

Hyperspectral Unmixing Geometrical, Statistical, and Sparse Regression-Based Approaches

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Hyperspectral imaging (and mixing)



Hyperspectral unmixing



VCA [Nascimento, B-D, 2005]

Outline

□ Mixing models

- Linear
- Nonlinear

□ Signal subspace identification

Unmixing

- Geometrical-based
- Statistical-based
- Sparse regression-based

J. M. Bioucas-Dias, A. Plaza, N. Dobigeon, M. Parente, Q. Du, P. Gader, and J. Chanussot, "Hyperspectral unmixing overview: geometrical, statistical, and sparse regression-based approaches", IEEE Journal of Selected Topics in Applied Earth Observations and Remote Sensing, vol. 5, no. 2, pp. 354-379, 2012.

W.-K. Ma, J. Bioucas-Dias, T.-H. Chan, N. Gillis, P. Gader, A. Plaza, A. Ambikapathi and C.-Y. Chi, "A signal processing perspective on hyperspectral unmixing", IEEE Signal Processing Magazine, Jan., 2014.

Linear mixing model (LMM)



$$\mathbf{r} = \sum_{i=1}^{p} \alpha_i \mathbf{m}_i \qquad \mathbf{m}_i = \begin{bmatrix} \rho_{i1} \\ \rho_{i2} \\ \vdots \\ \rho_{iL} \end{bmatrix}$$

 $\mathbf{r}=\mathbf{M}\alpha$

$$\mathbf{M} \equiv [\mathbf{m}_1, \mathbf{m}_2, \mathbf{m}_3] \qquad \boldsymbol{\alpha} = \begin{vmatrix} \alpha_1 \\ \alpha_2 \\ \alpha_2 \end{vmatrix}$$

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



Nonlinear mixing model

Intimate mixture (particulate media) Two-layers: canopies+ground





Radiative transfer theory

$$\mathbf{r} = f(\alpha, \theta)$$

material fractions

media parameters

$$\mathbf{r} = \sum_{i=1}^{p} \alpha_i \mathbf{m}_i + \sum_{\substack{i,j=1\\i\neq j}}^{p} \alpha_{i,j} \mathbf{m}_i \odot \mathbf{m}_j$$

single scattering double scattering

Schematic view of the unmixing process



Given N spectral vectors of dimension L:

$$Y = \left\{ y_i \in \mathbb{R}^L, i = 1, ..., N \right\}$$
ANC: abundance
nonnegative
constraint

Subject to the LMM: $y = M\alpha + n$, $\alpha \ge 0$, $1^T \alpha = 1$
ASC: abundance
sum-to-one
constraint

ANC: abundance
nonnegative
constraint

ASC: abundance

SLU is a blind source separation problem (BSS)

$$\mathbf{y} = \mathbf{M}\boldsymbol{\alpha} + \mathbf{n}$$
 dim $(\mathbf{M}) = [L \times p]$ $L \gg p$

Problem: Identify $\mbox{ span}\{M\}$ the subspace generated by the columns of M

Reasoning underlying DR

- 1. Lightens the computational complexity
- 2. Attenuates the noise power by a factor of p/L



Subspace identification algorithms

Exact ML solution [Scharf, 91] (known *p*, i.i.d. Gaussian noise)

- **PCA -** Principal component analysis (unknown *p*, i.i.d. noise)
- NAPC Noise adjusted principal components [Lee et al., 90]
- MNF Maximum noise fraction [Green et al., 88]
- HFC Harsanyi-Farrand-Chang [Harsanyi et al., 93]
- **NWHFC** [Chang, Du, 94]
- HySime Hyperspectral signal identification by minimum error [B-D, Nascimento, 08]
- GENE geometry-based estimation of number of endmembers [ArulMurugan, 13]
- RMT [Kritchman, Nadler, 2009], [Cawse et al., 11], [Halimi et al., 16]



Example (HySime)

 $L = 224 \quad p = 3$

 $\mathbf{n} \sim \mathcal{N}(\mathbf{0}, \sigma^2 \mathbf{I})$ $\sigma = 0.1$

Geometrical view of SLU



Inferring $\mathbf{M} \Leftrightarrow$ inferring the vertices of the simplex S_M

Classes of SLU problems



Unmixing frameworks

□ Geometrical (blind)

Exploits parallelisms between the linear mixing model and properties of convex sets

Application scenarios: pure pixels, pixels in facets

Statistical (blind, semi-blind)
 Approaches linear unmixing as a statistical inference problem
 Application scenarios: all

□ Sparse regression (semi-blind)

Approaches linear unmixing as a sparse regression problem **Application scenarios:** all

