Hyperspectral Unmixing Via Sparse Regression Optimization Problems and Algorithms

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Outline

□ Introduction to hyperspectral unmixing

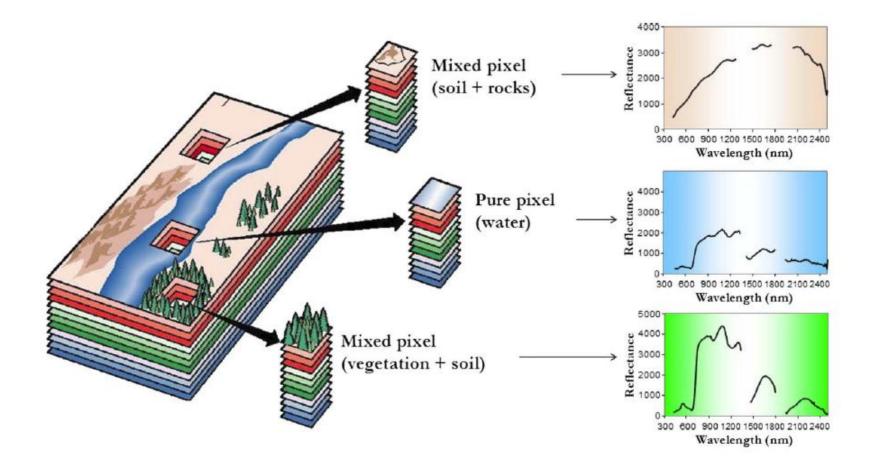
□ Hyperspectral unmixing via sparse regression.

□ Recovery guarantees/convex and nonconvex solvers

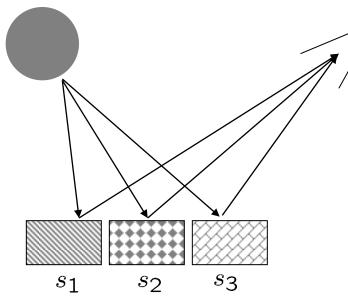
- □ Improving hyperspectral sparse regression
 - □ structured sparsity
 - □ dictionary pruning
- Solving convex sparse hyperspectral unmixing and related convex inverse problems with ADMM

Concluding remarks

Hyperspectral imaging (and mixing)



Linear mixing model (LMM)



$$\mathbf{y} = \sum_{i=1}^{p} s_i \boldsymbol{\rho}_i \qquad \boldsymbol{\rho}_i = \begin{bmatrix} \rho_{1i} \\ \rho_{2i} \\ \vdots \\ \rho_{mi} \end{bmatrix}$$

$$y = Ms$$
 $s = \begin{bmatrix} s \\ s \end{bmatrix}$

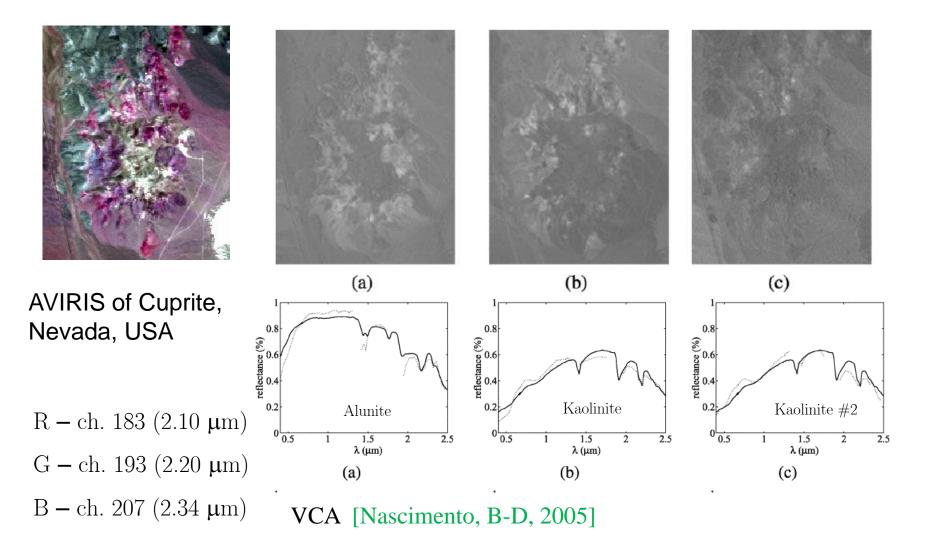
Incident radiation interacts only with one component (checkerboard type scenes)

$$\mathbf{M} \equiv [\boldsymbol{\rho}_1, \boldsymbol{\rho}_2, \boldsymbol{\rho}_3]$$

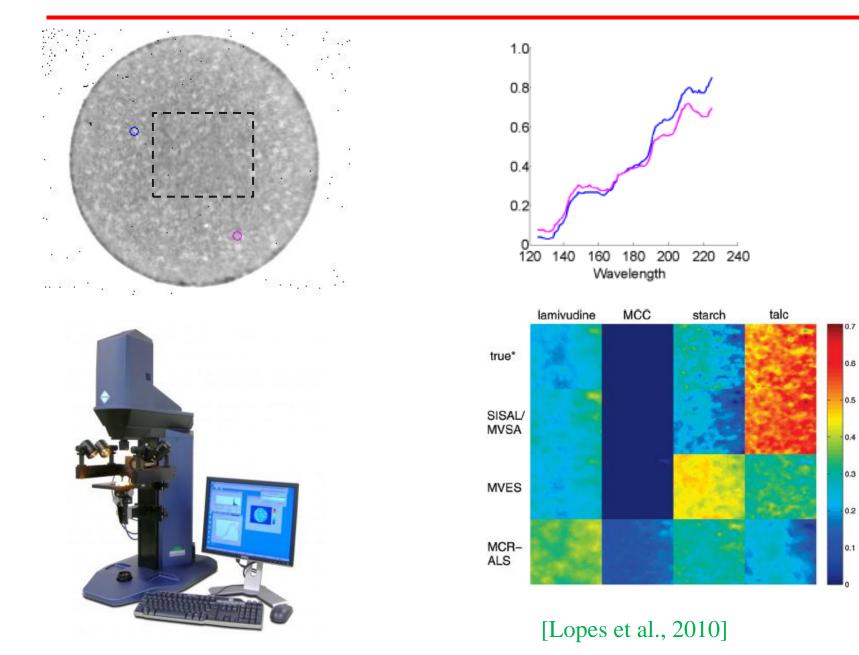
$$\mathbf{s} \equiv \begin{vmatrix} s_1 \\ s_2 \\ s_3 \end{vmatrix}$$

Hyperspectral linear $\hfill \hfill \hfill$

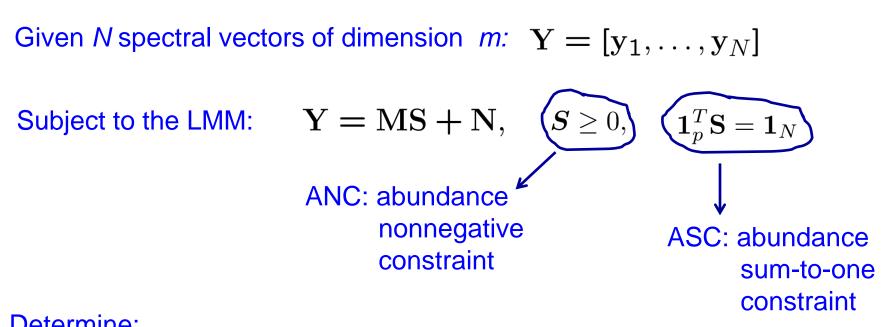
Hyperspectral unmixing



NIR tablet imaging



Spectral linear unmixing (SLU)



