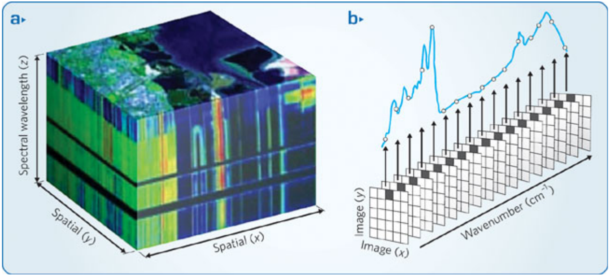
Linear Spectral Mixture Analysis (LSMA)

Bernard Lampe

November 14, 2018

Overview

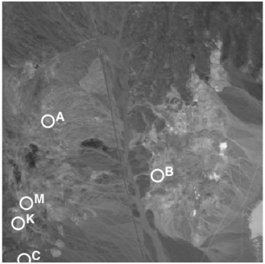
Hyperspectral Data



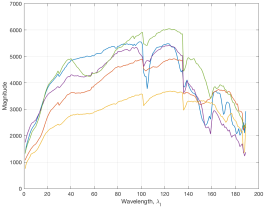
[David Bannon '09]

- Pixels are superpositions of a finite number of materials with non-negative reflectance (ANC) and sum-to-one (ASC) constraints
- Supervised: Applying FCLS and MFCLS to solve for abundance fractions
- Unsupervised: Applying NMF to solve unsupervised HSI unmixing

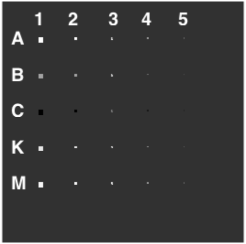
Synthetic Data



Cuprite Dimension 350x350x189



Plots of marked endmembers



Synthetic 200x200x189

Synthetic Data Descriptions

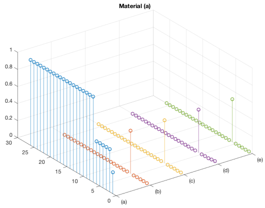
- TI2 = Target Implanted, no background, SNR = 20db
- TE2 = Target Embedded, with background, SNR = 20db
- Column 1, 4x4 Pure Pixel
- Column 2, 2x2 Pure Pixel
- Column 3, 2x2 Mixed Pixel, 50% $\mathbf{m}_i$, 50% $\mathbf{m}_j$
- Column 4, 1x1, Sub-pixel, 50% pixel, 50% background
- Column 5, 1x1, Sub-pixel, 25% pixel, 75% background
- Each row has one main material (A, B, C, K, M)

FCLS, Active Set Method

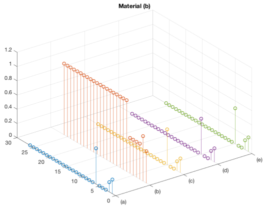
- Perform NCLS on the augmented pixel and endmember matrix
- Augment the pixel vector and endmember matrix to include ASC
- Active set corresponds to negative components in α
- Perform gradient descent on the active component dimensions only

$$\mathbf{s} = \begin{bmatrix} \delta \mathbf{r} \\ 1 \end{bmatrix}, \mathbf{N} = \begin{bmatrix} \delta \mathbf{M} \\ \mathbf{1}^T \end{bmatrix}$$

