#### Review and categorization of spectral processing methods

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Abstract. In this paper numerous known spectral analysis methodologies available to geologic remote sensing are reviewed. According to their requirement for reference data, the techniques are categorized into knowledge-based (KB) or data-driven (DD) approaches. The two categories are comparatively studied and their advantages, disadvantages, and major geologic outcomes are emphasized. Next ways to bridge between the spectral data and geochemical, mineralogic, and lithologic information are noted. Subsequently present and potential hybridization lines among the groups and sub-groups are discussed and at the end the challenges that spectral processing methods should meet are pointed out. In conclusion, hybridization of the two categories is proposed to be one of the lines of attack to yield the most robust processing methodologies, capable of fulfilling the demands of multi- and hyperspectral geological remote sensing.

Keywords: mineral mapping, algorithm, multispectral, hyperspectral, geologic remote sensing.

#### **1. Introduction**

Spectral processing (also known as spectral analysis) refers to "the extraction of quantitative and/or qualitative information from remotely sensed reflectance (or emittance) spectra based on the albedo- and wavelength-dependent properties of the material" (Mustard and Sunshine, 1999). It encompasses all the techniques proposed for detection, classification, identification, and quantification of materials in a given hyper- or multispectral scene (Chang, 2003; Schott, 2006).

There are several seminal review papers devoted to the topic of spectral analysis and geologic remote sensing (Bioucas-Dias et al., 2012; Cloutis, 1996; Keshava and Mustard, 2002; van der Meer et al., 2012). They are typically focused on the application of remote sensing in geology, or intensive in algorithm designs on spectral unmixing, or are not comprehensive and up to date. None of these reviews provide a categorization scheme for the vast spectral processing methodologies, nor study them in a comparative manner.

Methods can be grouped according to their date of emergence, (traditional, vs. advanced), presumed randomness (parametric, vs. non-parametric), the type of data it is applied to (multispectral vs. hyperspectral), the way pixels are treated (hard vs. soft classification), and the need for training data (supervised vs. unsupervised) (Landgrebe, 2003; Lu and Weng, 2007; Richards and Jia, 2006; Schott, 2006; Schowengerdt, 2007; Tso and Mather, 2009).

The bases in which a technique requires reference data or not to perform spectral processing is used here to establish the categorization. In the case of no reference data, the method is usually able to directly make use of spectral patterns available in a pixel spectrum. In contrast, there are those techniques that try to describe the spectral content of a pixel according to some predefined representative facts known as reference data, or endmembers. This initial difference gives rise to two distinct categories for the spectral processing methods: the knowledge-based approach (KBA), and the data-driven approach (DDA). Here we attempt to review and compare spectral processing methods that fall in both categories.

#### 2. Knowledge-based approach

KBA incorporates user knowledge about the spectral behavior of minerals to extract meaningful mineralogical information from individual spectrum. The building block of KBA is the distinct and diagnostic absorption features (position, depth, symmetry, and width) of different materials (Clark, 1999; Mustard and Sunshine, 1999; van der Meer, 2004). Here we have sorted out the methodologies into five different groups (Fig. 1).

#### 2.1 Band calculation

Band calculation intends to give an estimate of the gradient in the absorption feature using basic math operations. Band ratio (BR) uses the difference in reflectance between an absorption band and one of its shoulders (Goetz and Rowan, 1981), while relative absorption band-depth (RBD) uses an average of several channels (Crowley et al., 1989). Principal component analysis (PCA) makes use of the same spectral gradient, by projecting selected four bands into a new orthogonal space (Loughlin, 1991), whereas least-squares fitting (LS-Fit) predict the trend by polynomial modeling (Green and Craig, 1984).

The derivative of a spectrum involves the calculation of reflectance variation relative to the wavelength. In geology, derivative analysis (DA) is exploited for deriving parameters like band position and bandwidth from absorption features (Huguenin and Jones, 1986).

#### 2.2 Feature mapping

Generally every spectrum consists of three basic components: a continuum, absorption bands; and noise. To isolate the absorption, many KB methods require the continuum to be removed. For continuum removal (CR), a convex hull is fitted over the top of the spectrum using straight line segments, and then the original spectrum is divided to it (Clark and Roush, 1984; Kruse et al., 1993b). The continuum is also commonly removed in logarithmic reflectance ordinate (Sunshine et al., 1990).