Determine:

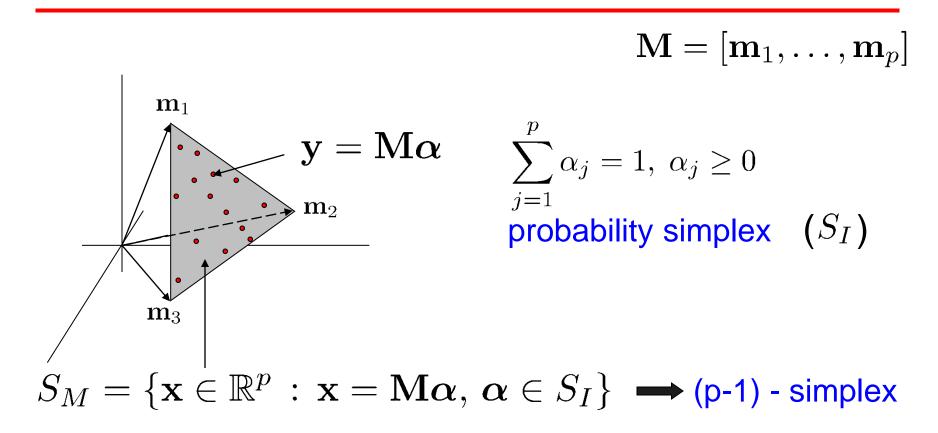
□ The mixing matrix **M** (*endmember spectra*)

 \Box The fractional abundance vectors S,



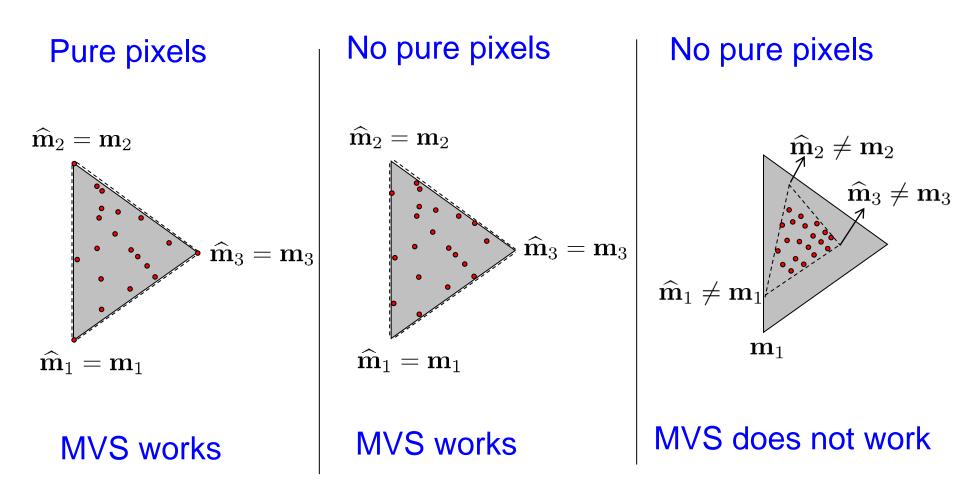
SLU is a blind source separation problem (BSS)

Geometrical view of SLU



Inferring **M** \Leftrightarrow inferring the vertices of the simplex S_M

Minimum volume simplex (MVS)

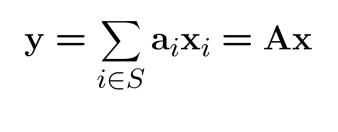


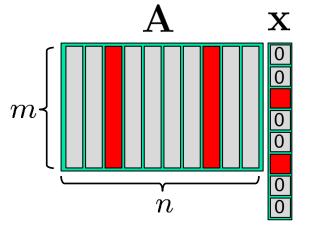
[B-D et al., IEEE JSTATRS, 2012]

Sparse regression-based SLU

Key observation: Spectral vectors can be expressed as linear combinations of a few pure spectral signatures obtained from a (potentially very large) spectral library

[Iordache, B-D, Plaza, 11, 12]





Unmixing: given y and A, find the sparsest solution of

$$y = Ax$$

Advantage: sidesteps endmember estimation

Disadvantage: Combinatorial problem !!!

Key result: a sparse signal is exactly recoverable from an underdetermined linear system of equations in a computationally efficient manner via convex/nonconvex programming [Candes, Romberg, Tao, 06] [Candes, Tao, 06] [Donoho, Tao, 06] [Blumensath, Davies, 09]

Let
$$\mathbf{A} \in \mathbb{R}^{m \times n}$$
, $m < n$, and \mathbf{x}^* , such that $\mathbf{A}\mathbf{x}^* = \mathbf{y}$

 \mathbf{x}^* is the unique solution of $\mathbf{A}\mathbf{x} = \mathbf{y}$ if $2\|\mathbf{x}^*\|_0 < \operatorname{spark}(\mathbf{A})$

 \mathbf{x}^{\ast} is the solution of the optimization problem

$$(P_0) \min_{\mathbf{x}} \|\mathbf{x}\|_0 \text{ subject to } \mathbf{A}\mathbf{x} = \mathbf{y}$$

Sparse reconstruction/compressive sensing

Optimization strategies to cope with P₀ NP-hardness

Convex relaxation

(BP – Basis Pursuit) [Chen et al., 2001] $\min_{\mathbf{x}} \|\mathbf{x}\|_1 \text{ st: } \mathbf{A}\mathbf{x} = \mathbf{y}$

(BPDN – BP denoising) $\min_{\mathbf{x}} \|\mathbf{x}\|_1 \text{ st: } \|\mathbf{A}\mathbf{x} - \mathbf{y}\|_2 \leq \delta$

(LASSO) [Tibshirani, 1996]
$$\min_{\mathbf{x}}(1/2) \|\mathbf{A}\mathbf{x} - \mathbf{y}\|_{2}^{2} + \lambda \|\mathbf{x}\|_{1}$$

Approximation algorithms

Bayesian CS [Ji et al., 2008]

CoSaMP – Compressive Sampling Matching Pursuit [Needell, Tropp, 2009]

IHT – Iterative Hard Thresholding [Blumensath, Davies, 09]

GDS - Gradient Descent Sparsification [Garg Khandekar, 2009]

HTP – Hard Thresholding Pursuit [Foucart, 10]

MP - Message Passing

[Villa Schniter, 2012]

Exact recovery of sparse vectors

Recovery guarantees: linked with the restricted isometric property (RIP)

Restricted isometric constant: $\delta_p(\mathbf{A}), \quad \mathbf{A} \in \mathbb{R}^{m \times n}$:

$$(1-\delta) \|\mathbf{x}\|_2 \le \|\mathbf{A}\mathbf{x}\| \le (1+\delta) \|\mathbf{x}\|_2, \quad \|\mathbf{x}\|_0 \le p$$

