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# Simplex Projection Methods for Selection of Endmembers in Hyperspectral Imagery

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**Abstract**— It is well known that performance of subpixel target detection algorithms depends on the choice of endmembers used to characterize the background and the target in hyperspectral imagery. In this paper, we investigate how well a set of endmembers characterizes a given set of spectra. We are assuming a fully constrained linear mixing model, and analyze the resulting residuals. To facilitate geometric and intuitive interpretation, we formulate the resulting constrained least-squares estimation problem in terms of projections on low-dimensional simplexes. Consequently, we define a family of simplex projection methods (SPM) for endmember selection. We give numerical results for two known endmember-selection procedures—the pixel purity index (PPI) and the maximum distance (MaxD) methods. Then we compare these results to those for a simple version of SMP, called the Farthest Pixel Selection (FPS) method. This new class of techniques promises to give better descriptions of the target and background regions than do current methods, which in turn should lead to more precise detection (with lower false alarm rates) of low-visibility small (subpixel) targets.

**Keywords:** *MaxD; PPI; endmembers; AVIRIS; hyperspectral imagery; linear mixing; fully constrained model; subpixel target detection*

## I. INTRODUCTION

It is well known that performance of subpixel target detection algorithms depends on the choice of endmembers used to characterize the background and the target in hyperspectral imagery [1]. The proper choice of endmembers also plays an important role in decomposing the observed hyperspectral scenes (by unmixing procedures) for the purpose of estimating abundances of the present materials. A poorly constructed set of endmembers often leads to incorrect estimation of material abundances. Slightly negative abundances are usually not a reason for significant concern. However, negative abundances of larger magnitude might cause significant distortions in further use of abundances for unmixing or for subpixel target detection.

In this paper, we investigate how well a set of endmembers characterizes a given set of spectra, such as background or target regions. We are assuming a linear mixing model with coefficients constrained to be positive fractions (between 0 and 1) that sum up to 1. Consequently, for a given set of spectra represented as a set of  $p$ -dimensional vectors (or points), we can define a convex hull (a “region”) generated by convex linear combinations of those vectors. When dealing with a set of background [target] spectra, we will call the convex hull a

background [target] region (rather than a background space or subspace, which could be confused with linear spaces).

In the terminology used in [2], endmembers can be derived from the image (image endmembers) or derived from a library or field reflectance spectra (reference endmembers). Analysis in this article is based on image endmembers. Also, we limit our investigation to the so-called native endmembers (i.e., vectors chosen from within the image spectra).

It is our view that in the target detection methods (which are the focus of this paper), the endmembers do not need to represent pure materials as long as they give a good representation of the background or target regions. It should also be recognized that the concept of a pure material is not always well defined. On the other hand, in the process of unmixing for the purpose of estimating material abundances, the physical interpretation of endmembers is more important.

The endmember coefficients (abundances) are estimated using the fully constrained least squares method, which is equivalent to projecting on a simplex. We use the projection terminology for ease of geometric and intuitive interpretation.

We investigate the distribution of the lengths of residual errors (distances between the spectra and their projections) to see how well a given set of endmembers characterizes a set of spectra. In order to minimize those distances, we introduce a family of simplex projection methods (SPM) for endmember selection and then further investigate one member of this family, called the Farthest Pixel Selection (FPS) method. We test it against two known methods—the Pixel Purity Index (PPI) method and the Maximum Distance (MaxD) method. The numerical results are obtained for an AVIRIS hyperspectral image (100 by 100 pixels) with 152 spectral bands (after the water bands are removed).

## II. DEFINITIONS

Consider a set of spectra  $\mathbf{x}_i, i = 1, \dots, N$ , where  $\mathbf{x}_i$ 's are  $p$ -dimensional vectors. Such sets may appear in the following contexts:

- A collection of  $N$  pixels in a spectral image
- A collection of target spectra generated under a variety of environmental conditions (such as atmospheric and illumination effects)
- A merged set of the target and image spectra.

