

An Overview on Hyperspectral Unmixing

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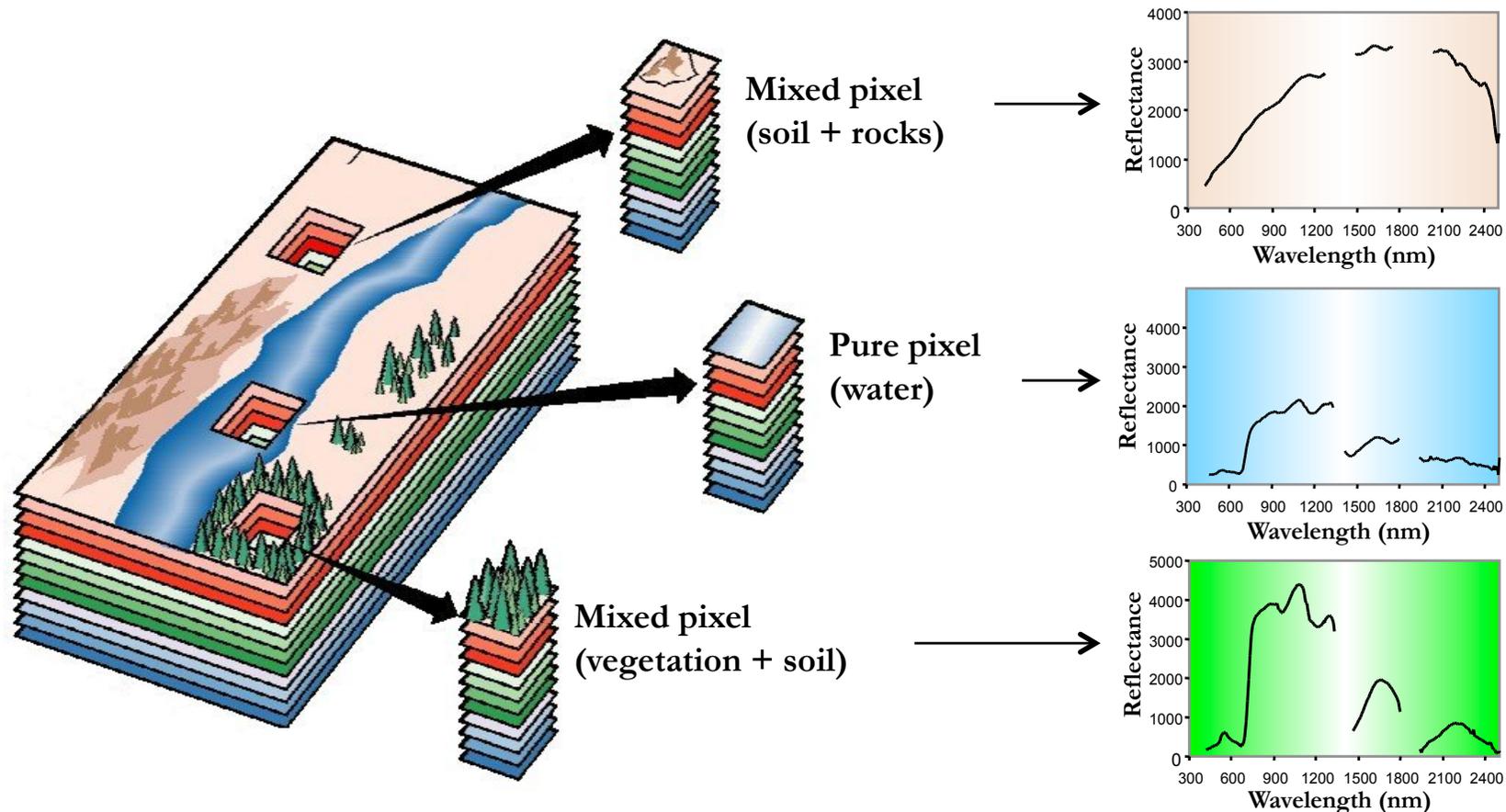
Grenoble – 11/12/2014

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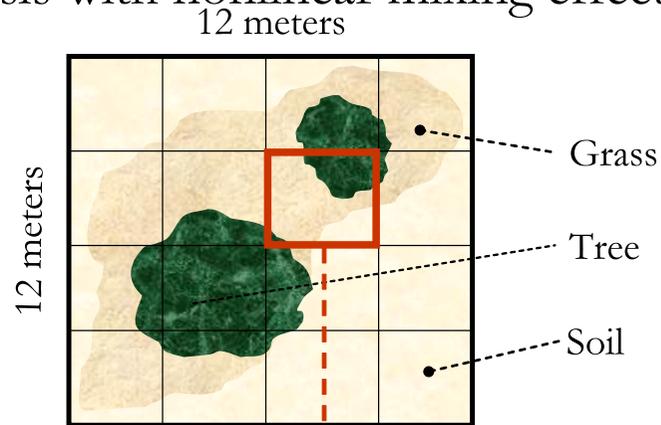
Introduction to spectral unmixing

- Mixed pixels are frequent in remotely sensed hyperspectral images due to insufficient *spatial resolution* of the imaging spectrometer, or due to *intimate mixing effects*.
- The rich spectral resolution available can be used to unmix hyperspectral pixels.



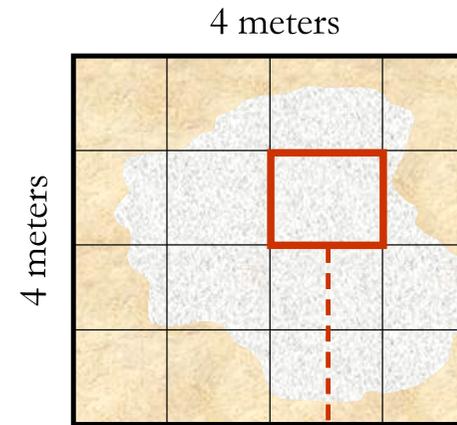
Introduction to spectral unmixing

- Mixed pixels can also be obtained with high spatial resolution data due to intimate mixtures, this means that increasing the spatial resolution does not solve the problem.
- The mixture problem can be approached in *macroscopic* fashion, this means that a few macroscopic components and their associated abundances should be derived.
- However, intimate mixtures happen at microscopic scales, thus complicating the analysis with nonlinear mixing effects.



Macroscopic mixture:

15% soil, 25% tree, 60% grass in a 3x3 meter-pixel

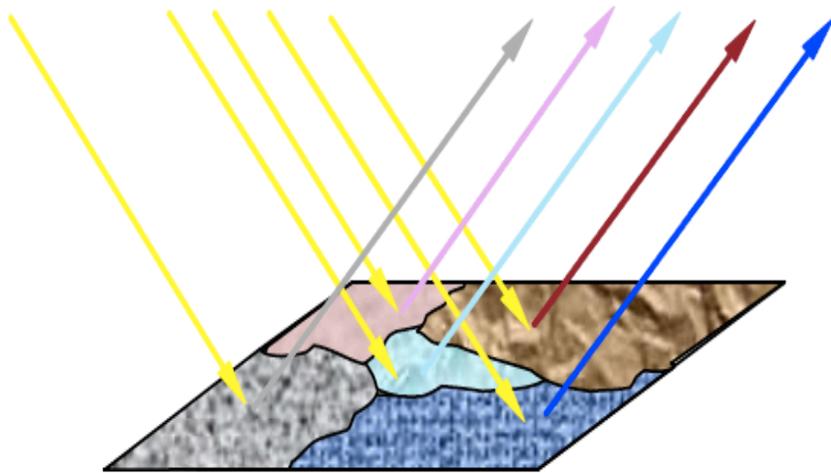


Intimate mixture:

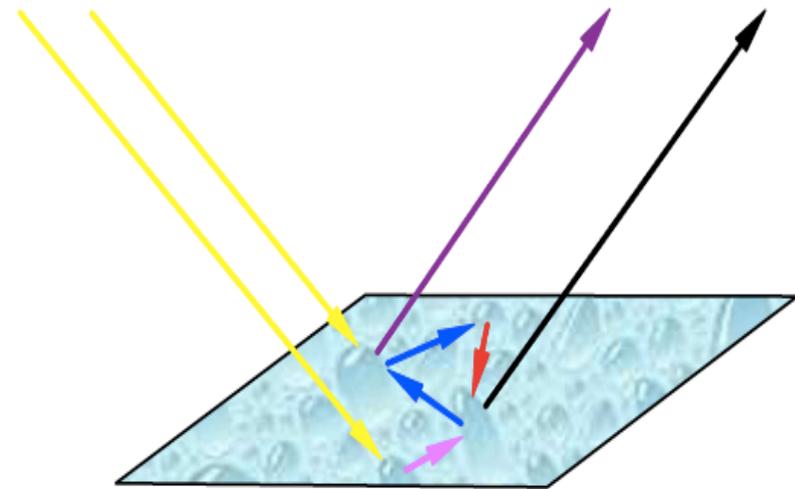
Minerals intimately mixed in a 1-meter pixel

Introduction to spectral unmixing

- In *linear* spectral unmixing, the macroscopically pure components are assumed to be homogeneously distributed in separate patches within the field of view.
- In *nonlinear* spectral unmixing, the microscopically pure components are intimately mixed inside the pixel. A challenge is how to derive the nonlinear function.
- Nonlinear spectral unmixing requires detailed *a priori* knowledge about the materials.



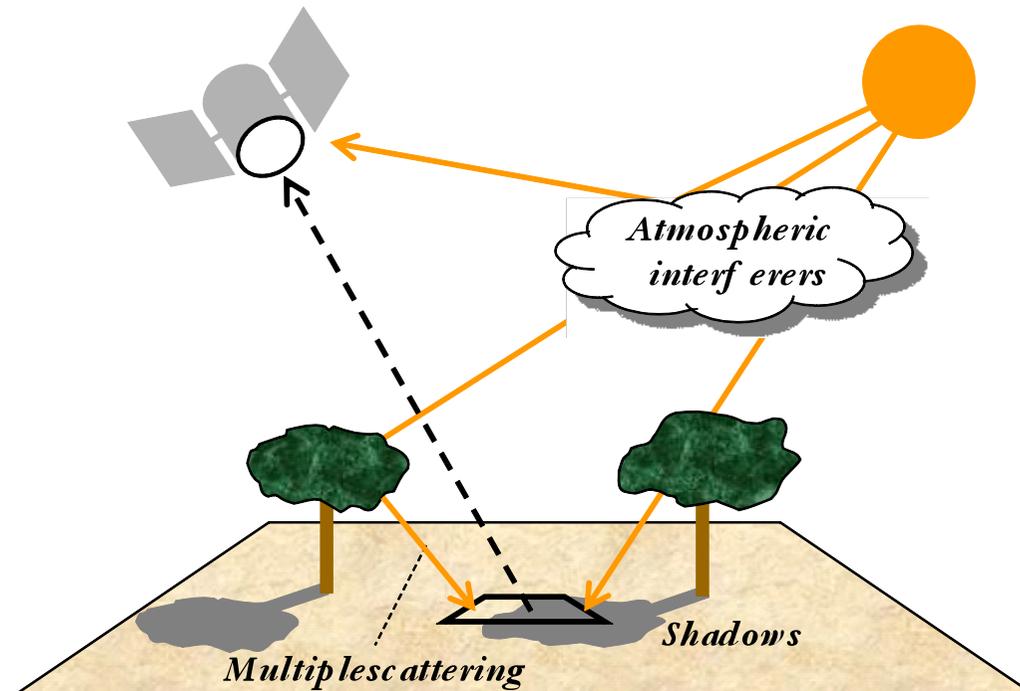
Linear interaction



Nonlinear interaction

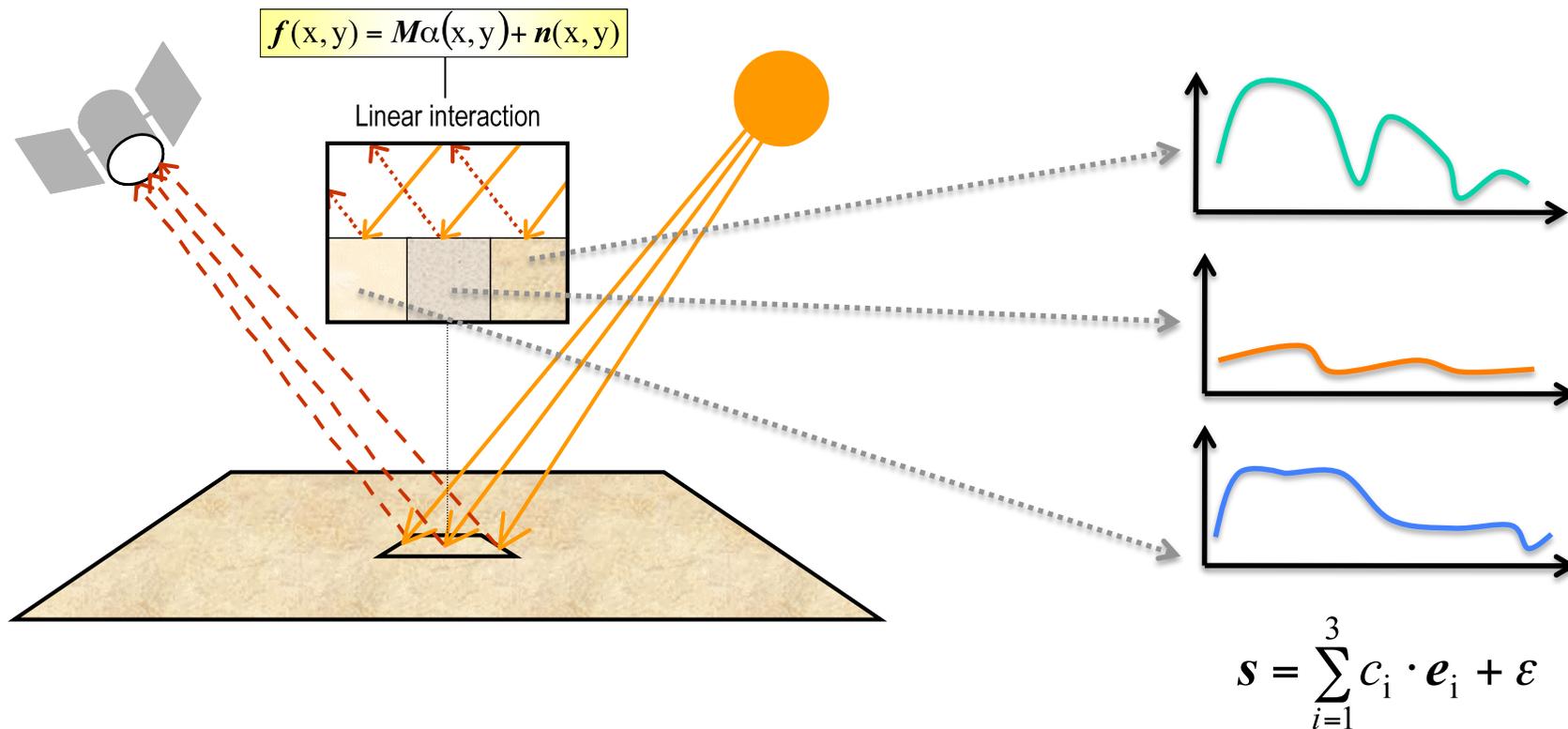
Introduction to spectral unmixing

- In addition to spectral mixing effects, there are many other *interferers* that can significantly affect the process of analyzing the remotely sensed hyperspectral data.
- For instance, *atmospheric interferers* are a potential source of errors in spectral unmixing.
- On the other hand, *multiple scattering* effects can also lead to model inaccuracies.
- Finally, shadows and variable *illumination* conditions should also be considered.



Introduction to spectral unmixing

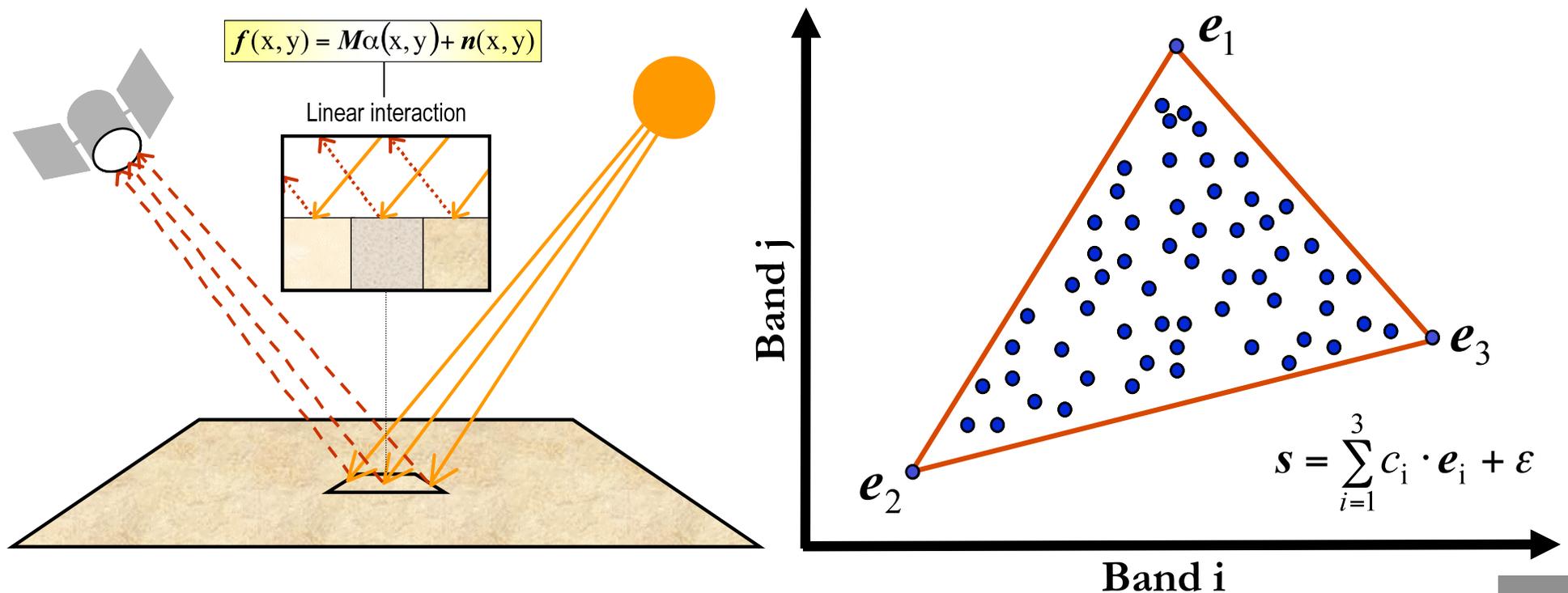
- In *linear* spectral unmixing, the goal is to find a set of macroscopically pure spectral components (called *endmembers*) that can be used to unmix all other pixels in the data.
- Unmixing amounts at finding the fractional coverage (*abundance*) of each endmember in each pixel of the scene, which can be approached as a *geometrical* problem:



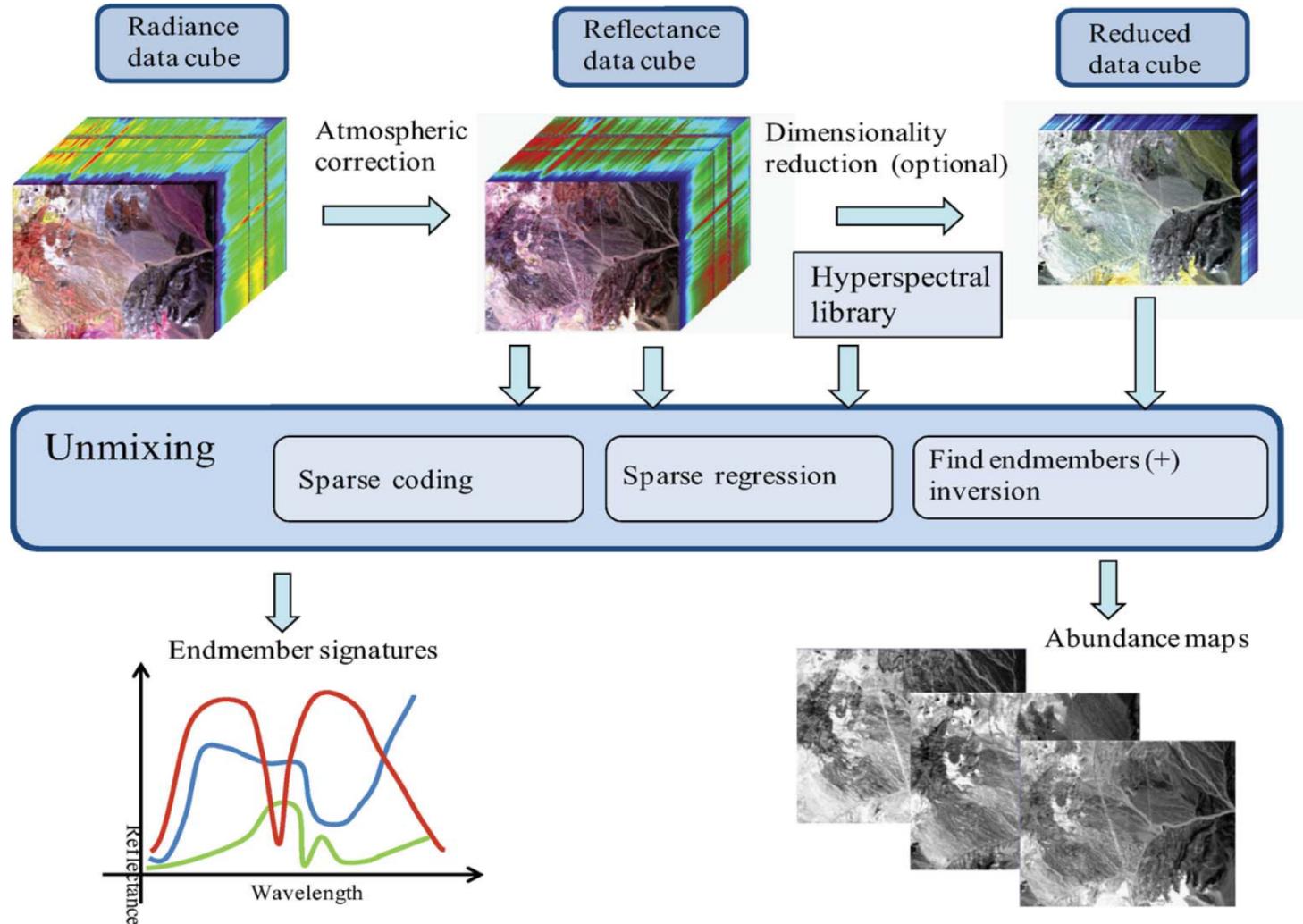
Introduction to spectral unmixing

Physical constraints:

- The spectra of the endmembers are non negative (a negative reflectance is not possible)
- Abundances are non negative (**non negativity constraint**)
- Abundances sum to one for each pixel (**sum to one constraint**)



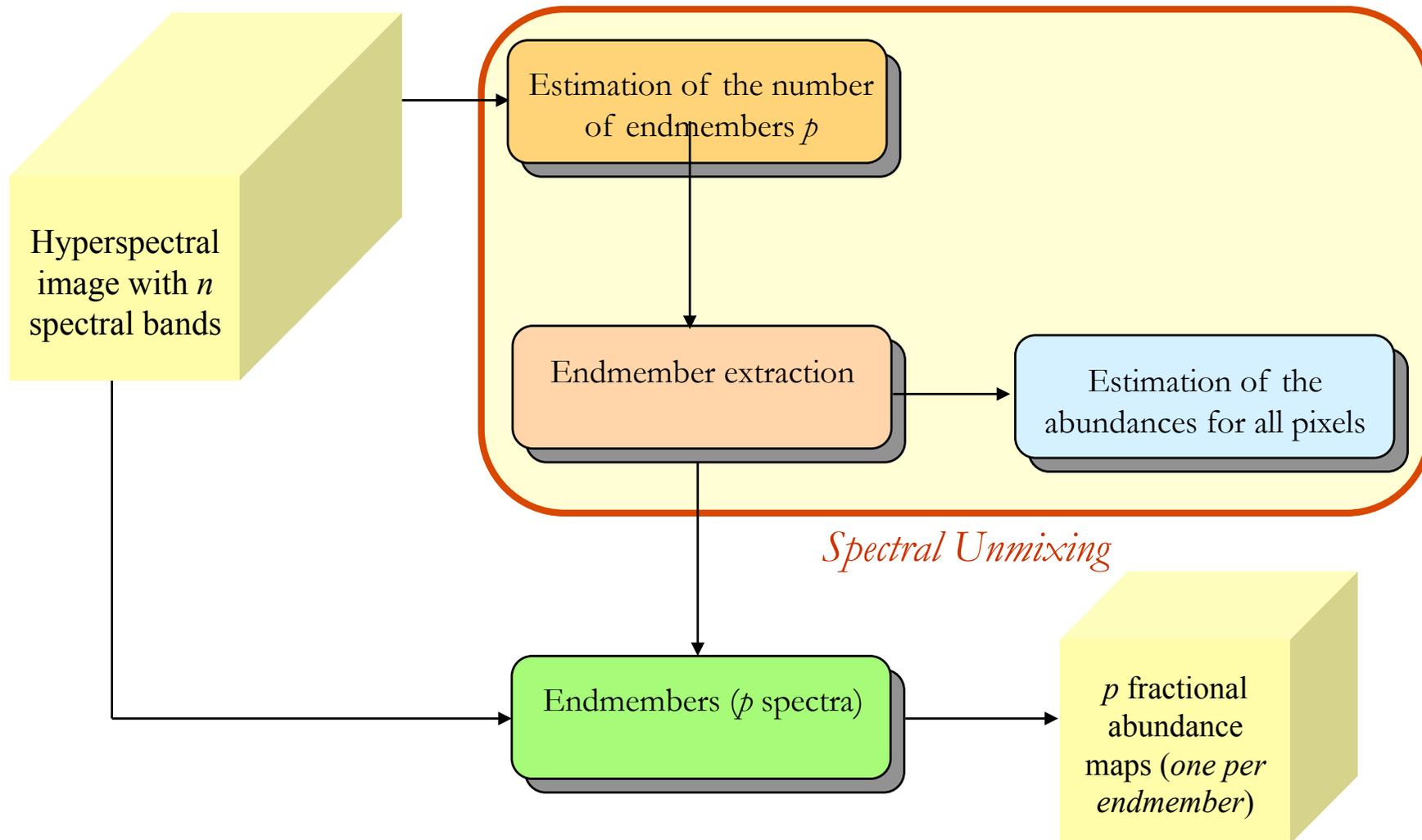
Introduction to spectral unmixing



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, April 2012.