Many SR algorithms ensure exact recovery provided that:

$$\delta_t(\mathbf{A}) \leq \delta_*$$
, for some t and δ_*

This condition is satisfied for random matrices provided that

$$m \simeq c \frac{t}{\delta_*^2} \log(n/t)$$

Algorit	hm	BP	НТР	CoSaMP	GDP	IHT
δ_t	$<\delta_*$	$\delta_{2s} < 0.465$	$\delta_{3s} < 0.577$	$\delta_{4s} < 0.384$	$\delta_{2s} < 0.333$	$\delta_{3s} < 0.555$
Ratio	t/δ_*^2	9.243	9	27.08	18	12

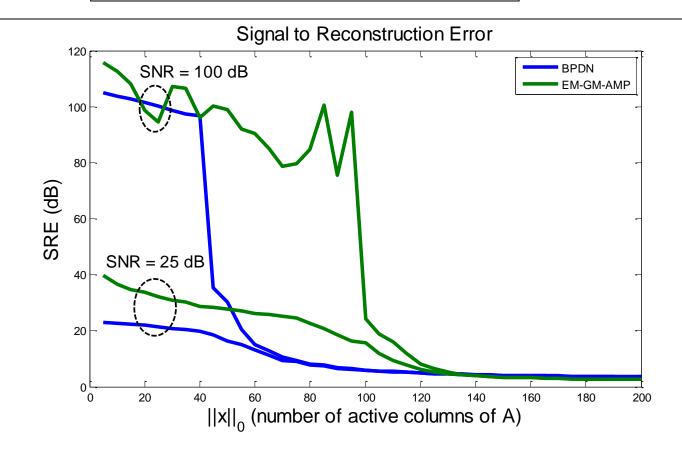
(from [Foucart, 10])

Example: Gaussian matrices; signed signals

$$\mathbf{A} \in \mathbb{R}^{m \times n}; \quad (m = 200, n = 400); \quad \mathcal{N}(0, 1); \text{ iid}; \quad x_i \sim \mathcal{N}(0, 1)$$

Algorithms:

(BPDN – SUnSAL) [B-D, Figueiredo, 2010] $\min_{\mathbf{x}} \|\mathbf{x}\|_1 \text{ st: } \|\mathbf{A}\mathbf{x} - \mathbf{y}\|_2 \leq \delta$ EM-BG-AMP [Villa Schniter, 2012]



Example: Gaussian matrices; non-negative signals

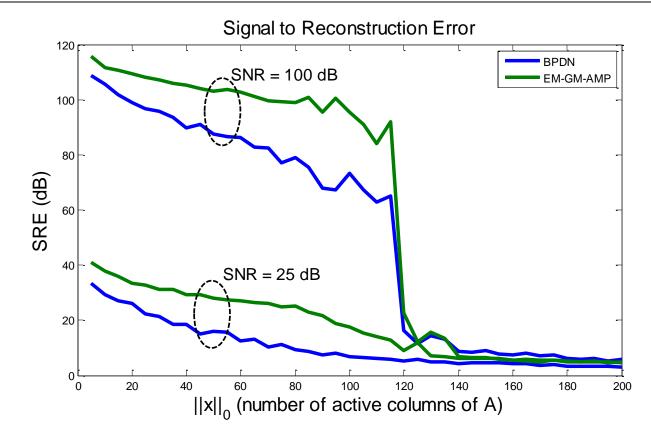
 $\mathbf{A} \in \mathbb{R}^{m \times n}$; $\mathcal{N}(0,1)$ iid; m = 200, n = 400; $x_i \sim \text{UD in the simplex}$

Algorithms:

(BPDN – SUnSAL)

$$\min_{\mathbf{x}} \|\mathbf{x}\|_1 \text{ st: } \|\mathbf{A}\mathbf{x} - \mathbf{y}\|_2 \le \delta, \ \mathbf{x} \ge \mathbf{0}$$

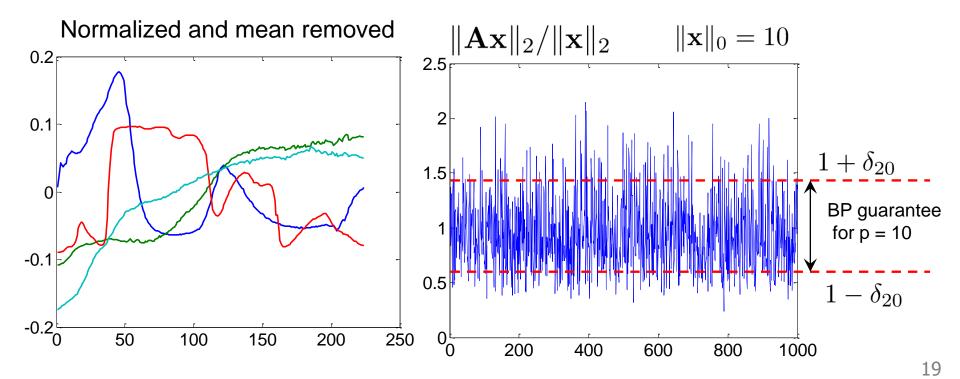
EM-BG-AMP



Hyperspectral libraries exhibit poor RI constants

(Mutal coherence close to 1 [Iordache, B-D, Plaza, 11, 12])

Illustration: $\mathbf{A} \in \mathbb{R}^{m \times n}$; subset from USGS; m = 200, n = 400

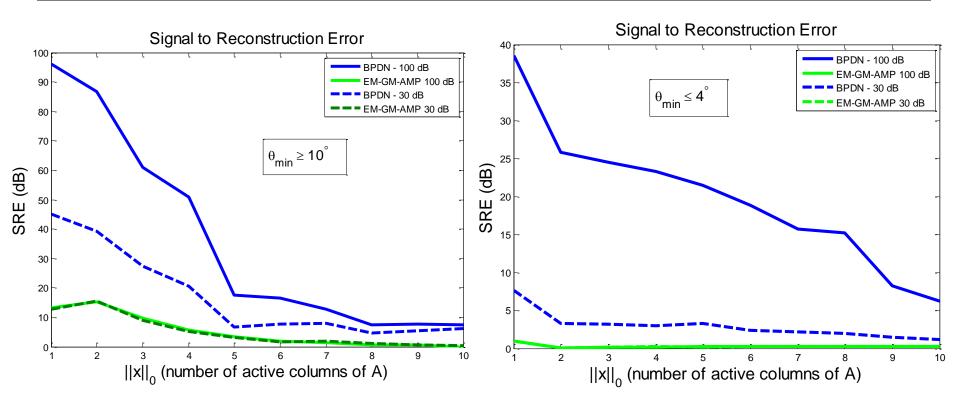


Example: Hyperspectral library; non-negative signals

 $\mathbf{A} \in \mathbb{R}^{m \times n};$ subset from USGS; m = 200, n = 300Illustration: Algorithms: (BPDN - SUnSAL)

