970 nm; (3) 2 470~2 500 nm. The eliminated water-absorption peaks wavebands and spectral curves after elimination are shown in Fig.1; the spectral curves after elimination are divided into three sections.

1.4 Analytical methods

In addition to direct analysis of soil reflectance, we use 14 transform types 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).

Transforming reflectance considers two aspects. On the 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.

| Description | Formula |
|-------------|---------|
| Reciprocal of \( R \) | \( 1/R \) |
| Reciprocal of \( \log R \) | \( 1/\log R \) |
| First derivative of \( R \) | \( R' \) |
| First derivative of \( \log R \) | \( (\log R)' \) |
| First derivative of \( \sqrt{R} \) | \( \sqrt{R}' \) |
| Second derivative of \( 1/R \) | \( (1/R)'' \) |
| Second derivative of \( 1/\log R \) | \( (1/\log R)'' \) |
| Logarithm of \( R \) | \( \log R \) |
| Square root of \( R \) | \( \sqrt{R} \) |
| First derivative of \( 1/R \) | \( (1/R)' \) |
| First derivative of \( 1/\log R \) | \( (1/\log R)' \) |
| Second derivative of \( R \) | \( R'' \) |
| Second derivative of \( \log R \) | \( (\log R)'' \) |
| Second derivative of \( \sqrt{R} \) | \( \sqrt{R}'' \) |
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 difference was calculated, but also the first-order and second-order difference of four transforms of reflectance (reciprocal, logarithm, logarithmic reciprocal and square root) were calculated. Statistical analytical technique was used to evaluate and compare their sensitivity as indicators of SOM.

1.4.1 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 difference. The calculative equations are:

$$R'(\lambda) = \frac{R(\lambda) - R(\lambda_{i+1})}{2\Delta\lambda}$$  \hspace{1cm} (2)

$$R''(\lambda) = \frac{R'(\lambda) - R'(\lambda_{i+1})}{2\Delta\lambda} = \frac{R(\lambda_{i+1}) - 2R(\lambda) + R(\lambda_{i-1})}{\Delta\lambda^2}$$  \hspace{1cm} (3)

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

1.4.2 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 with single correlation analysis in each waveband (Eq.(4)):

$$r_i = \frac{\text{cov}(R,OM)}{\sqrt{D(R)D(OM)}} = \frac{\sum_{n=1}^{N}(R_{ni} - \overline{R})(OM_{n} - \overline{OM})}{\sqrt{\sum_{n=1}^{N}(R_{ni} - \overline{R})^2 \sum_{n=1}^{N}(OM_{n} - \overline{OM})^2}}$$  \hspace{1cm} (4)

Here, $r_i$ is the single correlation coefficient between soil organic matter content $OM$ and spectral reflectance or its transforms (all denoted as $R$), $i$ is the serial number of waveband, $R_{ni}$ is the spectral reflectance (or its transforms) value at the $i^{th}$ waveband of the $n^{th}$ soil sample, $\overline{R}_{i}$ is the mean value of spectral reflectance (or its transforms) of $N$ soil samples at waveband $i$, $OM$ is the SOM content of the $n^{th}$ soil sample, $\overline{OM}$ is the actual measured mean for SOM content of $N$ soil samples, and $N$ equals to 174, the total number of soil samples.

1.4.3 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, 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, whose total is 134, possessing 77% of the total number), and the other was used to test the established regression model (called testing sample collection, whose total is 40, possessing 23% of the total number).

The stepwise regression analysis is a typical mathematical method used for selecting regression variables
in multiple linear regression models. Its basic idea is described as follows: the regression variables are selected one by one, and the selective qualification is their sum of partial regression square is remarkable; the selected variables performed significance tests one by one after the selection of each new variable, and the non-significant variables are removed. Repeat the process of selection, test and elimination until no variable can be selected or eliminated. When using the stepwise regression analysis to determine the 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 is a series of multiple linear equations containing different wave bands and corresponding validation coefficient $R^2$ (Eq.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 the regression effectiveness is rather bad, $R^2$ equals to 0 approximately, which manifests that the fitting value $\hat{Y}_i$ is irrelevant to the observed value $Y_i$ at all.

$$R^2 = \frac{\sum_{i=1}^{n} (\hat{Y}_i - \bar{Y})^2}{\sum_{i=1}^{n} (Y_i - \bar{Y})^2} = \frac{\sum_{i=1}^{n} (Y_i - \bar{Y})(\hat{Y}_i - \bar{Y})^2}{\sum_{i=1}^{n} (Y_i - \bar{Y})^2} = r_{Y\hat{Y}}^2 \quad (5)$$

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

$$Adjusted \ R^2 = 1 - \frac{\sum_{i=1}^{n} (Y_i - \hat{Y}_i)^2 / (n-k-1)}{\sum_{i=1}^{n} (Y_i - \bar{Y})^2 / (n-1)} \quad (6)$$

Here, $k$ is the amount of independent variables (number of selected wavebands), $n$ is the amount of observe objectives (number of samples). The amount of independent variables is more than 1, the value of $Adjusted \ R^2$ is less than the validation coefficient $R^2$.

As shown in the equations, the larger the $n$ is, the greater the difference between $R^2$ and $Adjusted \ R^2$ is.

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

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

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

After the establishment of the equation, the 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.

2 Analysis and results

2.1 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 350 nm~2500 nm was calculated according to Eq.4. The results indicated that, the transforms, except the logarithmic reciprocal of reflectance, increased the 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 (Fig.3). This also indicated that some subtle information obscured in original spectral data was amplified and made clear after differential transformation.