Introduction to spectral unmixing

- General scheme of Spectral Unmixing

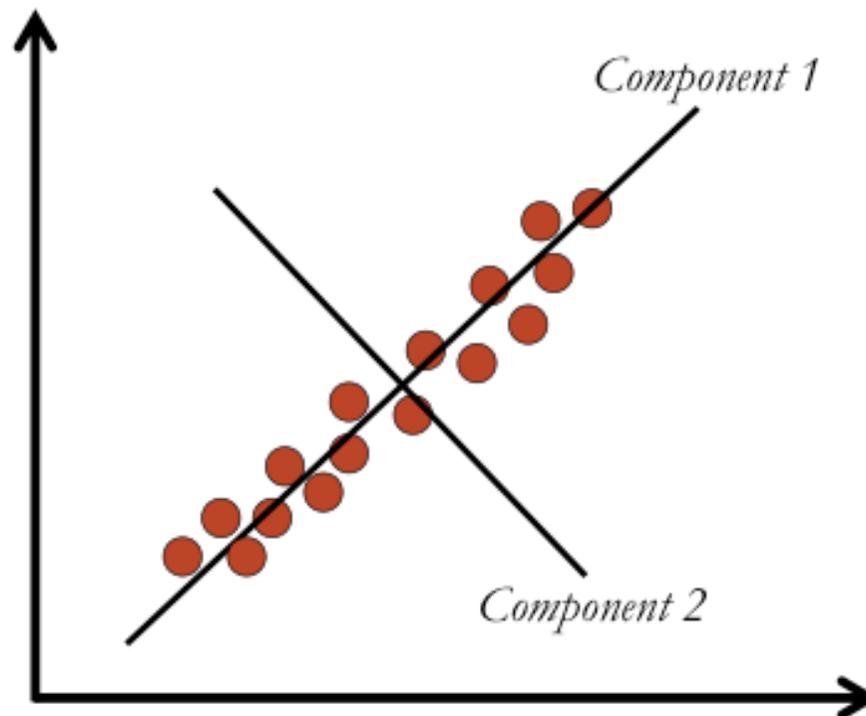


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 - 2.1. Classic methods for subspace estimation
 - 2.2. Hyperspectral subspace identification minimum error

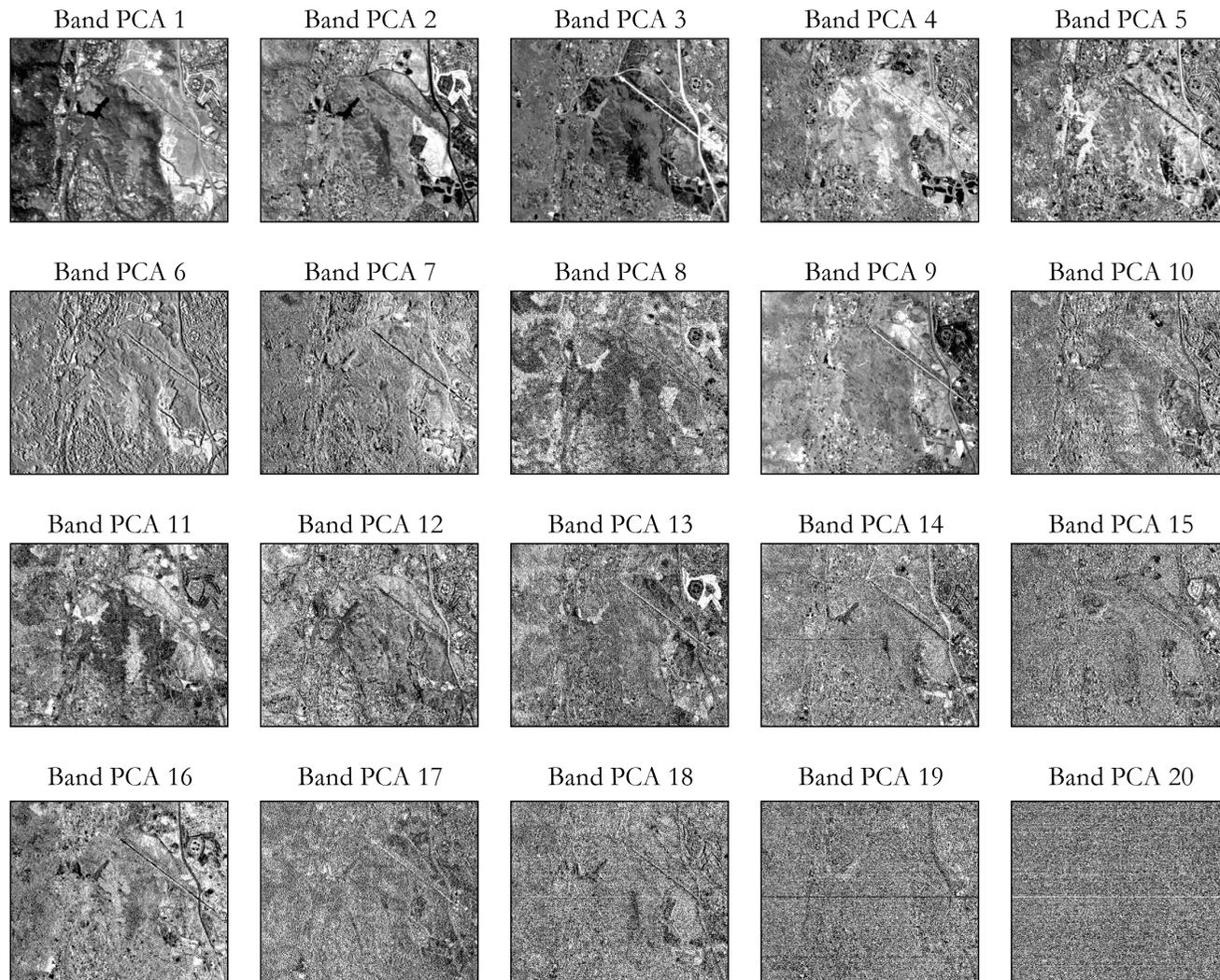
Classic methods for subspace estimation

- Determining the dimensionality of remotely sensed imagery is a challenging problem.
- The intrinsic dimensionality is defined as the minimum number of parameters needed to account for the observed properties of the data.
- Principal component analysis (PCA) transforms the data in a new coordinate system so that the number of significant components can be used as an estimate.



Classic methods for subspace estimation

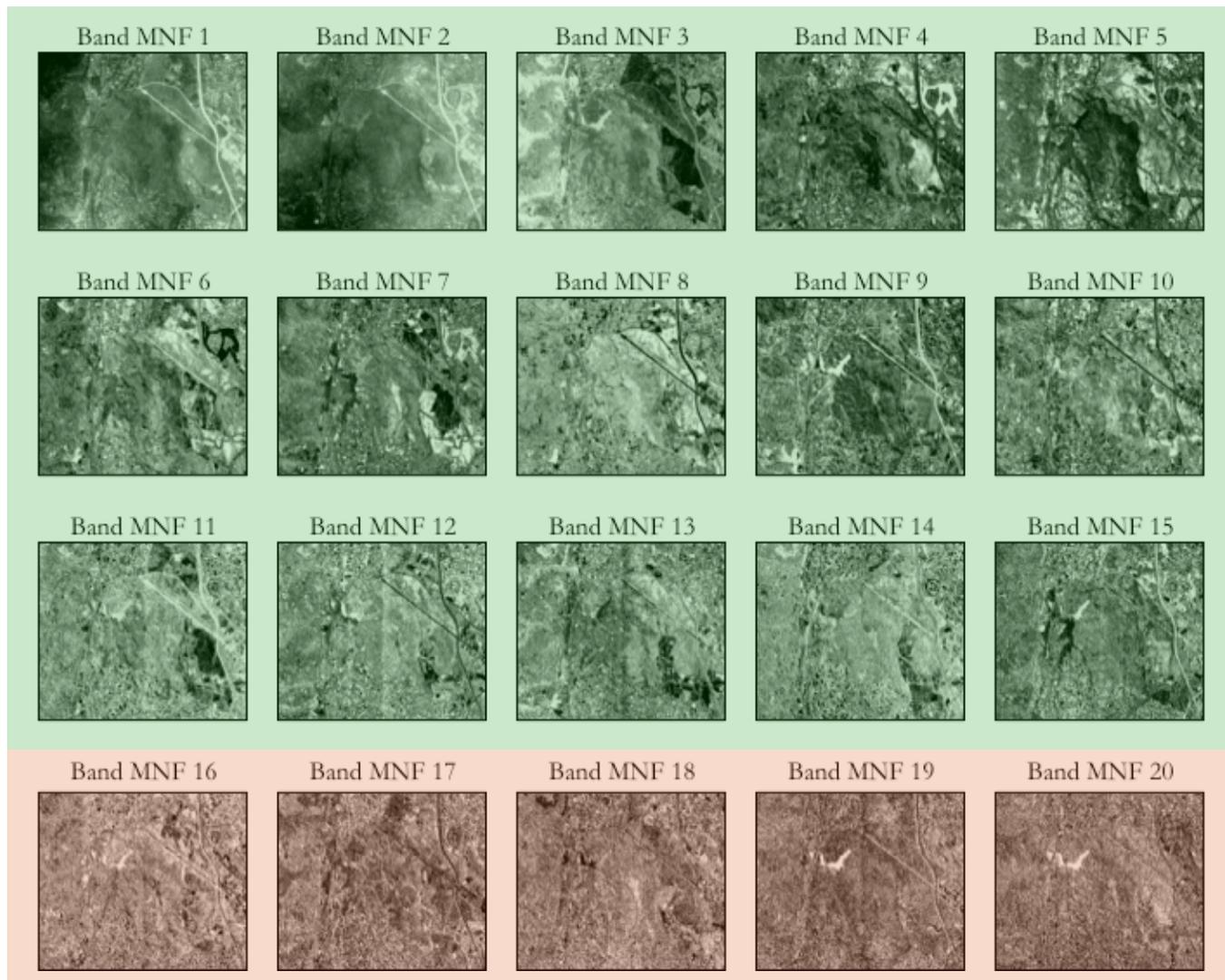
- The resulting PCA components are ordered in descending order of data variance:



Classic methods for subspace estimation

- Minimum noise fraction (MNF) orders the components in terms of signal to noise:

Signal



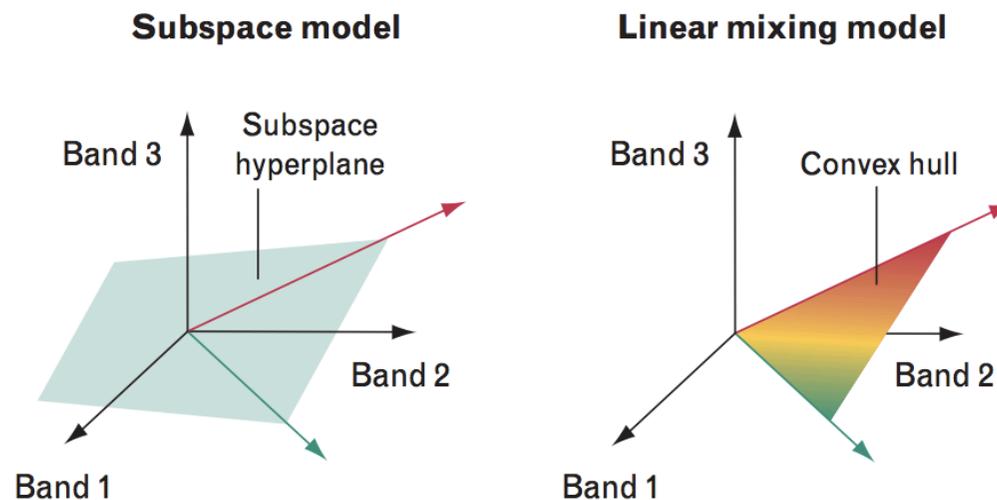
Noise

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HySime

- The idea of HySime is to find the first k eigenvectors that contain the most of data information, i.e., to find the k such that the mean square error (MSE) between the original data and its projection onto the eigenvector subspace is minimum.
- Subspace k is ranked in terms of data variance, but noise variance is not unitary in different directions and the contribution from signals may be smaller than from noise.
- HySime addresses this issue using subspace projection techniques, thus bringing an additional feature with regards to VD: the modelling of noise before the estimation.

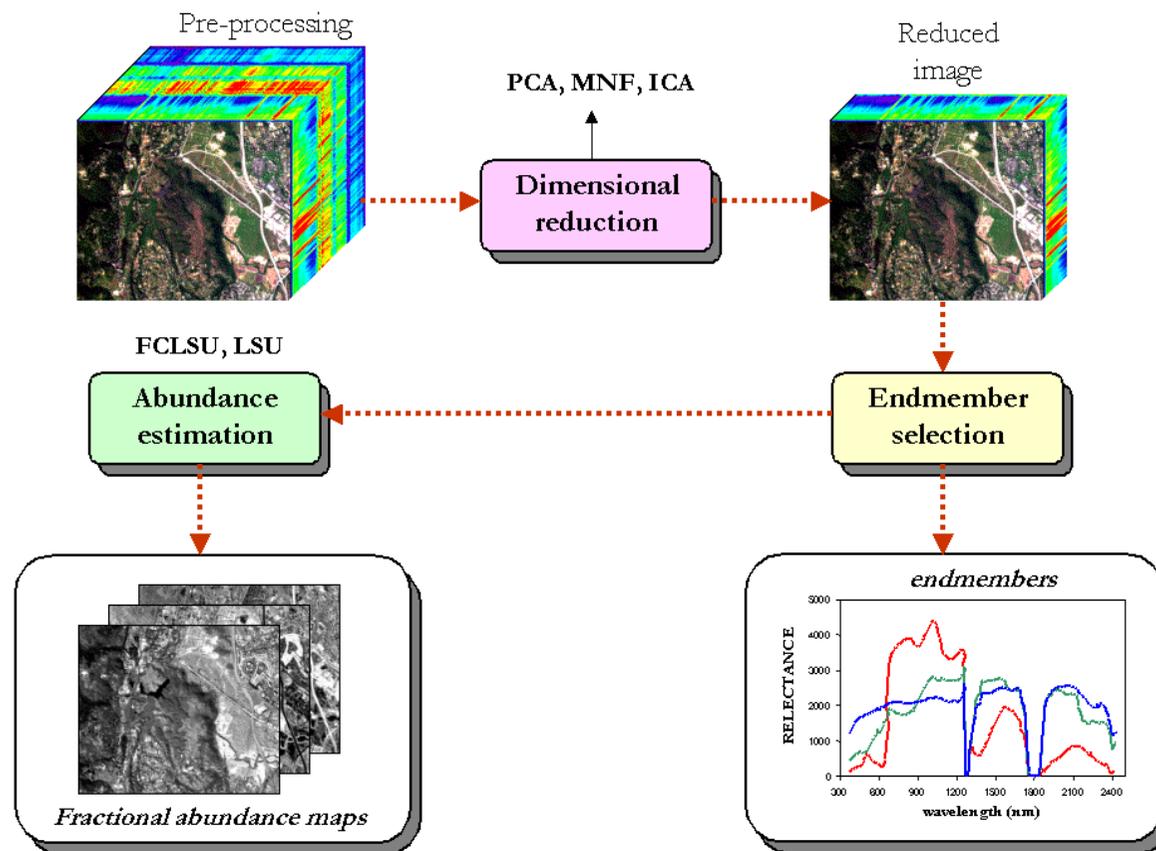


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 - 3.5. Comparative assessment using real data

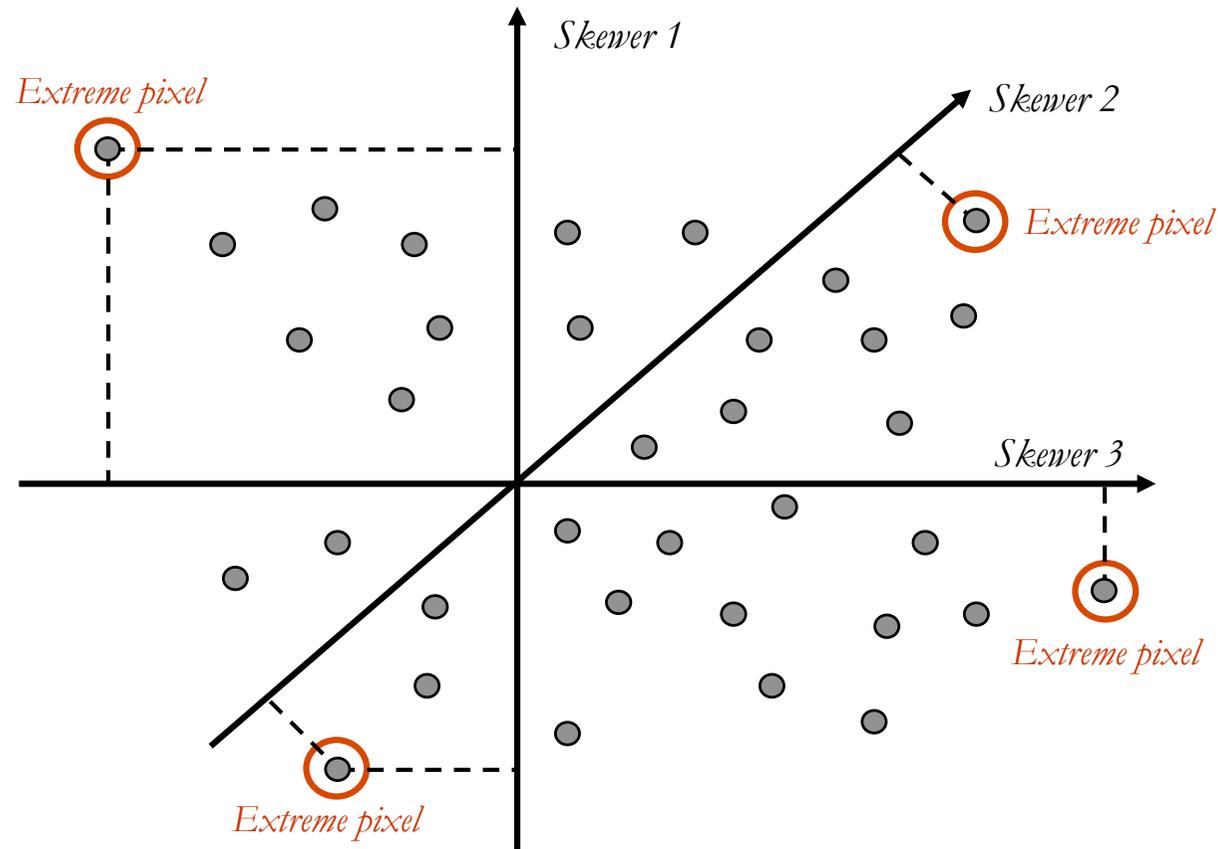
Classic methods for endmember extraction

- These methods assume a classic spectral unmixing chain made up of three stages: dimensional reduction, endmember selection and abundance estimation.
- Here, the endmembers are directly derived from the original hyperspectral scene.



Classic methods for endmember extraction

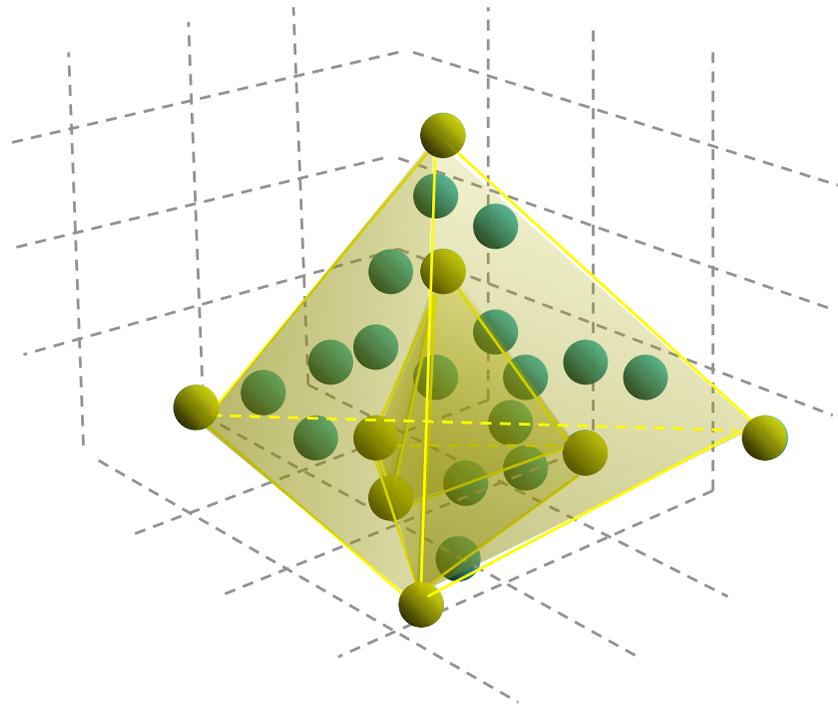
- The pixel purity index (PPI) is perhaps the most popular endmember extraction algorithm due to its availability in commercial software packages such as ENVI.