It is often convenient to define a relatively small set of spectra  $\mathbf{m}_1, \dots, \mathbf{m}_k$ , called endmembers, such that all  $N$  spectra  $\mathbf{x}_i$  can be represented (at least approximately) as linear combinations of the endmembers, that is,

$$\mathbf{x}_i = \sum_{j=1}^k a_{ij} \mathbf{m}_j + \boldsymbol{\varepsilon}_i \quad (1)$$

where  $a_{ij}$  are constants and  $\boldsymbol{\varepsilon}_i$  are approximation errors (residuals), which can be due to the noise in data or due to modeling error (or both). In the context of a spectral image, the linear combination (1) can be interpreted as representing a mixture of materials (defined by endmembers) contained in the image pixels, and the constants  $a_{ij}$  can be interpreted as abundances of those materials. This is why we are going to assume a convex linear combination in (1), that is,

$$a_{ij} \geq 0 \quad \text{and} \quad \sum_{j=1}^k a_{ij} = 1. \quad (2)$$

which is often called a fully constrained case [5]. Let us define a simplex  $M$  spanned over the endmembers  $\mathbf{m}_1, \dots, \mathbf{m}_k$  as

$$M = \left\{ \mathbf{x}: \mathbf{x} = \sum_{j=1}^k a_j \mathbf{m}_j, a_j \geq 0, \sum_{j=1}^k a_j = 1 \right\} \quad (3)$$

and define a projection of spectra  $\mathbf{x}$  onto  $M$  as a vector  $\mathbf{x}_M \in M$  such that

$$d(\mathbf{x}, \mathbf{x}_M) = \min \{ d(\mathbf{x}, \mathbf{z}), \mathbf{z} \in M \},$$

where  $d(\cdot, \cdot)$  is a distance between two vectors (points) in a  $p$ -dimensional space. A distance between  $\mathbf{x}$  and  $M$  can now be defined as

$$d(\mathbf{x}, M) = d(\mathbf{x}, \mathbf{x}_M).$$

Here, we will consider the case when  $d(\cdot, \cdot)$  is a Euclidian distance, that is,

$$d(\mathbf{x}, \mathbf{y}) = \sqrt{(\mathbf{x} - \mathbf{y})'(\mathbf{x} - \mathbf{y})}.$$

Once the endmembers  $\mathbf{m}_1, \dots, \mathbf{m}_k$  are defined, the coefficients  $a_{ij}$  can be estimated using the least squares method under the constraints (2), which is equivalent to projecting on the simplex (3) as described above.

Other distances can also be considered. For instance, when the noise in the image is known and its magnitude is large, a suitable distance might be a statistical (Mahalanobis) distance. More research is needed to investigate which distance is more appropriate in which cases.

### III. DIMENSIONALITY ADJUSTMENT

In order to adjust for dimensionality, we are defining an adjusted distance as

$$d_{adj}(\mathbf{x}, \mathbf{y}) = \frac{d(\mathbf{x}, \mathbf{y})}{\sqrt{p}}$$

Since all of our numerical calculations are performed in the same  $p$ -dimensional space, this dimensionality adjustment is

not really significant here. However, it makes it easier to interpret the numerical results. Please note that for two spectra differing by a shift of only one unit (up or down), the adjusted distance between the two spectra is equal to one unit (independent of dimensionality (number of spectral bands) used). The adjusted distance is also called root mean squared error by some authors (e.g., see [7]).

### IV. NUMERICAL RESULTS

In this section, we give some numerical results for evaluation of endmember sets generated by two methods: MaxD and PPI. An AVIRIS image consisting of 10,000 pixels (100x100) in 152 spectral bands is used here. No dimensionality reduction was performed. As many as 50 endmembers were generated using each of the two methods for the following reasons:

