Sparse Endmembers and Demixing

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This talk is based on joint work with Martin Ehler, who is currently at the University of Maryland, College Park and the National Institutes of Health.

Figure: Martin Ehler
Outline

1. Hyperspectral data and endmembers
   - Hyperspectral data
   - Endmembers

2. Sparse endmembers
   - Models
   - Theoretical underpinnings
   - Selecting the endmembers

3. Results
   - Urban
   - Smith
   - Final remarks
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Color image

Hyperspectral data and endmembers
Sparse endmembers
Results

Hyperspectral data
Endmembers

Sparse Endmembers and Demixing
Hyperspectral imagery data
Hyperspectral camera in action

Figure: http://www.diamond-sensing.com/uploads/media/Hyperspectral.jpg
Hyperspectral data cube
Overview of hyperspectral imagery data

- Hyperspectral imagery (HSI) data is characterized by the narrowness and contiguous nature of the measurements.
- HSI data sets are spectrally overdetermined, and thus provide ample spectral information to distinguish between spectrally similar (but unique) materials.
- HSI data sets can be useful for the following purposes:
  - target detection
  - material classification
  - material identification
  - mapping details of surface properties
Overview of hyperspectral imagery data

- Hyperspectral imagery (HSI) data is characterized by the narrowness and contiguous nature of the measurements.
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  - material classification
  - **material identification**
  - mapping details of surface properties
Assume our HSI data set is an $n_1 \times n_2 \times d$ cube.

- $n_1, n_2$ spatial dimensions.
- $n = n_1 n_2 =$ number of pixels.
- $d$ is the spectral dimension (so $d$ wavelengths measured).

$d$ is usually large, e.g., $d > 100$.

$n$ is usually very large, e.g., $n = \mathcal{O}(10^5)$ or even $n = \mathcal{O}(10^6)$.

Let $\mathcal{X} = \{x_i\}_{i=1}^n \subset \mathbb{R}^d$ denote the pixel vectors of the HSI data cube in set form.

Let $X = [x_1 \; x_2 \; \cdots \; x_n]$ be a $d \times n$ matrix where the columns $x_i$ of $X$ are the pixel vectors of the HSI data cube.
Endmembers

**Definition**

Endmembers are a collection of a scene's constituent spectra. If $\mathcal{E} = \{e_i\}_{i=1}^s \subset \mathbb{R}^d$ are endmembers corresponding to a data set $\mathcal{X}$, then there is some representation of each $x_i \in \mathcal{X}$ in terms of the elements of $\mathcal{E}$.

- Let $E = [e_1 \ e_2 \ \cdots \ e_s]$ be a $d \times s$ matrix where the columns $e_i$ of $E$ are the endmembers.
- $s$ is usually small, e.g., $s < d$.
- Many algorithms find the endmembers from within the data, so that $\mathcal{E} \subset \mathcal{X}$.
- One alternative is to find endmembers from a spectral library, $\mathcal{L}$, that can be used for multiple data sets.
Linear mixture model

- Given a data set $\mathcal{X}$ and corresponding endmembers $\mathcal{E}$, the linear mixture model states that:

$$x_i = \sum_{j=1}^{s} \alpha_{i,j} e_j + z_i, \quad \text{for all } x_i \in \mathcal{X}.$$  

- $\alpha_{i,j} \geq 0$ for all $i = 1, \ldots, n$ and $j = 1, \ldots, s$.
- $\sum_{j=1}^{s} \alpha_{i,j} = 1$ for all $i = 1, \ldots, n$.
- $z_i \in \mathbb{R}^d$ is a noise vector.
Visualization of the linear mixture model

Figure: The linear mixture model
Examples of endmember algorithms

Some endmember algorithms are the following:

- **N-FINDR [M. Winter]:** Finds the simplex of maximal volume that contains the data set $\mathcal{X}$; the vertices of this simplex are the endmembers.

- **SVDD [D. Tax and R. Duin]:** Obtains a spherical shaped boundary around the data set $\mathcal{X}$; support vectors, or endmembers, are derived from this description.