J. W. Boardman, F. A. Kruse and R. O. Green, "Mapping target signatures via partial unmixing of AVIRIS data," Proceedings of the Fifth JPL Airborne Earth Science Workshop, vol. 95, pp. 23-26, 1995.

Classic methods for endmember extraction

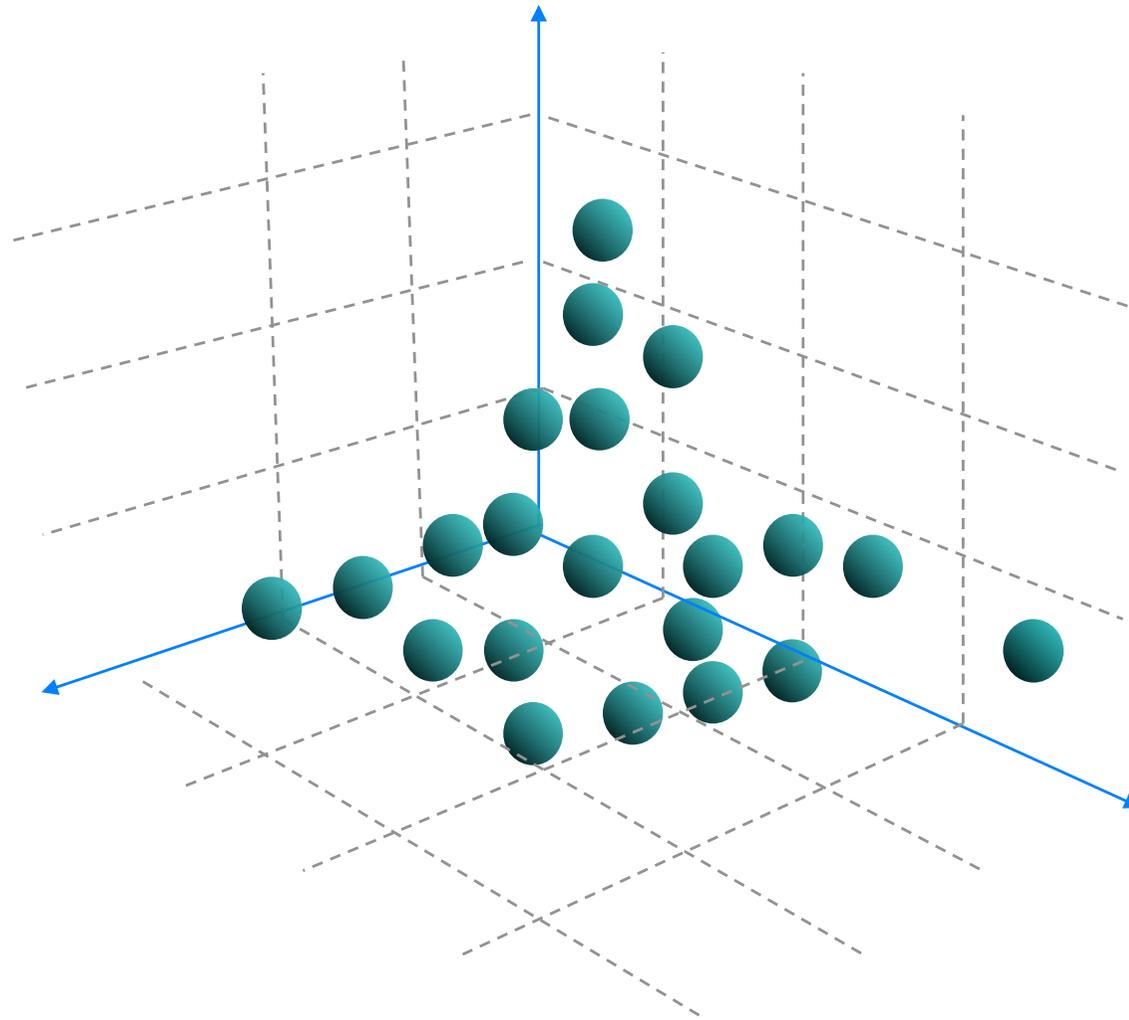
- The N-FINDR algorithm is also a very popular approach for endmember extraction.
- It assumes the presence of pure pixels in the original hyperspectral scene and further maximizes the volume that can be formed with pixel vectors in the data cube.



M. E. Winter, "N-FINDR: An algorithm for fast autonomous spectral endmember determination in hyperspectral data,"
Proceedings of SPIE, vol. 3753, pp. 266–270, Oct. 1999.

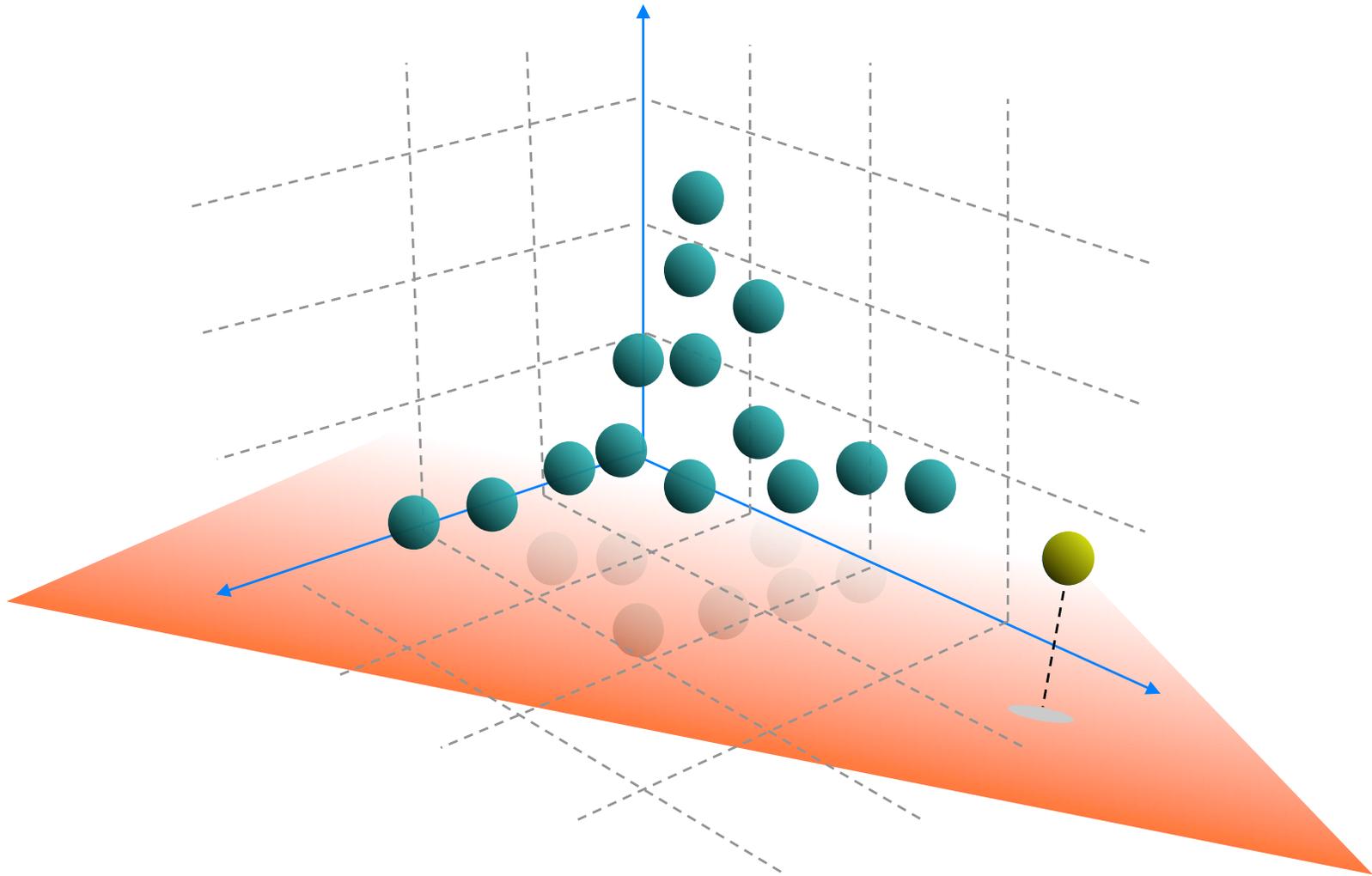
Classic methods for endmember extraction

- The orthogonal subspace projection (OSP) uses the concept of *orthogonal projections*:



Classic methods for endmember extraction

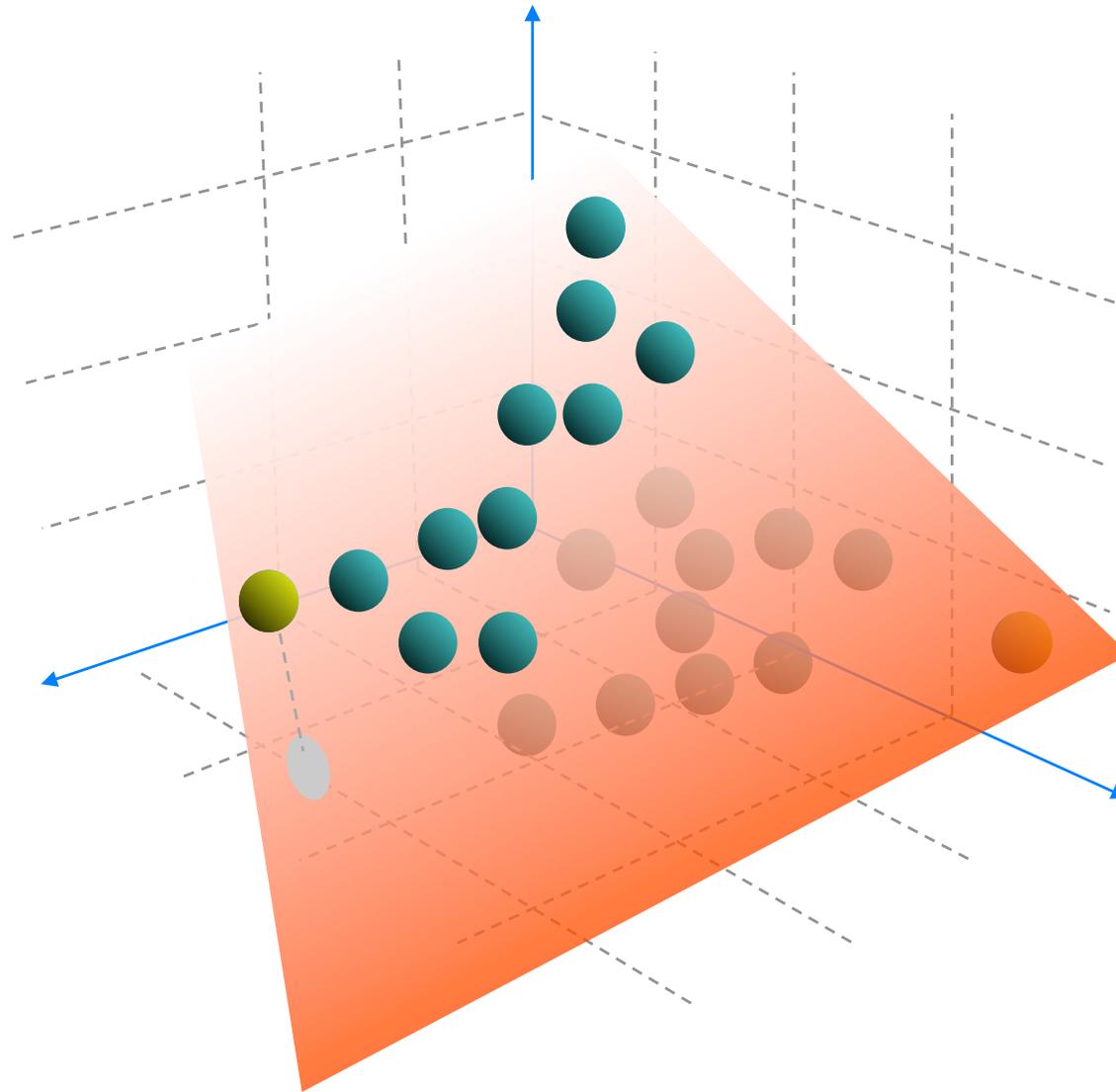
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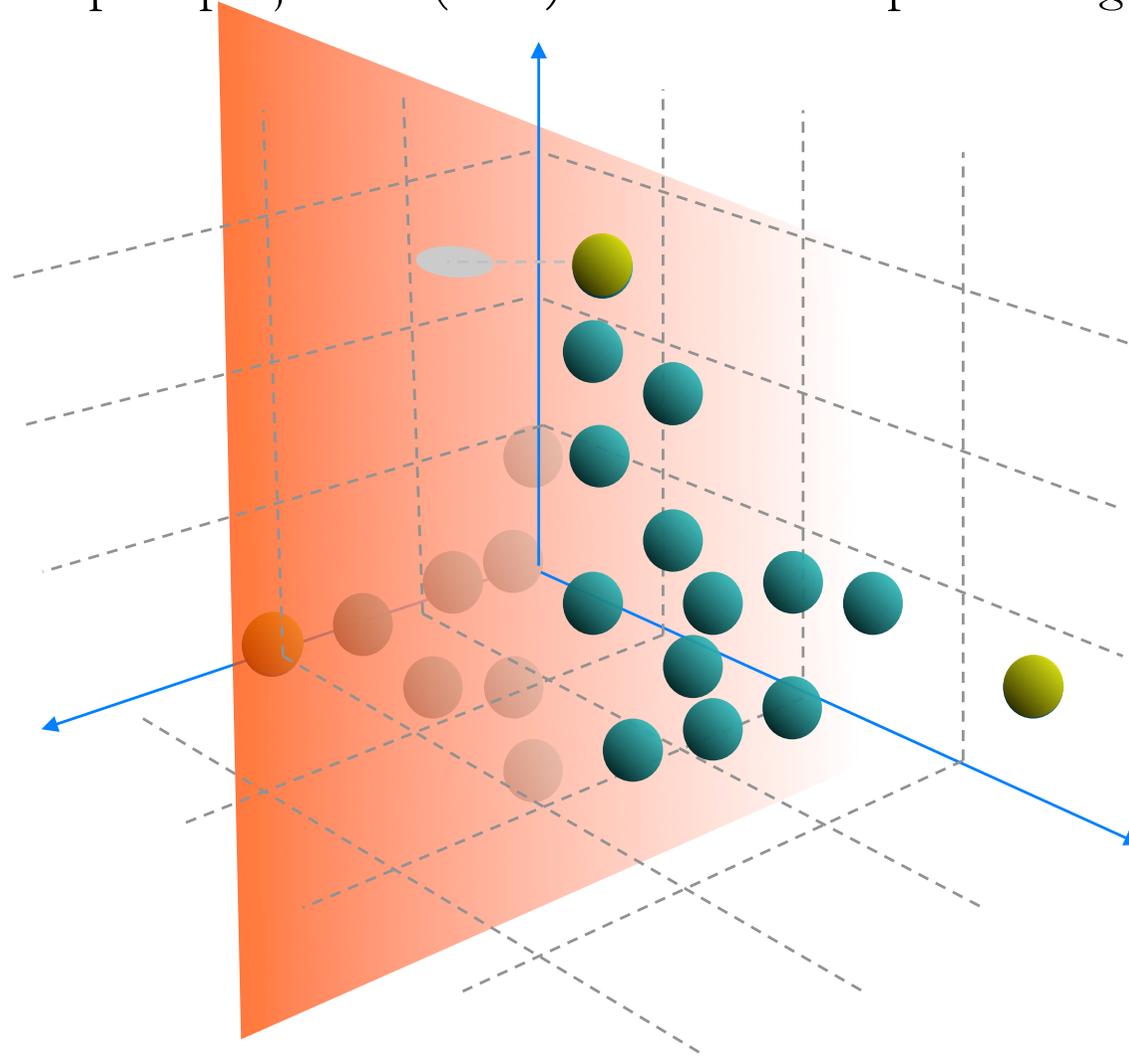
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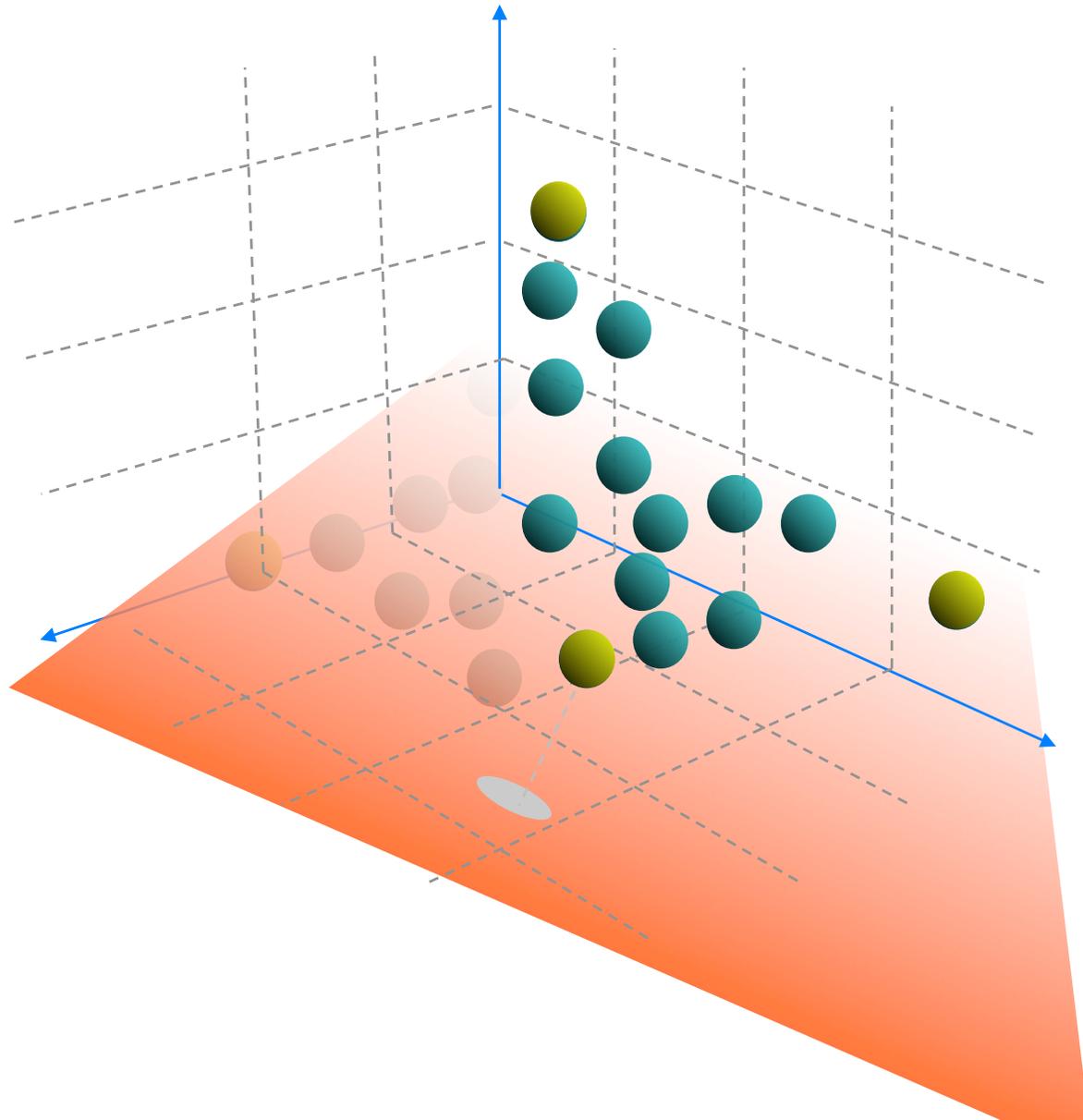
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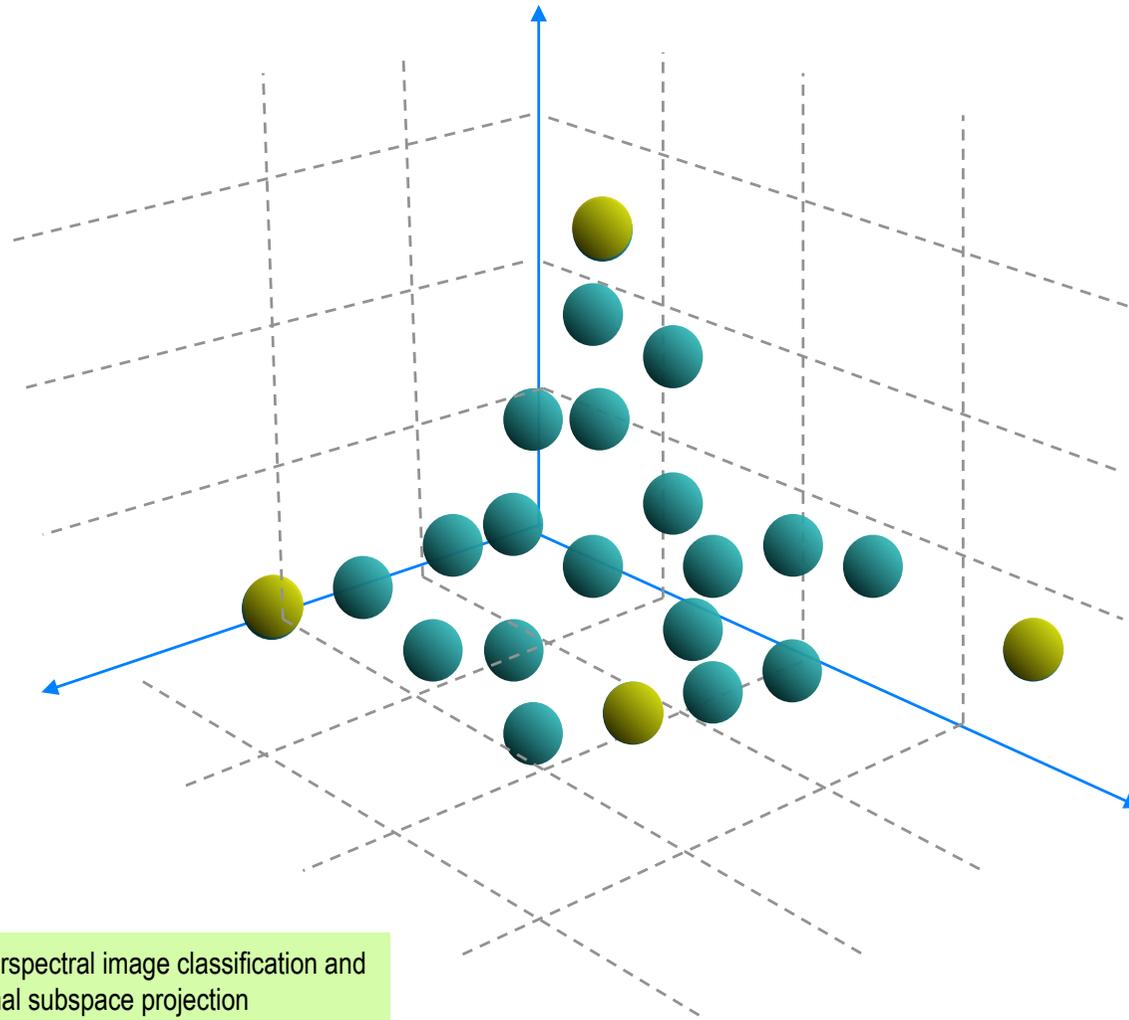
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Classic methods for endmember extraction

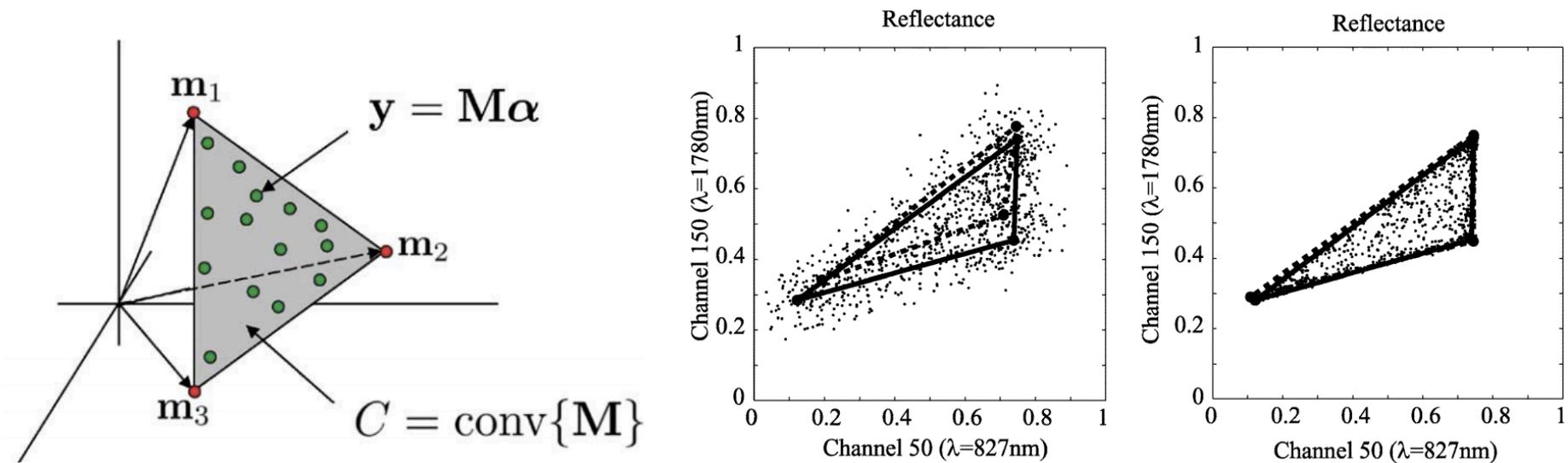
- The orthogonal subspace projection (OSP) uses the concept of *orthogonal projections*:



J. C. Harsanyi and C.-I. Chang, "Hyperspectral image classification and dimensionality reduction: an orthogonal subspace projection approach," *IEEE TGARS*, vol. 32, no. 4, pp. 779–785, 1994.

