AN OVERVIEW ON HYPERSPECTRAL UNMIXING: GEOMETRICAL, STATISTICAL, AND SPARSE REGRESSION BASED APPROACHES

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ABSTRACT

Hyperspectral instruments acquire electromagnetic energy scattered within their ground instantaneous field view in hundreds of spectral channels with high spectral resolution. Very often, however, owing to low spatial resolution of the scanner or to the presence of intimate mixtures (mixing of the materials at a very small scale) in the scene, the spectral vectors (collection of signals acquired at different spectral bands from a given pixel) acquired by the hyperspectral scanners are actually mixtures of the spectral signatures of the materials present in the scene.

Given a set of mixed spectral vectors, spectral mixture analysis (or spectral unmixing) aims at estimating the number of reference materials, also called *endmembers*, their spectral signatures, and their *fractional abundances*. Spectral unmixing is, thus, a source separation problem.

This paper presents an overview of the principal research directions in hyperspectral unmixing. The paper is organized into six main topics: **i**) mixing models, **ii**) signal subspace identification, **iii**) geometrical-based spectral unmixing, **iv**) statistical-based spectral unmixing, **v**) sparse regression-based unmixing, and **vi**) spatial-contextual information. For each topic, we summarize what is the mathematical problem involved and give relevant pointers to state-of-the-art algorithms to address these problems.

1. MIXING MODELS

Spectral unmixing is an important problem in hyperspectral data exploitation. Depending on the mixing scales at each pixel and on the geometry of the scene, the observed mixture is either linear or nonlinear [1], [2]. Linear mixing holds when the mixing scale is macroscopic and the incident light interacts with just one material, as it happens in checkerboard-type scenes [4]. Nonlinear mixing holds when the light suffers multiple scattering involving different materials [5].

- In a linear mixing scenario, the acquired spectral vectors are a linear combination of the endmember signatures present in the scene, weighted by the respective fractional abundances. The exploitation of this model, in spite of its simplicity, has fostered a huge amount of research leading to a plethora of unmixing algorithms developed under the geometrical or the statistical frameworks.
- In a nonlinear mixing scenario, the model for the scattered light is much more complex than its linear counterpart. Radiative transfer theory (RTT) is a well established model for the transfer of energy as photons interacts with the materials in the scene. The core of the RTT is a differential equation describing radiance collected by the sensor. It can be derived via the conservation of energy and the knowledge of the phase function, which represents the probability of light with a given propagation direction be scattered into a specified angle solid around a given scattering direction.

In this work, we provide an overview of current trends and techniques for analyzing hyperspectral data using spectral unmixing. Although previous efforts exist in the literature [1], none of them have been specifically focused on recent developments in spectral unmixing techniques. Taxonomies of unmixing algorithms have also been investigated in recent collaborative efforts[1]. In the present contribution, we specifically focus on the linear mixing model. The reason is that, despite its simplicity, it is an acceptable approximation of the light scattering mechanisms in many real scenarios. Furthermore, the linear mixing model constitutes the basis of many effective unmixing algorithms. This is to be contrasted with the nonlinear mixing model, where the inference of the spectral signatures and of material densities based on the RTT is a complex ill-posed problem, relying on scene parameters often very hard to obtain. A way to sidestep these difficulties is to formulate unmixing as regression problem based, for example, on neural networks or on kernels, in which the model parameters are learnt in a supervised fashion from a collection of examples (see [6] and references therein). Anyway, there are particular situations in which a nonlinear model can be converted into a linear one, as it it is the case of the two-stream method [4].

[1]http://www.hyperinet.eu

2. SIGNAL SUBSPACE IDENTIFICATION

The number of endmembers present in a given scene is, very often, much smaller than the number of available spectral bands. Therefore, spectral vectors generally lie in a lower-dimensional (linear) subspace. The identification of this subspace enables a more compact representation of spectral vectors, thus yielding gains in computational time and complexity, as well as in data storage and *signal-to-noise-ratio* (SNR). Furthermore, several unmixing algorithms only work on the signal subspace requiring, therefore, signal subspace identification as a first processing step.

Some well-known signal subspace identification algorithms are the *maximum noise fraction* (MNF) [7], the *noise adjusted principal components* (NAPC) [8], the *hyperspectral signal identification by minimum error* (Hysime) [11], the *Harsanyi-Farrand-Chang* (HFC) [9], and *virtual dimensionality* (VD) [10]. Topological methods which infer the data manifold –usually of lower dimension– such as independent component analysis, projection pursuit, and wavelet decomposition have also been introduced (see [12] and references therein).

3. LINEAR SPECTRAL UNMIXING

Linear spectral unmixing has been intensively researched in the recent years [1, 6, 12, 13]. Under this model, and assuming that the number of substances and their reflectance spectra are known, hyperspectral unmixing is a linear problem to which many solutions have been proposed (e.g., maximum likelihood estimation [14], spectral signature matching [15], spectral angle mapper [16], subspace projection methods [17, 18], and constrained least squares [19]).

