Subpixel Target Detection in Hyperspectral Imagery Using **Simplex Projections**

Peter Bajorski

School of Mathematical Sciences, Rochester Institute of Technology, USA Corresponding Author: Peter Bajorski

Abstract: In this paper, 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 two examples of SPMs—the Farthest Pixel Selection (FPS) method and the Stepwise Simplex Projection (SSP) method. The numerical examples using AVIRIS image data show that this new class of techniques gives better descriptions of the target and background regions than do current methods. This leads to more precise detection (with lower false alarm rates) of low-visibility small (subpixel) targets.

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I. Introduction

In this paper, we optimize a choice of a single endmember at each step by investigating its projection on a simplex generated by other endmembers. We call such algorithms Simplex Projection Methods (SPMs). The SPMs should lead to (but do not guarantee) better values of the summary measures.We consider two examples of SPMs-a forward method that we call the Farthest Pixel Selection (FPS) method and a stepwise method that we call the Stepwise Simplex Projection (SSP) method.

Farthest Pixel Selection (FPS) Method

The Farthest Pixel Selection (FPS) method is defined 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 as follows

$$\boldsymbol{M}_{k} = \left\{ \mathbf{x} : \ \mathbf{x} = \sum_{j=1}^{k} a_{j} \mathbf{m}_{j}, \ a_{j} \ge 0, \ \sum_{j=1}^{k} a_{j} = 1 \right\}$$
(1)

and select the spectra farthest from M_k as \mathbf{m}_{k+1} . Increase the value of k by 1.

4. Repeat step 3 until the desired number of endmembers is selected.

The FPS method is very similar to the Unsupervised FCLS (Fully Constrained Least Squares) introduced in [5] in terms of the resulting endmembers, assuming that the value of δ used in [5] is chosen appropriately ($\delta = 10^{-5}$ for the data set used here). The main difference is that we use this method only to identify endmembers, and then, for the purpose of target detection, we use only one detector (matched subspace detector) for all endmember selection techniques because our main goal is to investigate a wide range of these techniques without the confounding effect of the target detection method. On the other hand, in [5], the emphasis is on material quantification based on the estimates of the abundance coefficients a_{ii} , and the detection is based on the magnitude of the abundances.

Stepwise Simplex Projection (SSP) Method

The Stepwise Simplex Projection (SSP) method is similar to FPS. However, at each step we check if one of the previously chosen endmembers is sub-optimal in the sense that it is close to the simplex created by all other endmembers. In FPS, when a spectrum is chosen as an endmember, it is far from the simplex generated by previous endmembers, so it is usually an important addition. However, adding more endmembers may sometimes make the given endmember "obsolete," that is, less important than other endmembers. The SSP method is defined 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 (1), and select the spectra farthest from M_k as \mathbf{m}_{k+1} . This results in M_{k+1} generated by (k+1) endmembers.
- 4. For each of the (k+1) endmembers generating M_{k+1} , calculate its distance d_j , j = 1, ..., (k+1) to the simplex generated by the remaining k endmembers. The distance d_{k+1} was already calculated in the previous step.
- 5. If $\min\{d_j: 1 \le j \le k\} \ge d_{k+1}$, increase the value of k by 1, and continue with Step 3 using the endmembers identified so far. Otherwise (when $\min\{d_j: 1 \le j \le k\} < d_{k+1}$), eliminate the endmember with the smallest distance d_i , and continue with Step 3 using the remaining endmembers.
- 6. Repeat Steps 3 to 5 until the desired number of endmembers is selected.

The SSP method is not sequential because some of the previously chosen endmembers can be eliminated in Step 5.

Spatial Patterns

In addition to the histograms used so far, one could also investigate spatial relationships in the adjusted distances. We plotted 100 by 100 pixel images (not shown here) of the adjusted distances (often called RMSE images; for examples, see [8]). A desired pattern in such plots is randomness as opposed to observing some spatial patterns. All plots were confirming that a number of endmembers as small as 10 or 20 is not sufficient to eliminate strong spatial patterns. Even when 50 endmembers were used, some spatial patterns in adjusted distances were still left in the image.

II. Summary Measures for Simplexes

In order to investigate how our approximation depends on the number of endmembers and the method to generate the endmembers, it is convenient to consider summary measures of the approximation errors. We discuss and investigate the following four summary measures:

- Mean Distance (MD)
- Root Mean Squared Distance (RMSD)
- Maximum
- Percentile.

Mean Distance (MD)

The Mean Distance (MD) is defined as the average of adjusted distances, that is,

$$MD\{M\} = \frac{1}{n}\sum_{i=1}^{n} d_{adj}(\mathbf{x}_{i}, \mathbf{x}_{iM})$$

where \mathbf{x}_{iM} is a projection of \mathbf{x}_i onto the simplex M, as defined previously. Figure 1 shows that the two simplex projection methods are not much different as measured by MD, and they both are performing better than the two remaining methods. A disadvantage of MD as a measure of the approximation errors is that it may be insensitive to a relatively small fraction of spectra with large approximation errors. In subpixel target detection, we are often interested in a relatively small number of pixels (that contain the target), and we want to make sure that a significant majority of pixel spectra (or, even better, all of them) are well approximated. To address this issue, we introduce another measure in the next subsection.

