ABUNDANCE GUIDED ENDMEMBER SELECTION: AN ALGORITHM FOR UNMIXING HYPERSPECTRAL DATA

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ABSTRACT

Linear unmixing is a blind source separation problem that decomposes a hyperspectral image into the spectra of the material constituents of the scene and the abundance maps of those materials across that scene. A novel method for determining the material spectra from within the scene, AGES, is proposed based on the positional information contained within abundances generated by additivity-constrained inversion. This new approach is compared on both simulated and real data sets to the well established N-FINDR algorithm, comparing favorably in terms of computational complexity with the existing algorithm without significantly sacrificing accuracy. In addition, the algorithm has some desirable properties inherent in such an approach.

Index Terms— Hyperspectral, Unmixing, Endmember Determination, AGES

1. INTRODUCTION

Hyperspectral imaging is a form of imaging spectroscopy in which both spatial and spectral response information is captured from a scene, producing an image ‘cube’ [1]. While the exact number of bands required for an image to be classified as hyperspectral is not clearly defined, systems with tens [2] to hundreds [1] of contiguous bands have been labeled hyperspectral.

Such an approach greatly enhances one’s ability to discriminate between different materials within the scene [3] while requiring no preconceptions as to which bands will be useful for discrimination. This is not achieved without cost. The sheer volume of data produced means that algorithms that process this data are inherently computationally costly. This paper outlines the unmixing problem for hyperspectral data then proposes a novel means for the unsupervised unmixing of hyperspectral data; endmember determination, in which the signatures of the pure materials present in the scene are represented by pure pixels, the abundances, $a_i$, of those materials within each pixel. This process can generally be separated into three stages [6]: dimension reduction, in which the algorithm eliminates redundancy in the data; endmember determination, in which the signatures of the pure materials that make up the scene are determined; and inversion, whereby a (usually least-squares) process determines the abundances from the original data and the extracted endmembers.

2. HYPERSPECTRAL UNMIXING

Mixing models of hyperspectral data assume that the spectrum of every pixel within the scene is the result of a combination, usually linear, of the material constituents of that pixel [4, 5]:

$$x_i = Sa_i + n_i$$  \hspace{1cm} (1)

where:

- $x_i \in \mathbb{R}^3$ is the spectral signature measured for pixel $i$ with $\lambda$ bands,
- $S \in \mathbb{R}^{M \times 3}$ is the matrix of the spectral signatures of the $M$ materials that form the scene, known as the endmember matrix,
- $a_i \in \mathbb{R}^M$ is the proportion, or abundance, of each of the $M$ material constituents in pixel $i$. To be physically realizable, the abundances need to be non-negative and sum to one,
- $n_i \in \mathbb{R}^3$ is a (usually Gaussian distributed) noise vector.

The above model is known as the linear mixture model. Unmixing algorithms attempt to ‘unmix’ the data by determining the signatures of the materials that form the scene, $S$, and the abundances, $a_i$, of those materials within each pixel. This process exploits the structure of the data by expanding a simplex within the data points. After randomly choosing an initial set of pixels as endmember candidates, the algorithm calculates the volume of this simplex, and then tries each other data point in place of each vertex of the simplex one after the other. Any replacement that results in a volume increase is retained in the endmember set. Replacements continue until no further replacements increase the volume.

Despite the assumption inherent in this approach: that materials present in the scene are represented by pure pixels, the algorithm has flourished and a number of other algorithms now similarly search within the data for pure pixels to use as endmembers, such as Simplex Growing Algorithm (SGA) [15], Vertex Component Analysis (VCA) [16] and Unsupervised Fully Constrained Least Squares (UFCLS) [17].

3. GEOMETRIC UNMIXING ALGORITHMS

An important class of algorithms designed to perform endmember determination for unmixing is the group of geometric unmixing algorithms. These algorithms exploit the fact that the data in Eqn. 1 forms a convex set, specifically a simplex with the spectral signature of each pure material residing at one vertex of the set [5].

