Démélange parcimonieux et prise en compte de contraintes structurantes par optimisation globale

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Spectral unmixing [Singer and McCord, 1979]

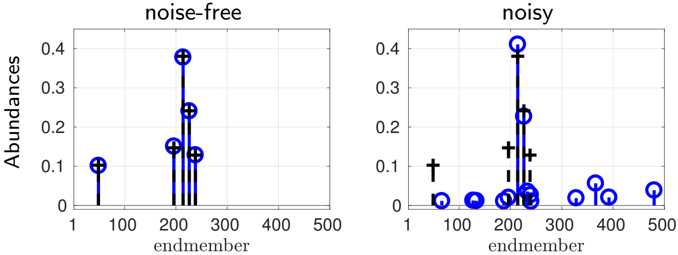
$$\boldsymbol{y} = \mathbf{S}\boldsymbol{a} \ (+ \ errors \ )$$

- $\boldsymbol{y}$: observed reflectance spectrum
- $\mathbf{S}$: dictionary of reflectance spectra
- $\boldsymbol{a}$: abundances (percentages) $\rightarrow a_n \in [0,1]$ and $\sum_n a_n = 1$

Standard approach: *Fully Constrained Least-Squares* (FCLS)

[Heinz and Chein-I-Chang, 2001]

$$\min_{\boldsymbol{a}\in[0,1]^N} \ \frac{1}{2}\|\boldsymbol{y} - \mathbf{S}\boldsymbol{a}\|^2 \ \text{ s.t. } \sum_{n=1}^{N} a_n = 1$$



Truth $+$, estimated $\circ$

More sophisticated estimates through Mixed Integer Programming (MIP)

$$\boldsymbol{y} = \mathbf{S}\boldsymbol{a} \; (+ \mathit{errors} \;)$$

- $\mathbf{S} \rightsquigarrow$ high number of endmembers
- Spectral variability [Zare and Ho, 2014, Meyer et al., 2016]

$\Rightarrow$ **add more constraints to the problem**

Models based on *binary variables* encoding the presence of each member in the data

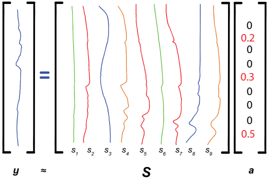
$$b_n = 1 \Leftrightarrow a_n \neq 0$$

$\rightsquigarrow$ reformulated as $0 \leq a_n \leq b_n$: Mixed Integer Programs

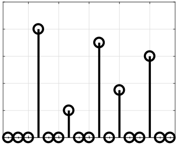
- Sparsity: most abundances are zero [Iordache et al., 2011]
- Structuration of the dictionary into groups [Meyer et al., 2016, Drumetz et al., 2019]
- Minimum values on the nonzero coefficients [never seen . . .]

Exact ℓ_0-norm sparsity

- *Only a small number of elementary spectra are used for representing the mixture*



$\rightarrow$ ***a*** must be sparse:



$$\boxed{\|\boldsymbol{a}\|_0 = \ \mathrm{Card}(n | a_n \neq 0) \leq K}$$

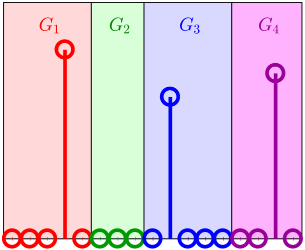
- Standard sparse methods perform poorly (ℓ_1-norm, greedy algorithms)

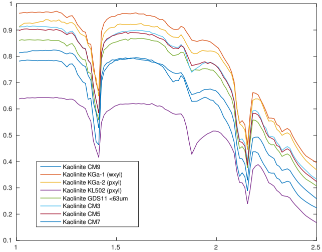
$\rightsquigarrow$ **Exact ℓ_0-norm constraint:**

$$\min_{\boldsymbol{a} \in [0,1]^N,\, \boldsymbol{b} \in \{0,1\}^N} \ \frac{1}{2} \|\boldsymbol{y} - \mathbf{S}\boldsymbol{a}\|^2 \text{ s.t. } \begin{cases} \mathbf{0} \leq \boldsymbol{a} \leq \boldsymbol{b} \\ \sum_{n=1}^{N} b_n \leq K \\ \sum_{n=1}^{N} a_n = 1 \end{cases}$$