Classic methods for endmember extraction

- Vertex component analysis (VCA) iteratively projects data onto a direction orthogonal to the subspace spanned by the endmembers which have been already determined.
- In this regard, the algorithm is similar to OSP with the main difference that VCA applies a noise characterization process in order to reduce the sensitivity to noise.
- This is done by using singular value decomposition (SVD) to obtain the projection that better represents the data in maximum-power sense.



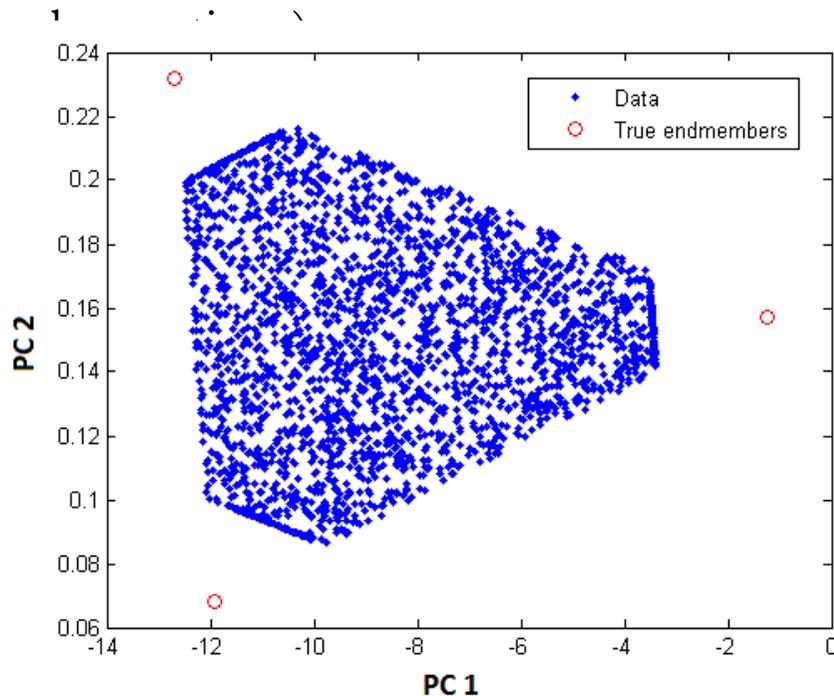
J. M. P. Nascimento and J. M. Bioucas-Dias, "Vertex component analysis: A fast algorithm to unmix hyperspectral data," *IEEE Transactions on Geoscience and Remote Sensing*, vol. 43, no. 4, pp. 898–910, 2005.

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Algorithms without pure pixel assumption

- What if the scene does not contain any pure signatures? (a very common scenario)
- In this case, the most feasible option is to use unmixing algorithms which *do not assume the presence of pure signatures* (these algorithms generate *virtual endmembers* located at the corners of the simplex with minimum volume that encloses all



ENDMEMBER IDENTIFICATION ALGORITHMS

Pure pixel assumption

- Convex geometry-based methods (OSP, N-FINDR, VCA)
- Spatial preprocessing (SPP, RBSPP, SSPP)
- Joint spatial-spectral methods (AMEE, SSEE)

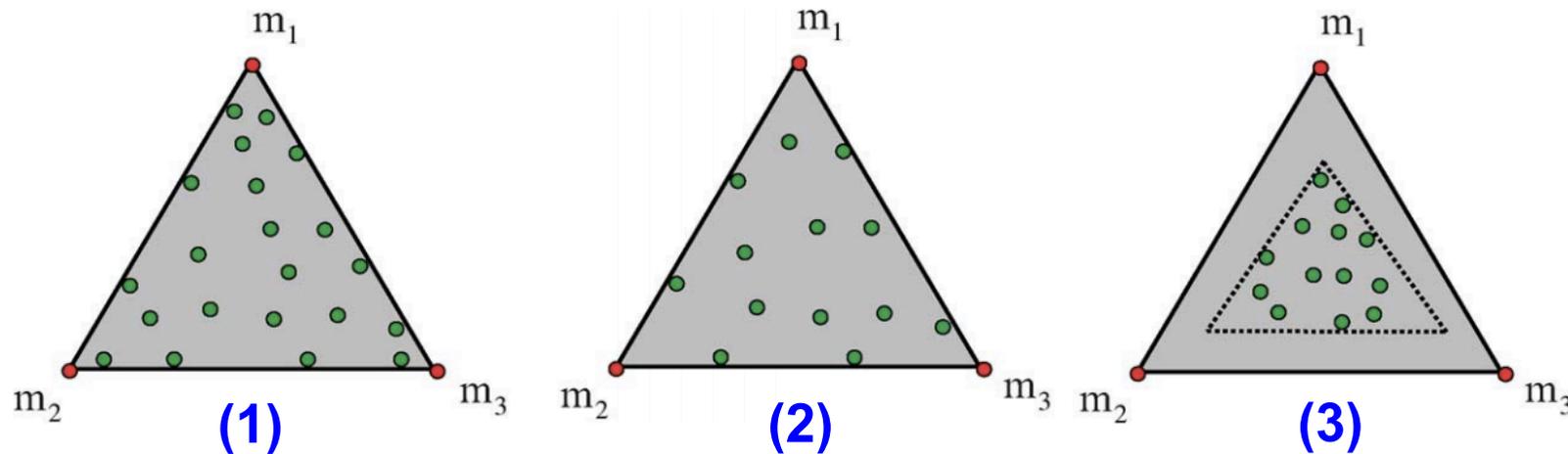
No pure assumption

- Minimum volume-based algorithms with different implementation options (MVSA, SISAL, MVC-NMF, ICE, SPICE, MVES, DECA)

E. M. T. Hendrix, I. Garcia, J. Plaza, G. Martin and A. Plaza, "A new minimum volume enclosing algorithm for endmember identification and abundance estimation in hyperspectral data," *IEEE Transactions on Geoscience and Remote Sensing*, vo. 50, no. 7, pp. 2744-2757, 2012.

Algorithms without pure pixel assumption

- In order to categorize algorithms, we may have three different situations in practice:
 - The data contains at least one pure pixel per endmember, i.e. there is at least one spectral vector in each vertex of the data simplex (pure pixel assumption).
 - The data does not contain pure pixels but contains at least $p - 1$ spectral vectors on each facet. In this case, we may fit a minimum volume simplex to the data.
 - The data is highly mixed, with no spectral vectors near the facets. In this case, minimum volume algorithms fail and we need to resort to a statistical framework.



J. M. Bioucas-Dias, A. Plaza, G. Camps-Valls, P. Scheunders, N. Nasrabadi and J. Chanussot, "Hyperspectral remote sensing data analysis and future challenges," *IEEE Geoscience and Remote Sensing Magazine*, vol. 1, no. 2, pp. 6-36, 2013.

Minimum Volume Algorithms

- From an optimization point of view, these algorithms are formulated as follows:

$$\min_{\mathbf{M}, \mathbf{A}} \|\mathbf{Y} - \mathbf{MA}\|_F^2 + \lambda V(\mathbf{M})$$

subject to: $\mathbf{A} \geq \mathbf{0}$, $\mathbf{1}_p^T \mathbf{A} = \mathbf{1}_n$,

- Here, the data term minimizes reconstruction error and the volume term promotes mixing matrices of minimum volume, with λ controlling their relative weight.
- This is the case of the *iterative constrained endmembers* (ICE) and the *minimum volume transform-nonnegative matrix factorization* (MVC-NMF) methods, whose main differences are related with the way they define the data volume term.
- The *sparsity-promoting* ICE (SPICE) is an extension of the ICE algorithm that incorporates sparsity-promoting priors aiming at finding the number of endmembers.

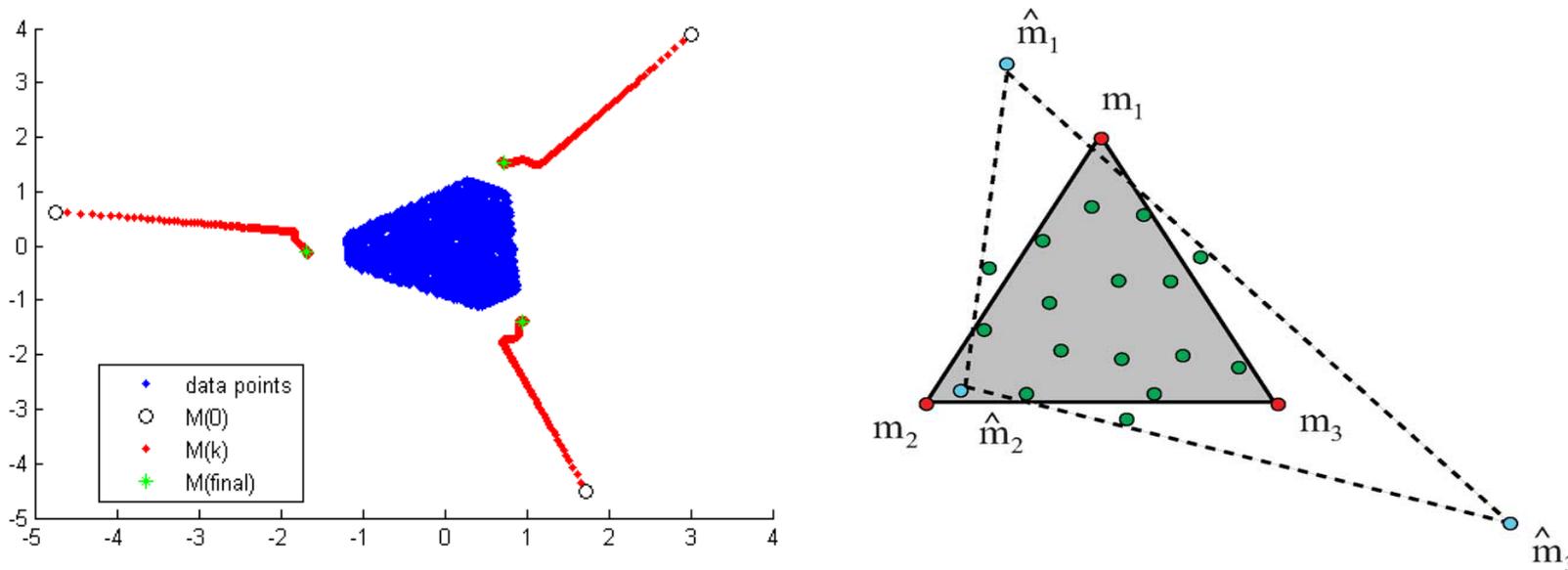
L. Miao and H. Qi, "Endmember extraction from highly mixed data using minimum volume constrained nonnegative matrix factorization," IEEE Transactions on Geoscience and Remote Sensing, vol. 45, no. 3, pp. 765–777, 2007.

M. Berman, H. Kiiveri, R. Lagerstrom, A. Ernst, R. Dunne, and J. F. Huntington, "ICE: A statistical approach to identifying endmembers in hyperspectral images," IEEE Transactions on Geoscience and Remote Sensing, vol. 42, no. 10, pp. 2085–2095, 2004.

A. Zare and P. Gader, "Sparsity promoting ICE detection for hyperspectral imagery," IEEE GRSL vol. 4, no. 3, pp. 446–450, 2007.

Minimum Volume Algorithms

- The minimum volume simplex analysis (MVSA/SISAL) algorithms follow a similar strategy, but allowing violations of the positivity constraint.
- This is because, due to the presence of noise or perturbations, spectral vectors may lie outside the true simplex.
- Both initialized with an inflated version of the solution provided by VCA algorithm.



J. Li and J. Bioucas-Dias, "Minimum volume simplex analysis: A fast algorithm to unmix hyperspectral data," in *Proceedings of the IEEE International Geoscience and Remote Sensing Symposium (IGARSS)*, vol. 3, pp. 250–253, 2008.

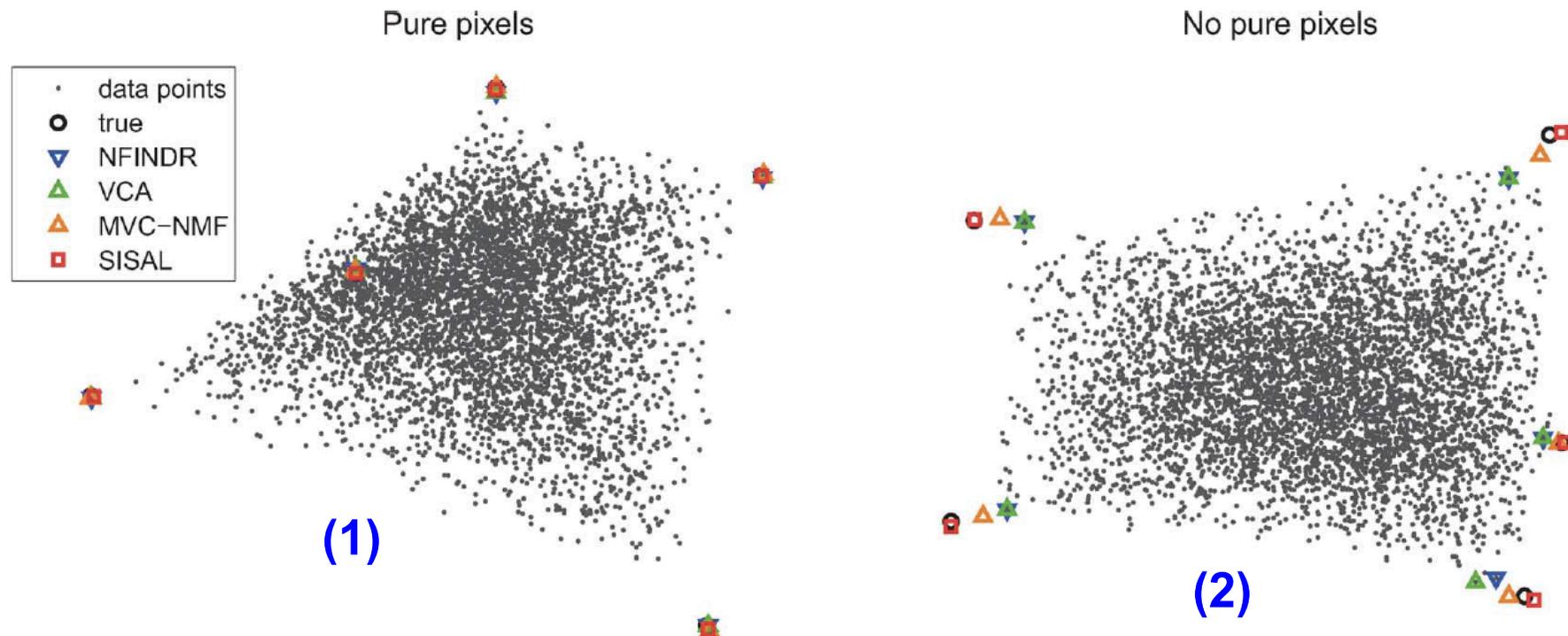
Statistical Algorithms

- When the data are highly mixed (no sufficient pixels in the facets), minimum volume algorithms fail and we need to resort to a statistical framework.
- This framework formulates unmixing as a statistical inference problem, usually adopting the Bayesian paradigm.
- A clear illustration of the potential of the Bayesian approach to cope with highly mixed data sets is provided (among several other strategies presented in the recent literature) by the *dependent component analysis* (DECA) algorithm.
- It automatically enforces the constraints of the abundance fractions namely non-negativity and constant sum when identifying the spectral endmembers.
- Finally, we note that most matrix factorization methods (e.g., MVC-NMF) may be also be formulated as Bayesian inference problems.
- This has the advantage of attaching meaning to the model parameters and providing a suitable framework to deal with them.

J.M. Bioucas-Dias and J. Nascimento, "Hyperspectral unmixing based on mixtures of Dirichlet components," *IEEE Transactions on Geoscience and Remote Sensing*, vol. 50, no. 3, pp. 863–878, 2012.

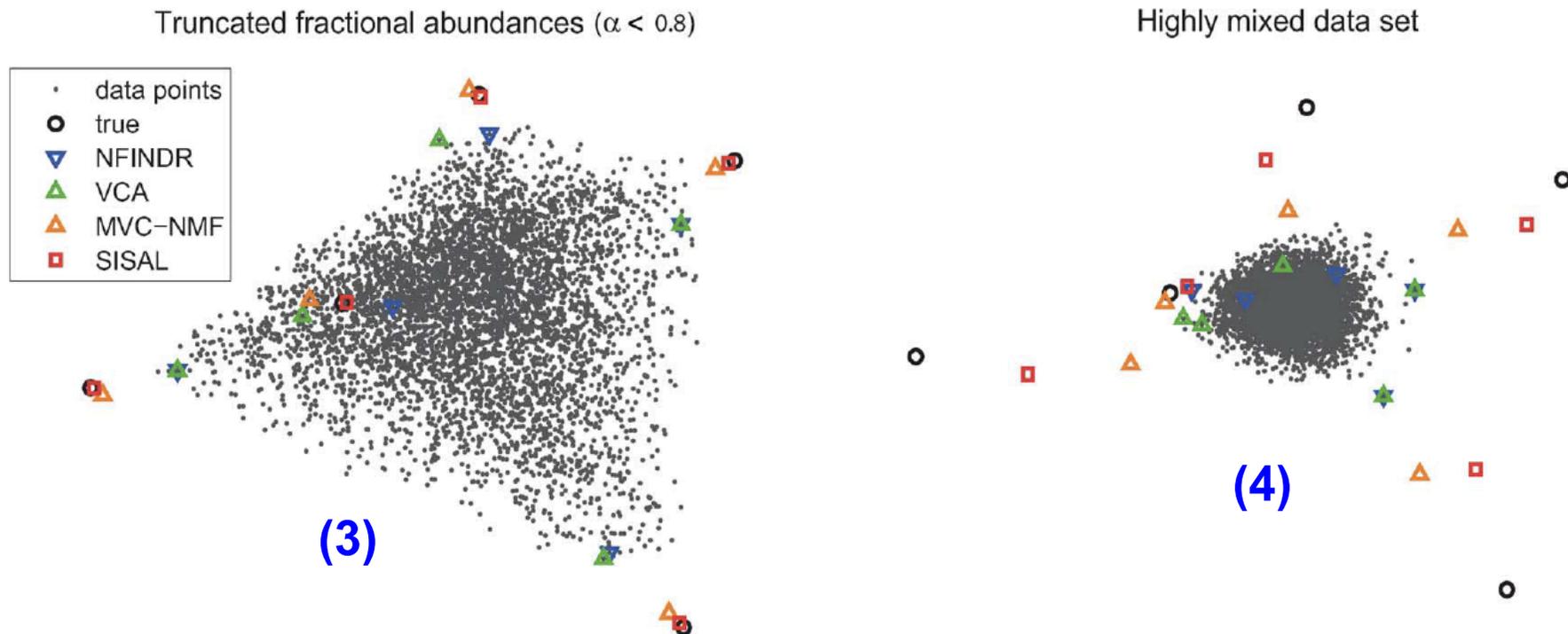
Unmixing example

- In the following, we illustrate the performance of techniques using a toy example.
- In scenarios (1) and (2), the algorithms can find the endmembers without difficulties.
- Scenario (1) is a case in which pure pixels are present in the data.
- Scenario (2) is a case without pure pixels but with spectral vectors on each facet.