One of the most popular algorithms of this class, both widely used in performance evaluations [7-9] and as a basis for modifications [10-12], is N-FINDR [13, 14]. This algorithm exploits the structure of the data by expanding a simplex within the data points. After randomly choosing an initial set of pixels as endmember candidates, the algorithm calculates the volume of this simplex, and then tries each other data point in place of each vertex of the simplex one after the other. Any replacement that results in a volume increase is retained in the endmember set. Replacements continue until no further replacements increase the volume.

3.1. Unmixing Exploiting Fully Constrained Inversion

A small collection of algorithms utilize the reconstruction error (RE), given in Eqn. 2 to select optimal endmember sets.

$$r_i = |x_i - \bar{x}_i|$$  \hspace{1cm} (2)

where:

- $r_i \in \mathbb{R}$ is the reconstruction error for pixel $i$,
- $\bar{x}_i \in \mathbb{R}^3$ is the reconstructed signal given by:

$$\bar{x}_i = Sa_i$$  \hspace{1cm} (3)
Examples of such algorithms include Iterated Constrained Endmembers (ICE) [7] and UFCLS [17]. Such approaches attempt to minimize the reconstruction error when the inversion process is fully constrained, that is that the abundances are both non-negative and sum to one (additivity). Under these circumstances, the reconstructed data fits perfectly within an $M-1$ dimensional simplex and all information about the quality of fit of the model to the data is contained within the reconstruction error.

The process of performing fully constrained unmixing is inherently computationally costly as the non-negativity constraint can only be achieved through iterative algorithms. Compounding this, ICE and UFCLS perform fully constrained inversion multiple times, once per iteration of the overall algorithm.

### 4. ABUNDANCE GUIDED ENDMEMBER SELECTION (AGES)

An alternative means of inversion forgoes the non-negativity constraint, allowing direct calculation of the abundances [4]:

$$c_i = u_i - (S^TS)^{-1}1(1^T(S^TS)^{-1}1)^{-1}(1^Tu_i - 1)$$  \hspace{1cm} (4)

where:

- $c_i \in \mathbb{R}^M$ are the additivity-constrained abundances for pixel $i$,
- $1 \in \mathbb{R}^M$ is a vector of ones,
- $u_i \in \mathbb{R}^M$ is the vector of unconstrained abundances obtained from:

$$u_i = (S^TS)^{-1}S^T \tilde{x}_i$$  \hspace{1cm} (5)

The reconstructed data points, substituting $c_i$ for $a_i$ in Eqn. 3, will no longer necessarily fall within a simplex formed from the endmembers. Instead, these points will now lie on a hyperplane through the set of $M$ endmembers, some of which will be enclosed by the current endmember estimate simplex and some will not. As a result, the RE becomes a less useful measure of the quality of the fit of the current endmember estimates.

Fortunately, this information is now contained within the abundances instead. Pixels with abundances outside of the range of 0 to 1 fall outside of the simplex. Indeed, the abundance of each pixel in a given endmember is closely related to the ratio of the perpendicular distance of that pixel and that endmember to the $M-2$ dimensional hyperplane through the remaining $M-1$ endmembers. Given two candidates for the $j^{th}$ endmember position, the current estimate, $e_j$, and a projected data point, $\tilde{x}_i$, the volumes of the simplex formed by selecting one over the other, $\text{Vol}(e_j)$ and $\text{Vol}(\tilde{x}_i)$, are related through the abundance of $e_j$ in pixel $i$:

$$|c_{ij}| = \frac{\text{Vol}(\tilde{x}_i)}{\text{Vol}(e_j)}$$  \hspace{1cm} (6)

Therefore, if the data was restricted to the hyperplane through the set of $M$ endmembers, the process of finding the largest simplex, given the additivity-constrained abundances would be straightforward. In real data, this is almost certainly not the case. However, one can look to the N-FINDR algorithm for a solution. It has been noted that the N-FINDR algorithm performs best in a reduced dimension subspace that can be obtained using an orthogonal subspace projection approach [11], such as Principal Components Analysis (PCA) or Minimum Noise Fraction (MNF) [18]. The use of PCA, as the least computationally intensive of the two, allows for the reduction of the dimension of the data to an $M$ dimensional subspace. Better yet, the use of the transform helps isolate the noise component out from the signal, meaning that the RE can be disregarded.

