

CONSIDERATIONS ON UNSUPERVISED SPECTRAL DATA UNMIXING AND COMPLEXITY PURSUIT

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1. INTRODUCTION

Hyperspectral sensors carry the distinctive advantage of recording hundreds of contiguous spectral images for the same scene providing an extraordinary amount of information that leads to precise differentiation of materials present in the scene even when such materials contribute only to few pixels [1]. With the advent of more and more powerful sensing platforms, coupled with reduction in manufacturing costs and diversification of technologies, hyperspectral imaging has become a powerful approach in remote sensing with applications spanning all traditional fields (such as agriculture, mining, military, resource management, etc.) as well as new ones (manufacturing quality control, pollution detection, health and life sciences, food safety etc.)

Fundamental to spectral imaging is the ability to correctly identify the materials by matching their lab collected spectral information (spectral signature) to the information collected in the images. Often, such direct match is not possible. Atmospheric conditions, sensor artifacts, differences in spectral resolution are only few of the factors that can affect a direct match. Furthermore, given low spatial resolution, pixels in the hyperspectral images represent mixtures of various materials. Correct extraction of the basic spectra from a mixture (also called spectra unmixing) is thus of key importance, unmixing being often found at the basis of any technique that uses hyperspectral images [1].

Given a hyperspectral data cube, unmixing is to the process of extracting a set of spectra, or endmembers and their corresponding abundances that indicate the contribution of the endmembers to each pixel vector in the cube. Both linear and non-linear mixing models have been developed, and active research continues to be performed in either direction [2]. Of particular interest is the use of unsupervised methods for unmixing. Unlike supervised approaches (that usually start with known endmembers and then use projections, spectral mapping or least squares to extract the abundances), in unsupervised unmixing, the assumption is that no prior knowledge of the endmembers can be used. The techniques need to approximate both the endmembers and the abundances. Recent unsupervised unmixing approaches have focused on inverse problems techniques derived from Independent Component Analysis (ICA) or Nonnegative Matrix Factorization (NMF)[2-4]. An ambitious approach, is relaxing ICA to refer not to independence of the components but to their spectral or spatial complexity. A class of

algorithms aiming to explore such complexity was recently proposed and shown to produce results superior to ICA [5,6].

In this paper we tackle the complexity based unmixing first proposed in [5] and develop new techniques that generalize the concept of spatial complexity to larger neighborhoods. Furthermore we assess the value of spatial complexity pursuit for small targets. Finally, we align the complexity based model with the linear mixing model by including additional conditions such as positivity and additivity.

2. COMPLEXITY BASED UNMIXING

Complexity of a signal originates in predictability, i.e. in the ability of previous observations to predict a new observation. The level of predictability for a signal \mathbf{s} is given by:

$$F(\mathbf{s}) = \ln \frac{\sum_{i=1}^n (\bar{s} - s_i)^2}{\sum_{i=1}^n (\tilde{s}_i - s_i)^2} \quad \text{where } \tilde{s}_i = \lambda \tilde{s}_{i-1} + (1 - \lambda) s_{i-1} \quad (1)$$

\bar{s} is the expected value for \mathbf{s} and λ is a value between 0 and 1. The formula provides a measure of the variation between adjacent observations compared to the overall variance. A signal with high F value means that the observations do not change suddenly but rather slowly. In turn, this means that the signal is less complex.

The predictability was extended to a two dimensional space [5]:

$$F(\mathbf{M}) = \ln \frac{\sum_{i,j=1}^{r,c} (\bar{m}_{ij} - m_{ij})^2}{\sum_{i,j=1}^{r,c} (\tilde{m}_{ij} - m_{ij})^2} \quad \text{where } \mathbf{M} \text{ is } r \times c \quad (2)$$

and \bar{m}_{ij} and \tilde{m}_{ij} are computed in a similar fashion as in Eq. 1 based on only the eight adjacent pixels (see Fig. 1a). In case of the expected value, the computation is done using each of these pixels equally weighted, whereas for \tilde{m}_{ij} the weights are the ones given in Fig. 1b

m_{i-lj-l}	m_{i-lj}	m_{i-lj+l}
m_{ij-l}	m_{ij}	m_{ij+l}
m_{i+lj-l}	m_{i+lj}	m_{i+lj+l}