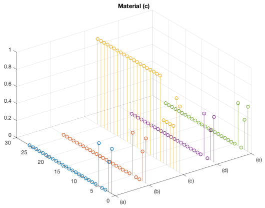
FCLS, Active Set Method, TI2 Results



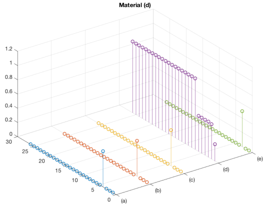
Material 1 in all rows



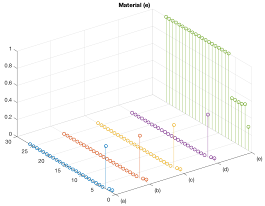
Material 2 in all rows



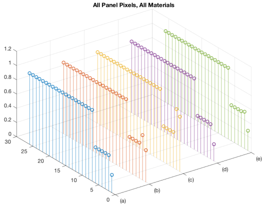
Material 3 in all rows



Material 4 in all rows

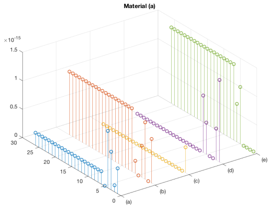


Material 5 in all rows

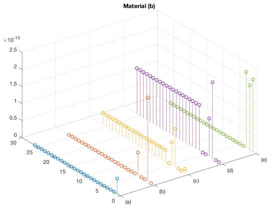


All Materials

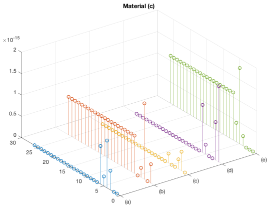
FCLS, Active Set Method, TE2 Results



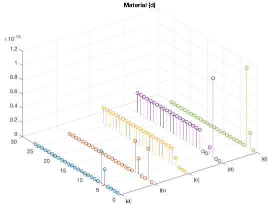
Material 1 in all rows



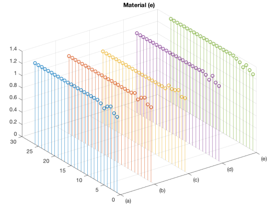
Material 2 in all rows



Material 3 in all rows



Material 4 in all rows



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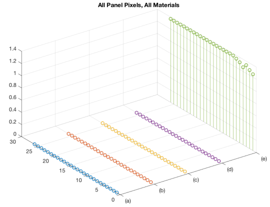


All Materials

FCLS, Geometric Method

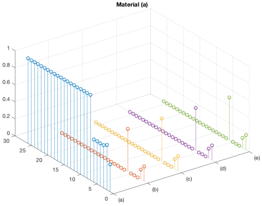
- Cramer's rule can be used to compute each component of α.
- The endmember matrix is augmented to add ASC.

$$\tilde{\mathbf{r}} = \begin{bmatrix} 1 \\ \mathbf{r} \end{bmatrix}, \tilde{\mathbf{M}} = \begin{bmatrix} 1 & 1 & \dots & 1 \\ \mathbf{m}_1 & \mathbf{m}_2 & \dots & \mathbf{m}_p \end{bmatrix}$$

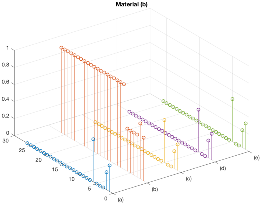
$$Vol(\tilde{\mathbf{m}}_1, \tilde{\mathbf{m}}_2, \dots, \tilde{\mathbf{m}}_p) = \frac{1}{(p-1)!} \sqrt{|\tilde{\mathbf{M}}^T \tilde{\mathbf{M}}|}$$

$$\alpha_i = \frac{Vol(\tilde{\mathbf{m}}_1, \dots, \tilde{\mathbf{m}}_{i-1}, \tilde{\mathbf{r}}, \tilde{\mathbf{m}}_{i+1}, \dots, \tilde{\mathbf{m}}_p)}{Vol(\tilde{\mathbf{m}}_1, \tilde{\mathbf{m}}_2, \dots, \tilde{\mathbf{m}}_p)}$$

