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Spectral unmixing based on a minimum volume simplicial enclosure model*

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Abstract This work describes the minimum volume enclosing simplex problem, which is known to be a multimodal Global Optimization problem. The problem has been used as a basis to estimate so-called endmember and abundance data in unmixing spectral data of hyperspectral sensors. This estimation problem is a big challenge. We explore the possibility of a new estimation algorithm using the minimum volume enclosing simplex problem. We investigate its behaviour numerically on designed instances comparing its outcomes with a maximum volume enclosed simplex approach which is used frequently in spectral unmixing.

Keywords: spectral unmixing, endmembers, principal components, optimization. minimum volume

1. Introduction

A challenging problem in having data from multispectral imaging sensors is to unfold them into components. We study here the possibility to do so using a minimum volume enclosing simplex approach. Hyperspectral sensors record scenes in which various disparate material substances contribute to the spectrum measured from a single pixel.

Spectral unmixing ([5]) is a term to denote a procedure to decompose a measured spectrum of a mixed pixel into a collection of constituent spectra (endmembers) and a set of corresponding fractions (abundances) that indicate the proportion of each endmember present in the pixel. Endmembers normally correspond to familiar macroscopic objects in the scene, such as water, soil, metal, or any natural or man-made material.

Many methods have been developed and tested to perform endmember extraction and unmixing, see [3] for an overview. We will focus on what is called linear unmixing and ask the question how one can recover the endmember and abundance data via unbiased estimators. One typically sees least squares approaches with the additional complication that the abundance estimate should lay on the unit simplex (nonnegativity). [4] takes an approach where two conflicting objectives, that of least squares and minimizing the volume of an enclosing simplex are combined in an objective function. Recently, [1] develop an approach where they apply sequential Linear programming to solve the minimum volume enclosing simplex problem. In this paper we use standard available nonlinear optimization algorithms to solve the problem.

The problem of enclosing a set of points with a minimum volume body leads usually to a Global Optimization problem; we will illustrate that for the generic simplicial enclosure

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this is the same. However, the use in spectral unmixing is far from worst case behaviour; instances are characterised by low noise and pixel data is well spread. A local search from a well designed starting body leads to the global optimum soon. We will take a hierarchical vision: First to minimize least squares using principal component analysis, which is very common in image data analysis and second, minimize the volume of an enclosing simplex in the reduced space. The question is how to use such an approach such that for linear mixture with white noise one obtains unbiased estimates of endmembers and abundance.

A benchmark method is to consider a maximum volume "inscribing" simplex looked for by the so-called N-FINDR algorithm [6]. Given the reduced data, in principle one looks for all combinations within the given pixels as candidate endmembers such that the resulting volume of the spanning simplex is maximum. If indeed the endmembers are present in the data and noise is low, the approach is very promising as analysed by [6]. We can use the results of such an approach to compare methods numerically.

2. Unmixing and minimum enclosing simplex

Let us assume that a hyperspectral scene contains m spectral bands and r pixel vectors. Each pixel vector in the scene (y_k) can be modeled using the following expression:

$$y_k = Xa_k + \epsilon \tag{1}$$

where y_k is $m \times 1$ observation bands, X is $m \times n$, bands of endmembers, a_k is $1 \times n$ abundance and ϵ is $m \times 1$ white noise with a standard deviation of σ. Our goal is to design a method for recovering "real" matrix X and abundance a_k of observed pixels y_k. To do so, usually two objectives are minimized: noise in a least squares way and the volume of the simplex spanned by the columns of matrix X. Moreover, the abundance should be positive for each pixel. The question is how to deal with least squares and minimum volume in such a way that the estimation is unbiased, i.e. the expected value of the estimator is the real value.

One should keep in mind that instances of the problem consisting of real images are characterized by pixels being mixtures of less than 4 constituents, i.e. vectors a_k have only a few positive values. The idea of least squares in the estimation procedure is, that often it is not know exactly how many endmembers, constituents, are involved in the data. Therefore application of principal component analysis is popular. Having n endmembers gives that one should discover an $n-1$ dimensional subspace that is responsible for the main variation and the rest of the m dimensional space is considered noise.