Group Exclusivity constraint (GE)

- *The spectral library may include different variations of a given mineral, but at most one may be activated in each group G_j*





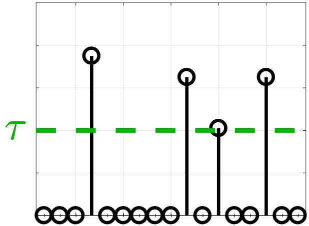
$\boxed{\|\boldsymbol{a}^{(j)}\|_0 \leq 1 \text{ in each group } Gj}$

$\rightsquigarrow$ **Also reformulated as MIP**

$$\min_{\boldsymbol{a}\in[0,1]^N,\ \boldsymbol{b}\in\{0,1\}^N} \frac{1}{2}\|\boldsymbol{y} - \mathbf{S}\boldsymbol{a}\|^2 \text{ s.t. } \begin{cases} \mathbf{0} \leq \boldsymbol{a} \leq \boldsymbol{b} \\ \sum_{i\in G_j} b_n \leq 1 \\ \sum_{n=1}^{N} a_n = 1 \end{cases}$$

Significant Abundances only

- *Non-zero abundances may exceed some threshold*



$$\boxed{a_n \neq 0 \Rightarrow a_n \geq \tau}$$

$\rightsquigarrow$ **Logical constraints**

$$\min_{\boldsymbol{a} \in [0,1]^N,\ \boldsymbol{b} \in \{0,1\}^N} \frac{1}{2} \|\boldsymbol{y} - \mathbf{S}\boldsymbol{a}\|^2 \ \text{ s.t. } \begin{cases} \tau \boldsymbol{b} \leq \boldsymbol{a} \leq \boldsymbol{b} \\ \sum_{n=1}^{N} a_n = 1 \end{cases}$$

Remark: also inducing sparsity ...

To sum up: reformulations as Mixed-integer Programs (MIPs)

- ℓ_0-norm sparsity

$$\min_{\boldsymbol{a}\in[0,1]^N,\, \boldsymbol{b}\in\{0,1\}^N} \frac{1}{2}\|\boldsymbol{y} - \mathbf{S}\boldsymbol{a}\|^2 \text{ s.t. } \begin{cases} \mathbf{0} \leq \boldsymbol{a} \leq \boldsymbol{b} \\ \sum_{n=1}^N b_n \leq K \\ \sum_{n=1}^N a_n = 1 \end{cases}$$

- Group Exclusivity

$$\min_{\boldsymbol{a}\in[0,1]^N,\, \boldsymbol{b}\in\{0,1\}^N} \frac{1}{2}\|\boldsymbol{y} - \mathbf{S}\boldsymbol{a}\|^2 \text{ s.t. } \begin{cases} \mathbf{0} \leq \boldsymbol{a} \leq \boldsymbol{b} \\ \sum_{i\in G_j} b_n \leq 1 \\ \sum_{n=1}^N a_n = 1 \end{cases}$$

- Significant Abundances

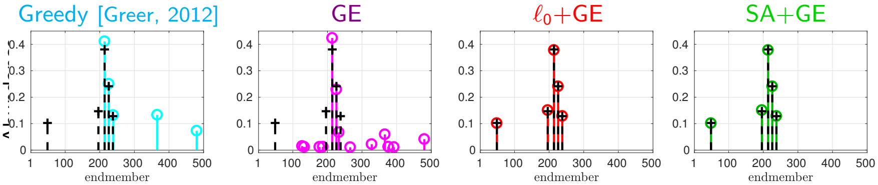
$$\min_{\boldsymbol{a}\in[0,1]^N,\, \boldsymbol{b}\in\{0,1\}^N} \frac{1}{2}\|\boldsymbol{y} - \mathbf{S}\boldsymbol{a}\|^2 \text{ s.t. } \begin{cases} \tau\boldsymbol{b} \leq \boldsymbol{a} \leq \boldsymbol{b} \\ \sum_{n=1}^N a_n = 1 \end{cases}$$