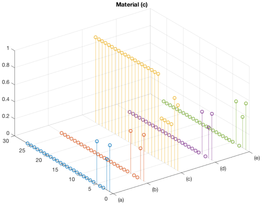
FCLS, Geometric Method, TI2 Results



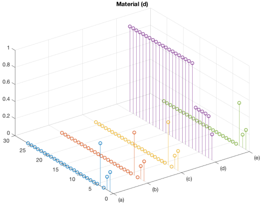
Material 1 in all rows



Material 2 in all rows



Material 3 in all rows



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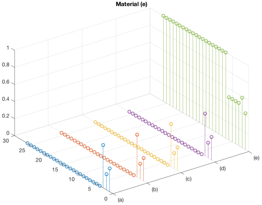
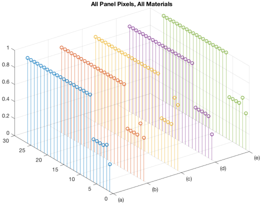
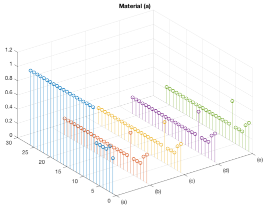


Material 5 in all rows

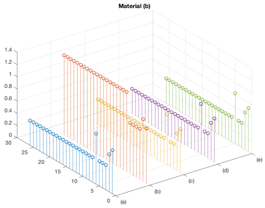


All Materials

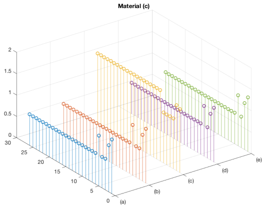
FCLS, Geometric Method, TE2 Results



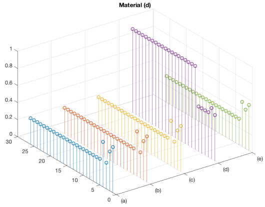
Material 1 in all rows



Material 2 in all rows



Material 3 in all rows



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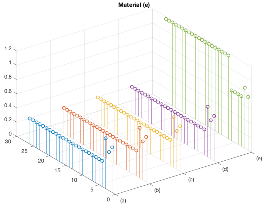

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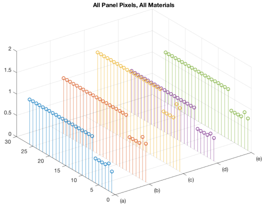


All Materials

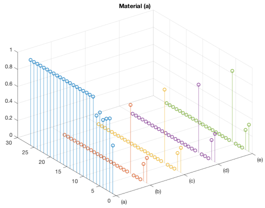
FCLS, OSP Method

- Compute $\delta_{\mathbf{m}_i} = \mathbf{P}_{\mathbf{U}}^{\perp}$ classifier for all $\mathbf{m}_i$
- Classification weight is abundance fraction
- Suppressing background leaves endmember contribution non-negative
- Normalized after classification

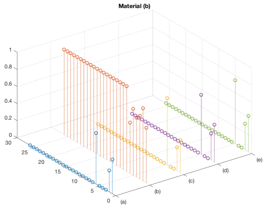
$$\tilde{\mathbf{M}} = [\mathbf{m}_1, ..., \mathbf{m}_{i-1}, \mathbf{m}_{i+1}, ..., \mathbf{m}_p]$$

$$\delta_{\mathbf{m}_i} = \mathbf{P}_{\mathbf{U}}^{\perp} = \mathbf{I} - \tilde{\mathbf{M}} \left(\tilde{\mathbf{M}}^T \tilde{\mathbf{M}} \right)^{-1} \tilde{\mathbf{M}}^T$$

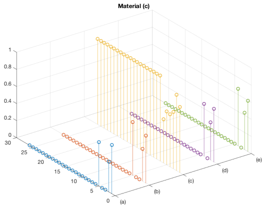
FCLS, OSP Method, TI2 Results



Material 1 in all rows



Material 2 in all rows



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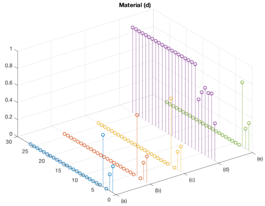

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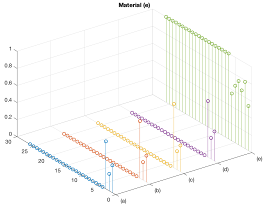

