Nonnegative Matrix Factorization (NMF)

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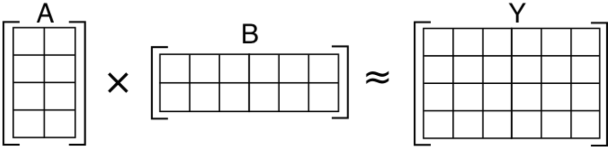
May 5, 2016

Overview

1. Theory
   - Model
   - Cost Function
   - Uniqueness
   - Algorithms
   - Performance
   - Diversity
2. Application
   - Description
3. Results
4. References



NMF Model

$$\mathbf{Y} = \mathbf{AB} + \mathbf{E},\ \mathbf{Y} \in \mathbb{R}^{M \times N}, \mathbf{A} \in \mathbb{R}^{M \times R}, \mathbf{B} \in \mathbb{R}^{R \times N}$$

$$Y_{ij} \approx \sum_{r=1}^{R} A_{ir} B_{rj}$$

- $\mathbf{Y}$ is a nonnegative data matrix
- $\mathbf{A}$ and $\mathbf{B}$ are nonnegative factor matrices
- $\mathbf{E}$ is an error matrix
- $\{\mathbf{a}_i\}$, columns of $\mathbf{A}$ are the basis vectors
- $\{\mathbf{b}_j\}$, columns of $\mathbf{B}$ are the coordinate vectors

Model Constraints of PCA, VQ, NMF, Dictionary Learning

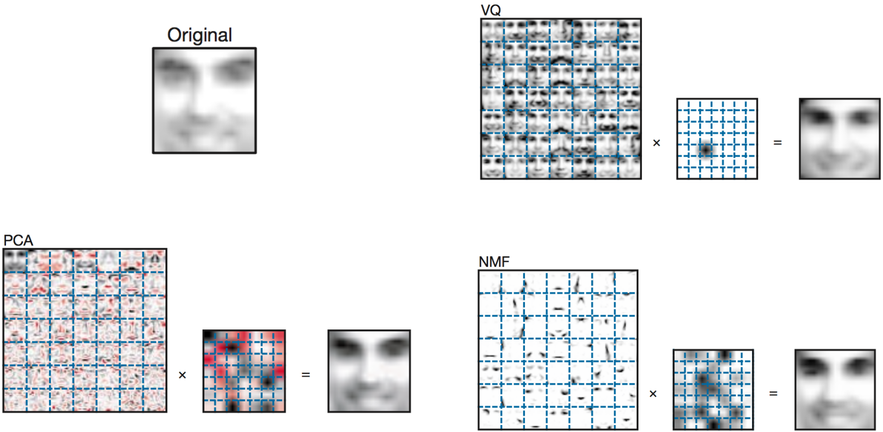
Different algorithms can be viewed as matrix decompositions with different constraints on $\mathbf{A}$ and $\mathbf{B}$.

- VQ require $\{\mathbf{a}_i\}$ to be quantized vectors, and $\{\mathbf{b}_j\}$ to be unitary
  - $\{\mathbf{a}_i\}$ are the centroids of the K-means algorithm
- PCA $\{\mathbf{a}_i\}$ are orthonormal, and $\mathbf{a}_1 = \arg\max_{\|\mathbf{a}_1\|} \mathrm{E}\{\mathbf{a}_1^T \mathbf{y}_i{}^2\}, \quad \forall i$
  - $\{\mathbf{a}_i\}$ are the eigenvectors of the correlation matrix
- NMF requires specification of R, and that $A_{ij} \geq 0$ and $B_{ij} \geq 0$
- Dictionary learning requires specification of R, and $A_{ij} \in \mathbb{R}$ and $B_{ij} \in \mathbb{R}$