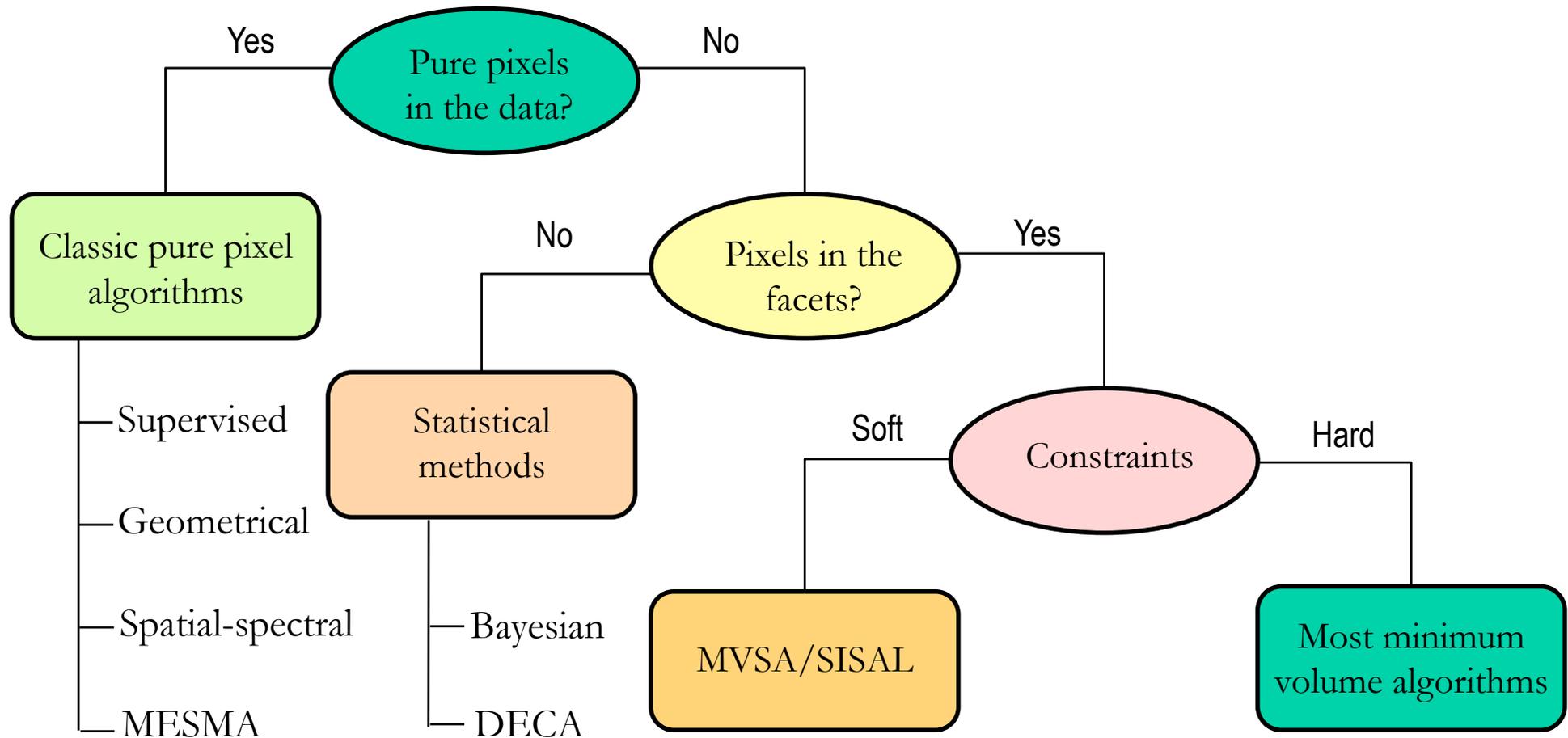


Unmixing example

- The most difficult scenarios arise when we consider highly mixed data.
- In scenario (3) we truncate the fractional abundances of (1) so that no pure pixels exist in the data. Unmixing still works if sufficient pixels are located on the facets.
- Scenario (4) is more difficult: in this case most algorithms fail since there are no sufficient spectral vectors in the facets and statistical techniques are required.



Summary of endmember extraction



Threat: when no pure pixels are present in the data, the spectral signatures derived may be unrealistic.

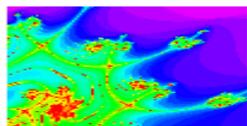
Opportunity: we have plenty of spectral libraries with realistic spectra available! Any chance to use them?

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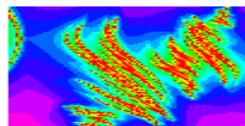
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Comparison using synthetic data

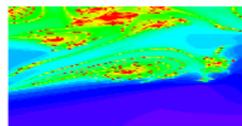
- Synthetic scenes have been generated using fractals to generate *random spatial patterns*.
- Each fractal image is divided into a set of classes or clusters.
- Mixed pixels generated inside each cluster using library signatures obtained from the U. S. Geological Survey (USGS) spectral library (<http://speclab.cr.usgs.gov>).
- Random noise in different signal-to-noise ratios (SNRs) is added to the scenes.



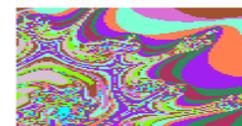
Fractal 1



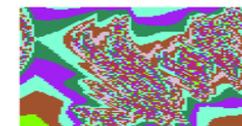
Fractal 2



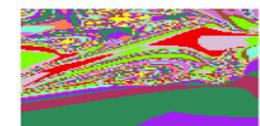
Fractal 3



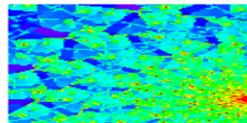
Clusters fractal 1



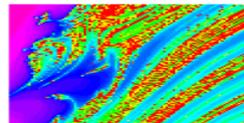
Clusters fractal 2



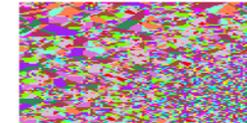
Clusters fractal 3



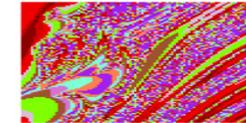
Fractal 4



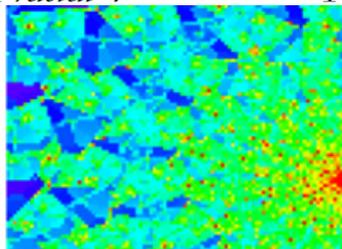
Fractal 5



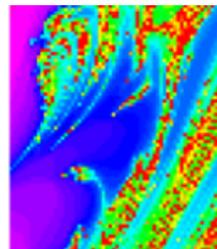
Clusters fractal 4



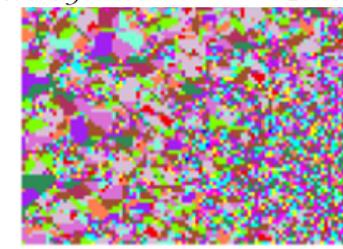
Clusters fractal 5



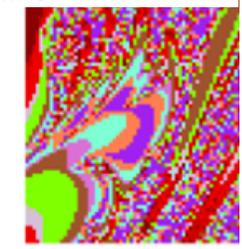
Fractal 4



Fractal 4



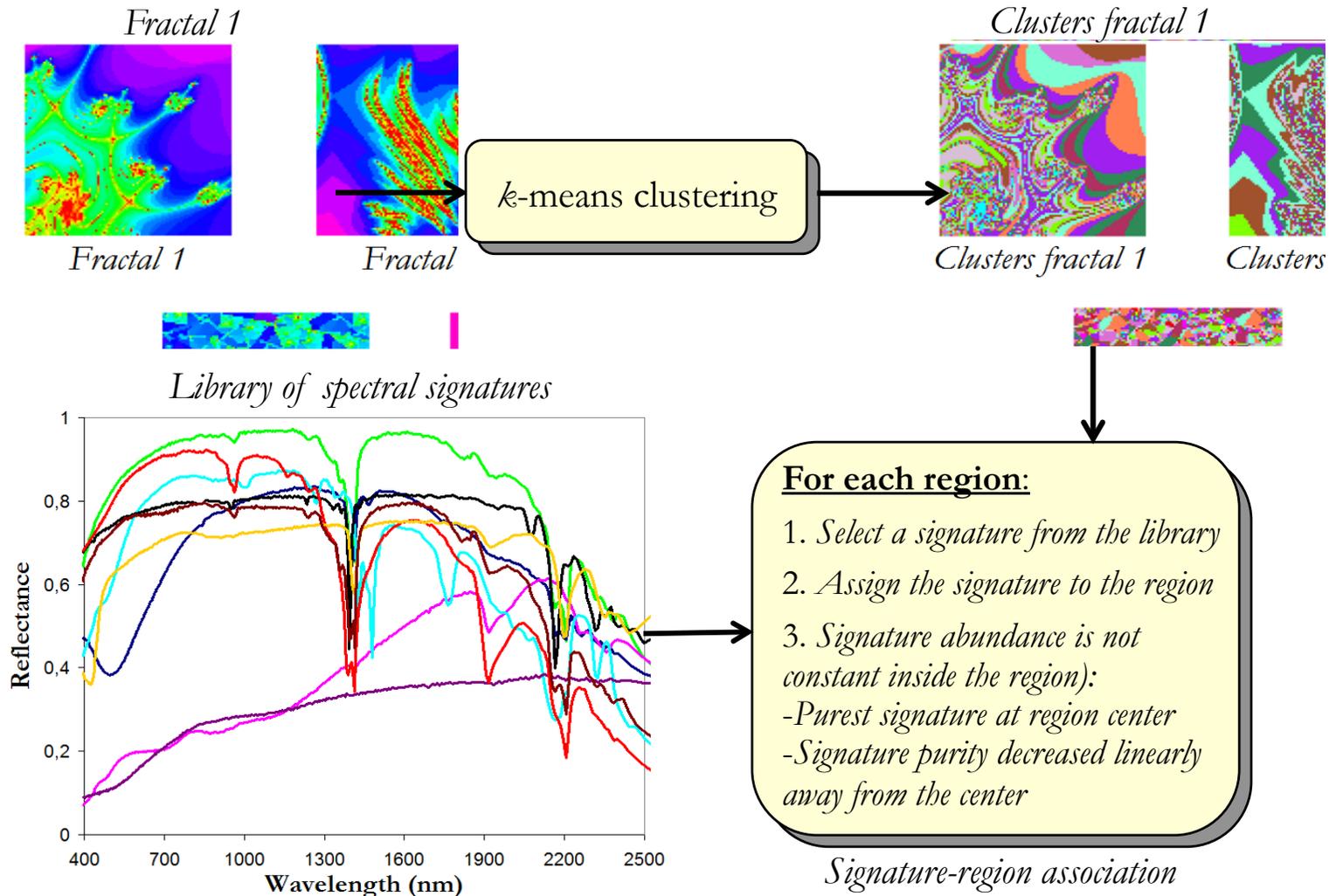
Clusters fractal 4



Clusters fractal 4

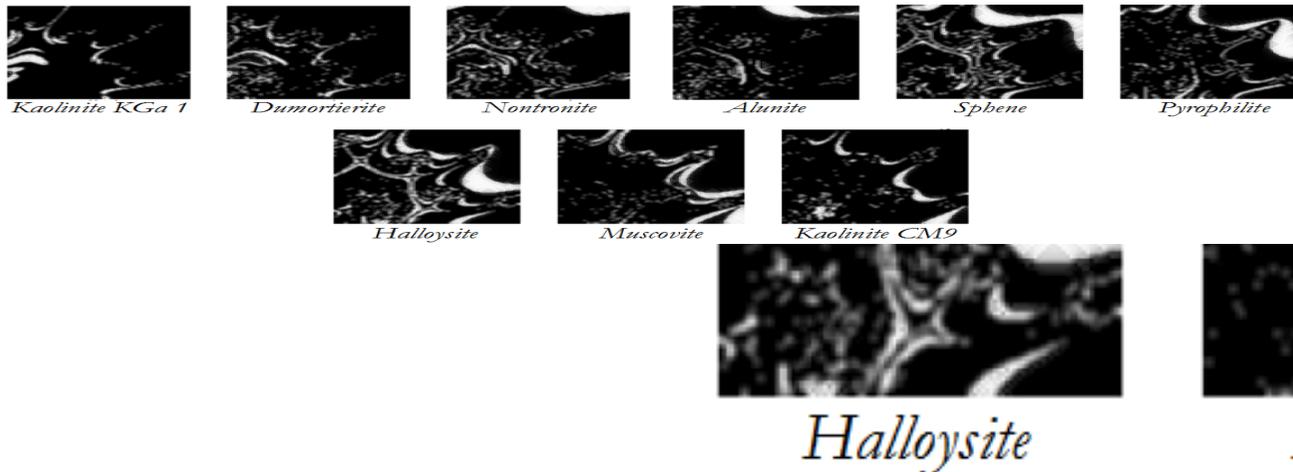
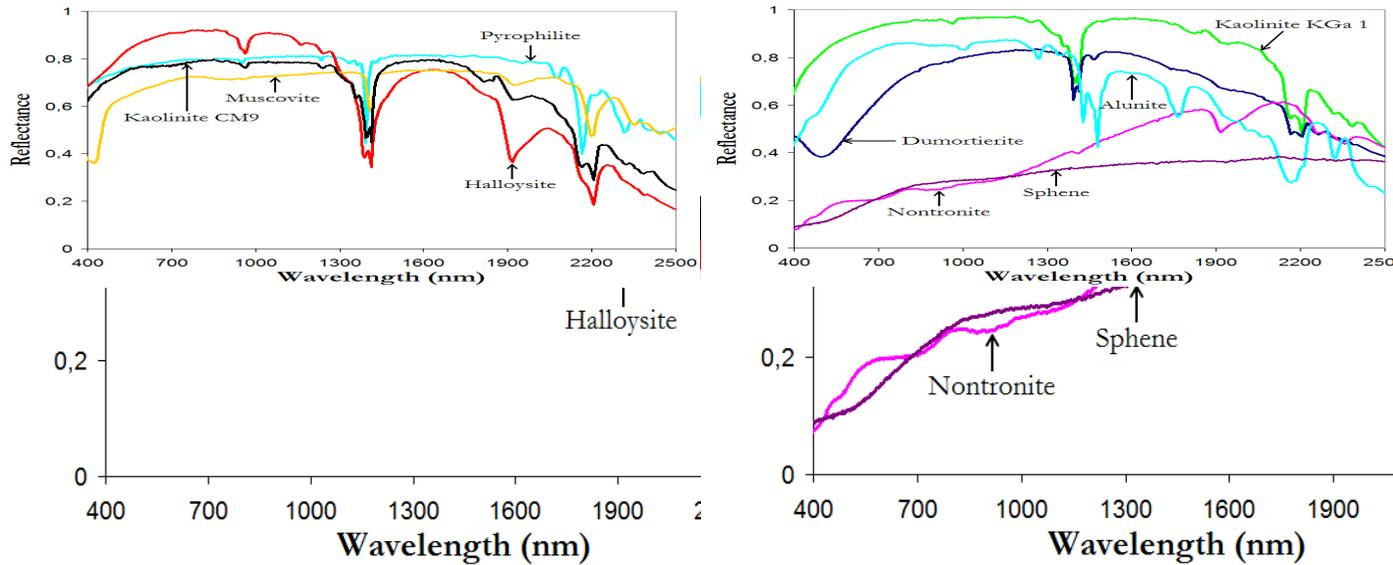
Comparison using synthetic data

- The simulation procedure is further illustrated in the following schematic diagram:



Comparison using synthetic data

- Scenes available online in HyperMix open tool: <http://www.hypercomp.es/hypermix>



Comparison using synthetic data

- Average spectral similarity (degrees) between USGS signatures and endmembers:

Algorithm	SNR=30:1	SNR=50:1	SNR=70:1	SNR=90:1	SNR=110:1	SNR= ∞
N-FINDR	2.089	0.464	0.384	0.389	0.362	0.362
OSP	2.118	0.452	0.350	0.361	0.345	0.365
VCA	2.188	0.520	0.368	0.434	0.436	0.400
MVC-NMF	1.558	0.384	0.383	0.351	0.374	0.316
MVES	12.569	1.436	0.279	0.085	0.042	0.108
MVSA	15.256	1.365	0.130	0.028	0.024	0.024
SISAL	12.754	1.256	0.206	0.142	0.212	0.154

- For very high noise ratios, most algorithms without the pure pixel assumption cannot derive good endmembers (minimum volume techniques are quite sensitive to noise).
- As the noise is reduced, the performance of the two kind of endmember algorithms (with and without the pure pixel assumption) becomes very similar and balanced.
- In optimal conditions, algorithms without the pure pixel assumption perform better.

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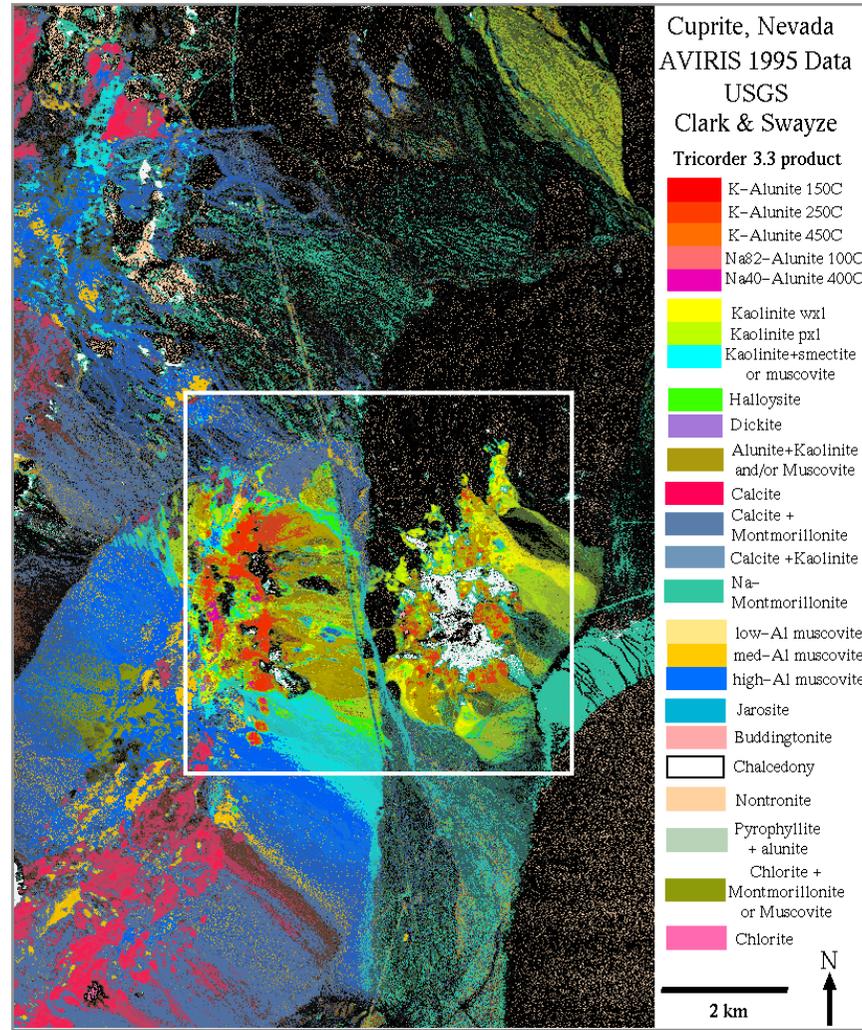
3. Endmember extraction
 - 3.1. Classic methods for endmember extraction
 - 3.2. Algorithms without the pure pixel assumption
 - 3.3. Comparative assessment using synthetic data
 - 3.4. Comparative assessment using real data

Comparison using real data

- We use the well-known AVIRIS Cuprite data set, a standard for unmixing evaluation.

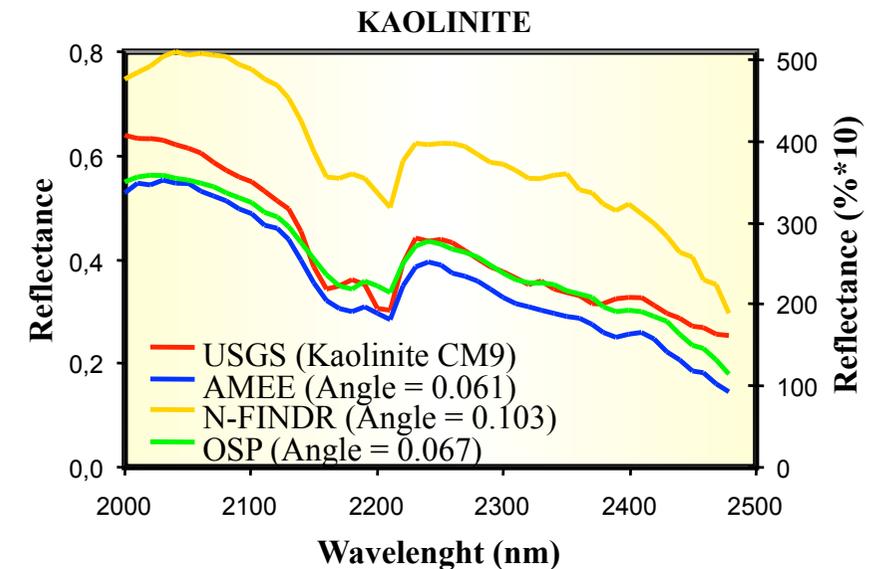
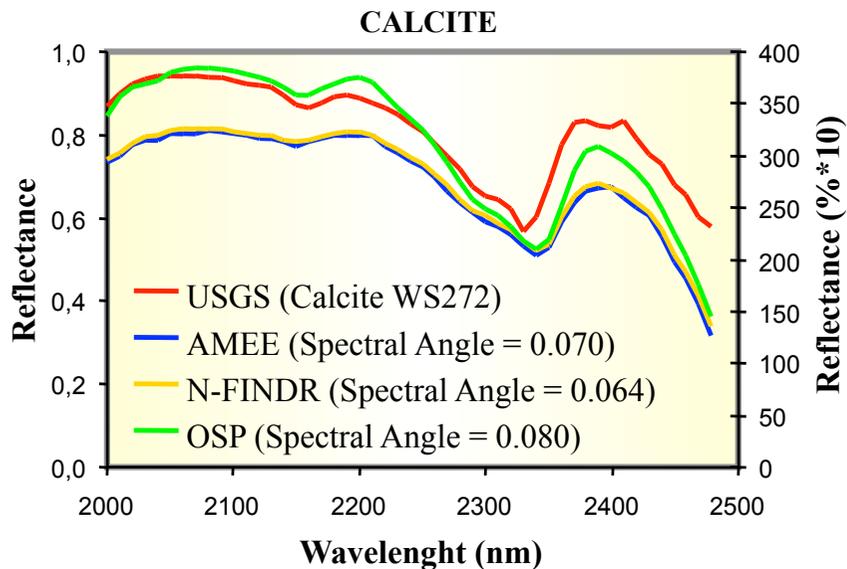
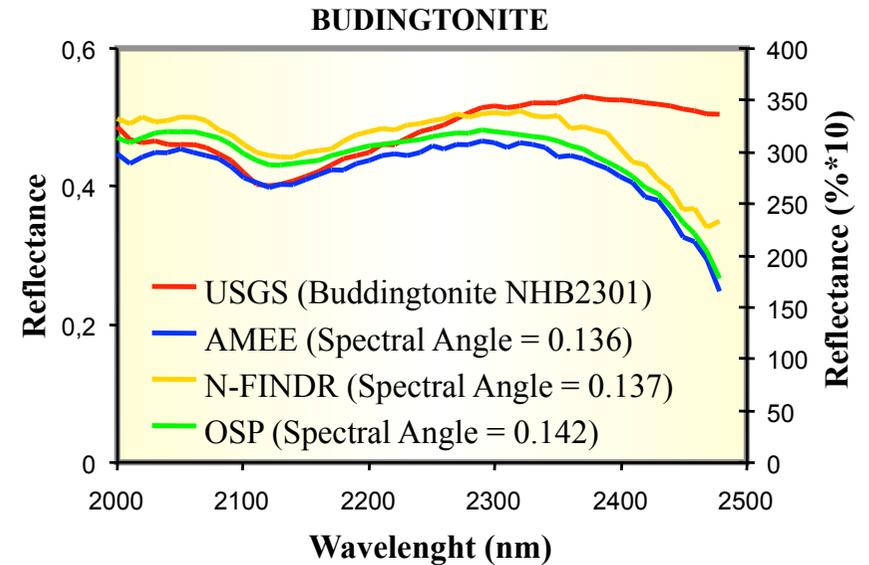
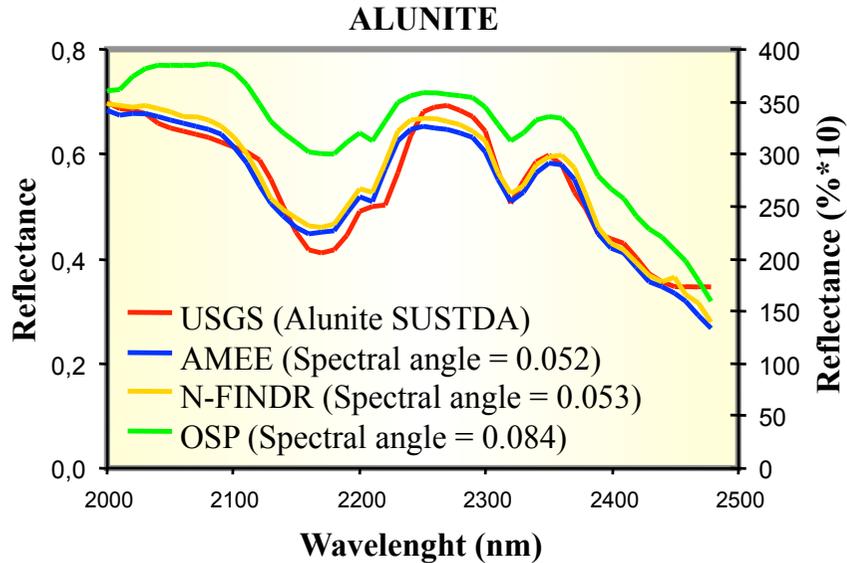