Hard assumption The data set contains at least one pure pixel of each material



PPI - [Boardman, 93]; N-FINDR - [Winter, 99]; IEA - [Neville *et al.*, 99];
AMEE - [Plaza *et al*, 02]; SMACC - [Gruninger *et al.*, 04]
VCA - [Nascimento, B-D, 03, 05]; SGA - [Chang *et al.*, 06]
AVMAX, SVMAX - [Chan, et al., 11]; RNMF- [Gillis & Vavasis, 12,14];
SD-SOMP, SD-ReOMP - [Fu et al.13, 15];

Simplex vertex pursuit



Unmixing example

HYDICE sensor $\mathbf{M} \in \mathbb{R}^{210 \times 6}$ $N = 500 \times 307$ resolution = 0.75m





Minimum-volume constrained nonnegative matrix factorization (MVC-NMF) (inspired by NMF [Lee, Seung, 01])

$$\begin{aligned} (\widehat{\mathbf{M}}, \widehat{\mathbf{S}}) &= \arg \min_{\mathbf{M} \in \mathbb{R}^{L \times p}, \mathbf{S} \in \mathbb{R}^{p \times N}} \frac{1}{2} \|\mathbf{Y} - \mathbf{M}\mathbf{S}\|_{F}^{2} + \tau V(\mathbf{M}) + \lambda \phi(\mathbf{S}) \\ \text{s.t.:} & \mathbf{M} \succeq 0, \ \mathbf{S} \succeq 0, \ \mathbf{1}^{T}\mathbf{S} = \mathbf{1}_{N}^{T}, \end{aligned}$$
 volume regularizer

DPFT - [Craig, 90]; **CCA** - [Perczel et al., 89] (seminal works on MVC) **ICE** - [Breman *et al.*, 2004] ($V(\mathbf{M}) \equiv \text{quadratic}, \phi = 0$); **MVC-NMF** - [Miao,Qi, 07] ($V(\mathbf{M}) = |\det(\mathbf{MM}^T)|, \phi = 0$); **SPICE** - [Zare, Gader, 2007] ($V(\mathbf{M}) \equiv \text{quadratic}, \phi \equiv \text{weighted } \ell_1$) **L1/2** - **NMF** - [Qian, Jia, Zhou, Robles-Kelly, 11] (V = 0, $\phi(\mathbf{S}) = \sum_{ij} |\alpha_{ij}|^{1/2}$) **CONMF** - [Li, B-D, Plaza, 12] ($V(\mathbf{M}) \equiv \text{quadratic}, \phi(\mathbf{S}) = ||\mathbf{S}||_{2,1}$)

Minimum volume simplex algorithms

MVSA – Minimum volume simplex analysis [Li, B-D, 08]

Optimization variable $\mathbf{Q} \equiv \mathbf{M}^{-1} \Rightarrow \mathbf{Q}\mathbf{Y} = \mathbf{S}$



MVSA solves a sequence of quadratic programs

MVES [Chan, Chi, Huang, Ma, 2009]

- Solves a sequence of linear programs by exploiting the cofactor expansion of det (Q)
- □ The existence of pure pixels is a sufficient condition for exact identification of the true endmembers

Robust minimum volume simplex algorithms: outliers





□ SISAL solves a sequence of convex subproblems using ADMM □ $(\lambda = \infty) \Rightarrow MVES \equiv (MVES, SISAL)$

Example: data set contains pure pixels

$$N = 5000 \quad p = 5 \quad \max_{\alpha_i} = 1, \text{ for } i = 1, \dots, p$$

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Time:

VCA \rightarrow 0.5 sec SISAL \rightarrow 2 sec

Example: Data set does not contain pure pixels

$$N = 5000$$
 $p = 5$ $\max_{\alpha_i} = 0.8$, for $i = 1, \dots, p$



No pure pixels and outliers

$$N = 1000$$
 $p = 3$ max = 0.8, for $i = 1, \dots, p$
no. outliers = 3



ERROR(mse): SISAL = 0.03 VCA = 0.88 NFINDR = 0.88 MVC-NMF = 0.90

TIMES (sec): SISAL = 0.61, VCA = 0.20 NFINDR = 0.25 MVC-NMF = 25

Real data: ArtImageDataA (converted into absorbance)



Geometrical Approaches: Limitations

□ determined by a small number of pixels; some may be outliers

□ MVS – Computationally heavy

PPI, N-FINDR, VCA, SGA, AMEE, SVMAX, AVMAX depend on the existence of pure pixels in the data

Do not work in highly mixed scenarios



Statistical approaches

- $\Box \text{ observation model} \qquad Y = MS + N$
- \Box prior (Bayesian framework) $p_S(S)p_M(M)$
- posterior density