Model Expressiveness

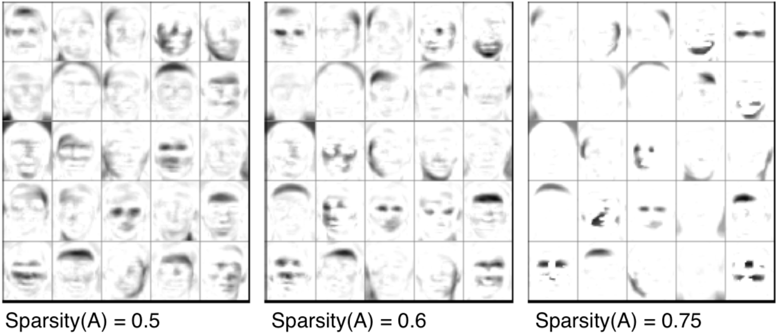
- PCA and ICA can add and subtract basis matrix vectors
- NMF can only add basis matrix vectors leading to "parts based" models
- NN-KSVD and non-negative dictionary learning are specific NMF factorizations

PCA, VQ and NMF Examples



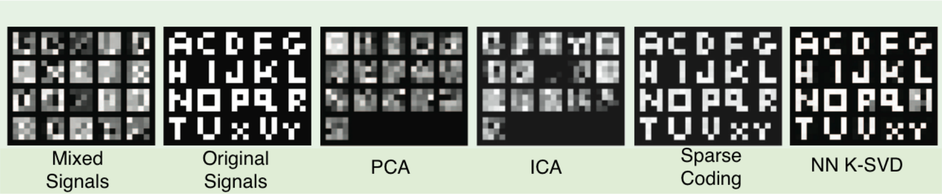
Basis matricies were trained with 2429, 19x19 pixel face images. [Lee and Seung '99]

NMF With Sparsity Example



[Hoyer '04]

Model Expressiveness Examples



[Ivana Tosic and Pascal Frossard '11]

- VQ, PCA and ICA have linearly independent vectors in the basis matrix
- PCA and ICA require $R \leq \min\{M, N\}$
- NMF can have linearly dependent vectors in the basis matrix

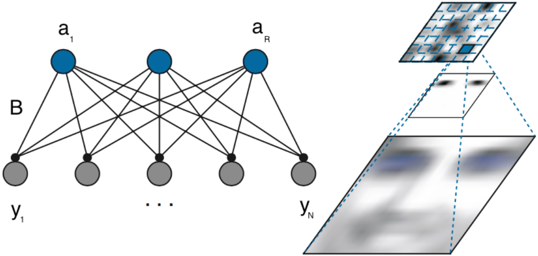
NMF as K-Means Clustering

$$J_{\text{K-means}} = \sum_{i=1}^{n} \min_{1 \le r \le R} \|\mathbf{y}_i - \mathbf{c}_r\|_F^2 = \sum_{r=1}^{R} \sum_{i \in C_r} \|\mathbf{y}_i - \mathbf{c}_r\|_F^2$$
$$= \sum_{i=1}^{n} \sum_{r=1}^{R} h_{ir} \|\mathbf{y}_i - \mathbf{c}_r\|_F^2 = \|\mathbf{Y} - \mathbf{AB}\|_F^2 = J_{nmf}$$

$$\mathbf{c}_r = \frac{1}{|C_r|} \sum_{i \in C_r} \mathbf{y}_i, \quad \mathbf{y}_i \in C_r, \quad h_{ir} = \{0, 1\}$$

- NMF can be considered a clustering of the data into R clusters with $\{\mathbf{a}_i\}$ centroids and $\{\mathbf{b}_j\}$ being unitary [C. Ding, et al '05]
- The centroids do not necessarily have to be positive, therefore this is refered to as "semi-NMF" or "relaxed-NMF"

NMF as Probabilistic Latent Variables



- Visible units $\{\mathbf{y}_i\}$ are connected to hidden latent variables $\{\mathbf{a}_j\}$ through weights in $\mathbf{B}$
- If $\{\mathbf{b}_j\}$ are normal, then $\{\mathbf{b}_j\}$ can be viewed as probability distributions
- If $J_{nmf} = D_{KL}(\mathbf{Y}\|\mathbf{AB})$, then the problem is exactly probabilistic latent semantic analysis [C.Ding '08]

Cost Functions

NMF is implemented by minimizing a non-convex cost function

- Euclidean Distance Minimization

$$J^*_{\mathrm{nmf}} = \arg\min_{\mathbf{A},\mathbf{B}} \frac{1}{2}||\mathbf{Y} - \mathbf{AB}||_2^2 \quad \text{s.t.} \quad \mathbf{A}, \mathbf{B} \geq 0$$