Fig. 1. Mean Distance (MD) as a function of the number (ranging from 4 to 50) of endmembers in the MaxD (solid line), PPI (dotted line), FPS (dotted-dashed line), and SSP (dashed line) simplexes.



The Root Mean Squared Distance (RMSD)

The RMSD is defined as

$$RMSD\left\{M\right\} = \sqrt{\frac{1}{n}\sum_{i=1}^{n} \left[d_{adj}\left(\mathbf{x}_{i}, \mathbf{x}_{iM}\right)\right]^{2}}$$

The RMSD is more sensitive than MD to large distances because the distances are squared. However, when only a small fraction of pixels has larger distances, this sensitivity may not have a significant impact on RMSD. This turns out to be the case for our numerical example, and a plot of RMSD for all four methods is very similar to Figure 1 and is not shown here.

Fig. 2.The Root Mean Squared Distance (RMSD) as a function of the number (ranging from 4 to 50) of endmembers in the MaxD (solid line), PPI (dotted line), FPS (dotted-dashed line), and SSP (dashed line) simplexes.



Figure 2 shows the relationships among the four endmember selection methods almost identical to those revealed by MD in Figure 1.

Maximum Distance

Both previous measures are based on averaging over the whole set of the image pixels. Since even small images usually have at least 10,000 pixels, the impact of a small fraction of pixels may be unnoticed when those measures are used. This is why it might be informative to use the maximum of the adjusted distances, that is,

$$\max\left\{d_{adj}\left(\mathbf{x}_{i},\mathbf{x}_{iM}\right):1\leq i\leq k\right\}$$

Fig. 3.The maximum adjusted distance as a function of the number (ranging from 4 to 50) of endmembers in the MaxD (solid line), PPI (dotted line), FPS (dotted-dashed line), and SSP (dashed line) simplexes.



Figure 3 shows the relationship among the four methods to be somewhat similar to that shown in Figures 1 and 2. One difference is that the PPI performs even worse when the maximum distance measure is used. The maximum adjusted distance may seem to be sensitive to the presence of outliers. As with any data, extreme outliers should be investigated. If they are a result of an error, then they can be removed. However, in practice, it is often difficult or impractical to make a decision about removing an outlier. An extreme outlier would most likely be identified as one of the endmembers. In that case, the adjusted distance of the outlying spectra to the endmember simplex would be zero, which would not interfere with any of the simplex measures defined here. Another issue is the impact of the outlier identified as an endmember on the target detection performance, which is discussed in the section on target detection.

The maximum adjusted distance used as a measure of approximation takes into account only the most extreme spectrum. One could argue that we are not very much concerned about a single spectrum in the whole image. To overcome this difficulty, we introduce one more measure in the next subsection.

Percentile (Quantile)

When we are concerned about a very small fraction of the image pixels, we can use a high percentile, for example, the 99.9 percentile of adjusted distances. This gives an adjusted distance such that only 0.1 percent of the image spectra (in our AVIRIS image, this means 10 spectra) are even farther from the endmember simplex. Figure 4 shows the relationship among the four methods to be very similar to that shown in Figure 3.





III. Conclusions on Summary Measures

For the AVIRIS data set used here, all four summary measures show similar relationships among the investigated endmember selection techniques. This strengthens the final conclusions about these relationships. We advocate using at least three of these summary measures in practice. The RMSD should be used to assess overall "goodness-of-fit" (with some penalty for very large approximation errors). The maximum distance and a high percentile should be used to evaluate whether the endmembers give a good approximation for all (or almost all) pixels.

IV. Non-native Endmembers

So far, we have used only the native endmember selection techniques, that is, techniques that select the endmembers from among the image spectra. One could also consider non-native endmembers, that is, p-dimensional vectors that are usually outside of the convex hull generated by the image spectra. Examples of methods generating non-native endmembers are the Minimum Volume Transforms (constructing the minimum volume simplex enclosing the data cloud) introduced in [13] and the Iterated Constrained Endmembers (ICE) introduced in [14]. The evaluation methods and summary metrics presented in previous sections can still be used for non-native sets of endmembers (or simplexes). However, they would need to be supplemented by metrics describing how "tightly" they enclose the data cloud. The non-native simplexes are likely to produce very small approximation errors (or even a perfect approximation with zero errors). However, the trade-off may be to include the regions in the p-dimensional space that are unlikely to represent real spectra or spectra of material actually present in an image. The Iterated Constrained Endmembers (ICE) method attempts to keep a balance between the endmember simplex that is large enough, but not too large. It is somewhat similar to a balance between a good fit to the data (small approximation errors) and an overfit (unrealistically small errors). The non-native endmembers are not investigated in this paper. However, in the next section, we suggest that non-native endmembers may help in resolving some of the issues encountered with the native endmembers.

V. Overall Conclusions and Future Work

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. 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 two examples from that family (FPS and SSP methods). Both simplex projection methods show promising performance, but still a relatively large number of endmembers is needed to obtain reasonably good approximations of all image pixels.

Further work is needed to see if the conclusions from this research also apply to

• other important detectors (especially those discussed in [11]), and

• other hyperspectral images.

Future work may also include investigation of other types of simplex projection methods.

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