(a)

0.05	0.2	0.05
0.2		0.2
0.05	0.2	0.05

(b)

Fig.1. a) Adjacent pixels contributing to estimation of m_{ij} b) weights used (from [5])

An extension to three dimensional predictability (as is the case of a hyperspectral cube) is also possible. A simple approach is to add up the predictability for each band. For a cube \mathbf{Y} formed of p bands, the predictability of the information in the cube is given by:

$$F(\mathbf{Y}) = \sum_{k=1}^p F(\mathbf{Y}_k) \quad (3)$$

Measures of predictability have been used for linear unmixing. In this case given the observed hyperspectral cube \mathbf{R} ($r \times c \times l$), we aim to find \mathbf{Y} ($r \times c \times p$) and \mathbf{W} ($l \times p$) such that:

$$\mathbf{Y} = \mathbf{WR} \quad (4)$$

In this case, \mathbf{Y} would constitute an estimate of the abundance of the endmembers and \mathbf{W} would constitute the pseudoinverse of the endmembers matrix \mathbf{M} :

$$\mathbf{R} \cong \mathbf{W}^{-1}\mathbf{Y} \quad (5)$$

The Spectral and Spatial Complexity Based Unmixing proposed in ?? is starting with random initial values for \mathbf{Y} and \mathbf{W} and then proceeds to maximizing [5]:

$$G(\mathbf{W}, \mathbf{M}) = \alpha F(\mathbf{Y}) - \beta \sum_{k=1}^p \ln \sum_{j=1}^l (\tilde{m}_{jk} - m_{jk})^2 \quad (6)$$

where α , and β are variable parameters, \mathbf{Y} is computed as in eq. 4, and m_{jk} refer to elements of \mathbf{M} .

The algorithm was tested on various hyperspectral data cubes as well on artificial data and shown to outperform various other techniques including regular and undercomplete ICA, constrained NMF and VCA (Vertex Component Analysis).

2. RETHINKING COMPLEXITY PURSUIT

A careful analysis of the algorithm above raises several questions. In the following we provide brief discussions of each of the issues, and indicate how our work improves upon previous research. Our experiments, some ongoing were performed on in house (produced using a Surface Optics hyperspectral camera) and commercially available data sets (HYDICE, AVIRIS).

2.1. Generalizing Neighborhoods

First, it is not clear why the neighborhood in Fig. 1 was chosen. In fact, the research suggested that spatial complexity can be further generalized to larger neighborhoods. In our research we expand the algorithm to additional neighborhood classes and compare the results with the original approach. Our contribution is the design of these neighborhoods as well as the generalization of computation for the weights for the new neighbors. To test our work we use similar experiments and show a deeper analysis of the impact of neighborhood size on the accuracy of unmixing.

Second, the use of spatial complexity for the abundances raises the question on how small targets will be correctly detected, since maximizing “smoothness” among abundances leads to such targets being assimilated to the background. The original research does not address this and the results published provide average accuracy scores that could not illustrate such situations. In our research we investigate the case of small targets and suggest

alternative approaches for the choice of neighborhoods. One such approach is the dynamic selection of neighborhood sizes.

2.2. Compatibility with Linear Mixing Model

At its basis, complexity pursuit solves a generic Blind Source Separation problem by imposing spatial smoothness constraints on its result. The pursuit of reduced spatial complexity for the abundances is augmented in eq. 6 by the pursuit of increased spectral smoothness for the endmember signatures. Indeed, a material spectra follows a smooth curve with many of its segment being highly correlated. However, in general, an inverse problem does not guarantee that the order of the produced components is the same as the order of the original sources (i.e. the spectral values resulted may not match the order of the spectral intervals. Similar behavior was observed in our previous work with ICA and NMF and a visual inspection of the results was required to identify the correct order of the spectral observations [7-9]. In our research with complexity based unmixing we perform a thorough analysis of the implications of such phenomenon and provide strategies for correct ordering of the extracted components.

Finally, we note that complexity pursuit does not guarantee that the resulting abundances are positive or that they add up to one, as required by the linear Mixing Model (LMM). We modified the algorithm in (6) to include positivity constraints on Y and also constraints of the additivity. Our results indicate improved accuracy.

3. REFERENCES

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