The resulting algorithm, dubbed Abundance Guided Endmember Selection (AGES), is summarized below:

1. Calculate the PCA transformation matrix, the eigenvectors corresponding to the $M$ largest eigenvalues of the scene covariance matrix: $P = \text{eig}(\overline{C}), P \in \mathbb{R}^{k \times M}$
2. Randomly select an initial set of pixels as endmember estimates, $S_i$
3. Calculate the image of $S$ on the reduced PCA space: $\tilde{S} = PP^T S$
4. Invert the data using Eqn. 4 with $\tilde{S}$ in place of $S$
5. Find the pixel with the largest magnitude abundance:
$$i,j = \text{argmax}_{i,j} |\tilde{c}_{ij}|$$
6. If $|\tilde{c}_{ij}| > \epsilon_{\text{thresh}}$, replace the $j^{th}$ endmember with the image of pixel $i$ in PCA space and go to 4, else, terminate.

The above algorithm is sensitive to the choice of initial pixels and so, similar to N-FINDR [13], AGES can be executed multiple times with different initial estimates, retaining the largest volume simplex, using the same volume calculation as N-FINDR.

From experience, an appropriate value of $\epsilon_{\text{thresh}}$ is 0.001. Smaller values risk the algorithm oscillating between two or more replacements instead of terminating. An additional prevention against oscillations used in the implementation of the algorithm is the restriction that the algorithm cannot replace the same endmember position twice in a row.

A mention should also be made of the fact that comparisons between derived endmembers and material spectra obtained from a different source, for example laboratory spectra, should use $S$ not $\tilde{S}$ unless the external spectra undergo the same transformation first.

### 5. EXPERIMENTAL METHODOLOGY

In order to validate the performance of the AGES algorithm the algorithm was executed on two sets of data: one simulated set, using varied numbers of endmembers and one real set of data. Due to the popularity of the N-FINDR algorithm, it was used as a benchmark against which AGES was compared. The implementation of N-FINDR used was based on the literature [13], not the commercial implementation, the details of which are unpublished. N-FINDR utilized PCA for dimension reduction.

The performance measures used to benchmark the algorithms were the simplex volume, calculated in the reduced PCA space, as per [13], and the Spectral Angle Mapper (SAM) measure of distance between the ground truth and derived material signatures:

$$\text{SAM}(a,b) = \arccos \left( \frac{a^T b}{\|a\| \cdot \|b\|} \right)$$  \hspace{1cm} (7)

Timing information was based on MATLAB implementations executed on an AMD Athlon 2600XP with 1GB of RAM.

#### 5.1. Simulated Data

Both algorithms were executed 100 times on 3 different simulated data scenes. Each scene consisted of a 100 by 100 pixel scene. The first scene contained 3 endmembers, the second: 5 and the third: 10. All bar one of the endmembers in each scene was given a single pure pixel and then the abundance of that endmember decreased linearly outwards from that centre until the abundance fell to zero. The final endmember was used to augment the decreased of every pixel to sum to one. The material spectra used to generate the scenes for the simulated data were taken from the AVIRIS 1995 USGS spectral library [19], consisting of 224 bands: Alunite AL706 (E1), Buddingtonite GDS85 (E2), Calcite CO2004 (E3), Chalcedony CU91-6A (E4), Jarosite GDS100 (E5), Kaolinite CM3 (E6), Montmorillonite CM20 (E7), Muscovite GDS107 (E8), Nanohematite BR93-34B2 (E9) and Nontronite NG-1.a (E10).
Additive Gaussian noise, \( n_{ij} \sim N(0, \sigma_N) \), was added independently to each band such that the signal to noise ratio (SNR = \( \frac{\mu}{\sigma_N} \)) of each band was 30.

