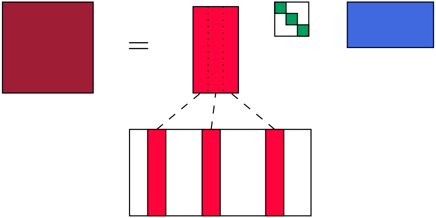
A New Approach to Dictionary-Based Nonnegative Matrix Factorization



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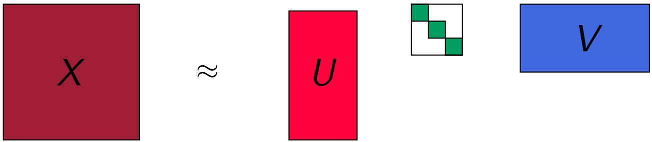
Nonnegative Matrix Factorization



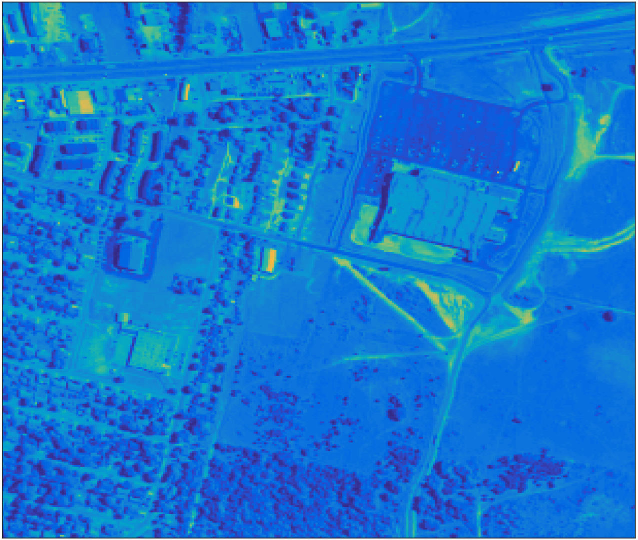
$$X \approx UV \iff X(:,j) \approx \sum_{k=1}^{k} U(:,k)V(k,j)\ \forall j.$$

where $U \geq 0$ and $V \geq 0$ element-wise.

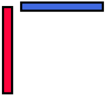
Uniqueness

The NMF of a nonnegative matrix X is **not unique** unless some harsh sparsity conditions on X are met [Donoho 2004, Laurberg 2008, Huang 2013].

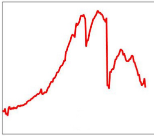
Application to spectral unmixing of HSIs



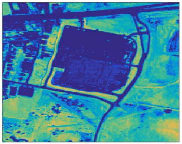
Application to spectral unmixing of HSIs

λ  $\approx \sum_{r=1}^{R}$ 

pixels



Spectre(λ)



Répartition spatiale(pixel)

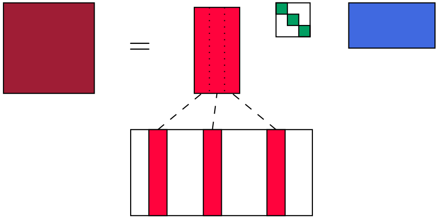
$$X \approx \sum_{r=1}^{R} \mathbf{u}_r \mathbf{v}_r \approx UV$$

Challenges

Identification problem: Which materials are present in the scene?

Unmixing problem: What is the composition of each pixel?

Additional hypotheses



$$X = UV \text{ where } U = D(:, \mathcal{K}) = DS$$

- Known Library of spectra.
- Pure pixels in the image $\leftrightarrow$ $D = X$

Uniqueness

DNMF is **unique** if spark$(D) \geq 2R$. If R is the rank of X, then this relaxes to spark$(D) \geq R + 1$. [Cohen 2017, others?]

State-of-the-art (non-exhaustive)

- **Continuous approaches ($X = DSV = DY$)**
  Lasso, GLUP [Ammanouil 2014], FGNSR [Gillis 2016]
  $+$ Robust, optimization criterion. $-$ Slow.
- **Greedy/Non-iterative method ($X = D(:, K)V$)**
  - Geometric algorithms (pure pixel hypothesis)
    N-FINDR [Winter 1999], VCA [Nascimento 2005], SPA [Gillis 2014, Businger Golub 1965]
  - Matching pursuit approaches
    SDSOMP[X.Fu 2013, Tropp 2006]

  $+$ Fast $-$ No explicit optimization criterion
- **Pixel-wise brute force algorithms**
  MESMA [Roberts 1998], MESLUM, AUTOMCU, AMUSES [Degerickx 2017]
  $+$ Flexible $-$ No low rank property, Slow.
- **Statistical methods**

Matching Pursuit ALS

An alternating nonnegative least squares method where U, $\mathcal{K}$ and V are estimated alternatively.

