# Deep/Machine Learning for Spectral Unmixing

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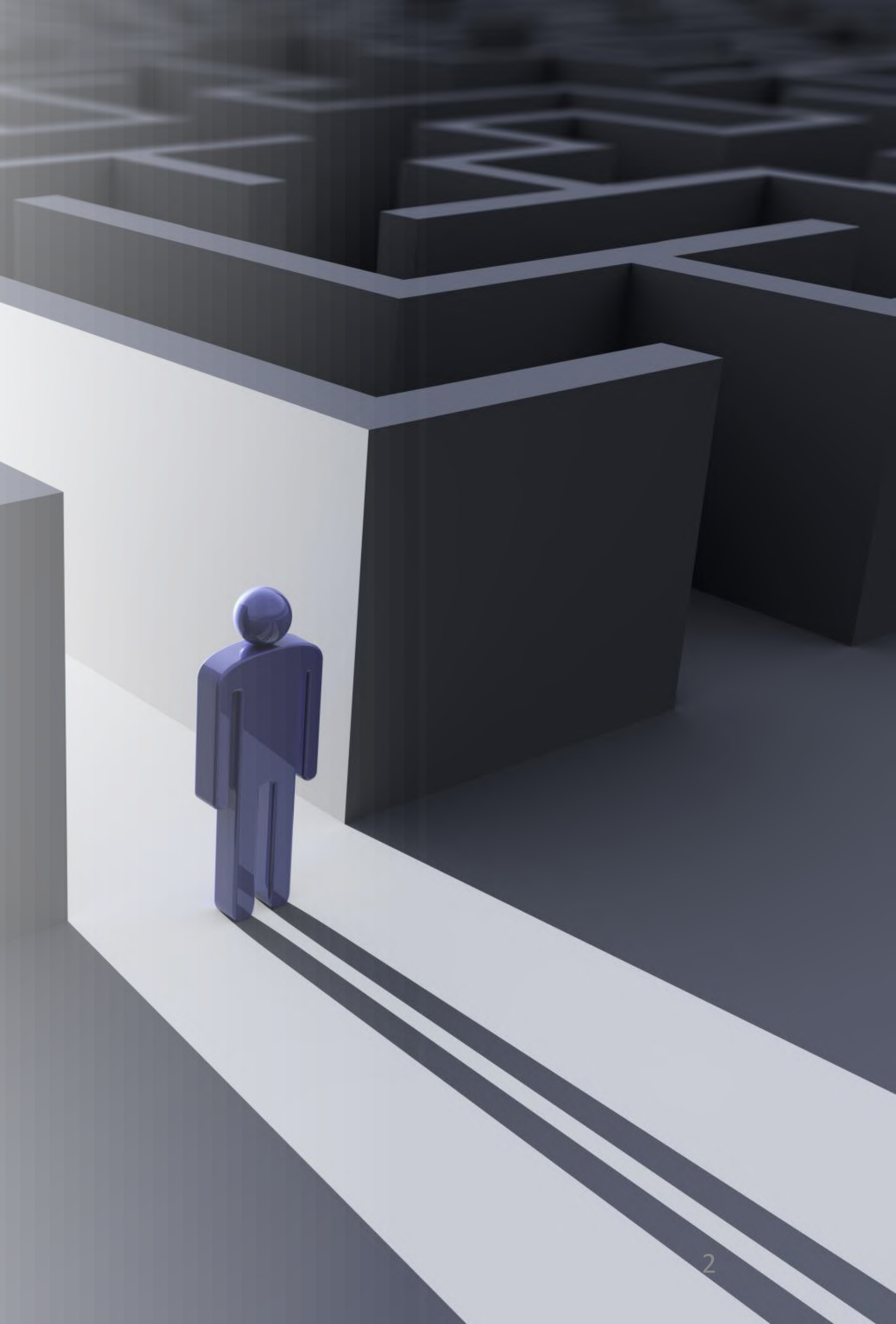
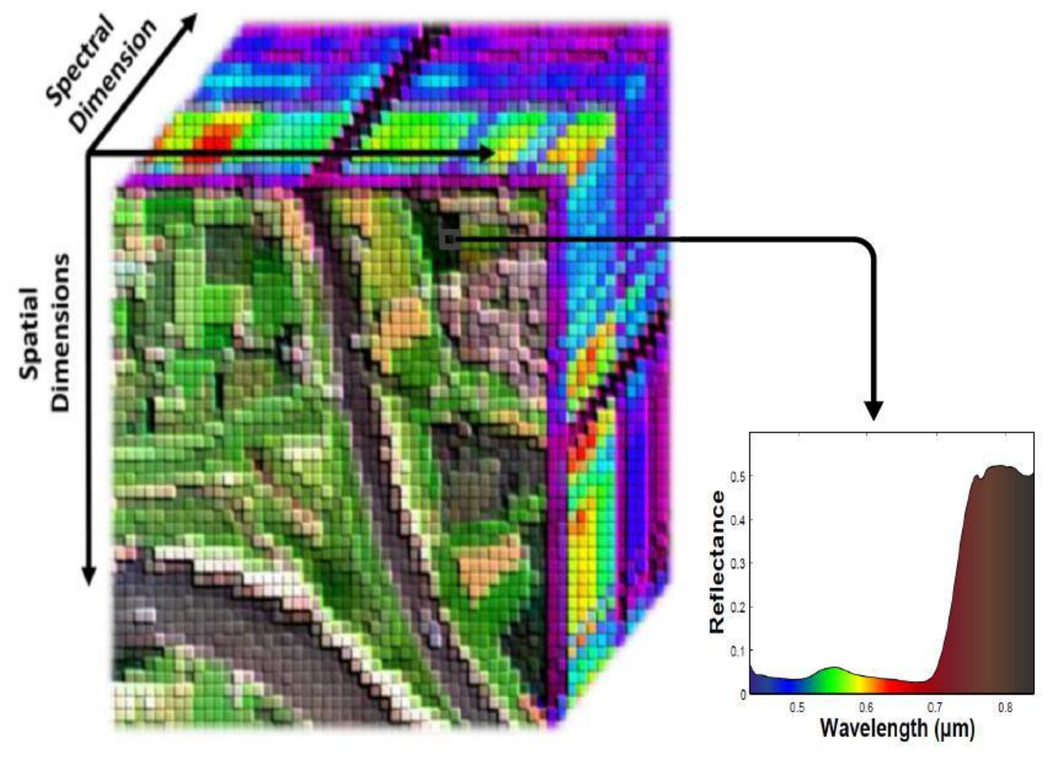
# Objectives