- Frobenius Distance Minimization

$$J^*_{\mathrm{nmf}} = \arg\min_{\mathbf{A},\mathbf{B}} \frac{1}{2}||\mathbf{Y} - \mathbf{AB}||_F^2 \quad \text{s.t.} \quad \mathbf{A}, \mathbf{B} \geq 0$$

- K-L Distance Minimization

$$J^*_{\mathrm{nmf}} = \arg\min_{\mathbf{A},\mathbf{B}} D_{KL}(\mathbf{Y}\|\mathbf{AB}) = \arg\min_{\mathbf{A},\mathbf{B}} \sum_{ij}(Y_{ij}\log\frac{Y_{ij}}{[\mathbf{AB}]_{ij}} - Y_{ij} + [\mathbf{AB}]_{ij})$$

Uniqueness

Factorization is not unique

$$\mathbf{Y} \approx (\mathbf{AT})(\mathbf{T}^{-1}\mathbf{B}) = \mathbf{A}'\mathbf{B}'$$

We can enforce a unique solution by including regularization (i.e., sparsity)

$$J^*_{\text{nmf}} = \arg\min_{\mathbf{A},\mathbf{B}} \frac{1}{2}\left|\left|\mathbf{Y} - \mathbf{AB}\right|\right|_2^2 + \lambda_0\|A\|_0 + \lambda_1\|B\|_0 \quad \text{s.t.} \quad \mathbf{A},\mathbf{B} \geq 0$$

If the sparsity of the **A** or **B** is low enough, then the solution is unique

$$\|\mathbf{B}\|_0 < \frac{R\ \text{spark}(\mathbf{A})}{2} \qquad \text{[Donoho and Elad '02]}$$

Spark is the smallest number of columns that are linearly dependent

$$\text{spark}(\mathbf{A}) = \min_{\mathbf{d}\neq 0} \|\mathbf{d}\|_0 \quad \text{s.t.} \quad \mathbf{Ad} = \mathbf{0}$$

Algorithms Used in Project

Optimization algorithms for NMF non-convex cost functions

- Alternating Least Squares (ALS)
  - J_{nmf} is minimized by alternating between **A** and **B**
  - J_{nmf} is minimized while holding **A** fixed and minimizing **B** and vise versa
- Multiplicative Update (MU)
  - J_{nmf} is minimized by fixing **A** and **B**
  - **A** and **B** are updated using a multiplicative update rule
- Hierarchical Alternating Least Squares (HALS)
  - J_{nmf} is minimized by fixing **A** and **B**
  - Only one column of **A** or **B** is updated using an update rule
- Multiplicative Update (MU) with Sparsity Constraint
  - J_{nmf} is minimized by fixing **A** and **B**
  - **A** and **B** are updated using a sparse multiplicative update rule

Alternating Least Squares Optimization

$$J_{\text{nmf}} = \arg\min_{\mathbf{A},\mathbf{B}} \frac{1}{2} \left|\left| \mathbf{Y} - \mathbf{AB} \right|\right|_2^2 \quad \text{s.t.} \quad \mathbf{A}, \mathbf{B} \geq 0$$

	Algorithm: Alternating Least Squares (ALS)
1:	Initialize **A** and **B**
2:	**Repeat**
3:	solve: $\arg\min_{\mathbf{B}} \frac{1}{2} \|\|\mathbf{Y} - \mathbf{AB}\|\|_2^2 \quad \text{s.t.} \quad \mathbf{A}, \mathbf{B} \geq 0$
4:	solve: $\arg\min_{\mathbf{A}} \frac{1}{2} \|\|\mathbf{Y} - \mathbf{AB}\|\|_2^2 \quad \text{s.t.} \quad \mathbf{A}, \mathbf{B} \geq 0$
5:	**Stopping Condition**

[Paatero and Tapper '94]

Multiplicative Update Optimization

$$J_{\text{nmf}} = \arg\min_{\mathbf{A},\mathbf{B}} \frac{1}{2} ||\mathbf{Y} - \mathbf{AB}||_2^2 \quad \text{s.t.} \quad \mathbf{A}, \mathbf{B} \geq 0$$