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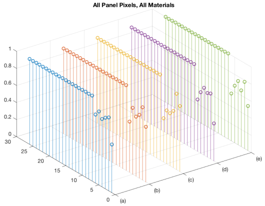
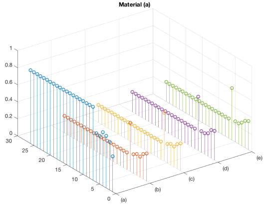
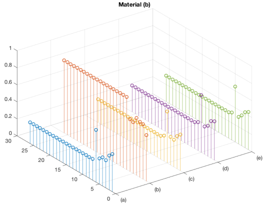


All Materials

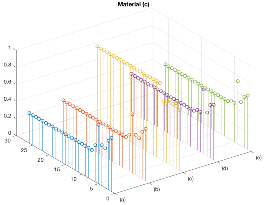
FCLS, OSP Method, TE2 Results



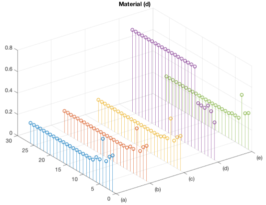
Material 1 in all rows



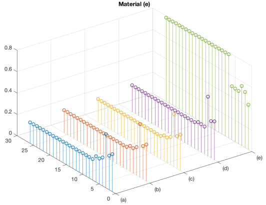
Material 2 in all rows



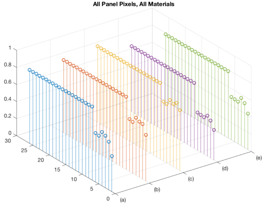
Material 3 in all rows



Material 4 in all rows



Material 5 in all rows



All Materials

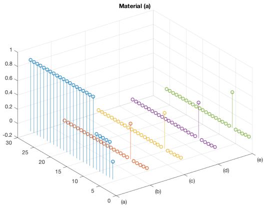
Modified FCLS Lagrange Multipler

- Initial condition is $\alpha^{MFCLS} = \alpha^{SCLS}$
- Compute λ_1 and λ_2 using constraints $\sum_{i=1}^{p} \alpha_i = 1$ and $\sum_{i=1}^{p} |\alpha_i| = 1$
- $\alpha^{MFCLS} = \alpha^{SCLS} - \left(\mathbf{M}^T\mathbf{M}\right)^{-1}\left[\lambda_1\mathbf{1} + \lambda_2 sign(\alpha^{SCLS})\right]$
- Iterate if any negative components left

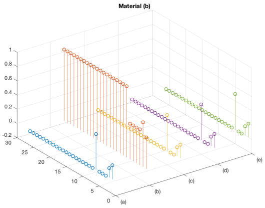
$$\begin{bmatrix} 1 - \mathbf{1}^T\alpha^{MFCLS} \\ 1 - sign(\alpha_{LS})^T\alpha^{MFCLS} \end{bmatrix} =$$

$$\begin{bmatrix} \mathbf{1}^T(\mathbf{M}^T\mathbf{M})^{-1}\mathbf{1} & \mathbf{1}^T(\mathbf{M}^T\mathbf{M})^{-1}sign(\alpha_{LS}) \\ sign(\alpha_{LS})^T(\mathbf{M}^T\mathbf{M})^{-1}\mathbf{1} & sign(\alpha_{LS}^T)(\mathbf{M}^T\mathbf{M})^{-1}sign(\alpha_{LS}) \end{bmatrix} \begin{bmatrix} \lambda_1 \\ \lambda_2 \end{bmatrix}$$

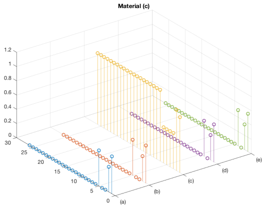
Modified FCLS Lagrange Multipler, TI2 Results