5.2. Real Data

Both algorithms were executed with 25 different initializations on a 350 by 350 pixel subsection of the 1997 AVIRIS Cuprite scene.

6. RESULTS AND DISCUSSION

6.1. Simulated Data

The N-FINDR algorithm produced the same set of endmembers in every trial for each scene. There was a slightly greater variation in the endmembers selected by AGES, however, the largest simplex result for AGES was identical to N-FINDR’s result. The volume of the endmember simplex and mean SAM angles to the ground truth endmembers are summarized in Tables I and II below. The quality of the N-FINDR and AGES results were very similar.

Table I Simplex volumes for AGES and N-FINDR on simulated data

<table>
<thead>
<tr>
<th>No. Materials</th>
<th>3</th>
<th>5</th>
<th>10</th>
</tr>
</thead>
<tbody>
<tr>
<td>N-FINDR</td>
<td>2.7020</td>
<td>0.3962</td>
<td>( \times 10^{-6} )</td>
</tr>
<tr>
<td>AGES Best</td>
<td>2.7020</td>
<td>0.3962</td>
<td>( \times 10^{-6} )</td>
</tr>
<tr>
<td>AGES Mean</td>
<td>2.7020</td>
<td>0.3961</td>
<td>( \times 10^{-6} )</td>
</tr>
</tbody>
</table>

Based on 1000 iterations on the simulated data, the mean time for one iteration was used with the number of iterations each algorithm took to converge to calculate the timing data in Table III.

Table III Shortest, mean and longest time (s) to converge

<table>
<thead>
<tr>
<th>No. Materials</th>
<th>3 Materials</th>
<th>5 Materials</th>
<th>10 Materials</th>
</tr>
</thead>
<tbody>
<tr>
<td>Shortest</td>
<td>7452</td>
<td>.1691</td>
<td>1.3668</td>
</tr>
<tr>
<td>Mean</td>
<td>8011</td>
<td>.1932</td>
<td>1.9613</td>
</tr>
<tr>
<td>Longest</td>
<td>1.1178</td>
<td>2.960</td>
<td>2.0502</td>
</tr>
</tbody>
</table>

The non-iterating portions of the algorithms, such as PCA and the inversion of results in N-FINDR took approximately 1 second.

6.2. Real Data

The volume of the simplex formed by the endmember sets was measured as each algorithm iterated for each of the 25 trials on the Cuprite subscene. The results for the best trial and the median volume for each algorithm with time are shown in Fig. 3.

Figure 3 Simplex volume vs. time for the best and median trials for N-FINDR and AGES on the Cuprite subscene

The AGES algorithm reached its maximum volume significantly quicker than the N-FINDR algorithm. The volume of AGES was commensurately lower. AGES assumes that no worthwhile information is contained in the RE. This assumption improves as the current simplex estimate becomes closer to the true simplex. Thus, the algorithm is sensitive to poor random initializations, making multiple executions more important. In addition, while the volume is a useful performance measure, the N-FINDR algorithm explicitly seeks to maximize this value and so this performance measure is inherently biased towards N-FINDR [9]. In contrast, the SAM angles from derived endmembers to materials known to reside within the scene suggest the performance of both algorithms is similar. The angles to spectra used as ground truth are shown in Table IV.

Table IV Mean SAM angles for (N)-FINDR and (A)GES

<table>
<thead>
<tr>
<th>No. Materials</th>
<th>3 Materials</th>
<th>5 Materials</th>
<th>10 Materials</th>
</tr>
</thead>
<tbody>
<tr>
<td>E1</td>
<td>.0328</td>
<td>.0328</td>
<td>.0321</td>
</tr>
<tr>
<td>E2</td>
<td>.0434</td>
<td>.0434</td>
<td>.0434</td>
</tr>
<tr>
<td>E3</td>
<td>.0314</td>
<td>.0314</td>
<td>.0300</td>
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<tr>
<td>E4</td>
<td>-</td>
<td>-</td>
<td>.0894</td>
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<td>E5</td>
<td>-</td>
<td>-</td>
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<td>-</td>
<td>-</td>
</tr>
<tr>
<td>E9</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>E10</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
</tbody>
</table>

The non-iterating portions of the algorithms, such as PCA and the inversion of results in N-FINDR took approximately 1 second.