- What is Unmixing? Why Unmixing?
- What is linear Unmixing? When can we use it?
- Pure pixel and Endmember Extraction
- No Pure Pixel Scenarios
- What is Spectral Variability?
- Difference between Supervised unmixing, Semisupervised (sparse) unmixing, and Blind Unmixing,
- Geometrical Unmixing
- Autoencoders and CNNs for Unmixing
- Hands-on and exercises. For this tutorial, we released an open-source python-based collection of unmixing approaches.



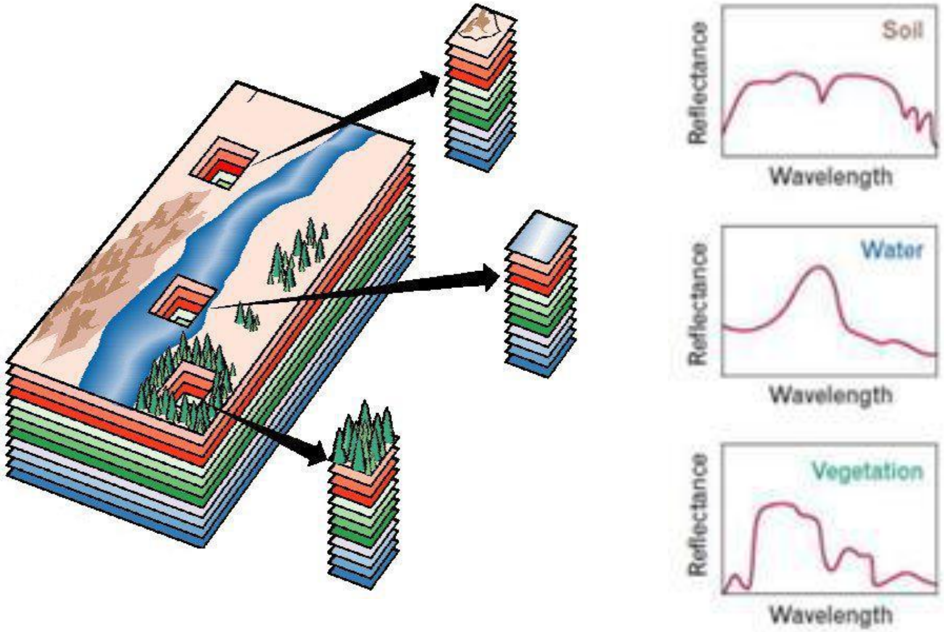
# Hyperspectral Image

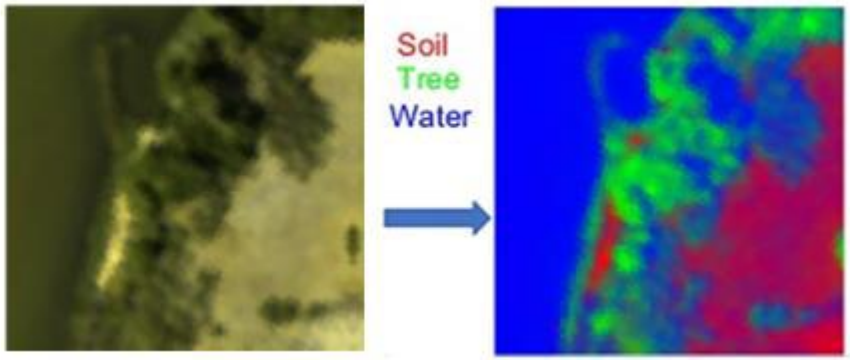



- **Hyperspectral cameras:** provide contiguous electromagnetic spectra ranging (often) from visible over near-infrared to shortwave infrared spectral bands (from 0.3 $\mu$m to 2.5 $\mu$m).
- The spectral signature: allowing to distinguish between materials with different characteristics.

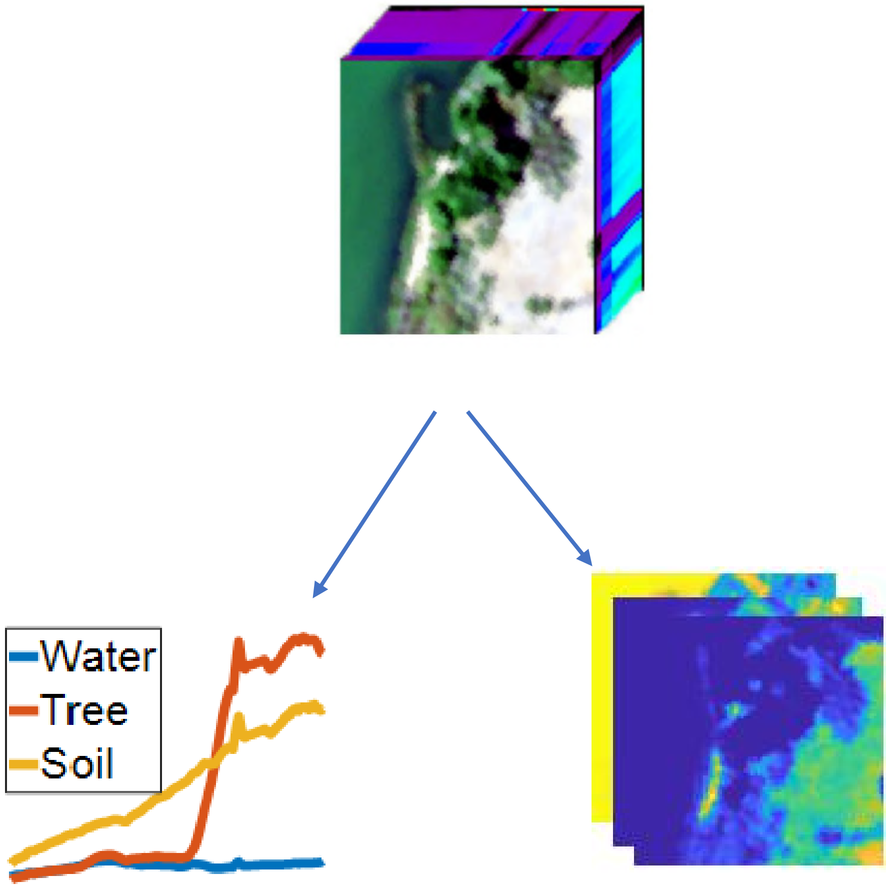
# Unmixing

- Estimating the fractional abundances of the pure spectra of constituent materials (called Endmembers) within a pixel