First of all the data are centralized by the mean $\overline{y}$, such that the columns of Y consist of centralized observations $y_k - \overline{y}$. The observed variation in the spectral data Y^TY is approximated by $(CZ)^TCZ$ where C is an $m \times (n-1)$ matrix of principal components and Z is $(n-1) \times r$ a so-called score matrix. In direction c_1 we have the biggest variation, in direction c_2 the second biggest etc. Essentially we have reduced model (1) to $z = Va + \xi$, where we expect the endmembers X to lay in the space $< C > +\overline{y}$ spanned by the columns of C. C represents an estimate of the space in which the endmember spectra X are located, $X = CV + \overline{y}$. To say it in another way, with absence of noise the estimate of C represents the space spanned by $X - \overline{y}\mathbf{1}^T$, where $\mathbf{1}$ is the all-ones vector of appropriate dimension. With noise, ξ is now the projection of ϵ on $< C >$ and therefore its components also form white noise. To be consistent, we should theoretically notice that $y = Cz + \overline{y} + \zeta$ where ζ is the part of ϵ projected on the orthoplement of $< C >$; $\epsilon = \xi + \zeta$. We will use the idea that the noise of z is componentwise independent.

We follow a two step approach often found in literature. First we estimate the space in which the n endmembers are lying. Secondly, in that space, we minimize the volume of the resulting simplex such that it encloses the projections of the observed bands of the pixels. The N-FINDR algorithm follows an approach where on the projected plane the volume of a simplex is maximized.

3. Minimum volume versus maximum volume simplices

The estimate of the matrix of endmembers $X = CV + \overline{y}$ appears from an estimate of V based on the projected bands (scores) Z. The problem of finding the minimum enclosing simplex of a set of points $z_k, k = 1, \ldots, r$ in $(n-1)$-dimensional space is

$$\min_V \{f(V) := \det \begin{pmatrix} V \\ \mathbf{1}^T \end{pmatrix}\} \texttt{ subject to } a_k = \begin{pmatrix} V \\ \mathbf{1}^T \end{pmatrix}^{-1} \begin{pmatrix} z_k \\ 1 \end{pmatrix} \geq 0, \;\; k = 1, \ldots, r \quad (2)$$

Enclosing with shapes may lead to GO problems. [2] give several examples for enclosing with spheres (the Chebychev problem) and with hyper-rectangles. The use of the minimum volume problem for endmember identification is illustrated next.

In general, we will call V the real values of endmembers defining simplex $S = conv(V)$ and use for the outer enclosing estimate $\hat{V}o$ and corresponding simplex $\hat{S}o$. In case all pixels would be convex combinations of (few) endmembers without any noise, the enclosing simplex $\hat{S}o$ obtains the endmembers V as vertices despite they do not appear in the pixels. Literature on spectral unmixing also uses a maximum volume simplex perspective. The idea is that pure pixels representing the endmembers are present in the data set Z. Consider the pixel data as a set $\mathbb{Z}$. One wants to find a subset $\mathbb{V}$ with $|\mathbb{V}| = n$ such that the corresponding simplex has maximum volume; i.e. $\max_{\mathbb{V} \subset \mathbb{Z}} \; f(V)$, where V is a matrix with the columns of $\mathbb{V}$. This defines a combinatorial optimization problem. The N-FINDR algorithm is a so-called local search heuristic in combinatorial optimisation context. We used a MATLAB implementation of N-FINDR as reference method to compare to MINVEST described in Section 4.

4. Minimum volume estimation procedure: MINVEST

The minimum volume simplex $\hat{S}o$ gives an accurate estimate of the endmembers if noise is absent. That is, sufficiently many pixels should lay on the boundary of S. Mathematically, this means that abundance values $a_{j,k} = 0$; i.e. pixel k does not contain any constituent j. In the hyperspectral image area, it is known that a pixel spectrum consists of a mix of at most 4 constituents. As soon as noise is added, one can approximate with probability theory the chance that a pixel lays outside S. Let ρ be an estimation of the fraction of pixels we expect to be interior with respect to S. An initial matrix V that does not include all pixels is generated. Iteratively the endmembers $\hat{V}$ are estimated from the minimum volume problem by solving (2) and the active pixels at its boundary are removed up to a ρ fraction is left over.

To recover the abundance values from the estimated endmembers V the term *linear spectral unmixing* (LSU) is used when nonnegativeness of estimated abundance is not taken into account. For the fraction of pixels located within simplex $\hat{S}$ we have automatically positive abundance values. For pixels z_k outside $\hat{S}$, we have at least one corresponding $a_{jk} < 0$. The term *fully constrained linear spectral unmixing* (FCLSU) is used if we want to force abundance values to be nonnegative. To do so we consider that the noise of z_k is componentwise independent we choose to project z_k on the facet of $\hat{S}$ closest to z_k and determine the abundance for the endmembers in the plane of that facet.