False color composite of 1997 flightline

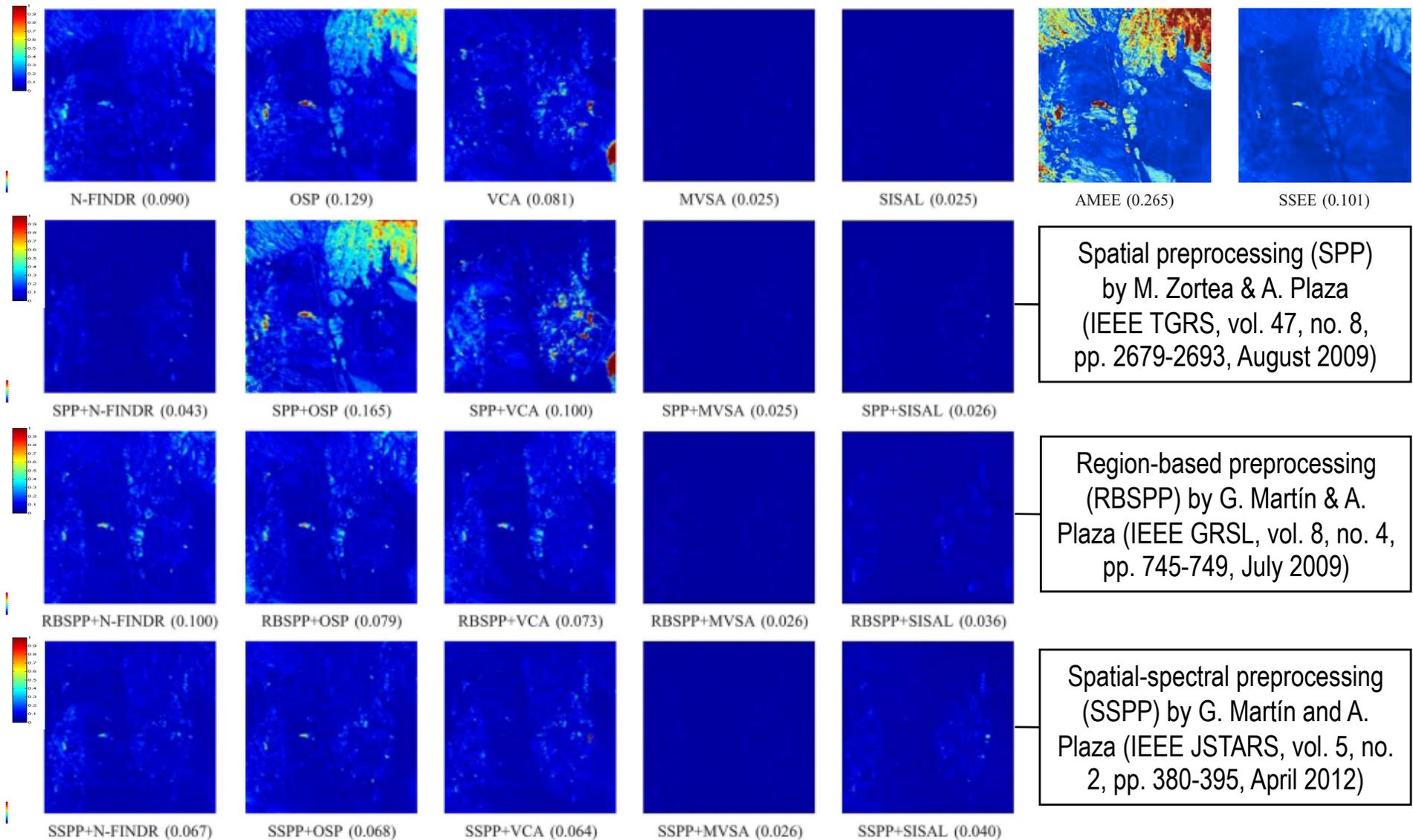


Map of materials (<http://speclab.cr.usgs.gov>)

Comparison using real data



Comparison using real data



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4. Abundance estimation

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4.2. Non-negative constrained least squares (NCLS)

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4.4. Remarks

Unconstrained least squares (UCLS)

- When all the endmember information (i.e., the number of endmembers and their spectral signatures) are known, abundances can be estimated by least squares.
- The idea is to find the abundances that minimize the reconstruction error obtained after approximating the original hyperspectral scene using a linear mixture model:

$$e = \|\mathbf{r} - \mathbf{M}\hat{\mathbf{a}}\|^2$$

- Here, the least squares solution is given by the following simple term:

$$\hat{\mathbf{a}} = (\mathbf{M}^T \mathbf{M})^{-1} \mathbf{M}^T \mathbf{r}$$

- However, this is an unconstrained solution which does not satisfy the abundance non-negativity (ANC) and the abundance sum-to-one constraints (ASC).

A. Plaza, G. Martin, J. Plaza, M. Zortea and S. Sanchez, "Recent developments in spectral unmixing and endmember extraction, in: *Optical Remote Sensing - Advances in Signal Processing and Exploitation Techniques*. Edited by S. Prasad, L. Bruce and J. Chanussot, Springer, 2011, ISBN: 978-3-642-1241-6, pp. 235-268.

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Non-negative constrained least squares

- If the ANC constraint needs to be satisfied, the problem of abundance estimation becomes a constrained optimization problem:

$$\min e = \min f(\boldsymbol{\alpha}) = \mathbf{r}^T \mathbf{r} - 2\mathbf{r}^T \mathbf{M}\boldsymbol{\alpha} + \boldsymbol{\alpha}^T \mathbf{M}^T \mathbf{M}\boldsymbol{\alpha}$$

$$\text{Subject to : } 0 \leq \alpha_i \leq 1, \text{ for } 1 \leq i \leq p$$

- This optimization problem with inequality constraints can be solved effectively by means of quadratic programming since the objective function is a quadratic function.
- However, imposing the ANC constraint can significantly increase the computational complexity of the abundance estimation problem.
- Normally the ASC constraint alone is not imposed, but in conjunction with the ANC.
- When both ASC and ANC constraints need to be imposed in the abundance estimation model, we have a fully constrained problem (more difficult to solve).

C.-I Chang and D. Heinz, "Constrained subpixel detection for remotely sensed images,"
IEEE Transactions on Geoscience and Remote Sensing, vol. 38, no. 3, pp. 1144-1159, May 2000.

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Fully constrained least squares unmixing

- If both the ANC and the ASC constraints need to be satisfied, the problem of abundance estimation becomes an even more complicated one:

$$\min e = \min f(\boldsymbol{\alpha}) = \mathbf{r}^T \mathbf{r} - 2\mathbf{r}^T \mathbf{M}\boldsymbol{\alpha} + \boldsymbol{\alpha}^T \mathbf{M}^T \mathbf{M}\boldsymbol{\alpha}$$

$$\text{Subject to : } \alpha_1 + \alpha_2 + \dots + \alpha_p = 1$$

$$0 \leq \alpha_i \leq 1, \text{ for } 1 \leq i \leq p$$

- Fortunately, the ASC can be easily included in the ANC-constrained formulation by simply adding a row vector with all elements set to one to the endmember matrix, adding an element one to the pixel vector, and solving the resulting least squares problem as follows:

$$\tilde{\mathbf{M}} = \begin{bmatrix} \mathbf{M} \\ \mathbf{1} \end{bmatrix} \quad \tilde{\mathbf{r}} = \begin{bmatrix} \mathbf{r} \\ 1 \end{bmatrix} \quad \tilde{\mathbf{r}} = \tilde{\mathbf{M}}\boldsymbol{\alpha} + \mathbf{n}$$

D. Heinz and C.-I Chang, "Fully constrained least squares linear spectral mixture analysis method for material quantification in hyperspectral imagery," *IEEE Transactions on Geoscience and Remote Sensing*, vol. 39, no. 3, pp. 529-545, 2001.

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- 4. Abundance estimation
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Remarks

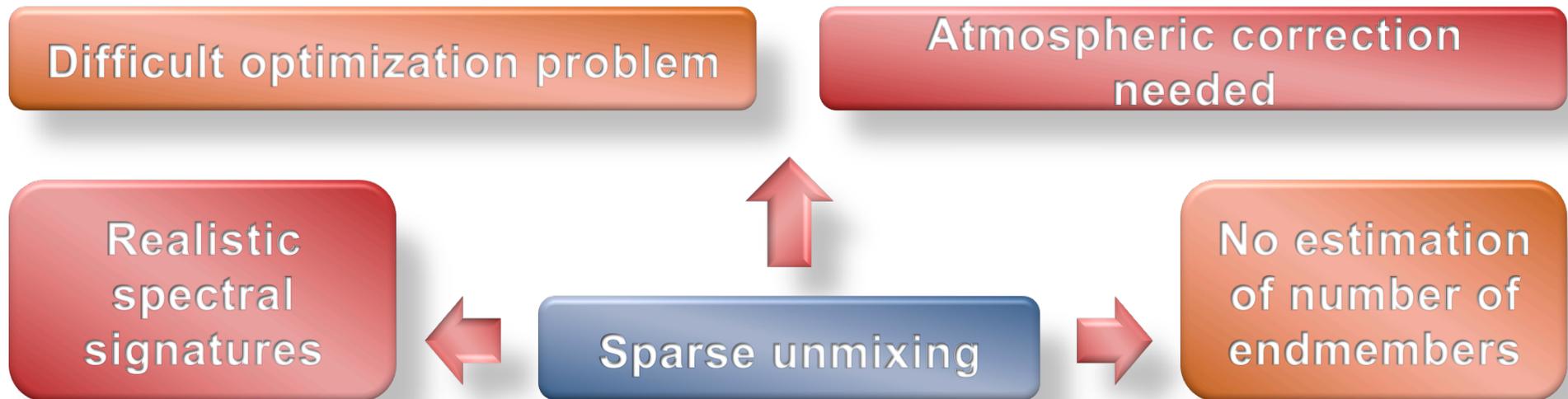
- Whether abundance constraints should be imposed or not depends on practical application. It has been argued that, if the linear mixture model is accurate, the two constraints should be satisfied automatically.
- In any event, the ANC is more important than the ASC. Due to noise and spectral variability, reinforcing the ASC may be prone to induce additional estimation error.
- When endmembers are unknown, endmember signatures should be extracted or estimated first. Some endmember extraction algorithms can provide abundance estimates simultaneously (e.g. algorithms without the pure pixel assumption).
- There exists another group of abundance estimation based on blind source separation, which does not require endmember signatures to be known *a priori*.
- Widely used matrix factorization-based blind source separation methods include independent component analysis (ICA) and non-negative matrix factorization (NMF), which have been mostly used in the context of unsupervised (*soft*) classification.
- If the linear assumption does not hold, nonlinear unmixing techniques should be used.

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Motivation

- Spectral unmixing algorithms **with the pure pixel assumption** require the presence of pure pixels in the scene for endmember extraction. Due to spatial resolution and mixing phenomena, this assumption cannot be always guaranteed.
- Spectral unmixing algorithms **without the pure pixel assumption** generate endmember signatures which often do not relate to real physical signatures.
- A possible solution is to use ground **spectral libraries** to perform spectral unmixing, but libraries are very large, hence the problem becomes sparse and difficult to solve. Another problem is the difference between the ground library and the image data.

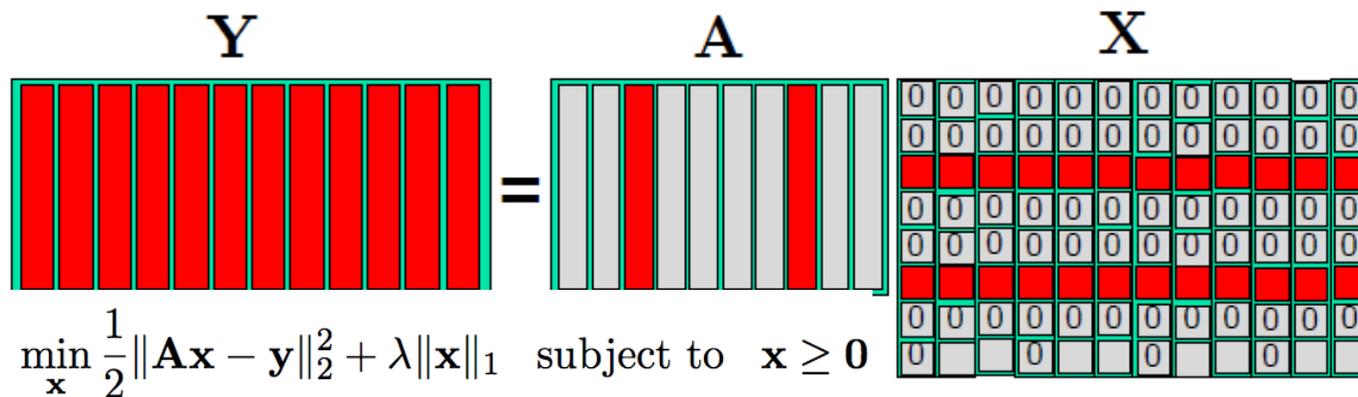


Sparse unmixing of hyperspectral data

- Pixel vectors can be expressed as *linear combinations* of a few pure spectral signatures obtained from a potentially very large spectral library of ground materials:

$$\mathbf{Y} = [\mathbf{y}_1, \dots, \mathbf{y}_n] \qquad \mathbf{Y} = \mathbf{A}\mathbf{X}$$

$$\mathbf{Y} \in \mathbb{R}^{L \times n} \quad \mathbf{A} \in \mathbb{R}^{L \times m} \quad \mathbf{X} \in \mathbb{R}^{m \times n}$$



- Advantage:** it sidesteps the *endmember extraction* (including number of endmembers)
- Disadvantage:** *combinatorial problem* (efficient solvers: SUnSAL and CSUnSAL)

D. Iordache, J. M. Bioucas-Dias and A. Plaza, "Sparse unmixing of hyperspectral data," *IEEE Transactions on Geoscience and Remote Sensing*, vol. 6, no. 6, pp. 2014-2039, June 2011.

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Total variation spatial regularization

- Consists of using a total variation (TV) regularizer to enforce spatial homogeneity by including this term in the original objective function:

$$\min_{\mathbf{X}} \frac{1}{2} \|\mathbf{A}\mathbf{X} - \mathbf{Y}\|_F^2 + \lambda \|\mathbf{X}\|_{1,1} + \lambda_{TV} \text{TV}(\mathbf{X}),$$

subject to $\mathbf{X} \geq 0$,

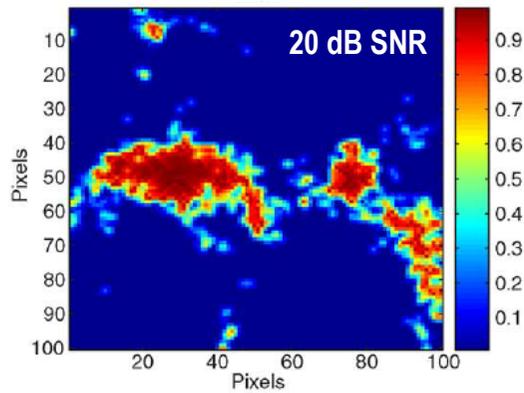
where the TV term promotes piecewise constant (or smooth) transitions in the fractional abundance of the same endmember among neighboring pixel:

$$\text{TV}(\mathbf{X}) \equiv \sum_{\{i,j\} \in \mathcal{E}} \|\mathbf{x}_i - \mathbf{x}_j\|_1$$

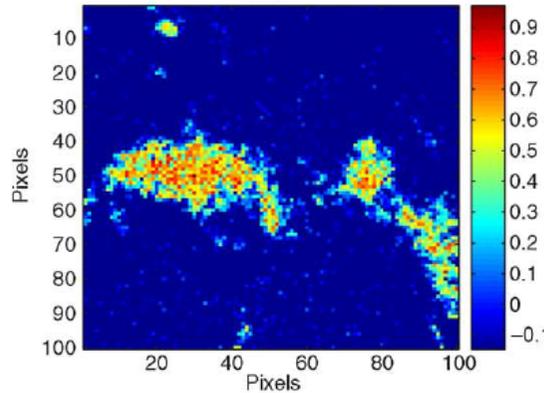
- The resulting SUnSAL-TV combines the idea of sparse unmixing with that of exploiting spatial-contextual information present in the hyperspectral images by including the TV regularizer on top of the sparse unmixing formulation.

Total variation spatial regularization

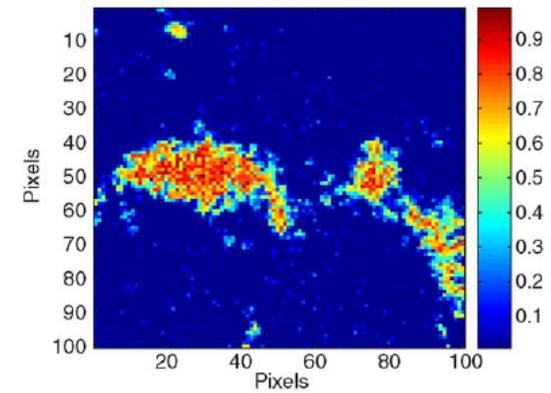
- It produces spatially smooth abundance fractions which improve sparse unmixing performance, even in very high noise conditions as illustrated in the example:



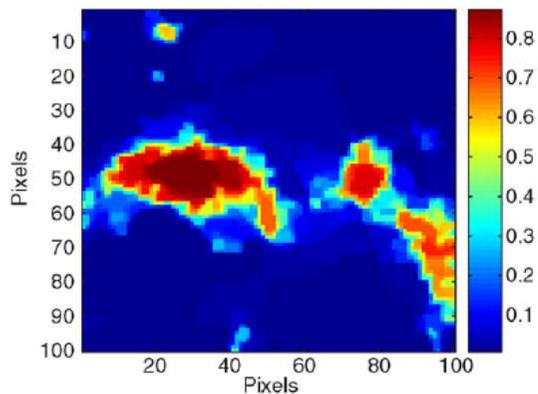
Ground-truth abundance



ANC-constrained (NCLS) estimate



SUnSAL (sparse) estimate

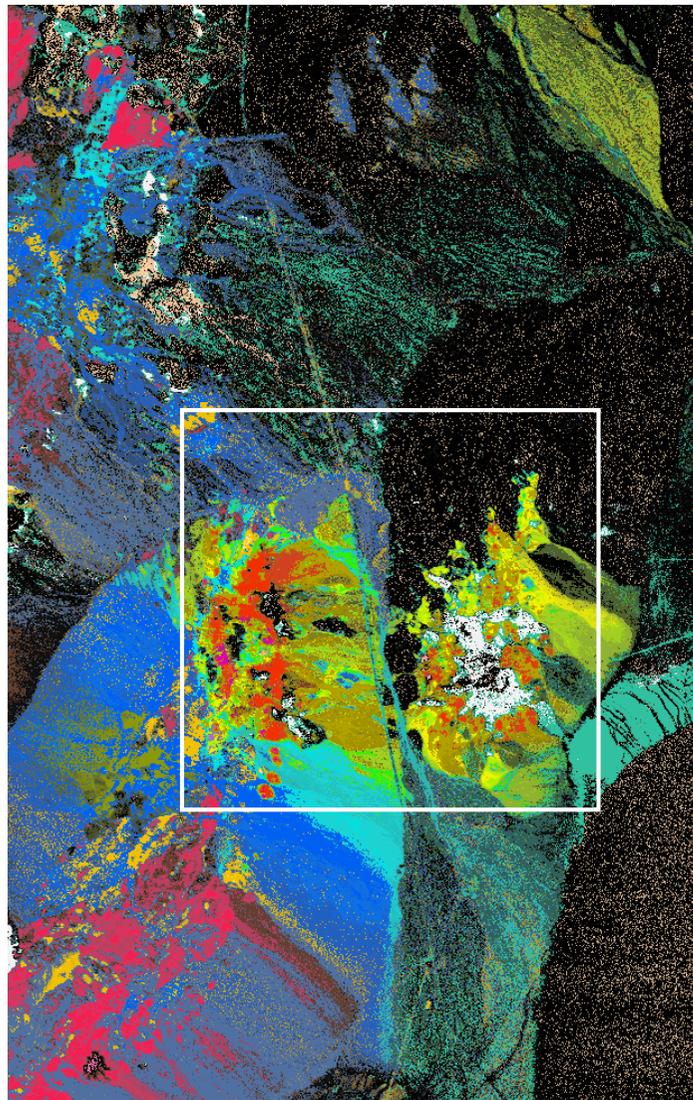


SUnSAL-TV estimate

M. D. Iordache, J. Bioucas-Dias and A. Plaza, "Total variation regularization in sparse hyperspectral unmixing," *IEEE GRSS Workshop on Hyperspectral Image and Signal Processing: Evolution in Remote Sensing*, Lisbon, Portugal, 2011.

D. Iordache, J. M. Bioucas-Dias and A. Plaza, "Total variation spatial regularization for sparse hyperspectral unmixing," *IEEE Transactions on Geoscience and Remote Sensing*, vol. 50, no. 11, pp. 4484-4502, November 2012.