	Algorithm: Multiplicative Update (MU)
1:	Initialize $\mathbf{A}^0$, $\mathbf{B}^0$, k = 0
2:	**Repeat**
3:	$A_{ir}^{k+1} = A_{ir}^{k} \frac{\left(\mathbf{Y}\mathbf{B}^k\right)_{ir}}{\left(\mathbf{A}^k (\mathbf{B}^k)^T \mathbf{B}^k\right)_{ir}}, \quad 1 \leq i \leq M, 1 \leq r \leq R$
4:	$B_{rj}^{k+1} = B_{rj}^{k} \frac{\left(\mathbf{Y}^T \mathbf{A}^{k+1}\right)_{rj}}{\left(\mathbf{B}^k (\mathbf{A}^{k+1})^T \mathbf{A}^{k+1}\right)_{rj}}, \quad 1 \leq j \leq N, 1 \leq r \leq R$
5:	$k = k + 1$
6:	**Stopping Condition**

[Lee and Seung '99]

	Algorithm: HALS / NN-KSVD
1:	Random Initialization of $\mathbf{A}^0$, J = 1
2:	**Repeat**
3:	Use pursuit algorithm to compute $\{\mathbf{b}_j\}$
	$\arg\min_{\mathbf{B}} \lvert\lvert \mathbf{Y}_i - \mathbf{AB} \rvert\rvert_2^2 \quad \lVert \mathbf{b} \rVert_0 \leq T_0$
4:	Update Stage: For k = 1, 2, . . . , R
	Define group that use $\{\mathbf{a}_k\} : w_k, i \in N, \mathbf{b}_i(k) \neq 0$
	Compute: $\mathbf{E}_k = \mathbf{Y} - (\mathbf{AB} - \mathbf{a}_k(\mathbf{b}^k)^T)$
	Restrict $\mathbf{E}_k$, choose only columns corresponding to w_k, get $\mathbf{E}_k^{w_k}$
	Apply SVD, $\mathbf{E}_k^{w_k} = \mathbf{U}\Delta\mathbf{V}^T, \quad \mathbf{a}_k = \mathbf{u}_1, \quad \mathbf{b}^k = \Delta(1,1)\mathbf{v}_1$
5:	$J = J + 1$
6:	**Stopping Condition**

[Michal Aharon, et al '06]

Multiplicative Update With Sparsity Optimization

$$J_{\text{nmf}} = \arg\min_{\mathbf{A},\mathbf{B}} \frac{1}{2}||\mathbf{Y} - \mathbf{AB}||_2^2 \quad \text{s.t.} \quad \mathbf{A}, \mathbf{B} \geq 0, \; S(\mathbf{a}_i) = S_a, \; S(\mathbf{b}_j) = S_b$$

$$S(\mathbf{x}) = \frac{\sqrt{n} - \|\mathbf{x}\|_1 / \|\mathbf{x}\|_2}{\sqrt{n} - 1} \quad \text{s.t.} \quad n = \dim(\mathbf{x})$$

	Algorithm: Multiplicative Update with Sparsity (MU)
1:	Initialize $\mathbf{A}^0$, $\mathbf{B}^0$, $k = 0$, $\mu_{\mathbf{A}}$, $\mu_{\mathbf{B}}$
2:	**Repeat**
3:	$\mathbf{A} = \mathbf{A} - \mu_{\mathbf{A}}(\mathbf{AB} - \mathbf{Y})\mathbf{B}^T$
4:	project: $\{\mathbf{a}_i\}$ s.t. $\|\mathbf{a}_i\|_1 = S_a$
5:	$\mathbf{B} = \mathbf{B} - \mu_{\mathbf{B}}\mathbf{A}^T(\mathbf{AB} - \mathbf{Y})$
6:	project: $\{\mathbf{b}_j\}$ s.t. $\|\mathbf{b}_j\|_1 = S_b$
7:	**Stopping Condition**

[Hoyer '04]

Performance

Big-O Complexity of NMF Algorithms

$$\mathbf{Y} = \mathbf{AB} + \mathbf{E},\ \mathbf{Y} \in \mathbb{R}^{M \times N}, \mathbf{A} \in \mathbb{R}^{M \times R}, \mathbf{B} \in \mathbb{R}^{R \times N}$$