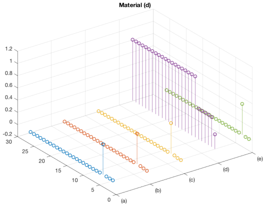
Material 1 in all rows



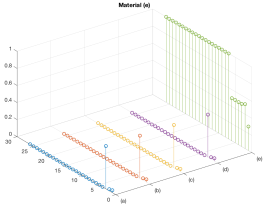
Material 2 in all rows



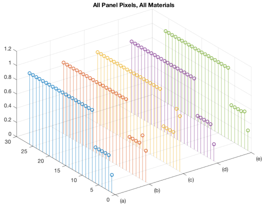
Material 3 in all rows



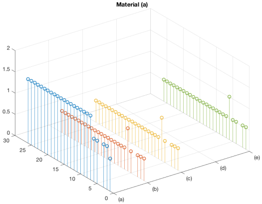
Material 4 in all rows



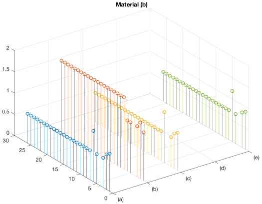
Material 5 in all rows



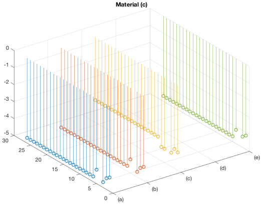
All Materials



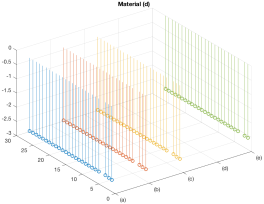
Material 1 in all rows



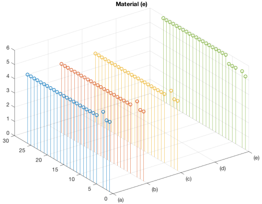
Material 2 in all rows



Material 3 in all rows



Material 4 in all rows



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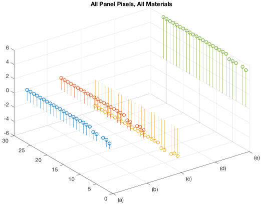


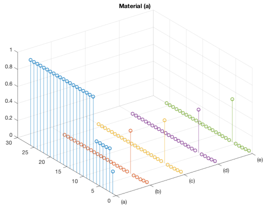
All Materials

MFCLS Iterative Algorithm

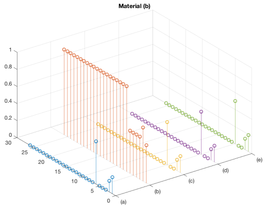
- Active set gradient descent method with augmented steering matrix to include ASC and AASC
- Augments the endmember and pixels to add ASC

$$\mathbf{s} = \begin{bmatrix} \delta\mathbf{r} \\ 1 \end{bmatrix}, \mathbf{N} = \begin{bmatrix} \delta\mathbf{M} \\ \mathbf{1}^T \end{bmatrix}$$

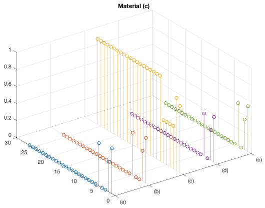
Modified FCLS Iterative, TI2 Results



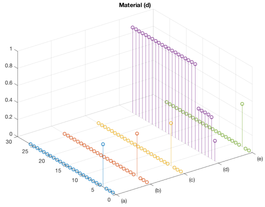
Material 1 in all rows



Material 2 in all rows



Material 3 in all rows



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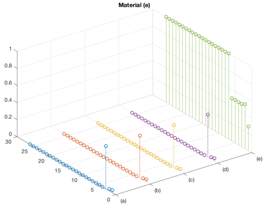

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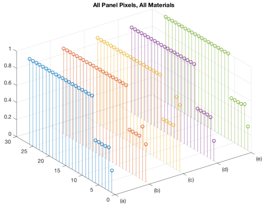
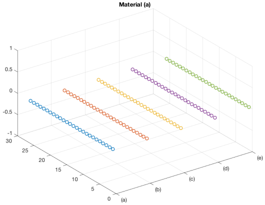
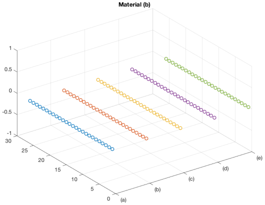