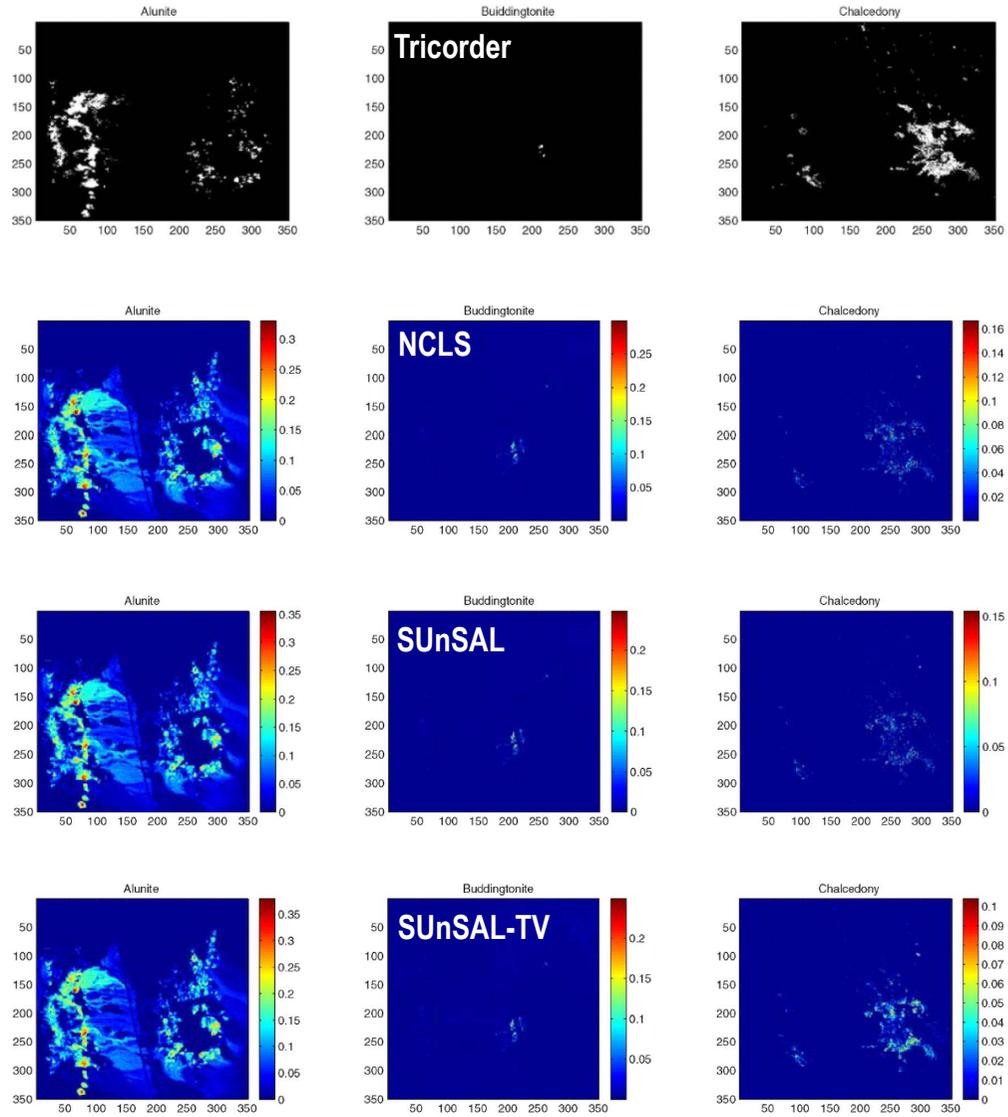
Total variation spatial regularization



Cuprite, Nevada
 AVIRIS 1995 Data
 USGS
 Clark & Swayze
 Tricorder 3.3 product

- K-Alunite 150C
- K-Alunite 250C
- K-Alunite 450C
- Na₂-Alunite 100C
- Na₄-Alunite 400C
- Kaolinite wxl
- Kaolinite pxl
- Kaolinite+smeectite or muscovite
- Halloysite
- Dickite
- Alunite+Kaolinite and/or Muscovite
- Calcite
- Calcite + Montmorillonite
- Calcite +Kaolinite
- Na-Montmorillonite
- low-Al muscovite
- med-Al muscovite
- high-Al muscovite
- Jarosite
- Buddingtonite
- Chalcedony
- Nontronite
- Pyrophyllite + alunite
- Chlorite + Montmorillonite or Muscovite
- Chlorite

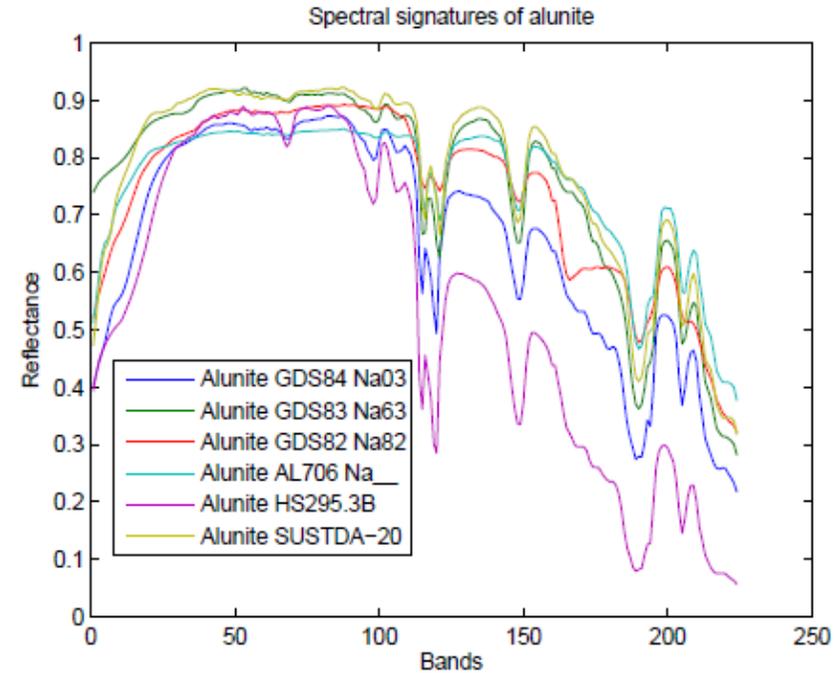
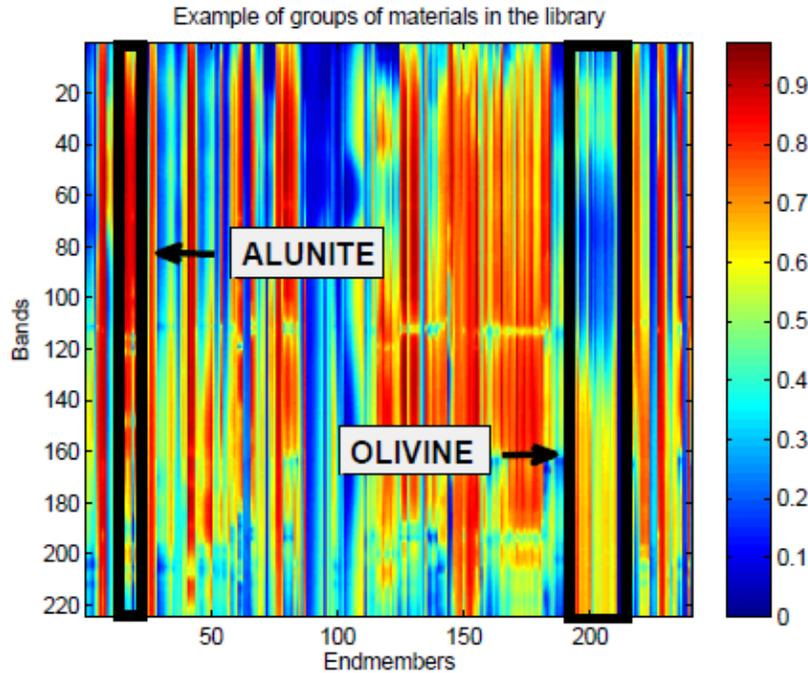
2 km 



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Group-based sparse unmixing

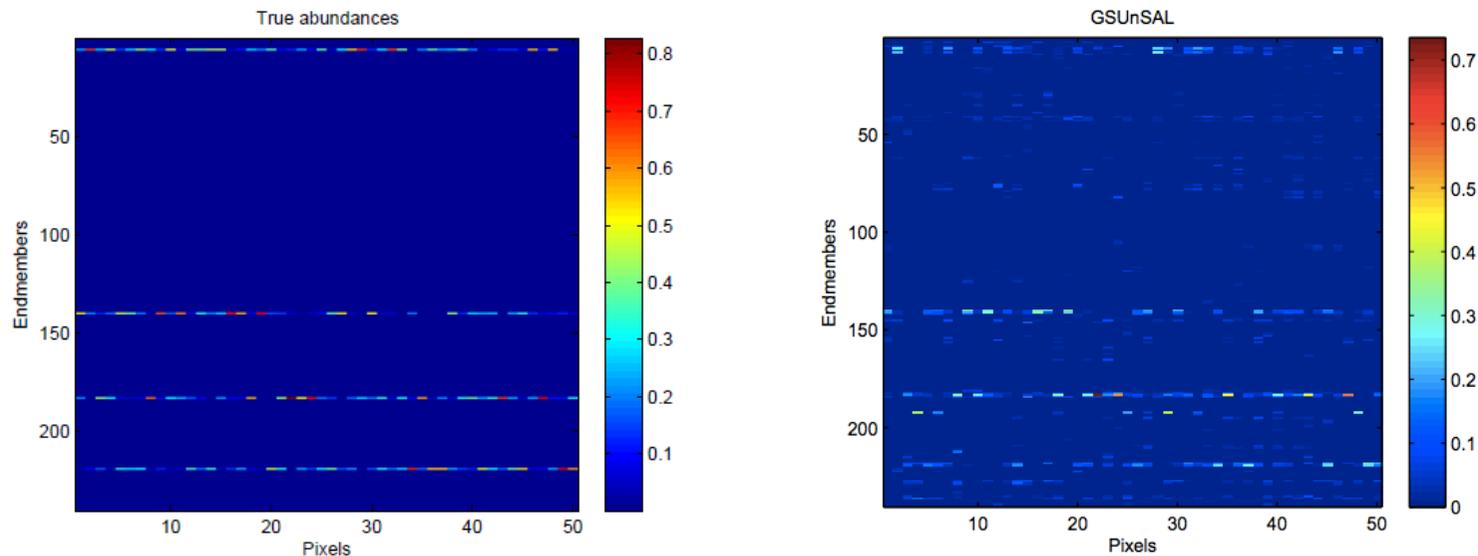


- It is observed that spectral libraries are generally organized in the form of *groups* with different variations of the same component (e.g. different mineral alterations).
- In this case, exploiting the inherent group structure present in spectral libraries can improve the results of sparse unmixing by selectively enforcing groups.
- This approach is similar to the use of *endmember bundles* but perhaps more refined.

Group-based sparse unmixing

- Including a group formulation can lead to an improvement in sparse unmixing.
- This is because spectral libraries are built in order to account for spectral variability.
- Group Lasso can be used to enforce sparsity based on groups
- Given the partition of the spectra \mathbf{A} in G groups, the retrieval of the abundance x can be obtained by solving:

$$\min_x \left\| y - \sum_{i=1}^G A_i x_i \right\|_2^2 + \lambda_1 \sum_{i=1}^G \|x_i\|_2 + \lambda_2 \|x\|_1$$



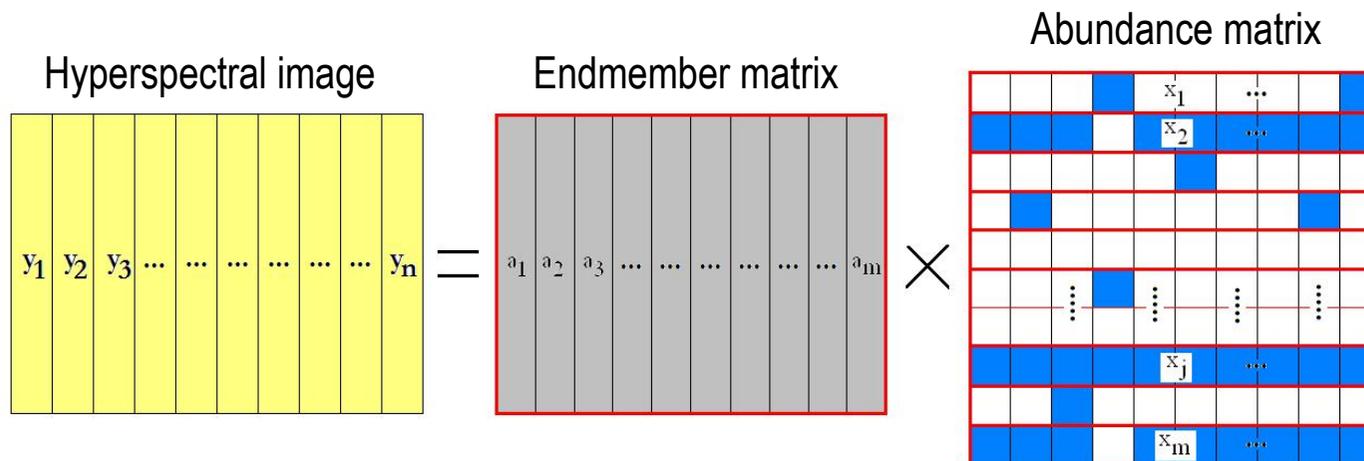
M. D. Iordache, J. Bioucas-Dias and A. Plaza, "Hyperspectral unmixing with sparse group Lasso," *Proceedings of the IEEE International Geoscience and Remote Sensing Symposium (IGARSS'11)*, vol. 1, pp. 3586-3589, Vancouver, Canada, 2011.

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Collaborative sparse unmixing

- Based on the concept of collaborativity, which forces the abundances of over-estimated endmembers to zero (number of endmembers in a scene is generally low).
- If the fractional abundances of the endmember signatures are expressed as a matrix with the number of columns equal to the number of pixels in the scene, there should be only a few lines with non-zero entries (corresponding to *active* endmembers).
- With this property, we no longer need to estimate the number of endmembers.



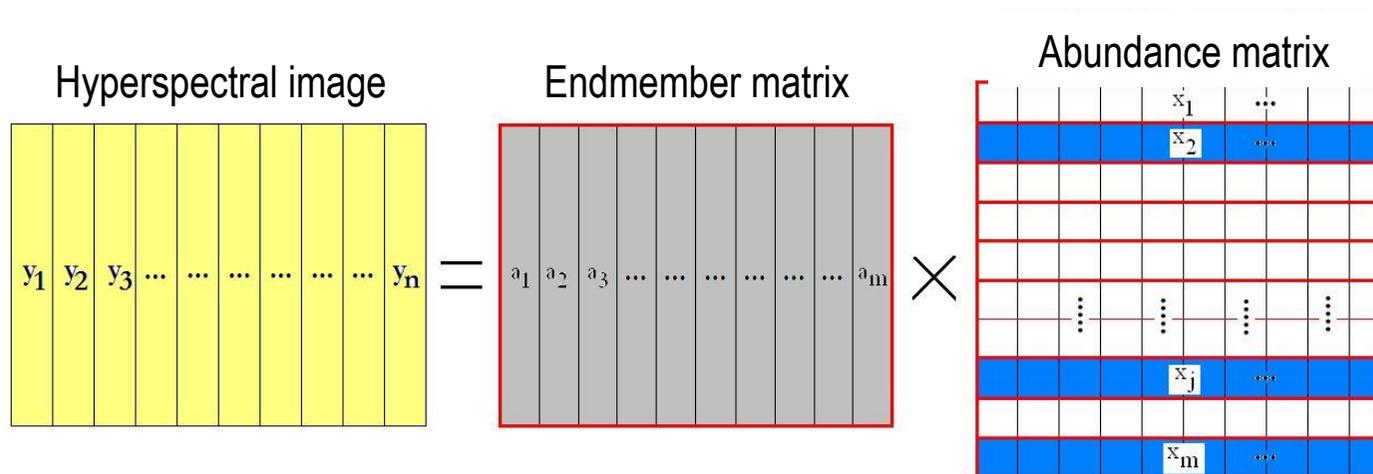
M. D. Iordache, J. M. Bioucas-Dias and A. Plaza, "Collaborative sparse regression for hyperspectral unmixing," *IEEE Transactions on Geoscience and Remote Sensing*, 2013.

Collaborative sparse unmixing

- Collaborativity is enforced by adding a mixed $l_{2,1}$ norm as a regularization term.
- The constraint acts on the rows $\{k\}$ of the abundance matrix \mathbf{X} .

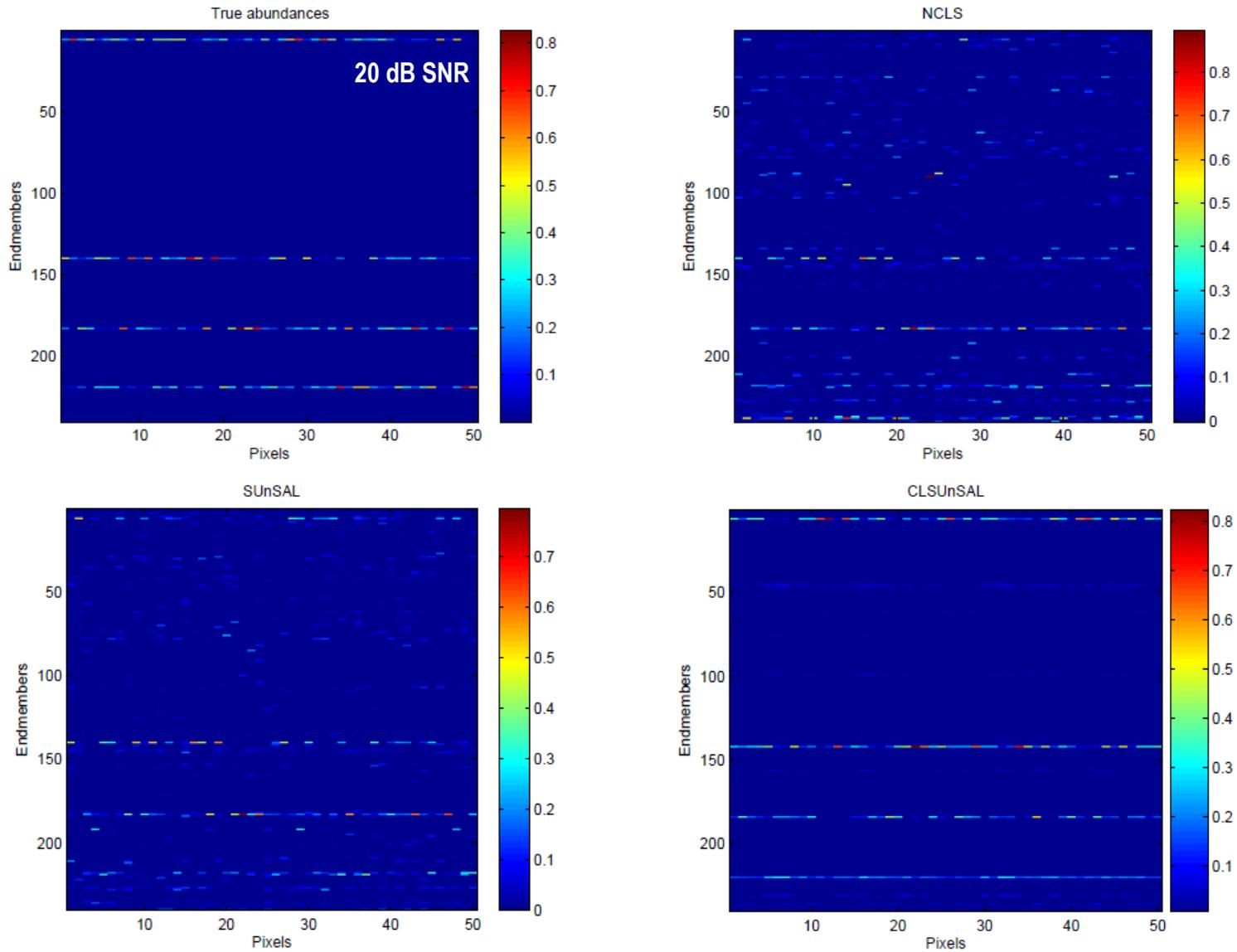
$$\min_{\mathbf{X}} \|\mathbf{A}\mathbf{X} - \mathbf{Y}\|_F^2 + \lambda \sum_{k=1}^m \|\mathbf{x}^k\|_2$$

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



M. D. Iordache, J. M. Bioucas-Dias and A. Plaza, "Collaborative sparse regression for hyperspectral unmixing," *IEEE Transactions on Geoscience and Remote Sensing*, 2013.

Collaborative sparse unmixing



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2. Estimation of the number of endmembers
3. Endmember extraction
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6. Summary and challenges

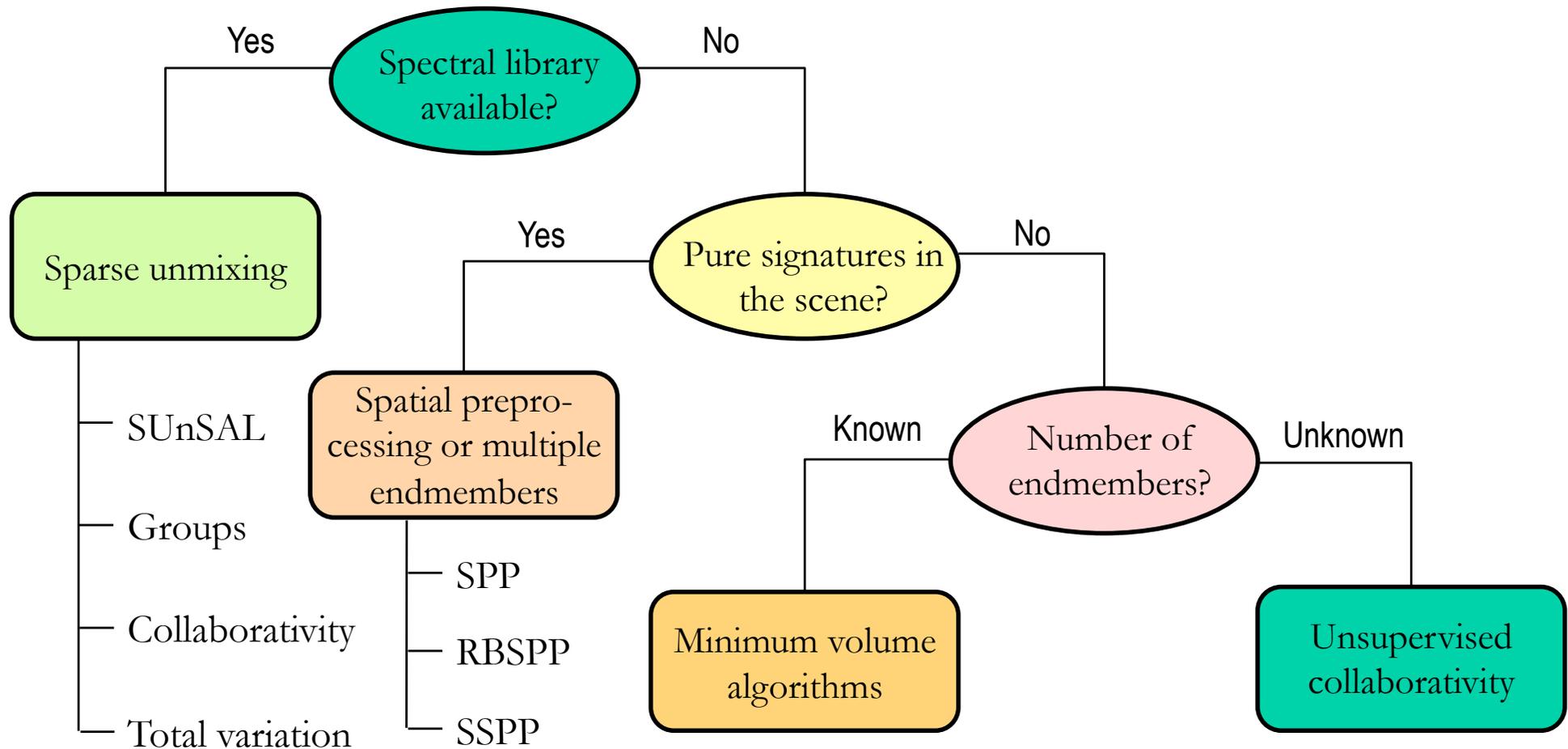
6.1. Summary

6.2. Non-linear unmixing

6.3. Spectral variability

6.4. Big-data problem

Summary and future directions



Threat: mixed pixels in real hyperspectral scenes may be nonlinear, hence the linear model may not hold.

Opportunity: develop more advanced nonlinear algorithms and techniques able to exploit spectral libraries.