The detection of absorption is the first step towards its quantification. Traditionally, this has been implemented manually, but there are now a number of algorithms for automatic absorption detection. The most popular is the DA (of different orders), which makes use of the depth in the spectrum (Huguenin and Jones, 1986). Also scale-space methods, such as spectral fingerprints (SFP) and maximum modulus wavelet transform (MMWT), are used to recover the inflection points related to the absorption (Hsu, 2003; Piech and Piech, 1990).

The shape and wavelength of absorbing bands is correlated to the mineralogical content a sample/target and its chemistry (Clark, 1999; Clark and Roush, 1984). Typically the abundance of a mineral is quantified by calculating the depth of its diagnostic absorption feature relative to the continuum background (Clark and Roush, 1984; Cudahy et al., 2008), whereas the compositional variation is attributed to the shifts in wavelength position. Methods like fitted polynomial (FP) are used for quantifying them (Cudahy et al., 2008).

In contrast, curve fitting techniques, such as the modified Gaussian model, strive to deconvolve the whole spectrum into three noted components (Sunshine et al., 1990).

#### **2.3 Expert systems**

The philosophy behind expert systems (ES) is to automate the process of mineral identification. This is achieved either by logical operator (LO) (Mars and Rowan, 2006) and decision tree (DT) partitioning techniques (Tso and Mather, 2009), or by systems that try to mimic human experts (Cudahy et al., 2008; Kruse et al., 1993b).

## 2.4 Wavelet analysis

Wavelet analysis (WA) decomposes a spectrum into a series of shifted and scaled versions of the mother wavelet function. Therefore narrow absorption features will be captured by low-scale and the continuum by higher scale wavelet components (Rivard et al., 2008).

#### 2.5 Scattering theory

Radiative transfer equation is suggested for describing the scattering behavior of light from particulate media. An approximate analytic solution to this equation is provided by what is

called scattering theory. The most popular of them are Hapke (Hapke, 1981), iso-grain (Hiroi and Pieters, 1992), and Shkuratov scattering theories (Shkuratov et al., 1999).



Figure 1. Taxonomic tree of the spectral processing methods as proposed and discussed in this paper. Abbreviations are given along the text.

### 3. Data-driven approach

DDA depends on reference data (spectra) to perform the processing. We have assigned the algorithm into two broad categories named "per-pixel", and "sub-pixel" (Fig. 1). The former compares each reference spectra to unknown pixels based on similarity metrics, statistics, or least-squares estimation, whereas the latter resolves pixel's content by multiple endmembers.

## 3.1 Similarity-based group

The spectral similarity techniques strive to find a measure of mathematical or physical similarity between a known reference spectrum, x, and unknown test (target) spectrum, y. There are a large number of methods in this group including binary encoding (BE), spectral angle mapper (SAM) (Kruse et al., 1993a), Euclidean distance (ED), spectral distance (SD) (Combe et al., 2005), spectral correlation mapper (SCM) (Carvalho Junior and Menezes, 2000), cross-correlogram spectral matching (CCSM) (van der Meer, 2006), as well as the spectral information divergence (SID) (Du et al., 2004). There are also algorithms like spectral similarity mapper (SSM), in which two measures are combined to generate a hybrid method.

#### **3.2 Least squares-based group**

Least squares regression techniques attempt to model dependent variables by the means of an independent variable. Spectral feature fitting (SFF) is a linear regression, whereas partial least square regression (PLSR) inherits features from PCA and multiple regression (Esbensen, 2006).

## 3.3 Training-based group

Traditional training-based classifiers aim to cluster the imagery by comparing the test spectrum with the training classes using a statistical criteria like the minimum distance (MD), Mahalanobis distance (MHD), and maximum likelihood (ML) (Landgrebe, 2003).

## 3.4 Learning-based group

Artificial neural networks (ANN) has the ability to learn the relationship between a set of example patterns, and then apply it to new input patterns (Mas and Flores, 2007). In remote sensing, ANN has been used as a supervised hard and soft classifier (Mas and Flores, 2007). Similarly support vector machines (SVM) draw on statistical learning theory for pattern recognition (Vapnik, 1998). Another non-parametric technique to note here is a variant of DT

known as random forests (RF), which is demonstrated to have superior performance (Cracknell and Reading, 2014).

## **3.5** Geostatistics-based group

Indicator kriging (IK) is the only geostatistical method in use for image classification and the extraction of absorption features for mineral mapping purposes (van der Meer, 1994).

