Study on Hyperspectral Characteristics and Content Estimation of Soil Iron Oxide

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Abstract. The iron oxide in the soil comes from the re-deposition of the weathering products of the parent material. It can be divided into free iron oxide (Fed) and amorphous iron oxide (FeO) according to chemical methods. The content of iron oxide in soil can be used as the soil type in soil system classification. Diagnostic indicators are considered to be a function of soil development and development. Although the traditional method for measuring iron oxide in soil has high precision, it is time-consuming and laborious, and it is impossible to obtain real-time monitoring data of soil physical and chemical properties in time. Hyperspectral remote sensing technology can quickly obtain the spectral information of soil by using hyperspectral instrument, combine the chemical data measured indoors with the physical model to establish the relationship between soil properties, realize the quantitative estimation of soil information, and have the tradition of rapid and current situation. The unparalleled advantages of soil iron oxide measurement methods provide broad application prospects for understanding soil iron oxide spectral information and its content prediction.

1. Introduction
The iron oxide in the soil comes from the re-deposition of the weathering products of the parent material. The iron oxide is chemically distinguished, including free iron oxide (Fed) and amorphous iron oxide (FeO). The ratio of amorphous iron oxide content to free iron oxide content can Characterize the activation degree of iron oxide [1, 2]. The content of iron oxide in soil can be used as a diagnostic indicator for determining soil type in soil system classification. At the same time, the quantity and shape of iron oxide in soil have significant influence on the physical, chemical and mineralogical properties of soil, often as a process of soil formation and formation. The reflection of the soil environment is considered to be a function of soil occurrence and development [3, 4]. Although the traditional method for measuring iron oxide in soil has high precision, it is time-consuming and laborious, and it is impossible to obtain real-time monitoring data of soil physical and
chemical properties in time. Hyperspectral remote sensing technology can quickly obtain the spectral information of soil by using hyperspectral instrument, combine the chemical data measured indoors with the physical model to establish the relationship between soil properties, realize the quantitative estimation of soil information, and have the tradition of rapid and current situation. The unparalleled advantages of soil iron oxide measurement methods provide broad application prospects for understanding soil iron oxide spectral information and its content prediction.

Previous studies have shown that iron oxides in soil have a great influence on the spectrum of the visible-near-infrared region, especially for the visible region, but for the near-infrared region, its presence will result in reflectivity throughout the band. Falling shows that iron oxide is an important factor affecting the hyperspectral properties [5, 6]. The parent material is the material basis of soil formation. The soil iron oxide is derived from the re-deposition of the weathering products of the parent material, and its content is greatly affected by the parent material. Using hyperspectral techniques to model and predict soil iron oxide content, soils with the same parent material should be considered. Only by determining the soil parent material and its mineral composition in the study area can a more accurate prediction model of iron oxide content be established.

2. Materials and methods

2.1. Soil sample collection
The tested soil samples were naturally air-dried in the room to remove impurities and passed through a 2 mm hole sieve for use. 10 g of the soil which has been sieved through a 2 mm sieve is ground and passed through a 0.149 mm sieve for the determination of iron oxide content in the soil. The content of iron oxide in soil was determined by inductively coupled plasma emission spectrometer (ICP-OES) using sodium dithionite-sodium citrate-sodium bicarbonate (DCB) leaching iron (Fed) and ammonium oxalate leaching iron (Feo).

| Statistical indexes | Max (g/kg) | Min (g/kg) | Mean (g/kg) | Standard deviation |
|---------------------|------------|------------|-------------|--------------------|
| FeO                 | 55.15      | 2.06       | 22.24       | 14.45              |

2.2. Spectral data determination
Soil reflectance spectroscopy was performed in the field using a high-density reflective probe equipped with an ASD Field Spec HR spectrometer. The wavelength range of the spectrometer is 350 ~ 2500 nm, the sampling bandwidth is 1.3 nm (350 ~ 1000 nm) and 2 nm (1000 ~ 2500 nm), and the sampling interval is 1 nm. High-density reflective probes can effectively avoid the effects of soil stray light and eliminate the effects of weather. 2cm front view area can avoid the soil in the stone tablets, crop roots, etc., see the parameters shown in Table 2.

| Length             | 10"(25.4 cm) |
|--------------------|--------------|
| Quality            | 1.5 lbs      |
| Voltage            | 12 ~ 18 VDC, 6.5W |
| Type               | Halogen bulb/1500h |
| Temperature        | 2901 +/-10%K |
| Spot size          | 10mm         |
2.3. Spectral data processing
Use the Spectrometer's own Trek Manager software to view and store sample data, and export the data to third-party software ViewSpecPro for subsequent processing. At this time, the spectral curve still has certain noise and step, and different forms of spectral processing are needed. The commonly used processing includes the elimination of outliers, spectral enhancement, spectral smoothing and denoising. This study uses Savitzky-Golay convolution smoothing (SG); first derivative (FD); second derivative (SD); standard normal variable transformation (SNV); continuum removal (Continuum Removed, CR); multiple scatter correction (MSC) and other processing methods.

3. Results and analysis
Partial least squares regression (PLSR): is a bilinear model widely used in visible-near-infrared spectroscopy and modeling. The algorithm is based on least squares (LS). Partial least squares regression combines information synthesis with screening techniques. Instead of directly considering the regression modeling of the set of dependent variables and the set of independent variables, it extracts several new comprehensive variables that have the best explanatory power for the system. Then they are modeled by regression. Regression modeling, data structure simplification, and correlation analysis between two sets of variables can be realized at the same time. The basic functions of the three analytical methods, principal component analysis, canonical correlation analysis and multiple linear regression, are integrated. The partial least squares method can avoid potential problems such as non-normal distribution of data, uncertainty of factor structure and inability to identify models. It solves the problem that the number of samples is less than the number of variables and multi-collinearity. Combine compression with regression while reducing spectral dimensions.