- For R = 1: "Easy", [Perron-Frobenius and Eckart-Young theorems '11]
- Rank($\mathbf{Y}$) = 2: Rank$_+$($\mathbf{Y}$) = 2, "Easy"
- Rank($\mathbf{Y}$) = R: $\mathcal{O}((M \times N)^{R^2})$, [Arora et al. '12, Moitra '13]

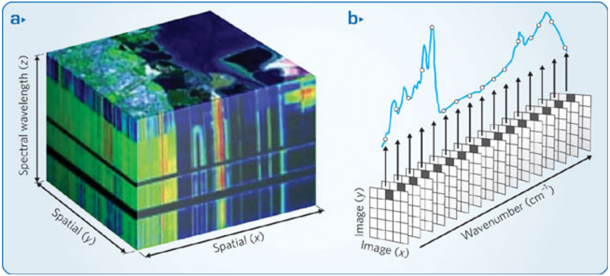
Algorithm	Complexity per iteration
ALS:	$\mathcal{O}(M \times N \times R)$
MU:	$\mathcal{O}(M \times N \times R)$
HALS:	$\mathcal{O}(M \times N \times R)$

[Guoxu Zhou, et al '14]

Other Methods

- Inexact Alternating Least Square (IALS)
- Accelerating Proximal Gradient (APG)
- Seperable NMF (Sep-NMF)
- Squential NMF (Seq-NMF)
- Multi-factor NMF (MF-NMF)
- NMF Based on Low Rank Approximations
- Non-negative Sparse Coding
- Many Others...

Problem Description



[David Bannon '09]

- HSI pixels are non-negative
- Pixels are superpositions of a finite number of materials with non-negative reflectance
- Applying NMF to solve the unsupervised HSI unmixing problem

Diversity in Hyperspectral Images (HSI)

- Minimize mutual coherence between $\{\mathbf{a}_i\}$

$$M(\{\mathbf{a}_i\}) = \max_{1 \leq i \neq j \leq R} \frac{|\mathbf{a}_i^T \mathbf{a}_j|}{\|\mathbf{a}_i\|_2 \|\mathbf{a}_j\|_2}$$

- Minimize sparsity of $\{\mathbf{b}_j\}$

$$1 \leq \|\mathbf{b}_j\|_0 \leq R$$

HSI Decomposition

- What are the basis vectors that "best" represent the image?
  - The material types can be represented by the columns of **A**
  - You can group and classify pixels from these types
- What are the coefficients for each pixel in the image?
  - The abundance fractions can be represented by the columns of **B**
- Each pixel in **Y** is then represented by a linear combination of **A** and columns of **B**

$$Y_{ij} \approx \sum_{r=1}^{R} A_{ir} B_{rj}$$

- The error due to approximation is

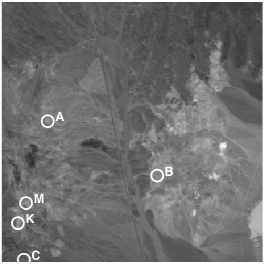
$$\mathbf{E} = \mathbf{Y} - \mathbf{AB}$$

Linear Unmixing

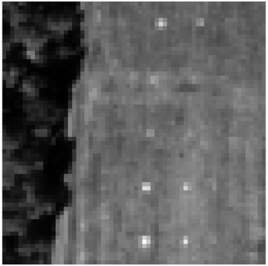
- What are the basis vectors that “best” represent the image?
  - The material types can be represented by the columns of **A**
  - You can group and classify pixels from these types
- What are the coefficients for each pixel in the image?
  - The abundance fractions can be represented by the columns of **B**
- Each pixel in **Y** is then represented by a linear combination of the columns of **A**