 $p_{M,S|Y}(\mathbf{M}, \mathbf{S}|\mathbf{Y}) = p_{Y|M,S}(\mathbf{Y}|\mathbf{M}, \mathbf{S})p_M(\mathbf{M})p_S(\mathbf{S})/p_Y(\mathbf{Y})$

□ inference

 $(\widehat{\mathbf{M}}, \widehat{\mathbf{S}})_{\mathrm{MAP}} \equiv \arg \max_{\mathbf{M}, \mathbf{S}} p_{M, S|Y}(\mathbf{M}, \mathbf{S}|\mathbf{Y})$ = $\arg \min - \log p_{Y|M, S}(\mathbf{Y}|\mathbf{M}, \mathbf{S}) - \log p_M(\mathbf{M}) - \log p_S(\mathbf{S})$

$$\widehat{\mathbf{M}}_{\text{MMSE}} \equiv \mathbb{E}[\mathbf{M}|\mathbf{Y}] = \int \mathbf{M} p_{M|Y}(\mathbf{M}|\mathbf{Y}) d\mathbf{M}$$
$$\widehat{\mathbf{S}}_{\text{MMSE}} \equiv \mathbb{E}[\mathbf{S}|\mathbf{Y}] = \int \mathbf{S} p_{S|Y}(\mathbf{S}|\mathbf{Y}) d\mathbf{S}.$$

Spectral linear unmixing and ICA/IFA

□ Formally, SLU is a linear source separation problem

□ Independent Component Analysis (ICA) come to mind

ICA
 Fastica, [Hyvarinen & Oja, 2000]
 Jade, [Cardoso, 1997]
 Bell and Sejnowski, [Bell and Sejnowski, 1995]

IFA

□ *IFA*, [Moulines *et al.*, 1997], [Attias, 1999]

$\mathbf{y} = \mathbf{M}\alpha + \mathbf{n}$

Assumptions

- 1. Fractional abundances (sources) are independent $p_{\alpha}(\alpha) = p_1(\alpha_1)p_2(\alpha_2)\dots p_k(\alpha_p)$
- 2. Non-Gaussian sources

Endmembers compete for the same area

$$\sum_{j=1}^{\kappa} \alpha_j = 1$$

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Sources are Dependent

ICA does not apply [Nascimento, B-D, 2005]

[Parra *et al.*, 00] (S- u.d. on the simplex, M- AR model, MAP)

[Moussaoui et al., 06,a,b], [Dobigeon et al., 09,a,b], [Dobigeon et al., 09,b], [Arngreen, 11]

- □ data term associated with the LMM
- \Box S–Uniform on the simplex
- □ conjugate prior distributions for some unknown parameters
- □ Infer MMSE estimates by Markov chain Monte Carlo algorithms

DECA - [Nascimento, B-D 09, 14]

- data term associated with a noiseless LMM
- □ S− Dirichlet mixture model
- □ MDL based inference of the number of Dirichlet modes
- □ MAP inference (GEM algorithm)

DECA – Dependent component analysis



DECA – Results on Cuprite







[Mittelman, Dobigeon, Hero, 12]

- □ data term associated with the LMM
- $\Box \quad \mathbf{S}-\text{ Dirichlet mixture model}$
- Latent label process enforcing adjacent pixels to have the same label
- spatial prior: tree-structured sticky hierarchical Dirichlet process (SHDP)
- □ MMSE inference by MCMC
- Model order inference (number of endmembers)

Sparse regression-based SLU

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

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

$$\mathbf{y} = \sum_{i \in S} \mathbf{a}_i \mathbf{x}_i = \mathbf{A} \mathbf{x}$$



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

$$y = Ax$$

□ Advantage: sidesteps endmember estimation

Disadvantage: Combinatorial problem !!!

CBPDN – Constrained basis pursuit denoising

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

Equivalent problem

$$\min_{\mathbf{x}}(1/2)\|\mathbf{y} - \mathbf{A}\mathbf{x}\|^2 + \lambda\|\mathbf{x}\|_1, \quad \mathbf{x} \ge 0$$

Striking result: In given circumstances, related with the coherence among the columns of matrix **A**, BP(DN) yields the sparsest solution ([Donoho 06], [Candès et al. 06]).