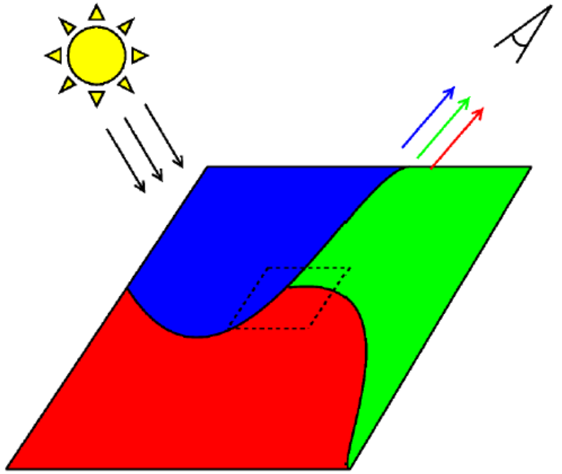



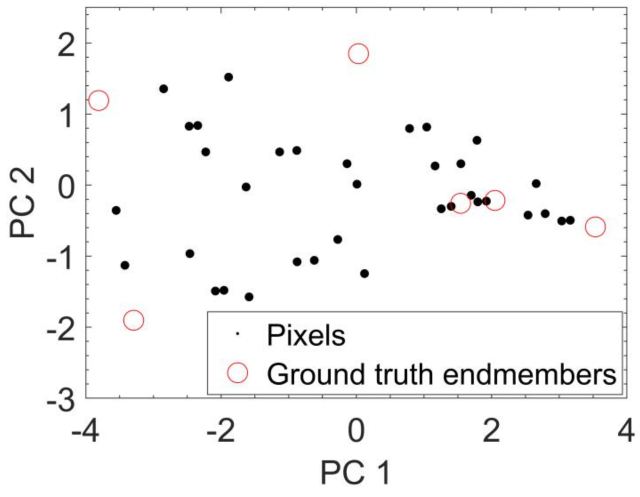
## Unmixing



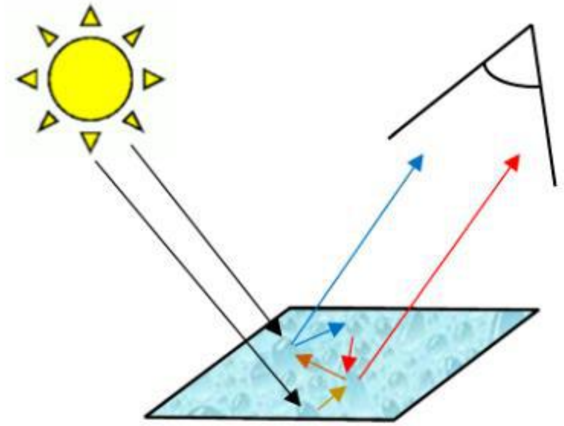

## Clustering/Unsupervised classification