- **Pixel Purity Index [J. Boardman]:** Repeatedly projects $d$–dimensional scatter plots onto a random unit vector; the extreme pixels in each projection are recorded and the total number of times each pixel is marked as extreme is noted.
Endmember coefficients

- After one finds an endmember set $E$, the coefficients $\{\alpha_{i,j}\}_{i,j=1}^{n,s}$ must be computed.

- Two common ways of computing the coefficients are the following:

  1. **Minimum error:**

     $$\alpha_{i,.} = \arg\min_{\tilde{\alpha}} \|x_i - E\tilde{\alpha}\|_2$$

  2. **Sparse:** let $\tau_i > 0$,

     $$\alpha_{i,.} = \arg\min_{\tilde{\alpha}} \|x_i - E\tilde{\alpha}\|_2^2 + \tau_i\|\tilde{\alpha}\|_1$$

- Note when solving either minimization problem, $\tilde{\alpha}$ is subject to the constraints of the linear mixture model.
A look ahead

- Even if one uses the sparse coefficient model, the endmember algorithm itself does not necessarily select the endmembers with sparsity in mind!
- The endmember algorithm presented in the next section is based on the sparse coefficient model.
- We will be searching for endmembers as a subset of $\mathcal{X}$, i.e., we assume that $\mathcal{E} \subset \mathcal{X}$. 
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A simplistic model

- Assume the linear mixture model, and furthermore suppose that $z_i = 0$ for all $i = 1, \ldots, n$.
- Define an $n \times n$ weight matrix, $W = (w_{i,j})$, as follows.
- Let $c : \mathbb{R}^n \rightarrow \mathbb{R}$ be a cost function.
- If possible,
  $$w_{i,*} = \arg \min_{\tilde{w}} c(\tilde{w}), \text{ subject to:}$$
  $$\sum_{j=1}^{n} \tilde{w}_j x_j = x_i$$
  $$\tilde{w}_j \geq 0 \text{ for all } j = 1, \ldots, n.$$  
  $$\sum_{j=1}^{n} \tilde{w}_j = 1$$
  $$\tilde{w}_i = 0$$
- Otherwise, $w_{i,*} = \delta_i$.
- We can extract the endmembers from the rows of $W$. Namely $x_i$ is an endmember if its corresponding weight row satisfies $w_{i,*} = \delta_i$. 

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Sparse Endmembers and Demixing
Observations on the previous model

- Notice that in the previous model we are representing each $x_i \in \mathcal{X}$ in terms of the dictionary, or finite frame,

$$\mathcal{X}^{(i)} = \mathcal{X} \setminus \{x_i\},$$

subject to the constraints of the linear mixture model.

- If the endmember set $\mathcal{E} \subset \mathcal{X}$ is sparse enough in the dictionary $\mathcal{X}$ (and thus in each $\mathcal{X}^{(i)}$ as well), then we could set the cost function as

$$c(\tilde{w}) = \|\tilde{w}\|_{\ell^0} = |\text{supp}(\tilde{w})|,$$

and expect that the support of each $w_{i,\cdot}$ lies within $\mathcal{E}$.

- Thus we could extract the endmembers from the columns of the weight matrix $W$ as well! In particular, if $\text{supp}(w_{\cdot,i}) \neq \emptyset$, then $x_i \in \mathcal{E}$.
In reality, the endmembers will not be quite so apparent.
Assume only part of the linear mixture model: remove the convexity (i.e. the sum to one) constraint.
Once again assume that \( z_i = 0 \) for all \( i = 1, \ldots, n \).
Suppose that \( s < d \ll n \), which makes \( E \) sparse in \( X \).
Define an \( n \times n \) weight matrix \( W = (w_{i,j}) \) as follows:

\[
\begin{align*}
    w_{i,\cdot} &= \arg\min_{\tilde{w}} \| \tilde{w} \|_{\ell^0}, \quad \text{subject to:} \\
    \sum_{j=1}^{n} \tilde{w}_j x_j &= x_i \\
    \tilde{w}_j &\geq 0 \text{ for all } j = 1, \ldots, n. \\
    \tilde{w}_i &= 0
\end{align*}
\]
Observations on the second model