## **3.6 Partial unmixing group**

In many applications, it is not essential to fully decipher a pixel's content, instead the aim is to detect the features of interest in an unknown background (Chang, 2003). Target detection algorithms include matched filtering (MF) (Boardman et al., 1995), constrained energy minimization (CEM) (Chang et al., 2000), orthogonal subspace projection (OSP) (Harsanyi and Chein, 1994), and adaptive coherence estimator (ACE) (Kraut et al., 2005), and mixture tuned matched filtering (MTMF) (Boardman, 1998).

## **3.7 Full unmixing group**

Full unmixing methods attempt to linearly decompose the pixel spectrum into a collection of deterministic endmembers and estimate their corresponding abundance (Adams et al., 1986). Linear spectral unmixing (LSU) (Boardman, 1989), independent component analysis (ICA) (Nascimento and Bioucas Dias, 2005), SVM (Camps-Valls and Bruzzone, 2009), Bayesian model (BM) (Dobigeon et al., 2008), ANN, and genetic algorithm (GA) are specifically adapted for unmixing process. To account for pixel-scale variability, iterative unmixing algorithms, including multiple endmember spectral mixture analysis (MESMA) (Roberts et al., 1998), iterative spectral unmixing (ISU) (van der Meer, 1999), iterative spectral mixture analysis (ISMA) (Rogge et al., 2006), simulated annealing (SA) (Debba et al., 2006), and endmember bundles (EB) (Bateson et al., 2000) have been developed.

# 4. The comparison of the approaches

KB and DD approaches originate from different disciplines, with dissimilar assumption and procedures. Nonetheless, both aim to decompose a multi- or hyperspectral signal into meaningful quantitative or qualitative geologic information. Accordingly it is possible to comparatively study them (table 1).

The KBA is physically-based and devised from concepts of spectroscopy. DDA is mathematically-based and relies on reference data for information extraction. It treats each pixel as a n-dimensional vector in feature space and attempts to model the "whole scene" variation by a set of endmembers. In contrast, KBA strives to describe the variation observed in a "single spectrum" through absorption band modeling in spectral space (Landgrebe, 2003). While the search for endmembers is automated in DDA, the detection of absorptions in KBA is mainly manual.

DDA properly implements both soft and hard classification and respectively yields "abundance image" and "thematic map" (Schott, 2006; Schowengerdt, 2007). The thematic map in geologic remote sensing includes a discriminated lithologic map obtained chiefly from the statistics-based algorithms. The abundance image, which represents the aerial fraction of an endmember in a pixel, is obtained from mixture-based category (Keshava and Mustard, 2002). The KBA in contrast is a soft classifier, because it pinpoints very specific spectral region for identification and/or quantification, hence raising the possibility for multiple mineral mapping using a single spectrum (Cudahy et al., 2008). Nevertheless where the absorption bands are overlapping, the KB algorithms are inevitably switched to a hard classifier. Generally, the conversion of KB methods into a hard classifier is challenging, because every case needs its own threshold, that is not always available, nor universal (Mars and Rowan, 2006). Other characteristics of the two approaches are summarized in table 1.

Parameter	approach	
	Knowledge-Based	Data-Driven
Domain	Spectral space (Spectral modeling)	Feature space (scene modeling)
Background theory	Spectroscopy (physical based)	Statistical/geometrical (mathematical)
Reference data	Not required	Is required
Input data	Reflectance/Emissivity	Reflectance/Emissivity /Radiance
Spectral band range	Partial (from 2-10 bands) MGM uses the full band	Full or partial
Feature selection criteria	Essential/Manual	Optional/ Interactive or automated
Treatment with pixels	Soft and hard	Hard and soft
Information unit	Absorption	Endmember/class
Required preparation	Absorption detection (assignment)	Endmember extraction/class definition
Preprocessing/normalization	CR (over the spectrum)	MNF, PCA, ICA (over the image)
Products	thematic maps, abundance image, composition and crystallinity maps	Thematic maps, abundance image
Main capability	Discrimination, classification, identification, quantification	Detection, classification, quantification
Abundance metric	Depth of absorption	Fraction of endmembers
Abundance quantity	Relative	Absolute
Sensitivity to noise	Very sensitive	Sensitive
Noise suppression	Spectral filters	Spatial/spectral filters
Error metric	Not available (except for MGM)	RMS error/ confusion matrix
	Simple, easy to execute, available to	More mature and robust, complicated,
Pros and cons	all, transferable between scales, less	expensive, unavailable, time
	robust results with MSI data	consuming