$$Y_{ij} \approx \sum_{r=1}^{R} A_{ir} B_{rj}$$

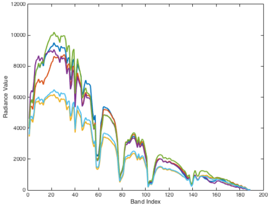
Collected and Synthetic Data



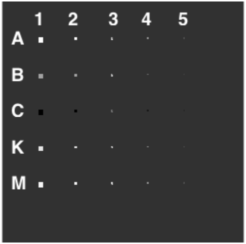
Cuprite Dimension 350x350x189



Hydice Dimension 64x64x169

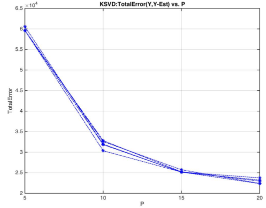


Plots of marked endmembers

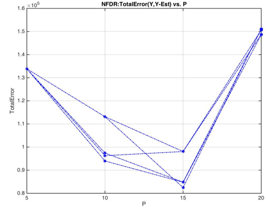


Synthetic 200x200x189

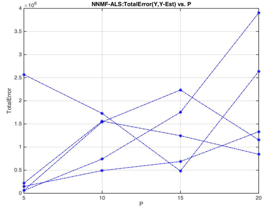
Numerical Error & Mutual Coherence



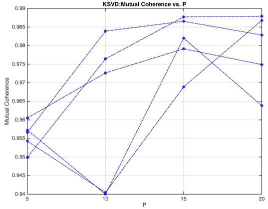
KSVD Error vs. P



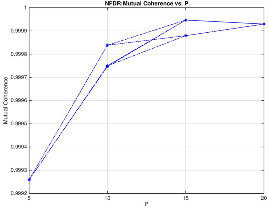
NFDR Error vs. P



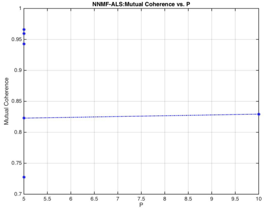
ALS Error vs. P



KSVD MC vs. P

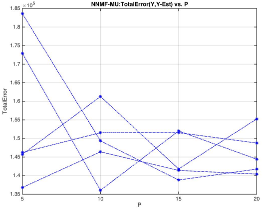


NFDR MC vs. P

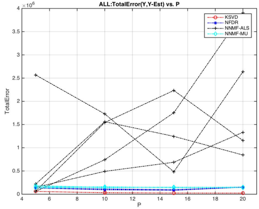


ALS MC vs. P

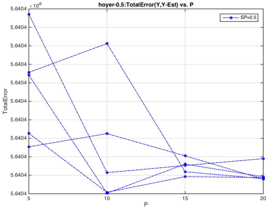
Numerical Error & Mutual Coherence



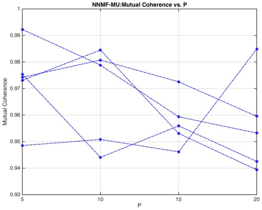
MU Error vs. P



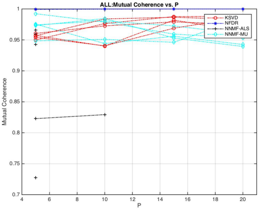
ALL Error vs. P



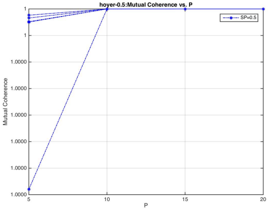
Hoyer 0.5 Error vs. P



MU MC vs. P

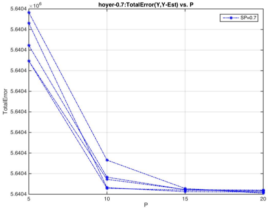


ALL MC vs. P

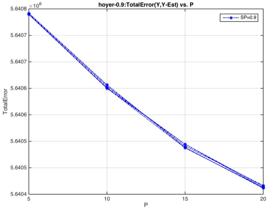


Hoyer 0.5 MC vs. P

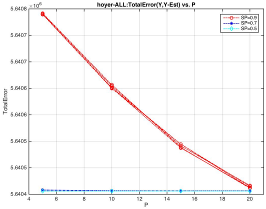
Numerical Error & Mutual Coherence



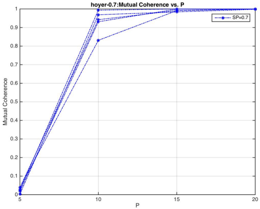
Hoyer 0.7 Error vs. P



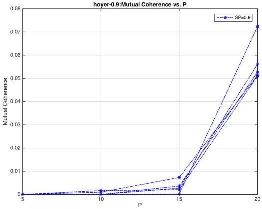
Hoyer 0.9 Error vs. P



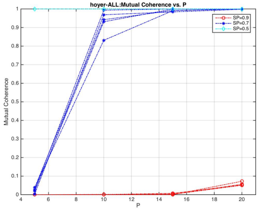
Hoyer All Error vs. P



Hoyer 0.7 MC vs. P

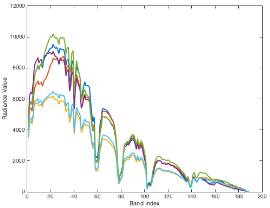


Hoyer 0.9 MC vs. P