Efficient solvers for CBPDN: SUNSAL, CSUNSAL [B-D, Figueiredo, 10]

Real data – AVIRIS Cuprite



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

Real data – AVIRIS Cuprite



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[Iordache, B-D, Plaza, 11, 12]
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Sparse reconstruction of hyperspectral data: Summary

Bad news: Hyperspectral libraries have poor RI constants

Good news: Hyperspectral mixtures are highly sparse, very often p · 5

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

Directio	ons 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)

$$\min_{\mathbf{X}} (1/2) \| \mathbf{A}\mathbf{X} - \mathbf{Y} \|_{F}^{2} + \lambda_{1} \| \mathbf{X} \|_{1} + \lambda_{2} \phi_{TV}(\mathbf{X}) \qquad \text{[Iordache, B-D, Plaza, 11]}$$
subject to: $\mathbf{X} \ge \mathbf{0}$

$$for a data interval in the second of the second of$$

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

Other Regularizers:

- vector total variation (VTV)! promotes piecewise smoo vectors [Bresson, Chan, 02], [Goldluecke et al., 12], [Yuan, Zhang, Shen, 12]
- convex generalizations of Total Variation based on the Structure Tensor [Lefkimmiatis et al., 13]
- □ sparse representation (2D, 3D) in the wavelet domain

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)

$$\begin{split} \min_{\mathbf{X}} (1/2) \| \mathbf{A} \mathbf{X} - \mathbf{Y} \|_{F}^{2} + \lambda \| \mathbf{X} \|_{2,1} & \| \mathbf{X} \|_{2,1} := \sum_{i=1}^{n} \| \mathbf{x}^{i} \|_{2} \\ \text{subject to: } \mathbf{X} \geq \mathbf{0}, \quad \mathbf{1}_{n}^{T} \mathbf{X} = \mathbf{1}_{N}^{T} \\ \text{[lordache, B-D, Plaza, 11, 12]} & [Turlach, Venables, Wright, 2004] \end{split}$$



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 MUSIC-CSR algorithm [lordahe, B-D, Plaza, 2013]

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 ($\geq 3^{\circ}$), Gaussian shaped noise, SNR = 25 dB, k = 5, m = 300,



Brief Concluding remarks

- □ HU is a hard inverse problem (noise, bad-conditioned direct operators, nonlinear mixing phenomena)
- HU calls for sophisticated math tools and framework (statistical inference, optimization, machine learning)
- The research efforts devoted to non-linear mixing models are increasing

Linear mixing

- Apply geometrical approaches when there are data vectors near or over the simplex facets
- Apply statistical methods in highly mixed data sets
- Apply sparse regression methods, if there exits a spectral library for the problem in hand

Spectral nonlinear unmixing (SNLU). Just a few topics

Detecting nonlinear mixtures in polynomial post-nonlinear mixing model, [Altmann, Dobigeon, Tourneret, 11,13]

$$\mathbf{y} = \mathbf{M} \boldsymbol{\alpha} + b(\mathbf{M} \boldsymbol{\alpha}) \odot (\mathbf{M} \boldsymbol{\alpha}) + \mathbf{n}$$

hypothesis test

Bilinear unmixing model, [Fan, Hu, Miller, Li, 09], [Nascimento, B-D, 09], [Halimi, Altmann, Dobigeon, Tourneret, 11,11]

$$\mathbf{y} = \sum_{i=1}^{p} \alpha_i \mathbf{m}_i + \sum_{i,j=1}^{p} \alpha_{i,j} \mathbf{m}_i \odot \mathbf{m}_j + \mathbf{n}$$

Kernel-based unmixing algorithms to specifically account for intimate mixtures [Broadwater, Chellappa, Burlina, 07], [Broadwater, Banerjee, 09,10, 11], [Chen, Richard, Ferrari, Honeine, 13]

N. Dobigeon, J.-Y. Tourneret, C. Richard, J. C. M. Bermudez, S. McLaughlin and A. O. Hero, "Nonlinear unmixing of hyperspectral images: models and algorithms," IEEE Signal Process. Magazine, vol. 31, no 1, pp. 82-94, 2014

R. Heylen, M.Parente, and P. Gader, "A review of nonlinear hyperspectral unmixing methods," Selected Topics in Applied Earth Observations and Remote Sensing, IEEE Journal of , vol.7, no.6, pp.1844-1868, 2014 $\mathbf{A} \in \mathbb{R}^{L \times m}$ (library, $p \ll L < m$, undetermined system) Problem – P0 $\min_{\mathbf{x}} \|\mathbf{x}\|_0$ subject to $\|\mathbf{y} - \mathbf{A}\mathbf{x}\|_2 \le \delta$, $\mathbf{x} \ge \mathbf{0}$, Very difficult (NP-hard)

Approximations to P0:

OMP – orthogonal matching pursuit [Pati *et al.,* 2003] BP – basis pursuit [Chen *et al.,* 2003] BPDN – basis pursuit denoising IHT (see [Blumensath, Davis, 11], [Kyrillidis, Cevher, 12])