Figure 1 Abundance maps for a series of simulated scenes with (left) three, (middle) five and (right) ten endmembers.
Table IV Mean SAM angles for the largest volume trial

<table>
<thead>
<tr>
<th>Material</th>
<th>N-FINDR</th>
<th>AGES</th>
</tr>
</thead>
<tbody>
<tr>
<td>Buddingtonite GDS85</td>
<td>0.0685</td>
<td>0.0685</td>
</tr>
<tr>
<td>Chaledony CU91-6A</td>
<td>0.1020</td>
<td>0.0859</td>
</tr>
<tr>
<td>Alunite CU91-217G1</td>
<td>0.1366</td>
<td>0.1395</td>
</tr>
<tr>
<td>Alunite CU91-5C-</td>
<td>0.1383</td>
<td>0.0860</td>
</tr>
<tr>
<td>Kaolinite CU00-19A</td>
<td>0.1052</td>
<td>0.0965</td>
</tr>
<tr>
<td>Kaol. + Smectite KLF508</td>
<td>0.0900</td>
<td>0.0900</td>
</tr>
<tr>
<td>Montmorillonite CU93-52A</td>
<td>0.0198</td>
<td>0.0213</td>
</tr>
<tr>
<td>Muscovite CU91-252D</td>
<td>0.0879</td>
<td>0.1030</td>
</tr>
<tr>
<td>Nontronite NG-1.a</td>
<td>0.0691</td>
<td>0.0632</td>
</tr>
<tr>
<td>Alun. + Kaol. MV00-11A</td>
<td>0.0672</td>
<td>0.0672</td>
</tr>
<tr>
<td>Calcite +Mont. GDS212</td>
<td>0.2216</td>
<td>0.2017</td>
</tr>
</tbody>
</table>

The timing information in Table V was calculated from the mean time per iteration over 100 iterations on the Cuprite scene and the number of iterations to converge.

Table V Time (s) to converge on the Cuprite subscene

<table>
<thead>
<tr>
<th></th>
<th>Shortest</th>
<th>Mean</th>
<th>Longest</th>
</tr>
</thead>
<tbody>
<tr>
<td>N-FINDR</td>
<td>433.1200</td>
<td>610.6992</td>
<td>866.2400</td>
</tr>
<tr>
<td>AGES</td>
<td>53.0100</td>
<td>65.3220</td>
<td>88.9200</td>
</tr>
</tbody>
</table>

The above timings confirm that AGES is significantly cheaper computationally than N-FINDR. An advantage of AGES not exploited in this investigation is that the algorithm is inherently parallelizable, as the bulk of the complexity is in the repeated abundance calculations and pixel abundances are independent of one another. By contrast, N-FINDR is inherently sequential.

Another advantage of the algorithm is that the abundance maps produced in each iteration are interpretable by the user and so AGES can display its progress as it iterates. On the Cuprite scene AGES produced a set of abundance maps every 1.71 seconds. This suggests, with modification, future applications where rows or columns are entering and leaving the data set over time.

7. CONCLUSION

A method for autonomously determining the material spectra present in a hyperspectral scene dubbed Abundance Guided Endmember Selection has been proposed. This algorithm exploits the geometric meaning of additivity constrained abundances and the properties of principal component spaces to provide an algorithm that allows for the unmixing of hyperspectral data with a relatively low computational complexity. The accuracy of AGES has been shown to be similar to the existing, popular N-FINDR algorithm on both simulated and real data, while proving significantly faster. In addition the algorithm has the potential for future parallelization and time-sensitive applications.

8. REFERENCES