Input: Initial U, V, $\mathcal{K}$ (Using e.g. SPA, VCA...).
while stopping criterion is not met,

- $\widehat{U} = \underset{U \geq 0}{\text{argmin}} \|X - UV\|_F^2$
- $\widehat{\mathcal{K}}(i) = \underset{j}{\text{argmax}}\ d_j^T \widehat{U}_i$
- $\widehat{V} = \underset{V \geq 0}{\text{argmin}} \|X - D(:, \mathcal{K})V\|_F^2$

Output: Selected atoms set $\mathcal{K}$ and abundances V.

Pros and Cons

Pros

- ✓ Can be adapted to N-way arrays.
- ✓ One iteration has the same complexity as geometric methods.
- ✓ Low memory requirements.
- ✓ Tries to minimize an explicit cost function.

Cons

- ✗ Very sensitive to initialization.
- ✗ No convergence proof.
- ✗ May be stuck in a local minimum.

Experiment on the URBAN HSI

	$r = 6$		$r = 8$	
	Time (s.)	Rel. err.	Time (s.)	Rel. err.
RAND-wo	0.00	7.87	0.00	11.66
d-RAND-wo	22.46 (13)	5.09	34.87 (18)	5.35
RAND-av	0.02	11.51	0.02	9.60
d-RAND-av	23.91 (13)	4.65	30.77 (15)	4.65
RAND-be	0.00	13.77	0.00	5.54
d-RAND-be	22.01 (11)	4.36	36.18 (19)	4.16
VCA	2.01	18.38	1.86	20.11
d-VCA	26.89 (15)	5.83	29.06 (14)	5.05
SPA	0.30	9.58	0.30	9.45
d-SPA	24.37 (13)	4.67	28.61 (14)	4.62
SNPA	24.34	9.63	36.72	5.64
d-SNPA	23.04 (13)	4.94	27.94 (13)	**3.97**
H2NMF	19.02	5.81	22.35	5.47
d-H2NMF	26.66 (15)	**4.05**	28.92 (14)	4.24
FGNSR-100	2.73	5.58	2.55	4.62
d-FGNSR-100	26.72 (14)	4.36	20.81 (8)	4.04

Table: Numerical results for the Urban data set.

Experiment on the URBAN HSI

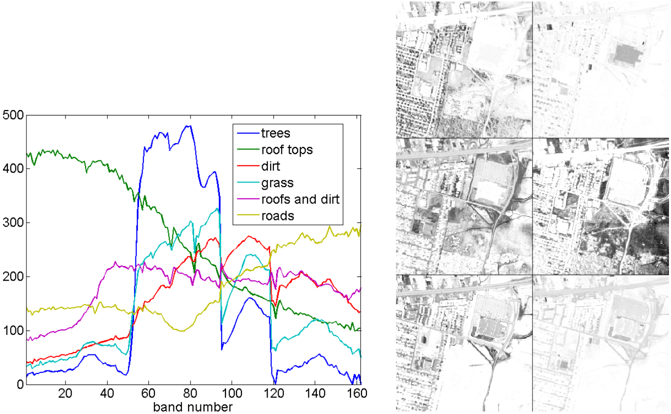


Figure: Spectral signatures and abundance maps identified using MPALS for the Urban data set with $r = 6$.

Conclusion and Perspectives

Conclusions

- MPALS is a relatively fast algorithm which outputs have small residuals.
- It can be easily modified to match more than one atom per spectra, and to satisfy specific constraints such as the sum to one of abundances.
- It is deterministic but very sensitive to initialization and the outputs are hard to predict with a random initialization.

Perspectives

- Use a three-way array adaptation of MPALS for fluorescence spectroscopy.
- Develop a multiple dictionary framework making use of MPALS.
- Refine MPALS with a soft version, or with convergence proofs.

Thank you for your attention!