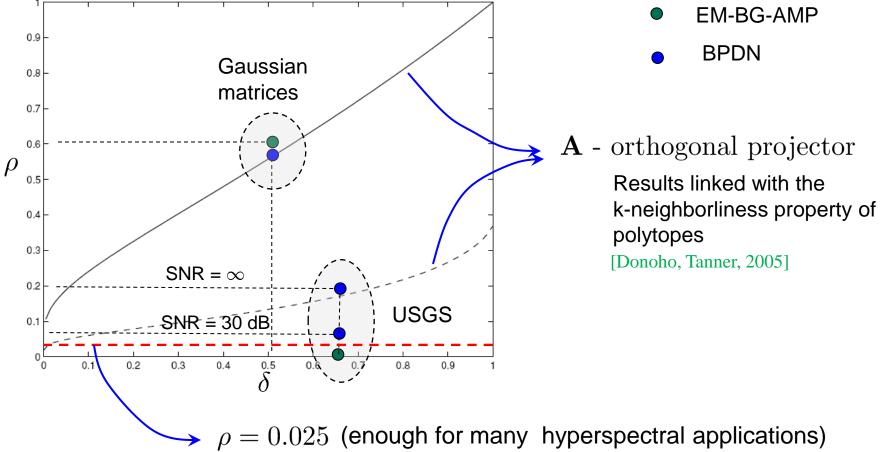
$$\min_{\mathbf{x}} \|\mathbf{x}\|_1 \text{ st: } \|\mathbf{A}\mathbf{x} - \mathbf{y}\|_2 \le \delta, \ \mathbf{x} \ge \mathbf{0}$$

EM-BG-AMP

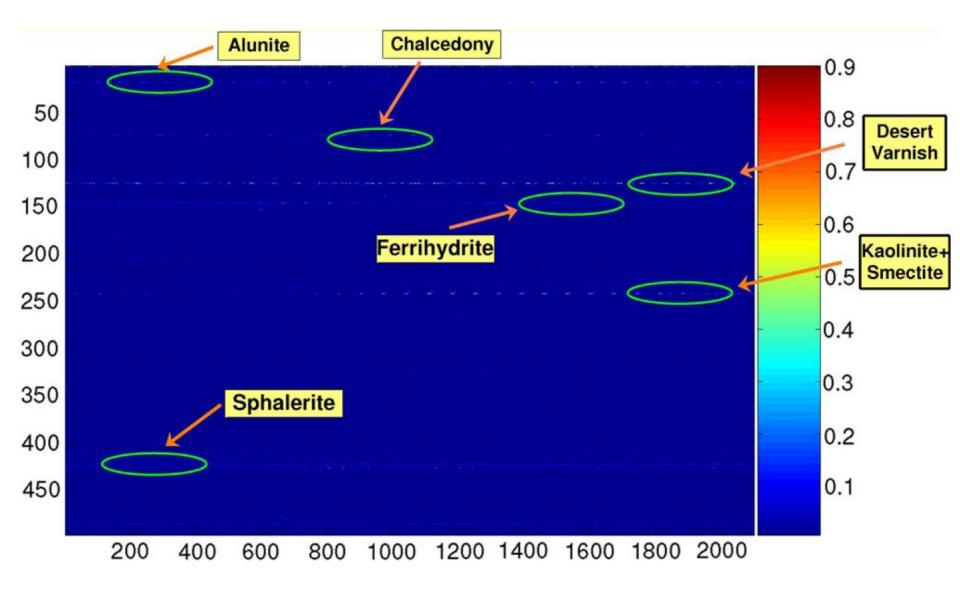


Phase transition curves

 $\ell_1, -/\ell_0$ equivalence for non-negative signals $(\mathbf{A} \in \mathbb{R}^{m \times n})$ $\delta = m/n$ undersamplig factor $\rho = \|\mathbf{x}\|_0/m$ fractional sparsity



Real data – AVIRIS Cuprite



Sparse reconstruction of hyperspectral data: Summary

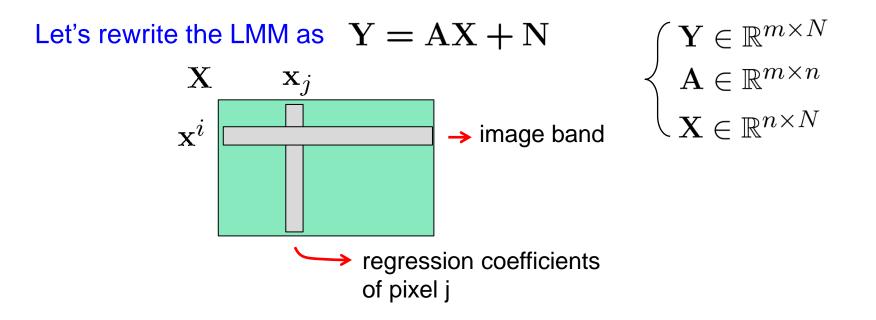
Bad news: Hyperspectral libraries have poor RI constants

Good news: Hyperspectral mixtures are highly sparse, very often $p \le 5$

Surprising fact: Convex programs (BP, BPDN, LASSO, ...) yield much better empirical performance than non-convex state-of-the-art competitors

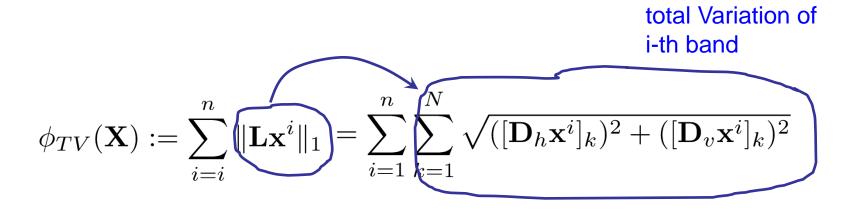
Directions to improve hyperspectral sparse reconstruction					
Structured sparsity + subspace structure (pixels in a give data set share the same support)					
Spatial contextual information (pixels belong to an image)					

Rationale: introduce new sparsity-inducing regularizers to counter the sparse regression limits imposed by the high coherence of the hyperspectral libraries.



$$\min_{\mathbf{X}} (1/2) \| \mathbf{A}\mathbf{X} - \mathbf{Y} \|_{F}^{2} + \lambda_{1} \| \mathbf{X} \|_{1} + \lambda_{2} \phi_{TV}(\mathbf{X}) \qquad \text{[Iordache, B-D, Plaza, 11]}$$

subject to: $\mathbf{X} \ge \mathbf{0}$



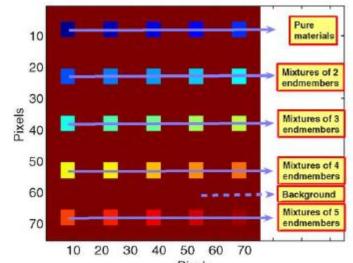
Related work

[Zhao, Wang, Huang, Ng, Plemmons, 12]

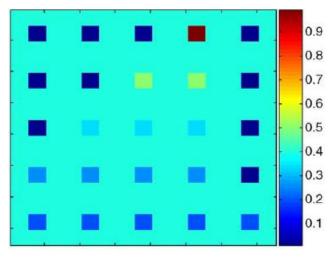
Ilustrative examples with simulated data : SUnSAL-TV