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.

2.2 Stepwise regression results

The 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: first, there exists an overfitting phenomenon in the establishment of the regression model. This phenomenon mainly appears while the sample size is less than the amount of wavebands. Then the spectral reflectance values may not be correlated with certain chemical composition while its noise pattern may be related to certain chemical composition. This kind of risk is increasing along with the increase of the number of wavebands. Second, the deficiency is highly correlated 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. In this condition, an input variable of the model possibly shields the effects of other variables on results. In short, the stepwise regression, as a fixed processing, has risks to users to a certain extent, because the regressive results are closely related to the initial model as well as the selective strategy for variables.

Considering the shortcomings of the stepwise regression analysis, this study first 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 number of input wavebands was reduced and overfitting phenomenon was avoided; on the other hand, the selection of input wavebands was 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 is divided into three sections after the elimination of water-absorption peaks. The longer the intervals among selected wavebands are, the weaker the correlation among them is. Accordingly, high correlation among selected variables (wavebands) was effectively prevented in this way.

Table 2 shows the regression equations used for the prediction of SOM from various transforms of reflectance. All equations were performed $F$-value test with significance level 0.001. As shown in Table 2, among all transforms, the first order difference 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 Figs. 4, 5, 6, 7.

### Table 2  Regression analytical result between different reflectance transforms and SOM content

| Transforms | Regression equations | $R^2$ | Adjusted $R^2$ | RMSE |
|------------|----------------------|-------|----------------|------|
| $X = R$    | $Y = 1.990 - 20.949X_{2139} + 22.318X_{1501}$ | 0.684 | 0.679 | 0.608 |
| $X = \sqrt{R}$ | $Y = 2.386 - 24.938X_{2139} + 24.689X_{1499}$ | 0.802 | 0.799 | 0.480 |
| $X = 1/R$  | $Y = 0.053 + 0.307X_{2277}$ | 0.789 | 0.787 | 0.486 |
| $X = (1/R)'$ | $Y = 1.029 - 12.359X_{2199} + 10.878X_{1604}$ | 0.851 | 0.849 | 0.417 |
| $X = (1/R)''$ | $Y = 0.581 - 362.003X_{1685} + 64.680X_{1145}$ | 0.840 | 0.837 | 0.432 |
| $X = \log{R}$ | $Y = 0.626 + 1308.365X_{2222} + 2027.007X_{1740} - 135.885X_{1672}$ | 0.706 | 0.699 | 0.586 |
| $X = (\log{R})'$ | $Y = 1.772 + 1004.071X_{2199} + 2893.272X_{1685} - 682.915X_{1681}$ | 0.888 | 0.885 | 0.360 |
| $X = (\log{R})''$ | $Y = 2.451 + 21952.91X_{1680} - 47995.4X_{1605}$ | 0.839 | 0.833 | 0.431 |
| $X = \sqrt{R}$ | $Y = 1.971 + 1399.130X_{2180} + 4260.033X_{1680} - 2459.097X_{1685}$ | 0.861 | 0.858 | 0.403 |
| $X = \sqrt{R}$ | $Y = 2.661 + 38552.8X_{1605} - 40731.4X_{1605}$ | 0.842 | 0.837 | 0.432 |
| $X = R'$  | $Y = 1.891 + 5024.556X_{1644} + 941.121X_{2197}$ | 0.789 | 0.782 | 0.500 |
| $X = R''$ | $Y = 2.305 + 13830.69X_{1687} + 52867.66X_{1725} - 35305.5X_{1629}$ | 0.754 | 0.748 | 0.537 |

### 3 Conclusion

(1) In the studied 350–2 500 nm wavelength range, the absorption peak of SOM does not exist. However, in the range of wavelength, spectral reflectance is negatively correlated with SOM content, and the highest correlation is near 675 nm. The results are consistent with the previous study\[14\], considering that SOM is negatively 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 \(1/\log R\) was inefficient for detecting SOM content. It cannot increase the correlation between spectral indicator and SOM content, but decrease their correlation. All the other transforms, such as reciprocal, logarithm, square root and difference, improve sensitivity to SOM content to different extents. The transform type of \((\log R)^{'}\) is the most significant among them. The logarithmic transform of reflectance reduces the effects of multiplicative factors induced by the changes of illumination conditions. However, it is insufficient to only perform logarithmic transform; the differential treatment is also needed to obtain better effect. Spectral differential technique can partially eliminate atmospheric effect; especially, the first order differential treatment can remove the effects of partially linear or approximately linear background and noise spectra on objective spectra.

(3) Overall, before performing the differential transform, the detecting ability of SOM content at visible light wavebands is stronger than that of bands, and the most sensitive band is near 675 nm; while after the spectral differential transform, the infrared bands become more sensitive, and the correlation coefficient between \((\log R)^{'}\) and SOM content is as high as 0.89 at 2 187 nm position, the maximum among the congeneric correlation coefficients.

(4) The optimal model for predicting SOM content is the regression equation composed with \((\log R)^{'}\) value at 849 nm, 1 681 nm and 2 187 nm wavebands as independent variables:

\[
Y = 1.772 + 1 \times 0.04071X_{2187} + 2 \times 893.272X_{849} - 1 \times 682.915X_{1681}
\]

Here, \(X = (\log R)^{'}\), \(Y\) is SOM content (%). The Adjusted \(R^2=0.885\) and \(RMSE=0.36\). It is the best 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, they are in essence selecting differential transforms for the logarithm of reflectance as variables. It is 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 prove this point.

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