All Materials

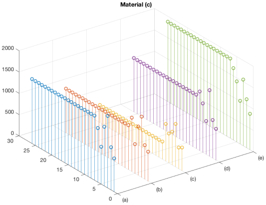
Modified FCLS Iterative, TE2 Results



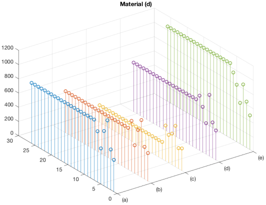
Material 1 in all rows



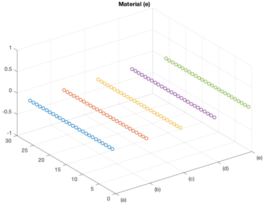
Material 2 in all rows



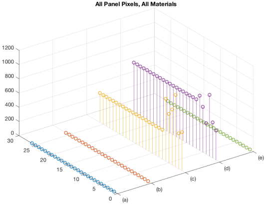
Material 3 in all rows



Material 4 in all rows



Material 5 in all rows



All Materials

Numerical Results, Accuracy and Timing

Table: I. Algorithm accuracy in MSE

	Active Set	Geometric	OSP	MFCLS 1	MFCLS 2
TI2	0.003489	0.00394	0.01672	0.003536	0.003538
TE2	0.709771	0.13506	0.02976	5.677302	143345.3

Table: II. Algorithm timing in seconds

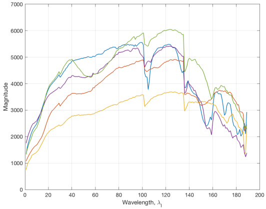
Active Set	Geometric	OSP	MFCLS 1	MFCLS 2
3.263822	1.762295	1.880125	2.453860	9.055446

Direct MNF

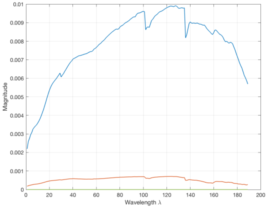
- Try and use MNF for FCLS
- Tried using augmented endmember matrix and pixels for ASC
- Also tried directly normalizing abundance on each iteration
- Tried both alternating least squares and multiplicative update
- Initialize the **W** matrix to **M**

$$\mathbf{s} = \begin{bmatrix} \delta \mathbf{r} \\ 1 \end{bmatrix}, \mathbf{N} = \begin{bmatrix} \delta \mathbf{M} \\ \mathbf{1}^T \end{bmatrix}$$