Original data cube

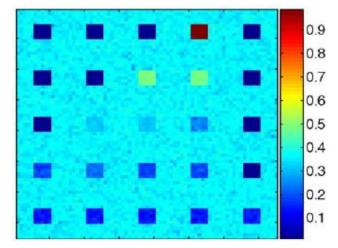


Original abundance of EM5

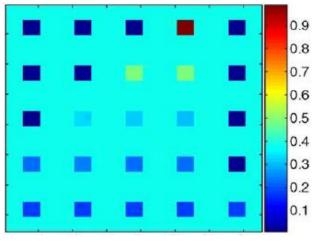


$$(m = 224, N = 75 \times 75, k = 5)$$

SUnSAL estimate



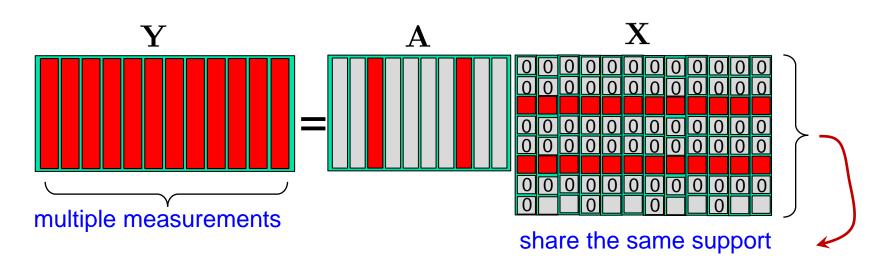
SUnSAL-TV estimate



Constrained colaborative sparse regression (CCSR)

$$\min_{\mathbf{X}} (1/2) \|\mathbf{A}\mathbf{X} - \mathbf{Y}\|_{F}^{2} + \lambda \|\mathbf{X}\|_{2,1} \qquad \|\mathbf{X}\|_{2,1} := \sum_{i=1}^{n} \|\mathbf{x}^{i}\|_{2}$$

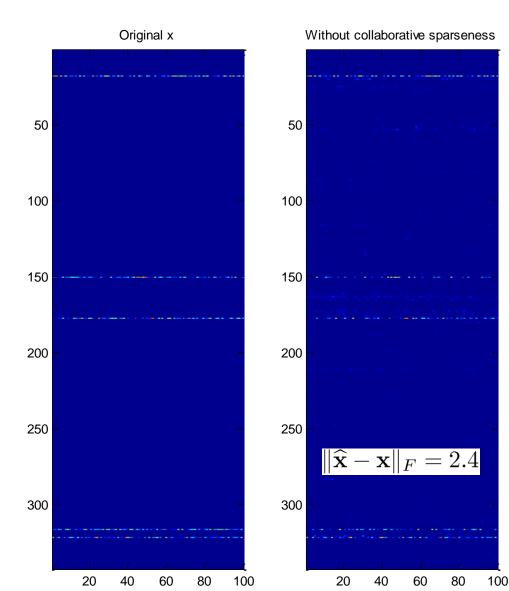
subject to: $\mathbf{X} \ge \mathbf{0}, \quad \mathbf{1}_{n}^{T}\mathbf{X} = \mathbf{1}_{N}^{T}$
[Iordache, B-D, Plaza, 11, 12] [Turlach, Venables, Wright, 2004]

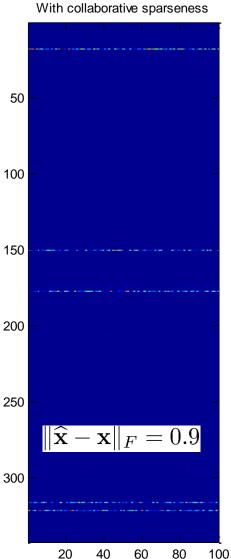


Theoretical guaranties (superiority of multichanel) : the probability of recovery failure decays exponentially in the number of channels. [Eldar, Rauhut, 11]

Ilustrative examples with simulated data : CSUnSAL

 $\mathbf{A} \in \mathbb{R}^{224 \times 350}$ (from USGS library) $\mathbf{x} \in \mathbb{R}^{350 \times 100}$ (sparsity k = 5)





SNR = 35dBtime = 10 sec The multiple measurement vector (MMV) problem

minimize $\|\mathbf{X}\|_0$

subject to: $\mathbf{Y} = \mathbf{A}\mathbf{X}$

 $\|\mathbf{X}\|_0$ - number of non-null rows of $~\mathbf{X}$

MMV has a unique solution iff

$$\|\mathbf{X}\|_0 < \frac{\operatorname{spark}(\mathbf{A}) + \operatorname{rank}(\mathbf{Y}) - 1}{2}$$

[Feng, 1997], [Chen, Huo, 2006], [Davies, Eldar, 2012]

MMV gain

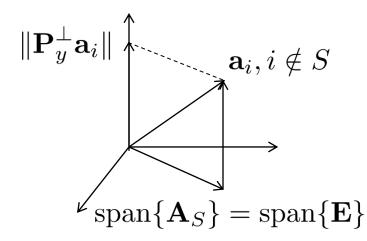
If $rank(\mathbf{Y}) = \|\mathbf{X}\|_0$, the above bound is achieved using the multiple sinal classification (MUSIC) algorithm

Endemember identification with MUSIC

$\mathbf{Y} = \mathbf{A}\mathbf{X}$ (noiseless measurements)

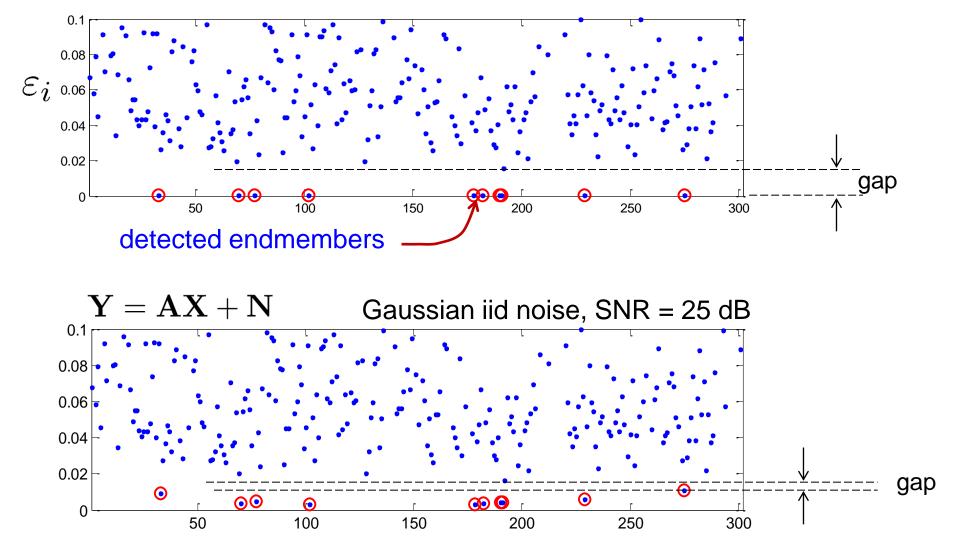
MUSIC algorithm

 Compute E = [e₁,...,e_p], the first *p* eigenvalues of R_y = YY^T/n
 Compute ε_i = ^{||P[⊥]_ya_i||}/_{||a_i||}, for i = 1,...,m and set M = A_S with S = {i : ε_i = 0, i = 1,...,m}