$\rightarrow$ Efficient resolution *via* numerical MIP solvers (ex. CPLEX)

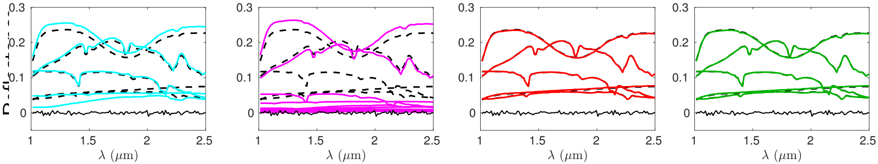
$\rightarrow$ These constraints can be mixed

Example of results (simulated data), $K = 5$ spectra, SNR$= 45$ dB

- *United States Geological Survey* database [Clark et al., 2003], 113 wavelengths from 1 to 2.5 μm
- Dictionary: $N = 481$ spectra and $J = 85$ groups corresponding to different minerals
- CPLEX MIP solver (`https://www.ibm.com/analytics/cplex-optimizer`, freely available for academics)



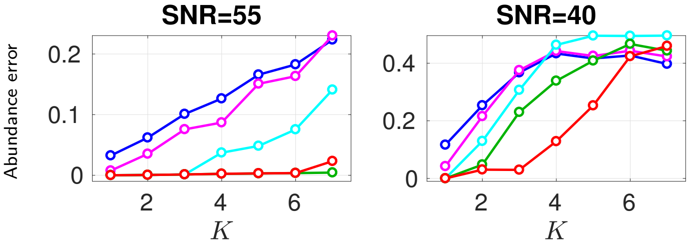
Estimated ($\circ$) and true ($+$) abundances.



Endmembers weighted by their abundances, and noise.

Average results (50 instances of each problem)

Quadratic error on abundances $E_Q = \|\widehat{\boldsymbol{a}} - \mathring{\boldsymbol{a}}\|_2^2$



FCLS (○), Greedy (○), GE (○), ℓ_0+GE (○), SA+GE (○)

Computing times (s)

	SNR	$K = 2$	$K = 4$	$K = 6$
ℓ_0+ GE	55dB	1.04	1.46	2.17
	50dB	1.23	4.25	123
	45dB	1.41	11.1	$547^{(4)}$
SA+GE	55dB	1.44	2.43	4.7
	50dB	6.98	16.7	$212^{(1)}$
	45dB	33	$204^{(1)}$	$681^{(5)}$

(In parentheses: number of instances where optimization did not terminate in 1000 s.)

Conclusions and perspectives

Global optimization through MIP-based formulations:

- $\rightsquigarrow$ allows *exact* modeling of sparsity
- $\rightsquigarrow$ flexible modeling of different kinds of constraints
- $\rightsquigarrow$ exact resolution is possible for problems of limited complexity (K/SNR)
- $\rightsquigarrow$ improves over standard methods, especially at high SNR

Perspectives:

- Evaluation and use on real data
- Reverse formulation: $\min_{\boldsymbol{a}} \|\boldsymbol{a}\|_0$ s.t. $\frac{1}{2}\|\boldsymbol{y} - \mathbf{S}\boldsymbol{a}\|^2 \leq \epsilon$
- Other kinds of constraints? *e.g.* social sparsity [Drumetz et al., 2019]
- Dedicated optimization strategies $\Rightarrow$ computing time $\searrow$

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