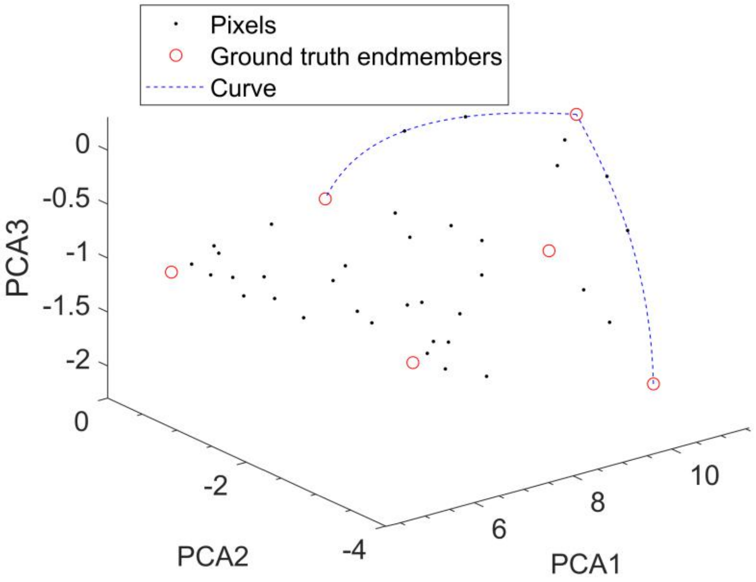
# Linear Unmixing



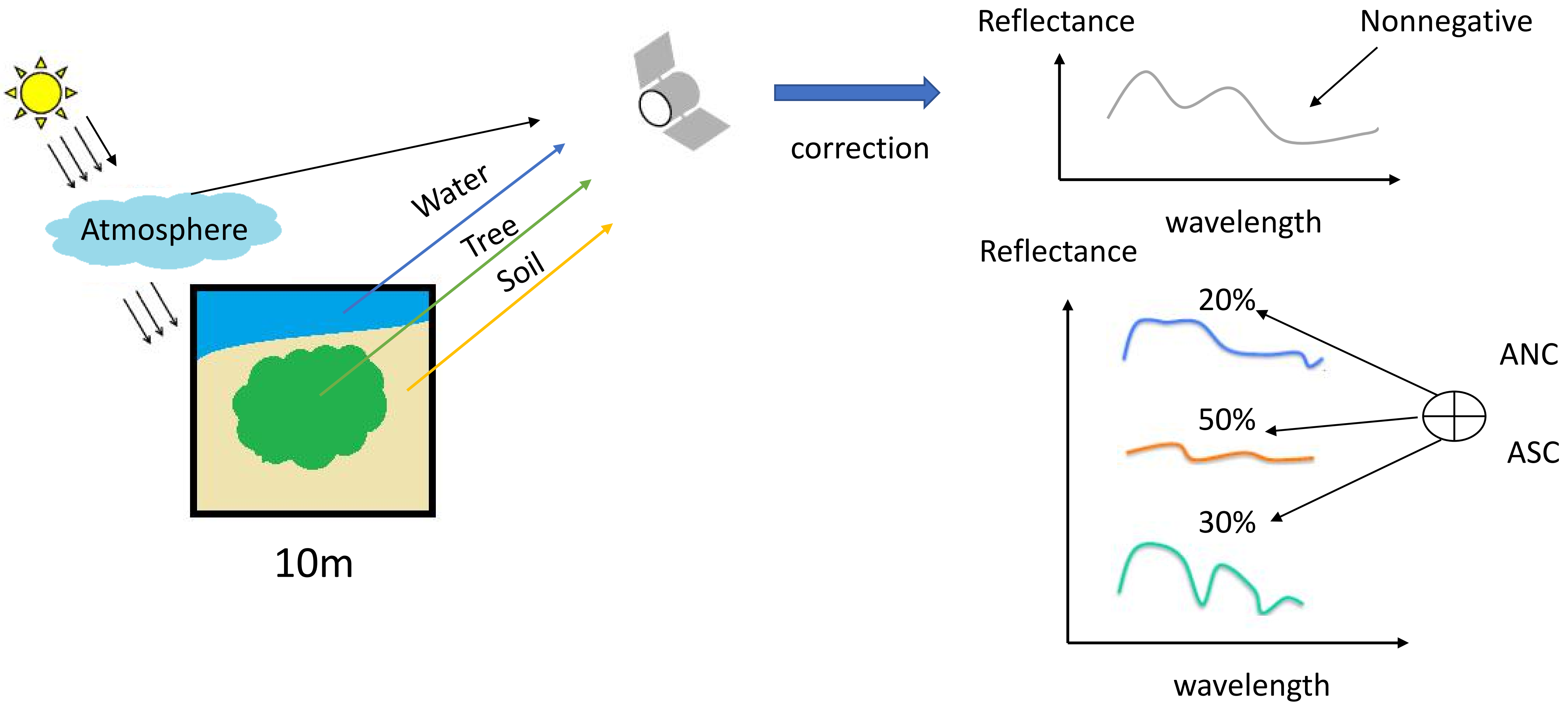



# Nonlinear Unmixing

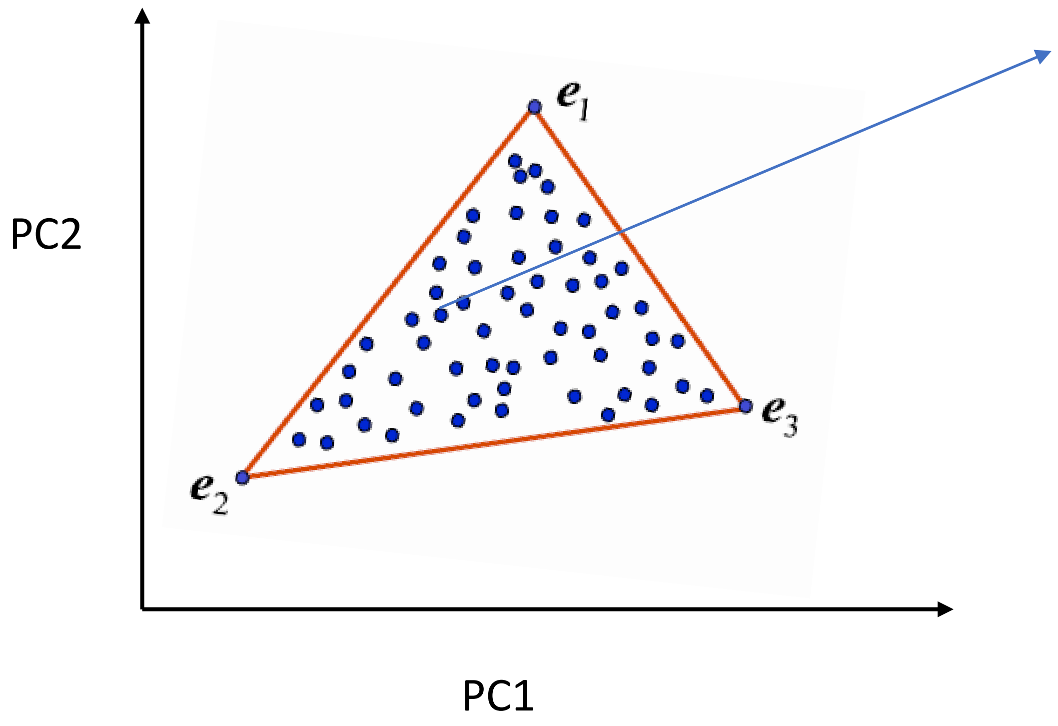




# Linear Unmixing



# Linear