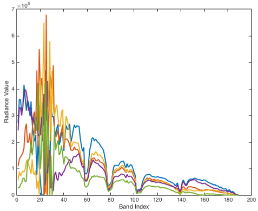


Hoyer All MC vs. P

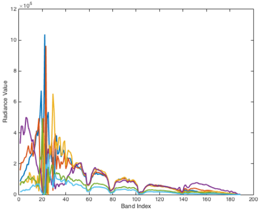
Reconstruction ALS and MU



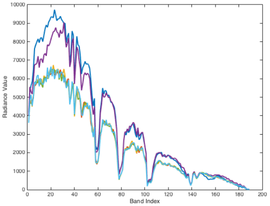
Original Radiance Data



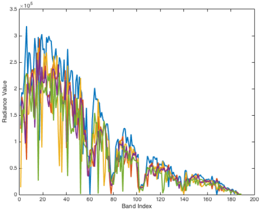
ALS Result



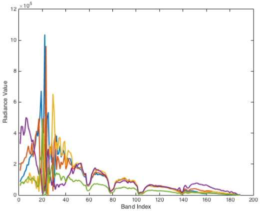
ALS/Mult Result



NFINDR Result

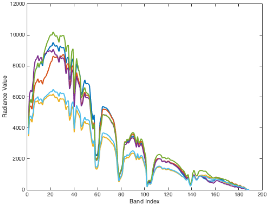


Multiplicative Result

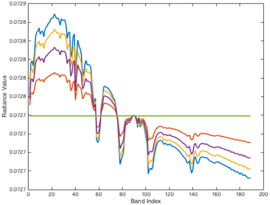


Mult/ALS Result

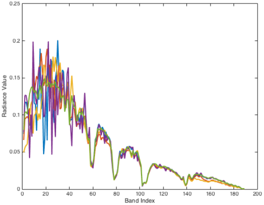
Reconstruction Hoyer and NN-KSVD



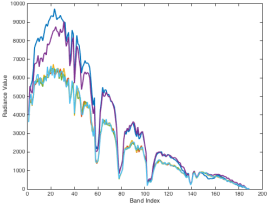
Original Radiance Data



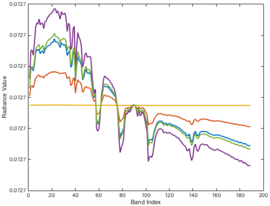
Hoyer (Sparsity $= 0.7$)



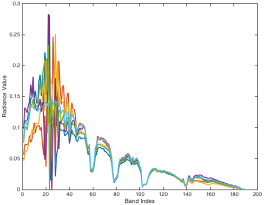
KSVD 10 Iterations



NFINDR Result



Hoyer (Sparsity $= 0.99$)



KSVD 250 Iterations

Algorithm Rankings

Criteria	**Best**				**Worst**
Abs Error	KSVD	NFINDR	MU	ALS	Hoyer
Repeatability	Hoyer	KSVD	NFINDR	MU	ALS
Increasing P	KSVD	Hoyer	NFINDR	ALS	MU
Shape	Hoyer	NFINDR	KSVD	ALS	MU
Run time	ALS	MU	Hoyer	NFINDR	KSVD

Conclusions

- NMF can be used to do linear unmixing of HSI data into constituent materials
- Scale and permutation ambiguity need application data to resolve
- Sparsity helps considerably with the uniqueness and repeatability
  - However, sparsity needs to be known a-priori
- Sparsity did resolve the shape better
  - However, Hoyer frequently converged to a uniform answer
- The run time of KSVD was much larger than the other algorithms

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