3.1. Analysis of Spectral Characteristics of Different Iron Oxide Contents
All soil samples were graded for iron oxide content, ie, the free iron content values were between 2.06~6.49, 6.62~12.27, 15.58~26.50, 26.54~34.75, 35.33~55.15 g/kg, respectively; the amorphous iron content was 0.32~4.32, 4.48~6.54, 6.67~8.43, 8.69~10.48, 11.59~38.33 g/kg. Then, the soil spectral curves in each level range are averaged to obtain a hyperspectral reflectance average curve under different iron oxide contents. All soil spectral data are imported into ENVI5.3 for continuum removal. The continuum curve can effectively amplify the absorption valley and the reflection peak, better reflect the spectral absorption characteristics, highlight the small changes in the position and shape of the absorption band, and return them. One to a consistent spectral background facilitates numerical comparison with other spectral features to extract feature bands.

3.2. Correlation analysis of soil TN and reflectance
After Savitzky-Golay convolution smoothing, the absolute value of the overall correlation coefficient is relatively small. In the 608~831nm, 989~1241nm band, the free iron content is significantly positively correlated with the reflectivity. The maximum correlation coefficient is in the 747nm band, only 0.324. After the first-order differential treatment, the free iron content is significantly positively correlated with the reflectivity in the 536~633nm and 656~735nm bands. In the 764~882nm, 1266~1387nm, 1652~1846nm, 2100~2202nm band, free iron the content was significantly negatively correlated with the reflectance, and the maximum correlation coefficient was 0.646 at 585 nm. After the second-order differential processing, the correlation coefficient jumps greatly, and the maximum correlation coefficient is in the 2187 nm band, which is -0.529. After the standard normal variable correction treatment, the correlation coefficient jumps greatly, and the maximum correlation coefficient is in the 2187 nm band, which is -0.529. After the standard normal variable correction treatment, the free iron content was significantly negatively correlated with the reflectance in the 467~547nm and 1862~2450nm bands. In the 588~831nm and 962~1375nm bands, the free iron content and reflectivity were significantly positive. Correlation, the maximum correlation coefficient is 0.655 in the 1153 nm band. After continuum removal treatment, the free iron content was significantly positively correlated with the reflectance in the bands of 611~736nm and 2112~2128nm, in the range of 400~553nm, 853~977nm, 1360~1587nm, 2138~2260nm, 2353~2396nm. The free iron
content was significantly negatively correlated with the reflectance, and the maximum correlation coefficient was in the 1380 nm band, which was -0.467.

3.3. Comparison of hyperspectral response bands of soil iron oxide

The maximum correlation coefficient after all treatments was significantly correlated at the 0.01 level. The best treatment for the correlation between free iron content and each wavelength is the multi-scattering correction CA method for the original spectrum, with a correlation coefficient of 0.667. The best correlation between the amorphous iron content and the respective wavelengths is the multi-scattering correction FM method for the original spectrum, with a correlation coefficient of -0.587. The best treatment method for iron oxide is to use the multi-scatter correction method. However, free iron is the multi-scatter correction CA method, and amorphous iron is the multi-scatter correction FM method. Therefore, based on the above research, the use of free iron (Fed) is diversified. The scatter-corrected CA method, amorphous iron (Feo) uses a multi-scatter correction FM method.

| Types of spectral parameters | (Fed) | (Feo) |
|-----------------------------|-------|-------|
|                            | Maximum positive correlation wave (nm) | Correlation coefficient | Maximum positive correlation wave (nm) | Correlation coefficient |
| SG                          | 747   | 0.324** | 2203   | -0.421** |
| FD                          | 585   | 0.646** | 1280   | -0.446** |
| SD                          | 2187  | -0.529** | 1882   | 0.538** |
| SNV                         | 1153  | 0.655** | 518    | -0.518** |
| CR                          | 1380  | -0.467** | 2451   | 0.327** |

4. Conclusion

(1) The spectral curve of soil iron oxide is in the range of 400–780nm, and the reflectivity increases with the increase of wavelength; in the range of 780–1300nm, the reflectivity decreases slowly and then rises sharply; in the range of 1400–1860nm, the reflectance curve It tends to be flat; in the range of 1920–2450nm, there are two repeated increases and then decreases in reflectivity. The absorption and reflection characteristics of the iron oxide spectral curve are mainly concentrated in the range of 400–1100nm. The specific response bands are concentrated in the reflection peaks and absorption valleys near 420nm, 480nm and 910nm. The magnitude of the reflection peak or absorption valley is related to the content of iron oxide.

(2) The reflectance of the original spectral data in the spectral range of 400–2450 nm after SG convolution smoothing, first-order differential, second-order differential, standard normal variable correction, continuum removal, and multi-scatter correction, respectively, and corresponding soil oxidation Correlation analysis of the iron content by band was performed, and the correlation was significantly enhanced, and both were significantly correlated at the 0.01 level. The best treatment method for the correlation between soil iron oxide content and each wavelength is to perform multi-scatter correction processing on the original spectrum. But the best way to improve correlation is not necessarily the best way to model

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