Given that linear spectral unmixing is a source separation problem, the independent component analysis (ICA) framework comes naturally to mind to unmix spectral data. However, the ICA crux assumption of source statistical independence is not satisfied in spectral applications, since the sources are fractions and, thus, non-negative and summing up to one. As a consequence, ICA-based algorithms have severe limitations in the area of spectral unmixing [3], and this has fostered new unmixing research directions taking into account geometric and statistical characteristics of hyperspectral sources.

To overcome the limitations of the ICA-based approaches to spectral unmixing, large research efforts have been devoted in the last decade to the development of unmixing algorithms targeted at spectral unmixing. Most of these algorithms adopt either a geometrical or a statistical framework [12, 13].

3.1. Geometrical based approaches: pure pixel based algorithms

The pure pixel based algorithms assume the presence in the data of at least one pure pixel per endmember, meaning that there is at least one spectral vector on each vertex of the data simplex. This assumption, though enabling the design of very efficient algorithms from the computational point of view, is a strong requisite that may not hold in many datasets. In any case, these algorithms find the set of purest available pixels in the data. Anyway, perhaps due to its computational lightness and clear conceptual meaning, they are, by far, the most widely used class of algorithms in linear hyperspectral unmixing applications. Relevant algorithms of this class are the *pixel purity index* (PPI), [20], N-FINDR [21], the *iterative error analysis* (IEA) [22], the *vertex component analysis* (VCA) [23], the *simplex growing algorithm* (SGA) [24], the *sequential maximum angle convex cone* (SMACC) [25], the *alternative volume maximization* (AVMAX) [26], and the *successive volume maximization* (AVMAX) [26].

3.2. Geometrical based approaches: Minimum volume based algorithms

The minimum volume (MV) approaches aim at finding the mixing matrix that minimizes the volume of the simplex defined by its columns and containing the observed spectral vectors. This is a nonconvex optimization problem much harder to solve than those considered in the previous subsection. Relevant algorithms of this class are the *convex cone analysis* (CCA) [27], the *iterative constrained endmembers* (ICE) [28], the *sparsity-promoting iterative constrained endmembers* (SPICE) [29], the *minimum volume transform-nonnegative matrix factorization* (MVC-NMF) [30], the *minimum volume simplex analysis* (MVSA) [31], the *minimum volume enclosing simplex* (MVES) [32], and the *simplex identification via variable splitting and augmented Lagrangian* (SISAL) [33].

3.3. Statistical methods

When the spectral mixtures are highly mixed, the geometrical based methods yield poor results because there are not enough spectral vectors in the simplex facets. In these cases, the statistical methods are a powerful alternative, which, usually, comes at the expense of higher computational complexity when compared with the geometrical based approaches.

Under the statistical framework, spectral unmixing is formulated as a statistical inference problem. Adopting a Bayesian perspective, the inference engine is the posterior density of the random objects to be estimated. Relevant examples of this approach are the *joint Bayesian endmember extraction and linear unmixing* [34], the *Bayesian analysis of spectral mixture data using Markov chain Monte Carlo methods* [35], the *Bayesian nonnegative matrix factorization* [36], the *dependent component analysis* DECA [37], and the em generalized bilinear model [38], which adopts a non-linear observation model accounting for double light interactions among the endmembers.

3.4. Sparse regression based unmixing

The spectral unmixing problem has recently been approached in a semi-supervised fashion, by assuming that the observed image signatures can be expressed as linear combinations of a number of pure spectral signatures known in advance [39, 40, 41] (*e.g.*, spectra collected on the ground by a field spectro-radiometer). Unmixing then amounts to finding the optimal subset of signatures in a (potentially very large) spectral library that can best model each mixed pixel in the scene [42]. In practice, this is a combinatorial problem which calls for efficient linear sparse regression techniques based on sparsity-inducing regularizers, since the number of endmembers participating in a mixed pixel is usually very small compared with the (ever-growing) dimensionality and availability of spectral libraries [1]. Linear sparse regression is an area of very active research with strong links to compressed sensing, basis pursuit, basis pursuit denoising, and matching pursuit [43].

A recent trend in sparse approximation is the learning of the regression dictionary from example data [44], [45]. These ideas have been recently applied with success in hyperspectral unmixing [46].

3.5. Incorporation of spatial-contextual information

Quite often, the hyperspectral vectors are organized into images and, thus, besides the spectral information, we have also spatial information: it is very likely that two neighboring pixels display similar properties. The exploitation of this contextual information is currently object of active research. Some examples of works including some sort of spatial information are the *spectral and spatial complexity-based hyperspectral unmixing* [47], the *automatic morphological endmember extraction* (AMEE) [48], ℓ_1 *unmixing and its application to hyperspectral image enhancement* [49], [50].

4. SUMMARY

This overview aims at describing the mathematical problems involved in the area of hyperspectral unmixing and summarizing state-of-the-art algorithms to address these problems. The compendium of techniques presented in this work reflects the increasing sophistication of a field that is rapidly maturing at the intersection of many different disciplines including physical modeling, signal and image processing, statistical inference, optimization, and computing developments.

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