**Evaluation of the effects of continuum removal on the accuracy of mineral spectral unmixing models**

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**ABSTRACT：**Precise abundance estimation of mineral composition is a tough problem, and spectral unmixing is no doubt one of the possible solutions to it. Spectral mixing model for minerals could be complex, and proper choice of unmixing model is essential for improvement of spectral unmixing accuracy. Continuum Removal (CR) is a commonly used spectroscopy analysis method, but also has been used in non-linear spectral unmixing applications. However, there has been little research on the effects of continuum removal on spectral unmixing models. In this paper, Linear Model and Non-linear Model of CR are applied in laboratory mineral powder spectra. Results show that for mineral powder mixture, CR Model could achieve much higher accuracy than Linear Model. So for dust covered surface of Moon or Mars, CR Model could have great potenial.

**1. INTRODUCTION**

Spectral unmixing is an effective tool for hyperspectral data, which could decompose a mixed pixel into a collection of constituents, or endmembers[1]. In geology remote sensing, spectral unmixing could be utilized to achieve the precise composition and distribution of minerals, which is widely used in satellite data, airborne data, field data, and core data[2,3].

Continuum Removal (CR) is a commonly used spectroscopy analysis method[4], but could also be applied in spectral unmixing as a pre-processing step. In geology research, continuum removal has been widely used in mineral abundance mapping on Earth [5], the Moon [6], Mars [7], etc.

Until now, little research has been done on the accuracy evaluation of non-linear unmixing models based on CR. In this paper, we will carry out spectral unmixing experiments on laboratory mineral mixtures. By comparison of the spectral unmixing accuracy and the reconstruction error, the effects of continuum removal on mineral spectral unmixing models will be evaluated.

**2. MATERIALS AND METHODS**

**2.1 Laboratory experimental data**

In the experiment, plaster and allochite samples were crushed into a powder, and a set of mixtures of different proportions were made, with accurate measurements taken using an electronic balance and graduated cylinder. The mineral mixture scheme is shown in Table 1.

**Table 1** Mineral mixture abundance

|  |  |  |
| --- | --- | --- |
| Mixture No. | Plaster | Allochite |
| 1234567 | 5%10%30%50%70%90%95% | 95%90%70%50%30%10%5% |

A SVC HR-1024 Hand-held Spectrometer covering the UV, visible, and NIR wavelengths from 350 nm to 2500 nm was used to measure the in situ reflectance with a 25° field of view at a distance of 1 m above the species. The spectral reflectance was calculated as the ratio of measured radiance to the radiance from a white standard reference panel. The spectral reflectance data were obtained between 9:00 pm and 12:00 pm, under dark conditions. To facilitate the subsequent derivation, the original reflectance spectra were resampled to 1-nm intervals.

**2.2 Methods**

Before spectral unmixing, we perform continuum removal, log operation and their combination on the data set to see their effects on the spectral mixing model. In order to compare the model accuracy, radiation transferring model of Hapke is also introduced and performed. For laboratory spectra and airborne hyperspectral image, different strategies of spectral unmixing and accuracy evaluation methods are used.

2.2.1 Continuum removal (CR)

The continuum is a function of nonselective absorption and scattering as well as broad wavelength selective absorptions [8]. These spectral properties define the continuum of a spectrum and are partially controlled by the physical properties of the surface (particle size, roughness, texture, etc.) and the chemical composition of the material [9]. Usually, the continuum is a convex hull fitted over the top of the spectrum. It consists of line segments connecting local maxima of the reflectance spectrum. The continuum removal spectrum is realized by using the following formula:

  (1)

where is the spectrum for which the continuum is removed, is the reflectance spectra, and  is the spectra continuum.

2.2.2 Fully Constraint Least Square (FCLS)

In the Linear Mixing Model (LMM), the reflectance of a pixel in each spectral band is expressed as a linear combination of the reflectance spectra of its component endmembers weighted by their proportions within the pixel [10]. When N endmembers exist, each having L bands, the LMM is expressed as

 (2)

where x is the pixel spectrum vector,  is the  matrix whose columns are the  endmembers, , ,  is the  fractional abundance vector whose entries are , , and  is the  observation noise vector. (spectral unmixing)

Usually, the LMM is subject to two constraints on the entries of . To be physically meaningful, none of the proportions should be negative (i.e. ). Secondly, the proportions should sum to unity (i.e. ). As for laboratory experimental data used here, the endmembers are fixed, so the above two constraints should be met and are added to the solving process.