**Table 1.** A comparison between different aspects of KB and DD approaches.

### 5. Hybrid methods

It is a known fact that a particular combination of multiple perspectives helps develop a more robust algorithm (Landgrebe, 2003; Schott, 2006). The tangible benefits of hybridization have been the motivation for various inter-group crossbreeding. For example, the CR procedure is coupled with an unmixing-like routine called canonical variates analysis (CVA) to get better results during mineral quantification (Berman et al., 1999). Elsewhere, the hybridization between linear mixture models and similarity measures has given rise to optimized cross correlation mixture (OCCM) analysis (Coulter, 2006). OCCM match the entire shape of each pixel spectra to a linearly synthesized mixture of endmember spectra using the SCM method.

The most advanced and rigorous processing methodologies, however, are achieved when two completely different perspectives (e.g. physically- and mathematically-based approach) inter-breed. On this basis, we conceived two major hybrid species:

- i) Those that incorporate the spectroscopy and mixing theory to build spectral libraries.
- ii) Those that supplement a priori geological knowledge with mixture theory.

The core of the first species is a highly enriched spectral library and a decision making mechanism to compare the image spectra with. One of the first of this kind was developed by Kruse et al. (Kruse et al., 1993b). The most sophisticated and successful form is indeed the Tetracorder package developed by the US geological survey (Clark et al., 2003). In this system the spectral library is enriched by binary, and ternary mineral mixtures and then are grouped based upon spectroscopic similarities. Two metrics, the goodness of fit (R<sup>2</sup>), and the band depth (D), are calculated on the basis of continuum removed image and library spectra, and then are used within an intelligent expert system decision-making framework to identify and map the geologic materials (Clark et al., 2003; Swayze et al., 2014).

Another similar hybrid system are described by Roy et al. (Roy et al., 2009) for the modeling of mantle, and crustal rocks. The state-of-the-art methodology of the first species belongs to hypersensitive mineral identification method (HMIM) (Sanga and Tachikawa, 2006). HMIM develops a very sophisticated spectral library for processing ASTER multispectral imagery by

simulating mixtures of 13 minerals for every 10% abundance using the iso-grain model cited above.

In many geological applications (e.g. mineral exploration and rock type classification), the type of target minerals and their associations are usually predictable. This *a priori* knowledge can be involved within the spectral processing chain. On other words, unmixing can be performed using the geologic context. In spite of the possible theoretical framework, hybrid methods of second species is yet to be developed.

### 6. Discussion and conclusion

Generally, all the spectral mapping techniques in geologic remote sensing domain aim to retrieve information about lithologic, mineralogic, or chemical content of the target. Regarding the mineralogic content, there are few accounts of the absolute accuracy and precision of the algorithms used for abundance estimation. While errors as big as 30% are reported, there are methods that maintain the error of estimation within 5-15% accuracy (Berman et al., 1999; Keshava and Mustard, 2002). Spectroscopy affords a unique opportunity to directly detect rare earth elements (REE). In the scarce literature on the subject, band depth has been the only method in use for REE characterization (Huntington et al., 2012). The other major/minor elements are normally modeled or predicted indirectly using regression techniques (Cloutis, 1996; Swayze et al., 2014; Tappert et al., 2011).

The extraction of meaningful information from imaging systems largely depends on the spectral processing methods. Despite important algorithm developments in recent years, there is still no universal and optimal recipe (neither from the knowledge-based, nor the data-driven approach) for remote identification, classification, and quantification of minerals and rocks. We anticipate that the next generation of spectral processing methods would come from hybridization between different disciplines. As discussed here, the two approaches that yield promising hybrid algorithms are spectral and feature domains. One such hybrid method can be "similarity-based unmixing", or "simulation-tuned similarity measurements" algorithms. The successful Tetracorder package is a good example of the latter solution.

As noted, current unmixing algorithms are not sensitive to the type of spectra (minerals) they are unmixing. Such knowledge can supplement the unmixing procedure to predict the proper and probable combinations of endmembers present in each pixel, which subsequently leads to better abundance estimation. This is what we call "unmixing in the geologic context"; a discipline-oriented hybrid method of second species.

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