- Notice that even the endmembers $e_i \in \mathcal{E}$ will have such a representation in the dictionary $\mathcal{X}\backslash\{e_i\}$.
- However, this representation will be a misrepresentation!
- For each $x_i \notin \mathcal{E}$ though, the support of $w_i \cdot$ will be contained in $\mathcal{E}$.
- Thus if the weight of the 'good' representations outweighs the 'bad' representations, then we will still extract the endmembers $\mathcal{E}$ from the columns of $W$.
- In particular, we know that for each $x_i \notin \mathcal{E}$, we have $\|w_i \cdot\|_{\ell^0} \leq s$.
- For $x_i \in \mathcal{E}$ though, we know that $\|w_i \cdot\|_{\ell^0} \leq n - s$.
- Also, due to the fact that $s \ll n$, we almost certainly have $\|w_i \cdot\|_{\ell^0} > s$.
- Thus we could extract the endmembers by selecting the $x_i \in \mathcal{X}$ corresponding to the largest $\|w_i \cdot\|_{\ell^0}$. 
Synthetic weight matrix

Figure: Weight matrix of synthetic data set
In practice of course, \( z_i \neq 0 \).

Furthermore, the \( \ell^0 \) pseudo-norm is computationally intensive, and so we turn to the \( \ell^1 \) norm.

In order to account for these two issues, we define our \( n \times n \) weight matrix \( W = (w_{i,j}) \) as follows:

\[
 w_{i,:} = \arg \min_{\tilde{w}} \| \tilde{w} \|_{\ell^1}, \quad \text{subject to: (1)}
\]

\[
 |x_i - X\tilde{w}|_{\ell^2} \leq \delta_i,
\]

\[
 \tilde{w}_j \geq 0 \quad \text{for all} \quad j = 1, \ldots, n,
\]

\[
 \tilde{w}_i = 0.
\]

Note that (1) can be replaced with:

\[
 w_{i,:} = \arg \min_{\tilde{w}} \| x_i - X\tilde{w} \|_{\ell^2}^2 + \lambda_i \| \tilde{w} \|_{\ell^1}, \quad \text{subject to: (2)}
\]

\[
 \tilde{w}_j \geq 0 \quad \text{for all} \quad j = 1, \ldots, n,
\]

\[
 \tilde{w}_i = 0.
\]
We use the second formulation of the noisy minimization, usually setting
\[
\lambda_i = (.01) \cdot (X^{(i)})^t x_i.
\]
\(\lambda_i\) controls the density of the weight matrix. Large values of \(\lambda_i\) will give less vectors in \(\mathcal{X}\) as possible endmembers.

In practice, if the non-negativity constraint is not enforced, the percentage of non-negative weights is around 0.01\%. Therefore this constraint can usually be removed in order to speed up run time.

There are (at least) two questions:

1. Are there any theoretical underpinnings to this approach?
2. How do we pick out the endmembers from \(W\)? In other words, which columns of \(W\) are the most significant?
Let $\Phi$ be a $d \times n$ dictionary.
Let $x_0 \in \mathbb{R}^d$ be a signal that has a sparse representation $\alpha_0 \in \mathbb{R}^n$ in $\Phi$, i.e. $x_0 = \Phi \alpha_0$.
Suppose all we have observed though is $x = x_0 + z$, where $z \in \mathbb{R}^d$ is noise vector satisfying $\|z\|_2 \leq \varepsilon$.
Define $\hat{\alpha}_{\delta,\varepsilon}$ as

$$
\hat{\alpha}_{\delta,\varepsilon} = \arg \min_{\tilde{\alpha}} \|\tilde{\alpha}\|_1 \text{ subject to } \|x - \Phi \tilde{\alpha}\|_2 \leq \delta.
$$
Theorem (Donoho, Elad, Temlyakov)

If $\Phi$ and $\alpha_0$ satisfy certain sparsity conditions, then

$$\|\hat{\alpha}_{\delta,\epsilon} - \alpha_0\|_{\ell^2} \leq C \cdot (\epsilon + \delta).$$