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6. Summary and challenges

6.1. Summary

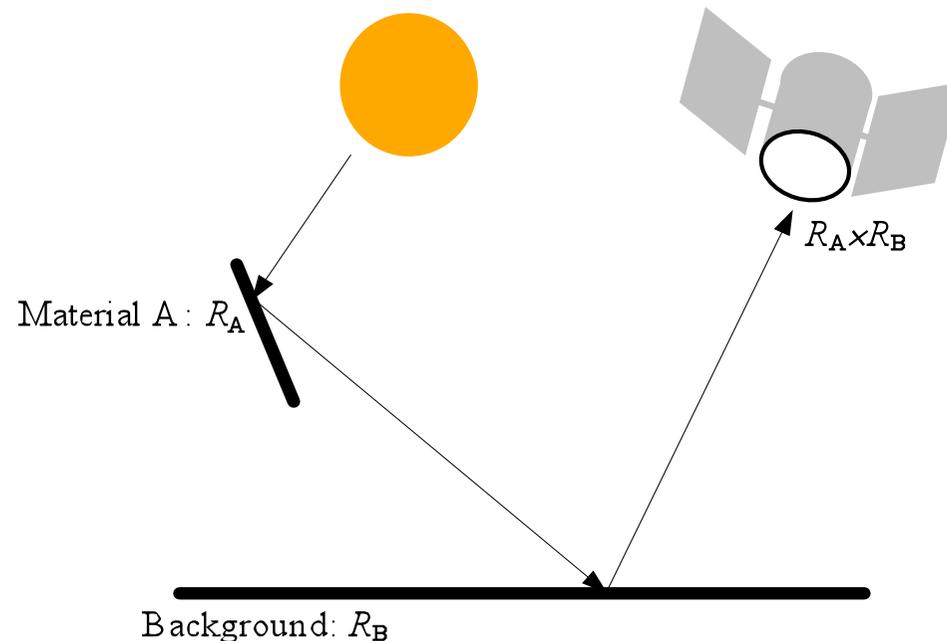
6.2. Non-linear unmixing

6.3. Spectral variability

6.4. Big-data problem

Simple nonlinear unmixing models

- Nonlinear mixing primarily occurs due to the multiple reflections between two or more surfaces. An example of the simplest multiple scattering is shown below.



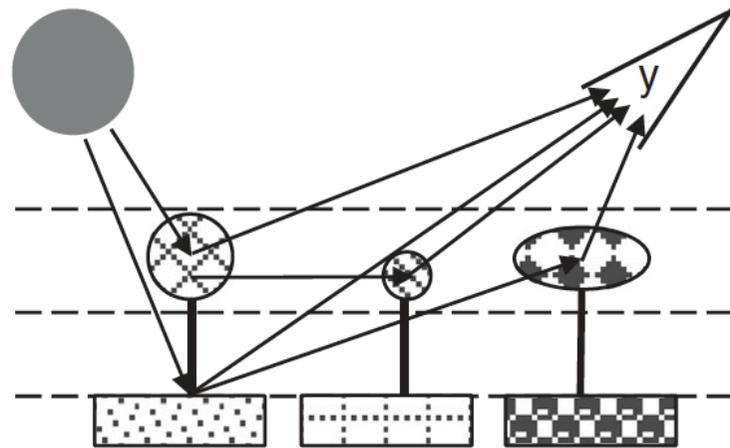
- The nonlinear scattering between surfaces can be approximated by a multiplication between the endmembers, so that endmember products are new “*endmembers*”.

N. Raksuntorn and Qian Du, “Nonlinear spectral mixture analysis for hyperspectral imagery in an unknown environment,” *IEEE Geoscience and Remote Sensing Letters*, vol. 7, no. 4, pp. 836-840, October 2010.

Simple nonlinear unmixing models

- Although this is a simplification, to avoid the complex physical models, usually simple strategies are applied using data-driven but physics inspired models.
- The bilinear model is valid when the scene can be partitioned in successive layers with similar scattering properties, for instance a two-layer scene can be modeled using single scattering (similar to linear mixture modeling) and multiplicative scattering.

Two-Layers: Canopies + Ground

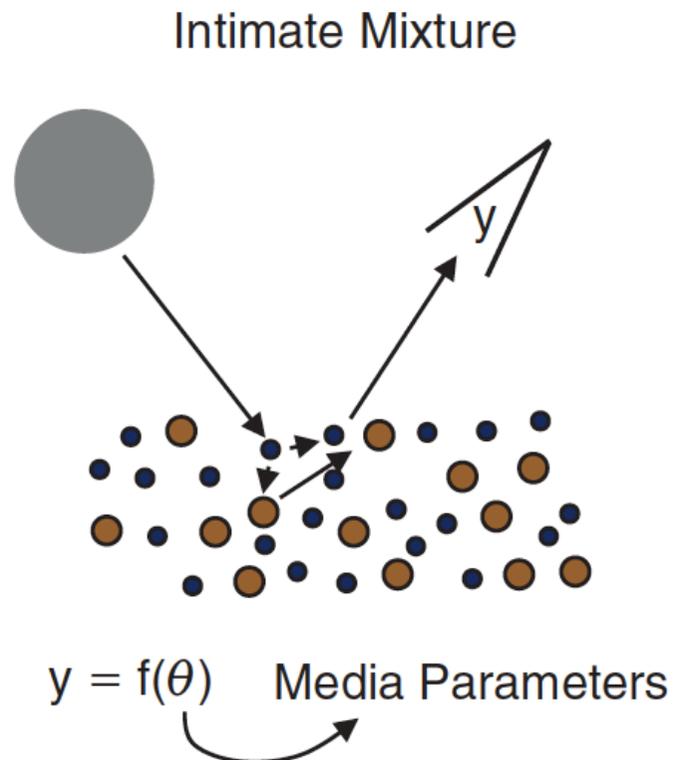


$$y = \underbrace{\sum_i \alpha_i \mathbf{m}_i}_{\text{Single Scattering}} + \underbrace{\sum_{i \neq j} \alpha_{ij} \mathbf{m}_i \odot \mathbf{m}_j}_{\text{Double Scattering}}$$

Single Scattering Double Scattering

Simple nonlinear unmixing models

- In the intimate model, the mixture occurs at a microscopic level.
- The Hapke approximation for intimate mixtures models the reflectance as a nonlinear function of a convex combination of the individual endmembers.
- Information about particle sizes and the media parameters is needed:



What has been done in practice?

- Strategies have successfully applied the bilinear model to treat the double scattering problem, such as Bayesian algorithms, where prior models are chosen to satisfy the positivity and sum-to-one constraints.
- On the other hand, kernel-based methods can design different types of (flexible) kernels to handle the problem of intimate mixtures.
- Other methods work directly on the nonlinear data manifold on which it can be shown that the concepts of convex geometry still hold.
- To cope with both scattering and intimate mixture problems simultaneously, machine learning technologies have been proposed, where training samples were used to train artificial neural networks (ANNs) for nonlinearities.
- A disadvantage of all the aforementioned methods is that they require detailed knowledge a priori about the endmember signatures.
- In summary, nonlinear unmixing remains a challenging (but very promising) research topic. Fully unsupervised nonlinear unmixing methods have very rarely been explored so far.

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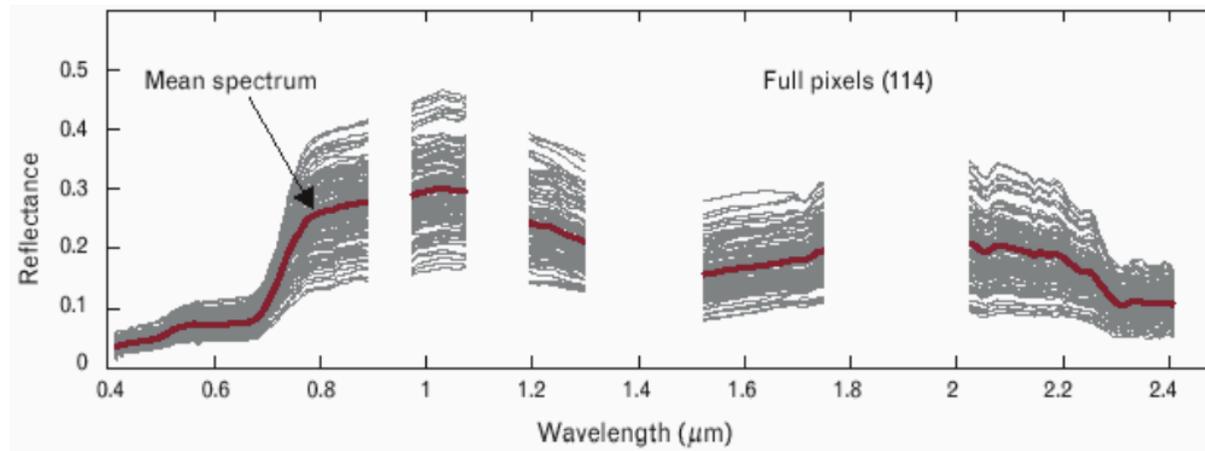
6.2. Non-linear unmixing

6.3. Spectral variability

6.4. Big-data problem

Multiple endmember spectral unmixing

- The shape of an endmember is fairly consistent, however the amplitude varies due to illumination conditions, spectral variability, topographic modulation and others.

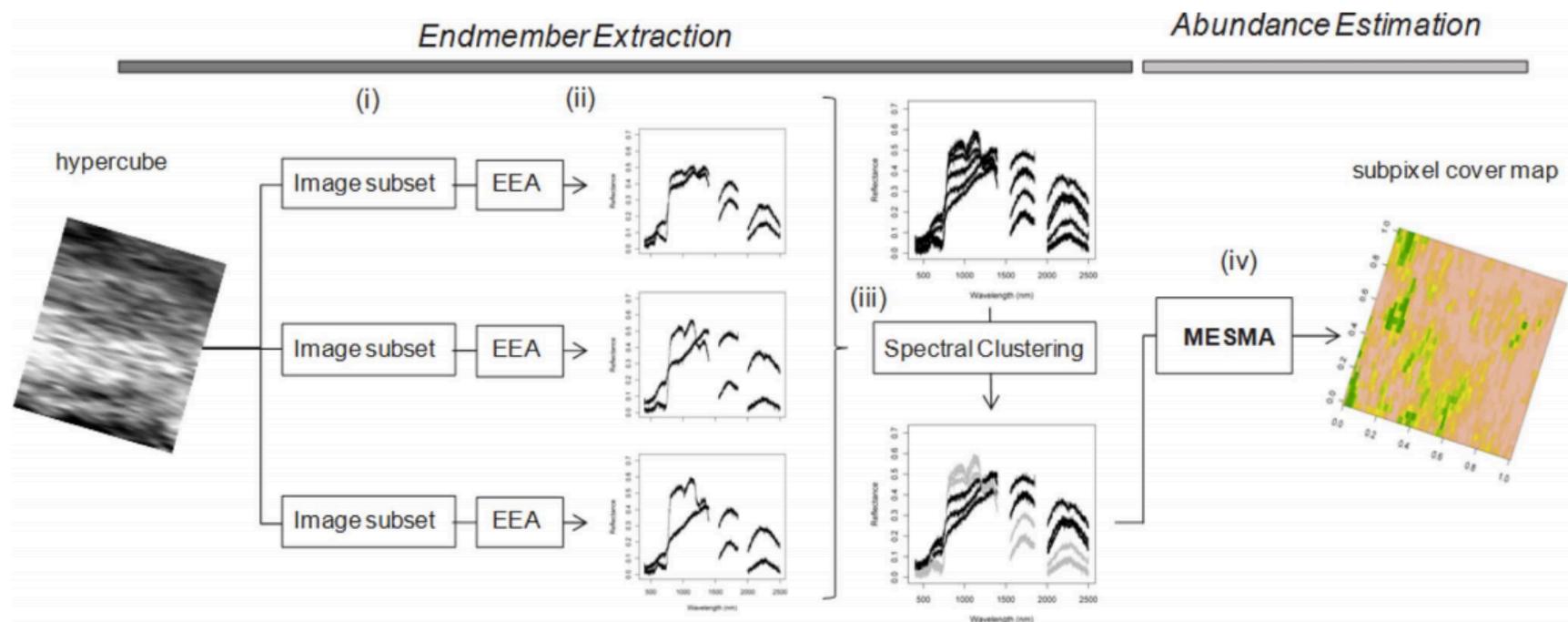


- This has been addressed with endmember bundles, which incorporate variability by representing each endmember by a set or bundle of spectra, each of which could reasonably be the reflectance of an instance of the endmember.
- Endmember unmixing needs to be extended to bundle unmixing. Using multiple signatures for each endmember class may provide more accurate fractions.

C. A. Bateson, G. P. Asner, and C. A. Wessman, "Endmember bundles: A new approach to incorporating endmember variability into spectral mixture analysis," *IEEE Transactions on Geoscience and Remote Sensing*, vol. 38, no. 2, pp. 1083-1094, 2000.

How to derive endmember bundles?

- The idea is to first subdivide the original hyperspectral image in a number of subsets.
- An endmember extraction algorithm is then applied to each of the obtained subsets.
- Endmember bundles are then constructed using a clustering algorithm, and fed to MESMA in order to provide a sub-pixel land cover distribution map.



B. Somers, M. Zortea, A. Plaza and G. P. Asner, "Automated extraction of image-based endmember bundles for improved spectral unmixing," *IEEE Journal of Selected Topics in Applied Earth Observations and Remote Sensing*, vol. 5, no. 2, pp. 396-408, April 2012.

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6.1. Summary

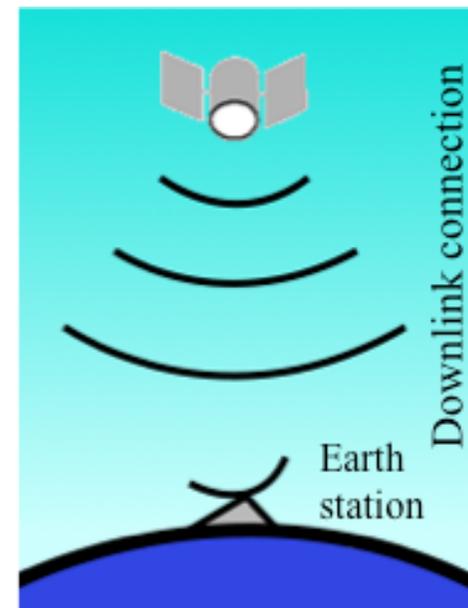
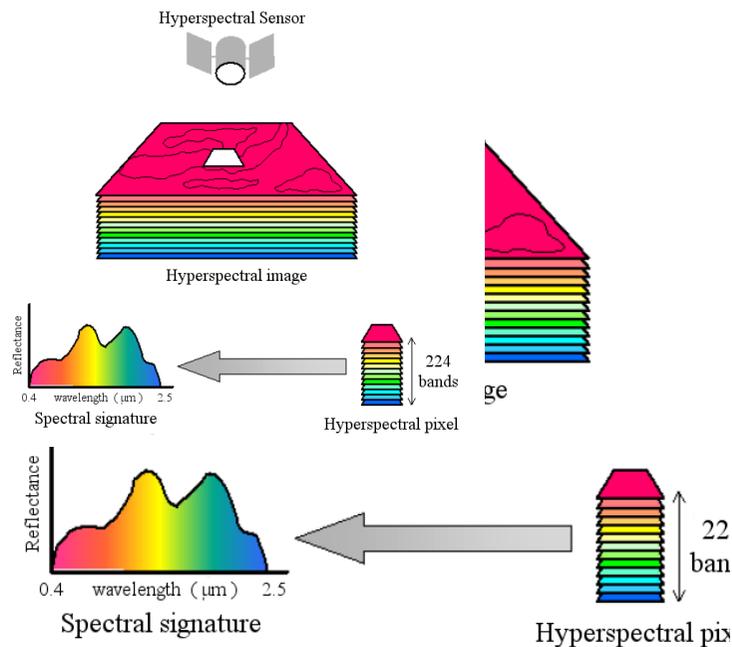
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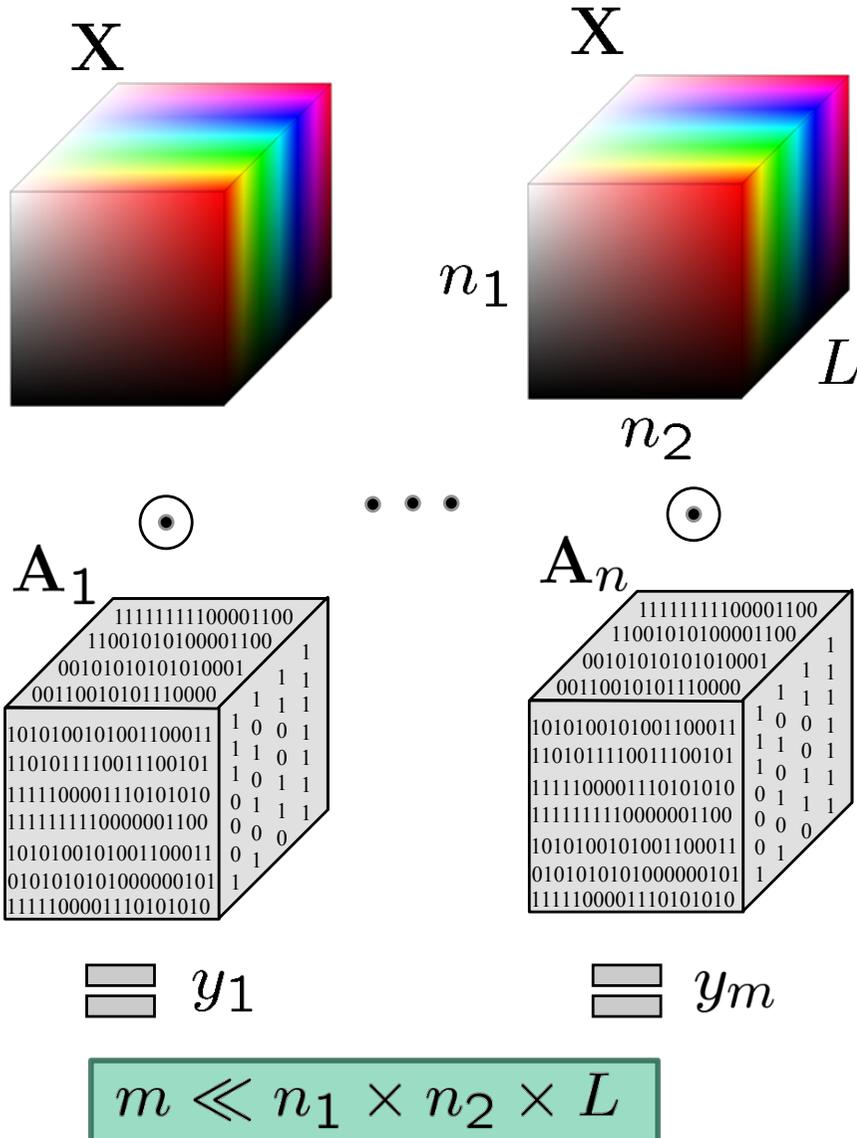
6.4. Big-data problem

Compressive sensing

- Hyperspectral sensor collects hundreds of bands at different wavelengths. The resulting data volume often comprises several Gigabytes per flight.
- However the bandwidth of the downlink connection between the sensor and the Earth station is reduced, which limits the amount of data that can be sent to Earth.
- Compressive sensing (CS) aims at reducing the amount of data that have to be measured in first place, thus reducing the amount of data that will be transmitted.



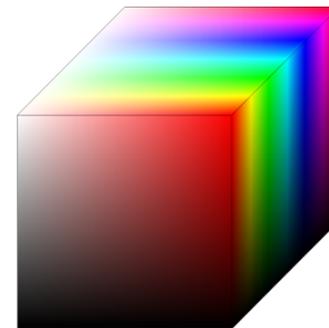
Compressive sensing



$\{y_1, \dots, y_m\}$ $\{A_1, \dots, A_m\}$

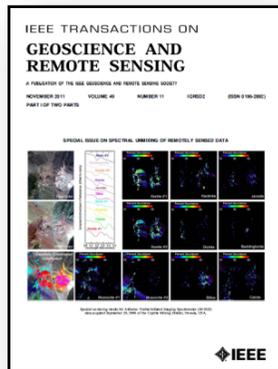


CS allows retrieving the original image from a small number of observations

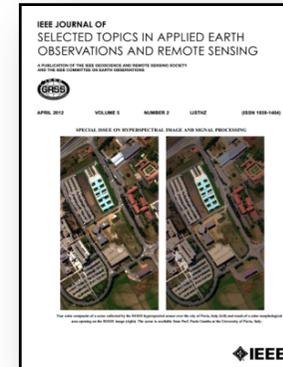


Perfect reconstruction

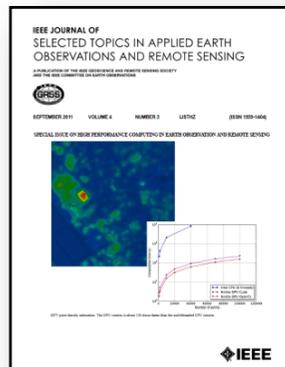
Further reading



A. Plaza, Q. Du, J. Bioucas-Dias, X. Jia and F. A. Kruse, Special issue on spectral unmixing of remotely sensed data, *IEEE Transactions on Geoscience and Remote Sensing*, vol. 49, no. 11, 2011



A. Plaza, J. Bioucas-Dias, A. Simic and W. Blackwell, Special issue on hyperspectral image and signal processing, *IEEE Journal of Selected Topics in Applied Earth Observations and Remote Sensing*, vol. 5, no. 2, 2012

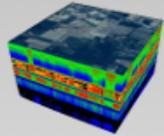


A. Plaza, Q. Du, Y.-L. Chang and R. L. King, Special issue on high performance computing in Earth observation and remote sensing. *IEEE Journal of Selected Topics in Applied Earth Observations and Remote Sensing*, vol. 4, no. 3, 2011



A. Plaza, J. Plaza, A. Paz and S. Sanchez. Parallel hyperspectral image and signal processing. *IEEE Signal Processing Magazine*, vol. 28, no. 3, pp. 119-126, May 2011 (top-ranked IEEE Journal)

The Hypermix open source toolbox



Hypermix

Developed by the Hyperspectral Computing Laboratory
University of Extremadura, Cáceres, Spain.

<http://www.hypercomp.es/hypermix>

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Welcome

Hypermix is a new open-source tool for remotely sensed hyperspectral image unmixing. It includes several popular algorithms covering different steps of the hyperspectral unmixing chain:

- **Estimation of the number of endmembers:**
 - Hyperspectral subspace identification algorithm (Hysime)
 - Virtual dimensionality (VD)
- **Endmember extraction.**
 - Orthogonal subspace projection (OSP)
 - N-FINDR algorithm
 - Vertex component analysis (VCA)
 - Spatial-spectral endmember extraction (SSEE)
 - Automatic morphological endmember extraction (AMEE)
 - Spatial pre-processing (SPP)
- **Abundance estimation.**
 - Linear spectral unmixing (LSU)
 - Non-negative constrained linear spectral unmixing (LSU)
 - Sum-to-one constrained linear spectral unmixing (SLSU)
 - Fully constrained linear spectral unmixing (FCLSU)

In addition, the tool includes techniques for dimensionality reduction and for quantitative and comparative evaluation of the results of spectral unmixing using reference spectral signatures in a library and other metrics such as the root mean square error (RMSE) in the reconstruction of the original scene using the results provided by the linear unmixing process. For additional details, please read the following [paper](#).