- The so-called “true” dimensionality of the image is difficult to establish in an objective way. The number  $(k-1)$  can be called true dimensionality of a set of spectra  $\mathbf{x}_i, i=1, \dots, N$ , if all approximation errors  $\boldsymbol{\varepsilon}_i$  in (1) are very small, and consequently, all spectra can be regarded as lying (approximately) in a  $(k-1)$  dimensional affine subspace generated by the endmembers  $\mathbf{m}_1, \dots, \mathbf{m}_k$ . Of course, the subjectivity of this definition is in establishing what it means that the vectors  $\boldsymbol{\varepsilon}_i$  are very small. We believe that the criterion of explaining a certain high percentage of variability (as used in PCA and SVD by some authors) is not sufficient here.
- If the true dimensionality  $(k-1)$  of the image is lower than 49, then the convex hull generated by 50 endmembers is no longer a simplex (after a projection to the  $(k-1)$  dimensional affine subspace) but rather a polyhedron (multi-dimensional polygon). We believe that such a polyhedron gives a more realistic approximation of the image cube. However, we still call this convex hull a simplex because it is a simplex in the original 152-dimensional space.
- Recent research (for example in [1]) indicates that relatively large numbers of endmembers are beneficial for performance of target detector algorithms.

#### A. Numerical Methods

In order to find the projection  $\mathbf{x}_M$  of a given spectra  $\mathbf{x}$ , we need to minimize the distance  $d(\mathbf{x}, \sum_{j=1}^k a_j \mathbf{m}_j)$  given the constraints  $a_j \geq 0, \sum_{j=1}^k a_j = 1$ . The square of the distance can be written as

$$d^2 \left( \mathbf{x}, \sum_{j=1}^k a_j \mathbf{m}_j \right) = \mathbf{x}^T \mathbf{x} - \mathbf{v}^T \mathbf{a} + \mathbf{a}^T \mathbf{Q} \mathbf{a}$$

where  $\mathbf{v}^T = 2\mathbf{x}^T \mathbf{B}$ ,  $\mathbf{Q} = \mathbf{B}^T \mathbf{B}$ , and  $\mathbf{B}$  is the matrix of endmembers  $\mathbf{m}_1, \dots, \mathbf{m}_k$  as columns. So, the minimization problem becomes a quadratic programming problem. In order

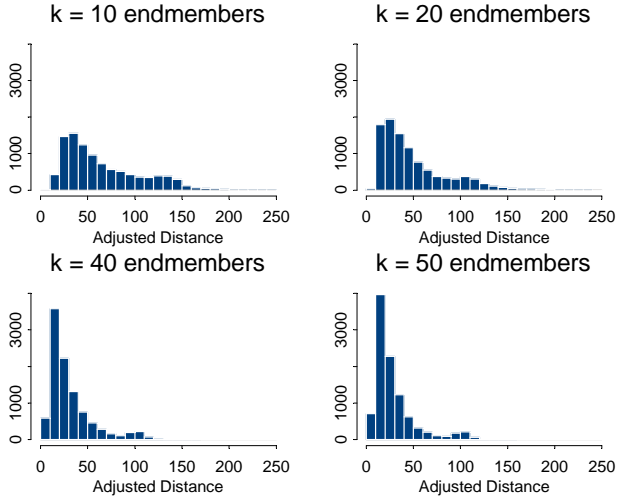


Figure 1. Histograms of adjusted distances of the image cube spectra from the simplexes  $M_k$  (defined by MaxD endmembers) for selected values of  $k$ . Vertical axes show frequencies.

to deal with the equality constraint  $\sum_{j=1}^k a_j = 1$ , the authors in [5] introduce a constant  $\delta$  (see formulas (17) and (18) in [5]). However, precision of results depends on the appropriate choice of  $\delta$ , which is quite inconvenient. Our approach is to eliminate  $a_k$  and introduce a new constraint  $\sum_{j=1}^{k-1} a_j \leq 1$ . The numerical results are obtained using S-plus function solve.QP for quadratic programming [6].