Examples (simulated data)

A – USGS (\geq 3°) p = 10, N=5000, X - uniform over the simplex, SNR = ∞ ,



Examples (simulated data)

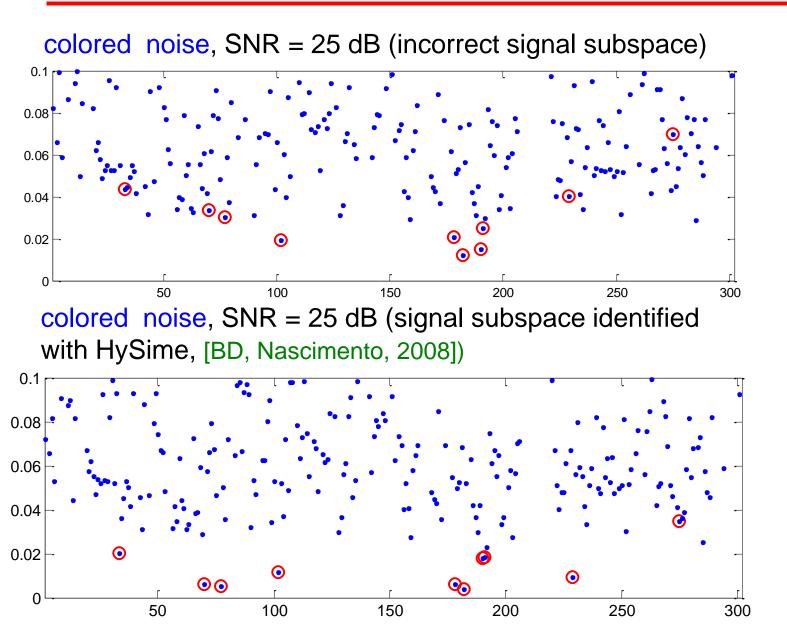
 $\mathbf{Y} = \mathbf{A}\mathbf{X} + \mathbf{N}$ colored noise, SNR = 25 dB0.1 0.08 0.06 0.04 0.02 $oldsymbol{O}$ \bigcirc 0 50 100 150 200 250 300

cause of the large projection errors: poor identification of the subspace signal

$$\mathbf{R}_{y} \simeq \mathbf{A}_{S} \mathbf{R}_{x} \mathbf{A}_{S}^{T} + \mathbf{R}_{n} \stackrel{\neq}{\rightarrow} \operatorname{span}{\mathbf{E}} \neq \operatorname{span}{\mathbf{A}_{S}}$$

cure: identify the signal subspace

Signal subspace identification



Proposed MUSIC – Colaborative SR algorithm

MUSIC-CSR algorithm [B-D, 2012]

- 1) Estimate the signal subspace $span{A_S}$ using, e.g. the HySime algorithm.
- 2) Compute $\varepsilon_i = \frac{\|\mathbf{P}_y^{\perp} \mathbf{a}_i\|}{\|\mathbf{a}_i\|}$, for $i = 1, \dots, m$ and define the index set $S = [i : \varepsilon_i \le \delta, i = 1, \dots, m]$
 - 3) Solve the colaborative sparse regression optimization

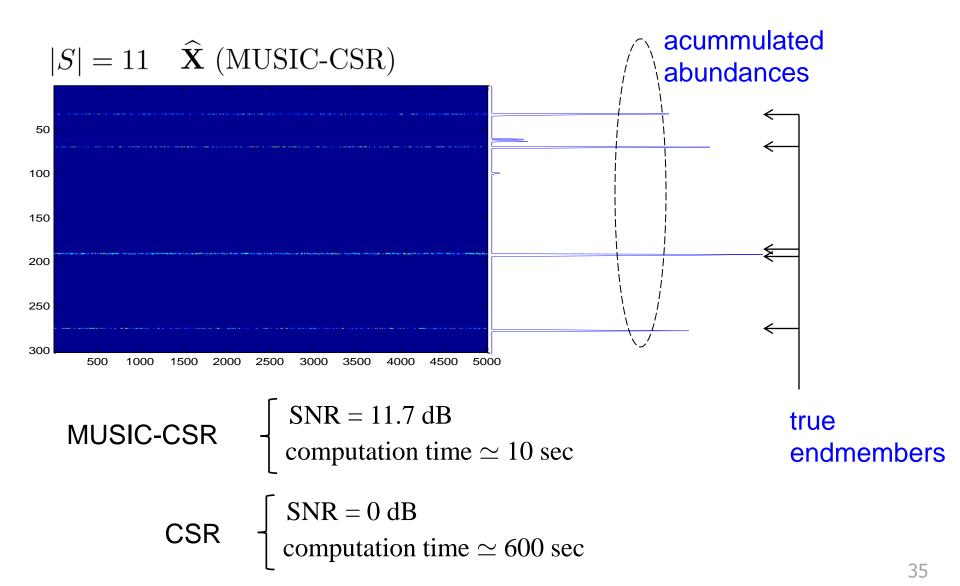
$$\begin{split} \min_{\mathbf{x}}(1/2) \|\mathbf{Y} - \mathbf{A}_{\mathbf{S}}\mathbf{X}\|^2 + \lambda \|\mathbf{X}\|_{2,1}, \quad \mathbf{X} \ge 0\\ \text{[B-D, Figueiredo, 2012]} \end{split}$$

Related work: CS-MUSIC [Kim, Lee, Ye, 2012]

(N < k and iid noise)

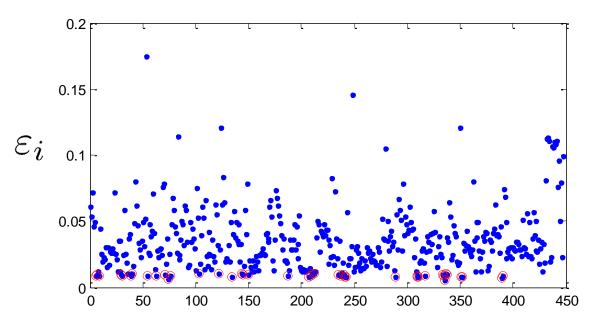
MUSIC – CSR results

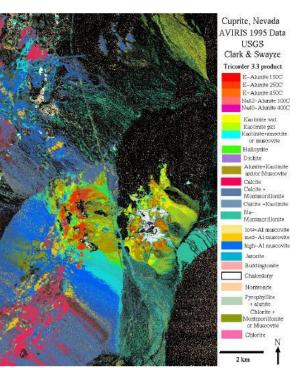
A – USGS (\geq 3°), Gaussian shaped noise, SNR = 25 dB, k = 5, m = 300,