**2.3 Workflow**

The workflow of laboratory is shown in Figure 1. To fully investigate the effects of CR, we set 2 conditions of pre-processing for the original reflectance data: CR and no processing at all (Linear Mixing Model). Then the processed data will be the input of FCLS, through which we could get the abundance estimation. Based on the estimated abundance and real abundance, unmixing accuracy evaluation will be carried out; meanwhile the mixing reconstruction error will be also calculated. Finally, based on the above results, the effects of the pre-processing methods will be comprehensively assessed.

**Figure 1.** The Workflow of Laboratory Data



**2.4 Accuracy assessment**

For the unmixing accuracy estimation, RMSE is used as the following formula:

 (3)

where  is the fraction residual error of each mixture, and  is the number of mixtures.

For the reconstruction error calculation, in order to eliminate the scale effects, NRMSE is introduced

 (4)

where  is the residual error at each wavelength, n is the number of wavelength,  is the highest value of all bands, and  is the lowest of all.

**3 RESULTS AND DISCUSSION**

**3.1 Unmixing accuracy estimation**

**Table 2** Results of abundance estimation of plaster

|  |  |  |
| --- | --- | --- |
| Mixture No. | Linear Model | CR Model |
| 1234567 | 0.03320.06730.19630.33670.52970.77660.8580 | 0.04850.10610.32180.51930.73290.89540.9445 |
| RMSE | 0.1143 | 0.017 |

The estimated abundances are shown in Table 2. As we perform FCLS on binary mixtures, the sum of abundance is one, and plaster and allochite share the same RMSE. So only the results for plaster are shown in Table 2. For Linear Model, the estimated abundances are far less than the actual values, and the RMSE is higher than 10%. This strongly indicates that Linear Model is not suitable for mineral powder mixtures. On the other hand, CR Model has very high accuracy, with RMSE less than 1.8%. This indicates that CR could effectively improve the accuracy of mineral spectral unmixing results.

**3.2 Reconstruction accuracy estimation**

The reconstructed spectra of the 2 models are shown in Figure 2. Comparing with the real spectra, we can distinguish the difference between them, and make estimation of the unmixing models. For Linear Model, the difference is mostly obvious, espectially when the fraction of the endmebers are equal. While for CR Model, the results are similar, hard to tell from visual directly.

**Figure 2.** The Reconstructed Spectra and Real Spectra of Laboratory Mineral Powders

(1st line: Linear Model; 2nd line: CR Model)





**Table 3** Comparison between reconstruction error and abundance estimation error

|  |  |  |
| --- | --- | --- |
|  | Linear Model | CR Model |
| NRMSE | 0.1122 | 0.062 |
| RMSE | 0.1143 | 0.017 |

To fully analyze the relationship between reconstruction error and abundance estimation accuracy, we also calculated the results of reconstruction error, and make a comparison between spectral unmixing accuracy and reconstruction error (shown in Table 3). Unsurprisingly, Linear Model has much higher reconstruction error than CR Model. However, the difference of reconstruction error between Linear Model and CR Model is not as obvious as unmixing accuracy. The intensity of CR spectra has no correlation with the original intensity, so the linear mixing results of CR spectra do not have clear physical meaning, which could explain the relatively poor performance of CR in reconstruction error. But CR could effectively extract the diagnostic absorption features, and the strength of absorption features has close relationship with the abundance of endmembers [11]. So although the modeled spectral of CR is not totally coincident with the actual mixing spectral at all wavelengths, which may be limited by the inaccurate definition of continuum, but near absorption features, the fitting result is very good (As is shown in Figure 2), and this special character ensured a high spectral unmixing accuracy.

**4 CONCLUSIONS**

The spectral mixing models for minerals can be quite complex and varied. Although CR has been used in mineral spectral unmixing, but little research has been done on its effects on the accuracy of spectral unmixing models. This paper carried out experiments on laboratory mineral mixtures based Linear Model and CR Model, and try to build a comprehensive accuracy evaluation system for them. The following conclusions are achieved:

1 For mineral powder mixture, continuum removal could effectively improve the spectral unmixing accuracy;

2 For mineral powder mixture, continuum removal could improve the reconstruction accuracy, although not very obviously;

3 CR Model has great potential for mineral spectral unmixing, especially for powder mixture, which is a close analogy of the surface of Moon or Mars;

In this passage, we only carried out experiments on laboratory powder mixtures. In future research, more types of mineral mixture will be dealed with, including airborne hyperspectral data, core imaging

spectrometer data, Lunar or Mars hyperspectral data, etc. A more comprehensive solution to mineral spectral mixture analysis will be available.

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