### B. MaxD Method

Fifty endmembers were found using the Maximum Distance (MaxD) method as described in [3] and [1]. For each  $k = 4, 5, \dots, 50$ , a simplex  $M_k$  was defined (as in (3)) by the first  $k$  of those identified endmembers. For each spectrum  $\mathbf{x}_i, i = 1, \dots, N = 10000$  from the image cube, we calculate the adjusted distance  $d_{adj}(\mathbf{x}_i, M_k)$  between the spectrum  $\mathbf{x}_i$  and the simplex  $M_k$ . The resulting distributions of  $N = 10000$  distances are represented by the histograms in Figure 1 for selected values of  $k = 10, 20, 40$ , and  $50$ . It is interesting to note that all adjusted distances  $d_{adj}(\mathbf{x}_i, M_k)$  are positive (different from zero) except for those spectra  $\mathbf{x}_i$  that create the simplex  $M_k$ . This means that all spectra in our image fall outside of the simplexes  $M_k$ . Clearly, this result is mainly related to the fact that these low-dimensional simplexes  $M_k$  have zero volume in the 152-dimensional space. However, we would expect a similar effect even if the dimensionality of the data set were reduced to  $(k-1)$ . This effect would be due to the co-called curse of dimensionality, which means that the high dimensional space is mostly empty.

It turns out that the maximum adjusted distance ranges from 230 to 154 units when  $k$  ranges between 20 and 50. We may then wonder how large the adjusted distance of 154 units really

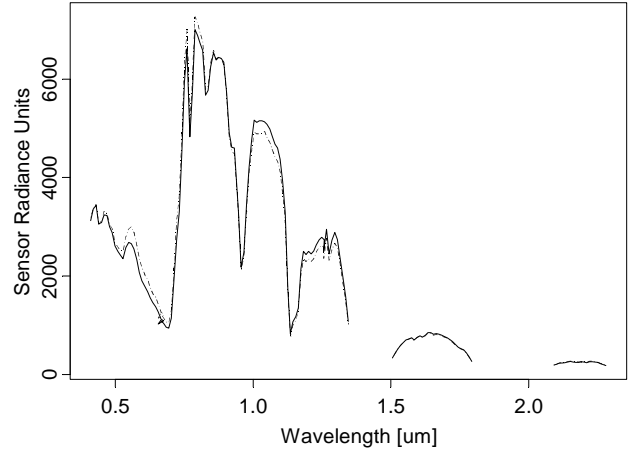


Figure 2. Spectra of a pixel (solid line) and its projection (dotted line) on the simplex defined by 50 MaxD endmembers. The adjusted distance between the two spectra is 154 units, and the angle between them is about 2.8 degrees, which is regarded as indicating a practically significant difference.

is. In order to answer this question, we compare the spectrum of a pixel farthest from  $M_{50}$  (as defined by 50 MaxD endmembers) and its projection on  $M_{50}$ . Figure 2 shows that the two spectra are quite different. Another popular measure is the angle between the two spectra treated as vectors. The angle for the two spectra from Figure 2 is about 2.8 degrees, which is regarded as indicating a significant difference between them.

### C. Pixel Purity Index (PPI) Method

In this section, the endmembers  $\mathbf{m}_1, \dots, \mathbf{m}_k, k = 50$ , were found using the Pixel Purity Index (PPI) method (see [4]), including the clustering as described in [1]. The resulting distributions of distances  $d_{adj}(\mathbf{x}_i, M_k), i = 1, \dots, N = 10000$ , are represented by the histograms in Figure 3 for selected values of  $k = 10, 20, 40$ , and  $50$ . These distributions are not much different from those in Figure 1. Note that the scale for all histograms is from 0 to 250 because most observations are in that range. However, the adjusted distances can be much larger in some cases. For instance, as many as 100 pixels are farther than 350 units from a simplex generated by  $k = 10$  PPI endmembers. Even though it may seem a small fraction of all image pixels, we still cannot ignore such discrepancies especially in the target detection problems where important image features are found in a very small fraction of the image.