Theorem (Donoho, Elad, Temlyakov)

If we exaggerate the noise level by setting $\delta = C' \cdot \epsilon$, where $C'$ is a particular constant dependent on $\Phi$ and $\alpha_0$, then

$$\text{supp}(\hat{\alpha}_{\delta,\epsilon}) \subset \text{supp}(\alpha_0).$$
Probabilistic results

- Again let $\Phi$ be a $d \times n$ dictionary.
- Let $x \in \mathbb{R}^d$ be our observed signal such that $x \approx \Phi \alpha$.
- Define $\hat{\alpha}_\varepsilon$ as

$$\hat{\alpha}_\varepsilon = \arg \min_{\tilde{\alpha}} \| \tilde{\alpha} \|_1 \quad \text{subject to} \quad \| x - \Phi \tilde{\alpha} \|_2 \leq \varepsilon.$$ 

**Theorem (Donoho)**

There exists $\rho > 0$ and $C > 0$ so that for all large $d$, the overwhelming majority of all $d \times n$ matrices $\Phi$ have the following property: For each vector $x$ admitting an approximation $\| x - \Phi \alpha_0 \|_2 \leq \varepsilon$, by some vector $\alpha_0$ obeying $\| \alpha_0 \|_0 < \rho d$, then

$$\| \hat{\alpha}_\varepsilon - \alpha_0 \|_2 \leq C \cdot \varepsilon.$$
Endmember selection

Given the weight matrix $W$, we select the endmembers $\mathcal{E} \subset \mathcal{X}$ according to two criterion on the columns of $W$.

1. Support size - should be large.
2. Intensity per weight - should also be large.
The exact method of selection

We rank the columns of $W$ according to the two criterion.

1. First sort the columns of $W$ according to their $\ell^0$ pseudo-norm, $\|w_{.,i}\|_{\ell^0}$. The larger the support, the better the rank (i.e., the more important that column is).
   - Columns with empty support are automatically discarded at this step.

2. Similarly, sort the columns according to the value of $\|w_{.,i}\|_{\ell^2}/\|w_{.,i}\|_{\ell^0}$. The larger the intensity per weight, the better the rank in this ordering.

3. Combine the two rankings to form a final ordering on the columns of $W$. The $s$ highest ranked columns in this ordering correspond to the $s$ endmembers in $E$. 

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Small subset of Urban

Figure: Small subset of Urban

- 50 × 50 pixels.
- 161 spectral dimensions.
Figure: Weight matrix of the Urban subset

- Number of nonzero columns: 31.
- Number of columns $w_{.,i}$ such that $\|w_{.,i}\|_{\ell^0} \geq 10$: 18.
Weight columns of the Urban subset

(a) $W$ column 1
(b) $W$ column 2
(c) $W$ column 3
(d) $W$ column 4
(e) $W$ column 5
(f) $W$ column 6
Weight columns of the Urban subset

(g) $W$ column 7
(h) $W$ column 8
(i) $W$ column 9
(j) $W$ column 10
(k) $W$ column 11
(l) $W$ column 12
Endmembers of the Urban subset

**Figure:** Endmembers of the Urban subset
Coefficients of the Urban subset

(a) Endmember 1
(b) $\ell^2$ coefficients
(c) $\ell^2 - \ell^1$ coefficients

(d) Endmember 2
(e) $\ell^2$ coefficients
(f) $\ell^2 - \ell^1$ coefficients


**Coefficients of the Urban subset**

(g) Endmember 3

(h) $\ell^2$ coefficients

(i) $\ell^2 - \ell^1$ coefficients

(j) Endmember 4

(k) $\ell^2$ coefficients

(l) $\ell^2 - \ell^1$ coefficients
The average $\ell^0$ norm per pixel of each coefficient set:

- $\ell^2$ coefficients: 1.9044.
- $\ell^2 - \ell^1$ coefficients: 1.9044.