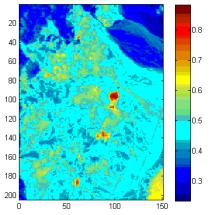
Results with CUPRITE

- size: 350x350 pixels
- spectral library: 302 materials (minerals) from the USGS library
- spectral bands: 188 out of 224 (noisy bands were removed)
- spectral range: 0.4 2.5 um
- spectral resolution: 10 nm
- "validation" map: Tetracorder***

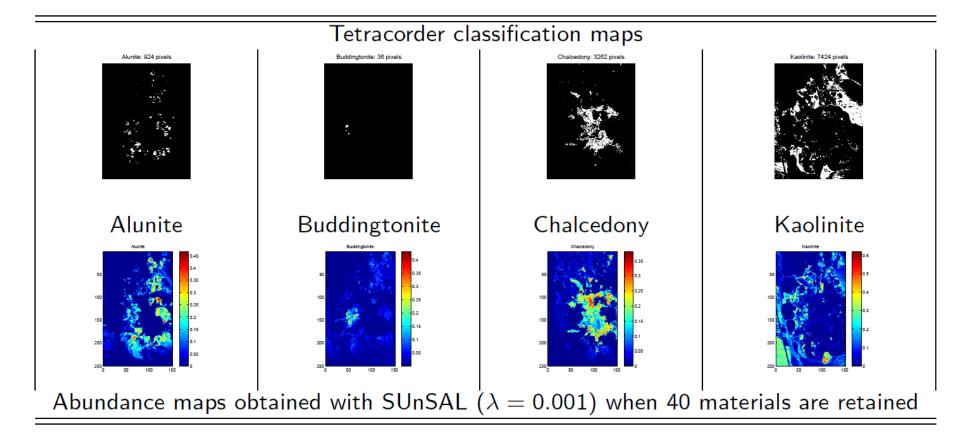






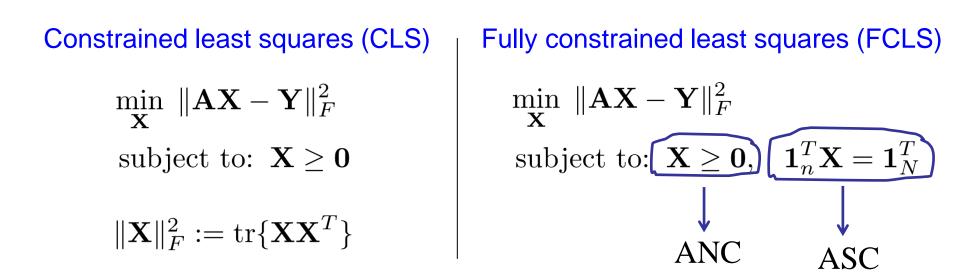


Results with real data



Note: Good spatial distribution of the endmembers *Processing times*: 2.6 ms/pixel using the full library; 0.22ms/pixels using the pruned library with 40 members

Convex optimization problems in SLU



Constrained sparse regression (CSR)

$$\min_{\mathbf{X}} (1/2) \| \mathbf{A}\mathbf{X} - \mathbf{Y} \|_F^2 + \lambda \| \mathbf{X} \|_1 \qquad \| \mathbf{X} \|_1 := \sum_{i=1}^N \| \mathbf{x}_i \|_1$$

subject to: $\mathbf{X} \ge \mathbf{0}$

Convex optimization problems in SLU

Constrained basis pursuit (CBP)	CBP denoising (CBPDN)
$\min_{\mathbf{X}} \ \mathbf{X}\ _1$	$\min_{\mathbf{X}} \ \mathbf{X}\ _1$
subject to: $\mathbf{A}\mathbf{X} = \mathbf{Y}, \ \mathbf{X} \ge 0$	subject to: $\ \mathbf{A}\mathbf{X} - \mathbf{Y}\ _F \leq \delta, \ \mathbf{X} \geq 0$

Constrained colaborative sparse regression (CCSR)

$$\min_{\mathbf{X}} (1/2) \| \mathbf{A}\mathbf{X} - \mathbf{Y} \|_F^2 + \lambda \| \mathbf{X} \|_{2,1} \qquad \| \mathbf{X} \|_{2,1} := \sum_{i=1}^n \| \mathbf{x}^i \|_2$$

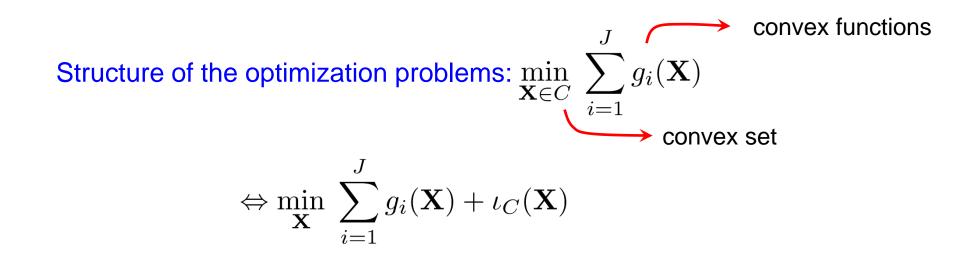
subject to: $\mathbf{X} \ge \mathbf{0}, \quad \mathbf{1}_n^T \mathbf{X} = \mathbf{1}_N^T$

Constrained total variation (CTV)

$$\min_{\mathbf{X}} (1/2) \|\mathbf{A}\mathbf{X} - \mathbf{Y}\|_F^2 + \lambda_1 \|\mathbf{X}\|_1 + \lambda_2 \phi_{TV}(\mathbf{X})$$

subject to: $\mathbf{X} \ge \mathbf{0}$

Convex optimization problems in SLU



Source of difficulties: large scale ($n \times N \gtrsim 10^7$); nonsmoothness

Line of attack: alternating direction method of multiplies (ADMM) [Glowinski, Marrocco, 75], [Gabay, Mercier, 76]

Alternating Direction Method of Multipliers (ADMM)

Unconstrained (convex) optimization problem: $\min_{\mathbf{z}\in\mathbb{R}^d}~f_1(\mathbf{z})+f_2(\mathbf{G}\,\mathbf{z})$

ADMM [Glowinski, Marrocco, 75], [Gabay, Mercier, 76]

$$\begin{aligned} \mathbf{z}_{k+1} &= \arg\min_{\mathbf{z}} f_1(\mathbf{z}) + \frac{\mu}{2} \|\mathbf{G} \,\mathbf{z} - \mathbf{u}_k - \mathbf{d}_k\|^2 \\ \mathbf{u}_{k+1} &= \arg\min_{\mathbf{u}} f_2(\mathbf{u}) + \frac{\mu}{2} \|\mathbf{G} \,\mathbf{z}_{k+1} - \mathbf{u} - \mathbf{d}_k\|^2 \\ \mathbf{d}_{k+1} &= \mathbf{d}_k - (\mathbf{G} \,\mathbf{z}_{k+1} - \mathbf{u}_{k+1}) \end{aligned}$$

Interpretations: variable splitting + augmented Lagrangian + NLBGS; Douglas-Rachford splitting on the dual [Eckstein, Bertsekas, 92]; split-Bregman approach [Goldstein, Osher, 08] Consider the problem

$$\min_{\mathbf{z}\in\mathbb{R}^d} f_1(\mathbf{z}) + f_2(\mathbf{G}\,\mathbf{z})$$

Let f_1 and f_2 be closed, proper, and convex and G have full column rank.