## V. SIMPLEX PROJECTION METHODS (SPM)

Since our emphasis is on having small adjusted distances  $d_{adj}(\mathbf{x}_i, M_k)$ , it makes sense to consider a summary measure of those adjusted distances and then minimize it by the appropriate choice of endmembers. Examples of the summary measures could be the mean, a high percentage (e.g., 99.5%) quantile (percentile), or a maximum value. Since it would not be feasible to check all possible sets of spectra as endmembers, we need to rely on some heuristic procedures to minimize a summary measure. Natural choices in this case would be some

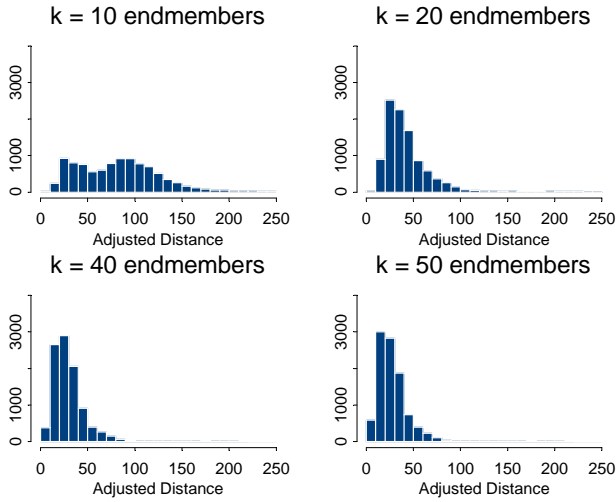


Figure 3. Histograms of adjusted distances of the image cube spectra from the simplexes  $M_k$  (defined by PPI endmembers) for selected values of  $k$ . Vertical axes show frequencies.

forward, backward, or stepwise procedures.

In this brief note, we consider only one example of a forward method based on the maximum (over all spectra) of adjusted distances. We call it the Farthest Pixel Selection (FPS) method, and we define it as follows

1. Select the longest spectra vector as  $\mathbf{m}_1$  (first endmember).
2. Select the spectra farthest from  $\mathbf{m}_1$  as  $\mathbf{m}_2$ . Set  $k = 2$ .
3. Define  $M_k$  according to (3), and select the spectra farthest from  $M_k$  as  $\mathbf{m}_{k+1}$ .
4. Repeat step 3 until the desired number of endmembers is selected.

This method turns out to be almost identical with Unsupervised FCLS (fully constrained least squares) introduced in [5].

Figure 4 shows the adjusted distances that are significantly smaller than those for MaxD and PPI methods in Figures 1 and 3, respectively.

## VI. CONCLUSIONS

There is a prevailing perception in the current literature that a relatively small set of endmembers (from 5 to 10) can be used to describe an image through a linear mixing model (1). Our numerical results indicate that the resulting approximation may not be sufficient for many applications. We observe significant differences between the observed spectra and the modeled spectra (convex linear combinations of endmembers), even for as many as 20 or 40 endmembers (depending on the method used). In order to find endmembers that more closely estimate the image spectra, we introduce a family of simplex projection methods and investigate one example from that family (FPS method). The FPS method shows performance better than that of the MaxD and PPI methods, but still a relatively large number of endmembers is needed to obtain reasonably good approximations of all image pixels.

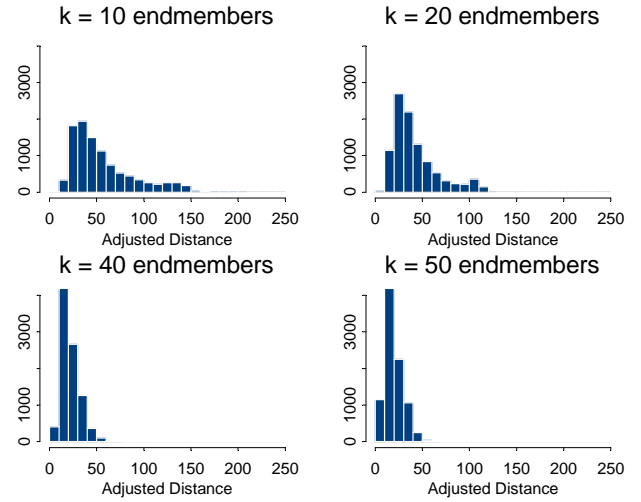


Figure 4. Histograms of adjusted distances of the image cube spectra from the simplexes  $M_k$  (defined by FPS endmembers) for selected values of  $k$ . Vertical axes show frequencies.

Further work may include investigation of

- the spatial structure of residual errors,
- other types of simplex projection methods, and
- target detection performance of the resulting endmembers.

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