Note though that the $\ell^2$ coefficients though do a better job of putting different materials with different endmembers!
Large data sets

- For large data sets, e.g. $n \geq 10^4$, computing the weight matrix $W$ may be too time intensive.
- In order to get around this problem, we sample the data set uniformly at random; call this sample $Y \subset X$.
- We then compute the weight matrix for $Y$, and in turn select the endmembers from $Y$ as well.
- The coefficients for the whole data set $X$ are then computed from these endmembers.
Figure: Urban: http://www.agc.army.mil/Hypercube/index.html

- 307 \times 307 \text{ pixels.}
- 161 \text{ spectral dimensions.}
- Sample size: 4000 \text{ pixels}
The weight matrix, $W$, of Urban had the following statistics:

- Number of nonzero columns: 90.
- Number of columns $w_{i,i}$ such that $\|w_{i,i}\|_{\ell^0} \geq 10$: 50.
Coefficients of Urban

(a) Endmember 1
(b) $\ell^2$ coefficients
(c) $\ell^2 - \ell^1$ coefficients

(d) Endmember 2
(e) $\ell^2$ coefficients
(f) $\ell^2 - \ell^1$ coefficients
Coefficients of Urban

(g) Endmember 3

(h) $\ell^2$ coefficients

(i) $\ell^2 - \ell^1$ coefficients

(j) Endmember 4

(k) $\ell^2$ coefficients

(l) $\ell^2 - \ell^1$ coefficients
Coefficients of Urban

(m) Endmember 5
(n) \( \ell^2 \) coefficients
(o) \( \ell^2 - \ell^1 \) coefficients

(p) Endmember 6
(q) \( \ell^2 \) coefficients
(r) \( \ell^2 - \ell^1 \) coefficients
Coefficients of Urban

(s) Endmember 7  
(t) $\ell^2$ coefficients  
(u) $\ell^2 - \ell^1$ coefficients

(v) Endmember 8  
(w) $\ell^2$ coefficients  
(x) $\ell^2 - \ell^1$ coefficients
Sparsity statistics for Urban

The average $\ell^0$ norm per pixel of each coefficient set:

- $\ell^2$ coefficients: 3.8503.
- $\ell^2 - \ell^1$ coefficients: 2.7217.
Figure: Smith

- $679 \times 944$ pixels (497182 nonzero pixels).
- 110 spectral dimensions.
- Sample size: 5000 pixels.
The weight matrix, $W$, of Smith had the following statistics:

- Number of nonzero columns: 23.
- Number of columns $w_{.,i}$ such that $\|w_{.,i}\|_{\ell^0} \geq 10$: 16.
Endmembers of Smith

Figure: Endmembers of Smith
Coefficients of Smith

(a) Endmember 1  
(b) $\ell^2$ coefficients

(c) Endmember 2  
(d) $\ell^2$ coefficients
Coefficients of Smith

(e) Endmember 3

(f) \( \ell^2 \) coefficients

(g) Endmember 4

(h) \( \ell^2 \) coefficients
Coefﬁcients of Smith

(i) Endmember 5

(j) $\ell^2$ coefficients

(k) Endmember 6

(l) $\ell^2$ coefficients
Sparsity statistics for Smith

- The average $\ell^0$ norm per pixel of the $\ell^2$ coefficients: 2.5063.
Extension to spectral libraries

- We can easily extend this method to search for endmembers from a spectral library, $\mathcal{L}$.
- In fact, by computing the weight matrix, $W$, with dictionary
  \[ \Phi = \mathcal{X}^{(i)} \cup \mathcal{L}, \]
  we can search simultaneously for endmembers from both the given data set and the spectral library.
- Note that we would only compute weights for $x_i \in \mathcal{X}$. 
For the future

Things we are working on:

- Developing more intricate and realistic models in which it is possible to obtain provable results.
- Consider smarter sampling methods that ideally would:
  - Reduce randomness in the endmember output.
  - Facilitate further gains in sparsity when computing the weight matrix, $W$.
- Continue to run trials on both real and synthetic data sets, and in particular, branch out to biomedical imaging.
- Systematically compare with other endmember methods.
Thank you for your time!