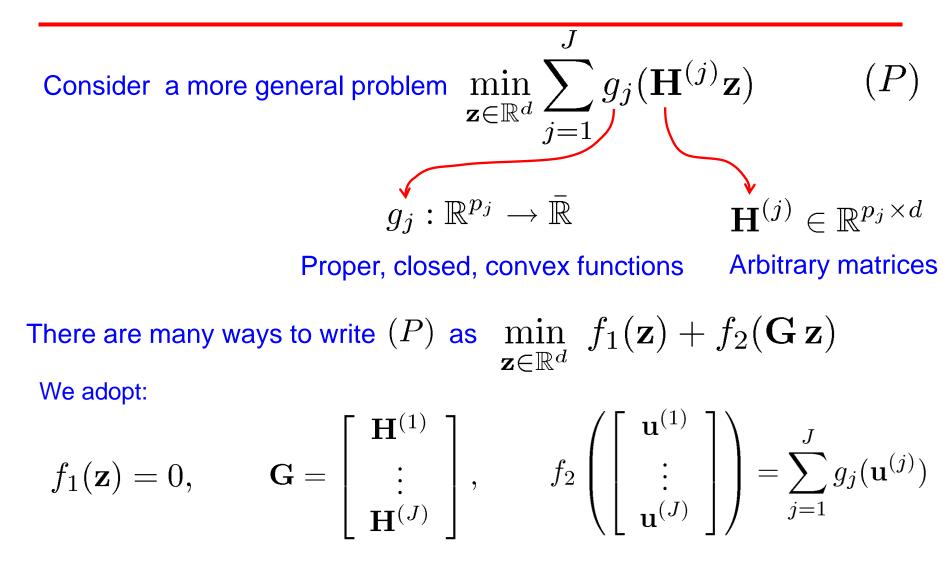
Let $(\mathbf{z}_k, k = 0, 1, 2, ...)$ be the sequence produced by ADMM, with $\mu > 0$, then, if the problem has a solution, say $\overline{\mathbf{Z}}$, then

$$\lim_{k\to\infty}\mathbf{z}_k=\bar{\mathbf{z}}$$

The theorem also allows for inexact minimizations, as long as the errors are absolutely summable.

Convergence rate: $O(1/\varepsilon)$ [He, Yuan, 2011]

ADMM for two or more functions [Figueiredo, B-D, 09]



Another approach in [Goldfarb, Ma, 09, 11]

Applying ADMM to more than two functions

$$\begin{aligned} \mathbf{z}_{k+1} &= \left[\sum_{j=1}^{J} (\mathbf{H}^{(j)})^* \mathbf{H}^{(j)} \right]^{-1} \left(\sum_{j=1}^{J} (\mathbf{H}^{(j)})^* \left(\mathbf{u}_k^{(j)} + \mathbf{d}_k^{(j)} \right) \right) \\ \mathbf{u}_{k+1}^{(1)} &= \arg\min_{\mathbf{u}} g_1(\mathbf{u}) + \frac{\mu}{2} \| \mathbf{u} - \mathbf{H}^{(1)} \mathbf{z}_{k+1} + \mathbf{d}_k^{(1)} \|^2 = \operatorname{prox}_{g_1/\mu} \mathbf{H}^{(1)} \mathbf{z}_{k+1} - \mathbf{d}_k^{(j)}) \\ &\vdots &\vdots &\vdots \\ \mathbf{u}_{k+1}^{(J)} &= \arg\min_{\mathbf{u}} g_J(\mathbf{u}) + \frac{\mu}{2} \| \mathbf{u} - \mathbf{H}^{(J)} \mathbf{z}_{k+1} + \mathbf{d}_k^{(J)} \|^2 = \operatorname{prox}_{g_1/\mu} \mathbf{H}^{(1)} \mathbf{z}_{k+1} - \mathbf{d}_k^{(j)}) \\ \mathbf{d}_{k+1}^{(1)} &= \mathbf{d}_k^{(1)} - (\mathbf{H}^{(1)} \mathbf{z}_{k+1} - \mathbf{u}_{k+1}^{(1)}) \\ &\vdots &\vdots \\ \mathbf{d}_{k+1}^{(J)} &= \mathbf{d}_k^{(J)} - (\mathbf{H}^{(J)} \mathbf{z}_{k+1} - \mathbf{u}_{k+1}^{(J)}) \end{aligned}$$

Conditions for easy applicability:

inexpensive proximity operators

inexpensive matrix inversion

Constrained sparse regression (CSR)

Problem
$$\min_{\mathbf{X}} (1/2) \| \mathbf{A} \mathbf{X} - \mathbf{Y} \|_{F}^{2} + \lambda \| \mathbf{X} \|_{1}$$
, subject to: $\mathbf{X} \ge \mathbf{0}$
Equivalent formulation $\min_{\mathbf{X}} (1/2) \| \mathbf{A} \mathbf{X} - \mathbf{Y} \|_{F}^{2} + \lambda \| \mathbf{X} \|_{1} + \iota_{\mathbb{R}_{+}}(\mathbf{X})$
indicator of the first orthant
Template: $\min_{\mathbf{X}} \sum_{j=1}^{J=3} g_{j}(\mathbf{H}^{(j)} \mathbf{X})$
Mapping:
 $\mathbf{H}^{(1)} = \mathbf{A}, \quad g_{1}(\mathbf{Z}) = (1/2) \| \mathbf{Z} - \mathbf{Y} \|_{F}^{2}$
 $\mathbf{H}^{(2)} = \mathbf{I}, \quad g_{2}(\mathbf{Z}) = \lambda \| \mathbf{Z} \|_{1}$
 $\mathbf{H}^{(2)} = \mathbf{I}, \quad g_{2}(\mathbf{Z}) = \lambda \| \mathbf{Z} \|_{1}$
 $\mathbf{H}^{(3)} = \mathbf{I}, \quad g_{3}(\mathbf{Z}) = \iota_{\mathbb{R}_{+}}(\mathbf{Z})$
Matrix inversion can be precomputed
(typical sizes 200~300 x 500~1000)
 $\begin{bmatrix} \sum_{j=1}^{J} (\mathbf{H}^{(j)})^{*} \mathbf{H}^{(j)} \end{bmatrix}^{-1} = \begin{bmatrix} \mathbf{A}^{T} \mathbf{A} + 2\mathbf{I} \end{bmatrix}^{-1}$

Spectral unmixing by split augmented Lagrangian (SUnSAL) [B-D, Figueiredo, 2010] Related algorithm (split-Bregman view) in [Szlam, Guo, Osher, 2010]

Concluding remarks

Sparse regression framework, used with care, yields effective hyperspectral unmixing results.

Critical factors

- High mutual coherence of the hyperspectral libraries
- Non-linear mixing and noise
- Acquisition and calibration of hyperspectral libraries

Favorable factors

- □ Hyperspectral mixtures are highly sparse
- ADMM is a very flexible and efficient tool solving the hyperspectral sparse regression optimization problems

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