Inversion of soil heavy metals in Guanzhong area of Shaanxi based on VIS-NIR spectroscopy

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Abstract. This study takes soil Cr, Mn, Ni and Cu from the Guanzhong area as the research object. Using the ASD Fieldspec4 spectrometer to acquire soil spectra and perform different forms of data transformation, and partial least squares regression (PLSR) method was used to establish the calibration-validation model. The results indicated: (i) after the differentiation of the spectrum and the transformation of MSC, NOR, SNV, etc., the signal response strength is enhanced; (ii) The determination coefficients of Cr, Mn, Ni, and Cu are 0.7002, 0.7852, 0.6857, and 0.8036, respectively; (iii) The results show that the spectral predictive model have quickly obtain the distribution of heavy metals in the study area.

1. Introduction

Soil is a layer of loose matter on the surface of the earth. It is composed of various granular minerals, organic matter, water, air, microorganisms, etc., and can grow plants [1]. With the development of human society, agriculture and agriculture, and the development of urbanization, human factors have caused heavy metal pollution in the soil, which is an environmental problem that cannot be ignored in the world today [2], [3]. Heavy metals are mostly non-ferrous metals, which are widely used in human production and life, and are accompanied by serious environmental pollution that emphasizes metals [4]. The development and smelting of colored heavy metal deposits is the most important source of pollution for the discharge of heavy metals into the environment. Industrial and mining enterprises that discharge heavy metals into the environment, such as mining, mineral processing, metallurgy, electroplating, electrician, dyes, textiles, and oil refining. Traditional heavy metal detection methods are time consuming and laborious, and are prone to environmental pollution.

However, with the continuous development of spectroscopy, Domestic and foreign scholars based on soil reflectance spectral features, combined with multivariate statistical methods to establish predictive models, combined Vis-NIR spectroscopy with soil heavy content has been widely. Kemper inverts the content of As, Hg and Pb in the soil of the mining area by using reflectance spectroscopy.
Moros et al. established the relationship between heavy metals and organic matter through soil spectroscopy, and established a partial least squares prediction model based on Vis-NIR to build the monitoring of metals in the study area.

Soil heterogeneity due to large differences in soil and time, different soil parent materials and soil use types, soil pollution levels are different. Therefore, the spectral response of the soil is different. Based on the above research, a total of 44 soil samples from the Guanzhong area of Shaanxi Province were collected. Chemical methods were used to obtain heavy metal content in the soil and spectrometers were used to measure spectral reflectance. Combined with different differential forms of the spectrum, SNV, MSC, NOR

Based on the above research, chemical methods were used to obtain heavy metal content in the soil and spectrometers were used to measure spectral reflectance. Combined with different differential forms of spectra, SNV, MSC, NOR for spectral feature enhancement, PLSR was used to establish a heavy metal inversion model in the study area.

2. Materials and methods

2.1. Soil sample collection

The study area is located in the Guanzhong area of Shaanxi Province (Fufeng, Yangling, Wugong), and the main soil type is bauxite. At the time of sampling, the position of the sampling point is recorded using the Global Positioning System. A total of 44 soil layers (about 1 kg) were collected from the soil surface, and the debris such as gravel and roots were removed. After air drying, the sieve was passed through a 0.149 mm sieve. The samples were separated by a quarter method, one for the acquisition of indoor heavy metal content and one for the collection of spectral data.

| Element | Max (mg/kg) | Min (mg/kg) | Mean (mg/kg) | SD (mg/kg) |
|---------|-------------|-------------|--------------|------------|
| Cr      | 20.0        | 16.1        | 18.0         | 0.96       |
| Mn      | 310         | 249         | 274          | 13.60      |
| Ni      | 14.1        | 11.0        | 12.8         | 0.71       |
| Cu      | 8.4         | 6.4         | 7.3          | 0.46       |

2.2. Spectral data determination and preprocessing

Soil spectra were acquired using an ASD Field spec4 spectrometer with a spectral range of 350-2500 nm and a resolution of 1 nm. Use high-density probes when measuring soil. In order to reduce spectral noise, the spectral signal-to-noise ratio is improved. In this study, SG convolution smoothing, FD, SD, absorbance are used to reduce the influence of noise, and at the same time, the response characteristic band of heavy metals is obtained.

3. Results and analysis

3.1. Correlation Analysis

Correlation is significantly improved after multiple forms of transformation of heavy metal reflectance spectra compared to the original spectral correlation, Results are shown in Figure 1. The results show that after the FD and SD of the spectroscopy, the correlation effect is the best, and the FD optimal. Similarly, the correlation coefficients of Mn, Ni and the FD were all significantly correlated, and the values were 0.76 and -0.63, respectively. The correlation coefficients of Cr, Cu, and SD were -0.61 and -0.65, respectively.
Figure 1. Correlation coefficient between nine heavy metals and reflection spectra and their different transformations

3.2. Model establishment and comparison
Using PLSR to establish four prediction models for heavy metals with different transformations, including R, FD, SD, and Abs. The best calibration and validation accuracy of heavy metals Cr, Mn, Ni and Cu in all optimal PLSR models are 0.7002, 0.7852, 0.6857, and 0.8036, respectively. By comparing, the chemistry values and predicted of Hg has good regression results. According to the statistic results, the best PLSR of four heavy metal elements is ranked: Cu > Mn > Ni > Cr.

4. Conclusion
The different forms of transformation of the original spectrum enhance the spectral response. At the same time, the characteristic band of the element can be obtained after correlation analysis with the element content. The heavy metal inversion model established in this study can be well applied to this study.

Acknowledgments
This work was financially supported by the Fund Project of Shaanxi Key Laboratory of Land Consolidation (2018-TD02) and Pre-research project (2019-NBYY-03). We gratefully acknowledge the Institute of Land Engineering and Technology, Shaanxi Provincial Land Engineering Construction Group, Xi’an, China.
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