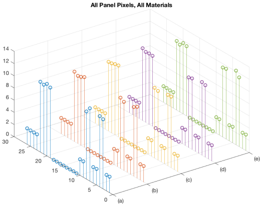
TI2 Direct NMF



Ground Truth Endmembers

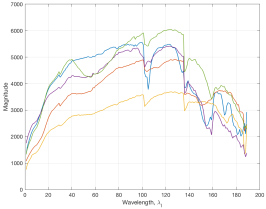


NMF Computed Endmembers

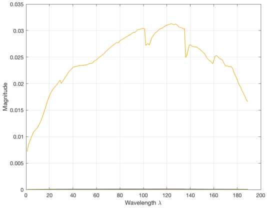


NMF Computed Abundance

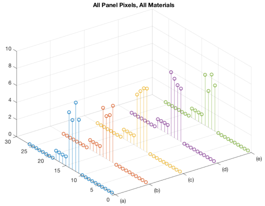
TE2 Direct NMF



Ground Truth Endmembers



NMF Computed Endmembers



NMF Computed Abundance

NMF Hoyer Sparsity Algorithm

Algorithm: NMF with sparseness constraints

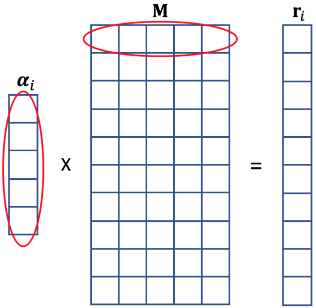
1. Initialize $\mathbf{W}$ and $\mathbf{H}$ to random positive matrices
2. If sparseness constraints on $\mathbf{W}$ apply, then project each column of $\mathbf{W}$ to be non-negative, have unchanged L_2 norm, but L_1 norm set to achieve desired sparseness
3. If sparseness constraints on $\mathbf{H}$ apply, then project each row of $\mathbf{H}$ to be non-negative, have unit L_2 norm, and L_1 norm set to achieve desired sparseness
4. Iterate
   (a) If sparseness constraints on $\mathbf{W}$ apply,
      i. Set $\mathbf{W} := \mathbf{W} - \mu_{\mathbf{W}}(\mathbf{WH} - \mathbf{V})\mathbf{H}^T$
      ii. Project each column of $\mathbf{W}$ to be non-negative, have unchanged L_2 norm, but L_1 norm set to achieve desired sparseness

   else take standard multiplicative step $\mathbf{W} := \mathbf{W} \otimes (\mathbf{VH}^T) \oslash (\mathbf{WHH}^T)$

   (b) If sparseness constraints on $\mathbf{H}$ apply,
      i. Set $\mathbf{H} := \mathbf{H} - \mu_{\mathbf{H}}\mathbf{W}^T(\mathbf{WH} - \mathbf{V})$
      ii. Project each row of $\mathbf{H}$ to be non-negative, have unit L_2 norm, and L_1 norm set to achieve desired sparseness

   else take standard multiplicative step $\mathbf{H} := \mathbf{H} \otimes (\mathbf{W}^T\mathbf{V}) \oslash (\mathbf{W}^T\mathbf{WH})$

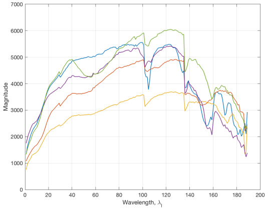
NMF Hoyer Sparsity Algorithm



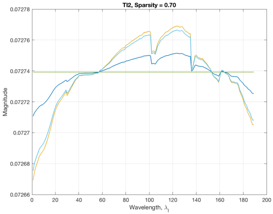
$$\text{sparseness}(\boldsymbol{\alpha}_i) = \frac{\sqrt{n} - \|\boldsymbol{\alpha}_i\|_1 / \|\boldsymbol{\alpha}_i\|_2}{\sqrt{n} - 1}$$

- High sparsity applied to abundance fractions columns $\boldsymbol{\alpha}_i$
- Low sparsity applied to rows of $\mathbf{M}$
- Problem is one sparsity is applied across all endmembers and another across all abundances

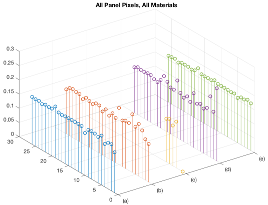
TI2 NMF with Hoyer Sparsity = 0.7, Normalized ASC



Ground Truth Endmembers

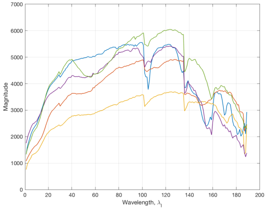


NMF Computed Endmembers

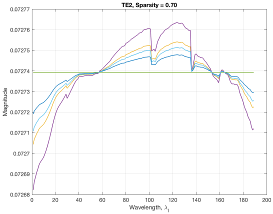


NMF Computed Abundance

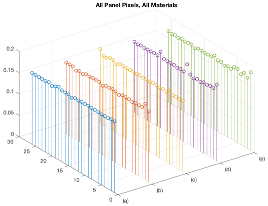
TE2 NMF with Hoyer Sparsity = 0.7, Normalized ASC