5. Computer simulated data experiments and conclusions

Computer simulations have been carried out in order to evaluate the accuracy of MINVEST in comparison with N-FINDR in highly controlled analysis scenarios. The quality of estimation $\hat{V}$ ($\hat{A}$) of V (A) is measured as the standard deviation estimate assuming $\hat{V}$ ($\hat{A}$) is unbiased, also called root mean squared error (RMSE). To distinguish, we will use σ_A if $\hat{A}$ is generated by LSU and σ_{Ap} if $\hat{A}$ is generated by FCLSU We show the results obtained from a case with $n = 5$

endmembers and $r = 500$ pixels. To mimic the idea of combinations of a few constituents, a ground truth abundance matrix A is generated consisting for 50% of mixtures of 2 endmembers and for 50% of mixtures of 3 endmembers. They are generated uniformly over the unit simplex. The score matrix Z as input for the estimation is taken as $Z = VA + \sigma \cdot \xi$, where ξ is standard white noise. The choice of the parameter value for ρ is determined by the data $\rho = 18.25\%$. Given that performance indicators depend on pseudo-randomly drawn white noise, for each ground-truth matrix A we replicated white noise 100 times.

Table 1. (RMSE) of endmembers V and abundance A obtained by N-FINDR and MINVEST given noise σ.

	N-FINDR					MINVEST				
σ	0.01	0.1	0.2	0.5	0.7	0.01	0.1	0.2	0.5	0.7
σ_V	.030	.118	.233	.857	1.359	.013	.111	.194	.486	.922
σ_A	.011	.063	.114	.259	.323	.007	.058	.105	.204	.266
σ_{Ap}	.008	.048	.092	.224	.281	.005	.048	.086	.174	.234

The measured performance for N-FINDR and MINVEST is given in Table 1. It shows standard deviation estimates σ_V of endmembers and σ_A of fractional abundances calculated via LSU and via fully constrained spectral unmixing (FCLSU). One can observe that the standard deviation of the estimates is in the same order of magnitude as that of noise. This means that the procedures give results as accurate as the input data. Deviation of endmembers and abundances estimations provided by N-FINDR are higher than those obtained with MINVEST. Other scenarios with and without pure pixels have been generated and evaluated.

The following can be concluded: (1) The problem of unmixing hyperspectral data may be a hard to solve problem. (2) The minimum volume simplicial enclosure problem is a Global Optimization problem where the number of optima depends in worst case on the number of points in the convex hull of the instance. (3) The resulting simplex of the (combinatorial) maximum volume simplex problem is enclosed in the result of the minimum volume enclosing simplex problem. (4) Local search from a good starting simplex leads in general to the global optimum for the case of spectral unmixing due to well spread data in the originating simplex and low noise in practice. (5) The new MINVEST algorithm does not require pure pixels to be present in the scene of the instance unlike the N-FINDR algorithm. (6) In the case of having no noise and well spread data over the boundary of the spectral simplex, MINVEST recovers the original endmembers and ground truth abundance. (7) The RMSE performance indicator is sensitive to scaling in its use for measuring abundance discrepancies. (8) The results of MINVEST seems more correlated to ground truth abundance data than the ones of N-FINDR.

References

[1] T.H. Chan, C.Y. Chi, Y.M. Huang, and W.K. Ma. Convex analysis based minimum-volume enclosing simplex algorithm for hyperspectral unmixing. In *Proceedings of the 2009 IEEE international conference on Acoustics, Speech and Signal Processing*, pages 1089–1092. IEEE, Piscataway, 2009.

[2] E. M.T. Hendrix and B.G. Toth. *Introduction to Nonlinear and Global Optimization*. Springer, Cambridge, 2010.

[3] N Keshava. A survey of spectral unmixing algorithms. *Lincoln Laboratory Journal*, 14:55–78, 2003.

[4] L. Miao and H. Qi. Endmember extraction from highly mixed data using minimum volume constrained nonnegative matrix factorization. *IEEE Transactions on Geoscience and Remote Sensing*, 45:765–777, 2007.

[5] A. Plaza, P. Martinez, R. Perez, and J. Plaza. A quantitative and comparative analysis of endmember extraction algorithms from hyperspectral data. *IEEE Transactions on Geoscience and Remote Sensing*, 42(3):650–663, 2004.

[6] M. E. Winter. N-FINDR: an algorithm for fast autonomous spectral end-member determination in hyperspectral data. *Proc. SPIE Image Spectrometry V*, 3753:266–277, 2003.