Ground Truth Endmembers

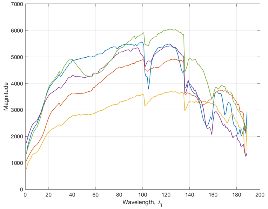


NMF Computed Endmembers

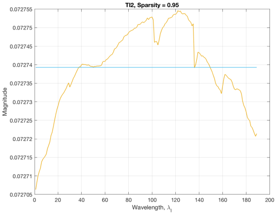


NMF Computed Abundance

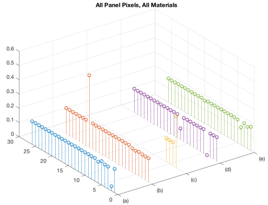
TI2 NMF with Hoyer Sparsity = 0.95, Normalized ASC



Ground Truth Endmembers

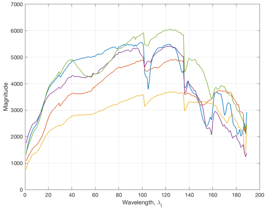


NMF Computed Endmembers

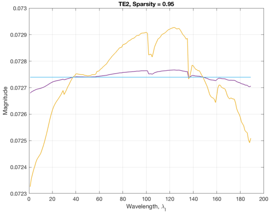


NMF Computed Abundance

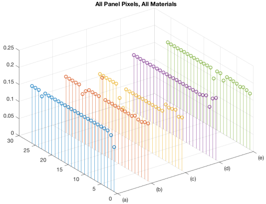
TE2 NMF with Hoyer Sparsity = 0.95, Normalized ASC



Ground Truth Endmembers



NMF Computed Endmembers



NMF Computed Abundance

Minimum Volume Constrained NMF

- Minimize the LSE subject to ANC and ASC and minimum volume
- Algorithm in paper uses gradient descent of objective function and PCA projection to measure volume
- At each iteration impose the ASC via abundance matrix augmentation

$$min\{f(\mathbf{M},\mathbf{A}) = 1/2\|\mathbf{R}-\mathbf{M}\mathbf{A}\|_F^2 + \lambda Vol(\mathbf{M})\}$$
$$\mathbf{M} \succeq 0, \mathbf{A} \succeq 0, \mathbf{1}^T\mathbf{A} = \mathbf{1}$$

Minimum Volume Constrained NMF

Algorithm 1: Minimum volume constrained NMF

Data : Non-negative mixture data $\mathbf{X} \in \mathbf{R}^{l \times N}$ with each column being an observation vector, and the number of endmembers c.

Result: Two non-negative matrices $\mathbf{A} \in \mathbf{R}^{l \times c}$ and $\mathbf{S} \in \mathbf{R}^{c \times N}$ with sum-to-one constraint $\mathbf{1}^T\mathbf{S} = \mathbf{1}^T$.

//Initialization
Initialize $\mathbf{A}$ by randomly selecting c data points to form its columns,
$\mathbf{S} = \underline{\mathbf{0}}$, which is a zero matrix;
Set iteration index $k = 0$;

//main loop
while *stop condition is not met* **do**
- $\mathbf{A}^{k+1} = \max(\mathbf{0},\ \mathbf{A}^k - \alpha^k \nabla_{\mathbf{A}} f(\mathbf{A}^k, \mathbf{S}^k))$;
- $\mathbf{S}^{k+1} = \max(\mathbf{0},\ \mathbf{S}^k - \beta^k \nabla_{\mathbf{S}} f(\mathbf{A}^{k+1}, \mathbf{S}^k))$;
- Scale columns of $\mathbf{S}$ to sum to unity;
- Increase k by 1.

end

Conclusions

- FCLS and MFCLS works well with TI2
  - TI2 pixels are in the range space of the endmembers
- FCLS and MFCLS does not work well for TE2
  - TE2 pixels are not in the range space of the endmembers because of the background
- NMF can be used to do linear unmixing of HSI data into constituent materials
  - Other constraints are necessary to produce good results

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