Unmixing



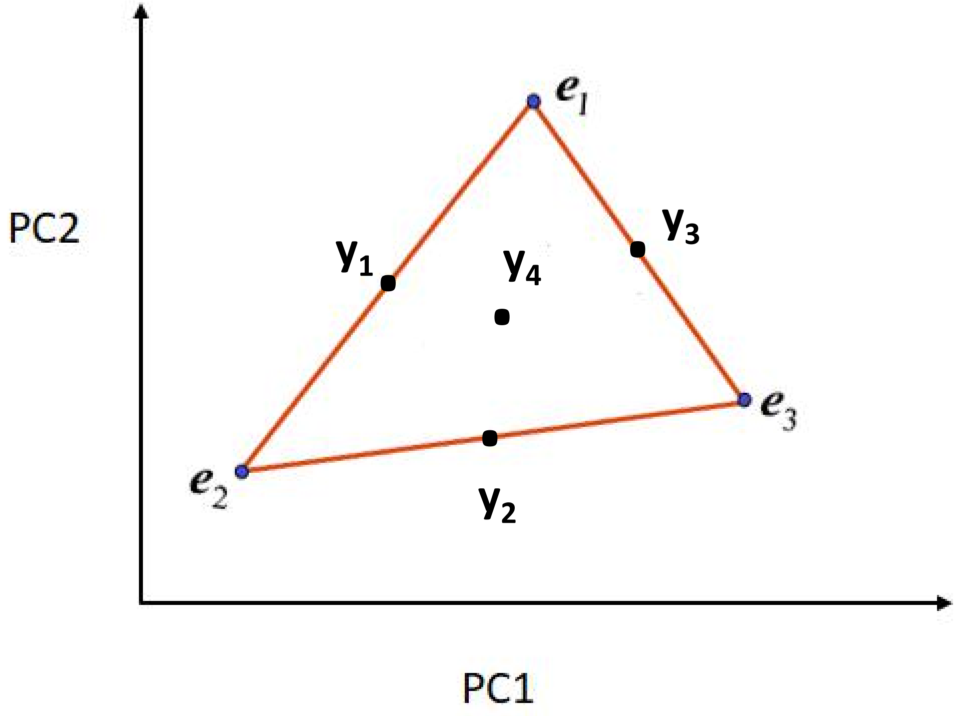

$$\boldsymbol{y} = \boldsymbol{E}\boldsymbol{a} + \boldsymbol{n} \quad \text{s.t.} \quad \sum_{i=1}^{r} a_i = 1, a_i \geq 0, i = 1, .., r$$

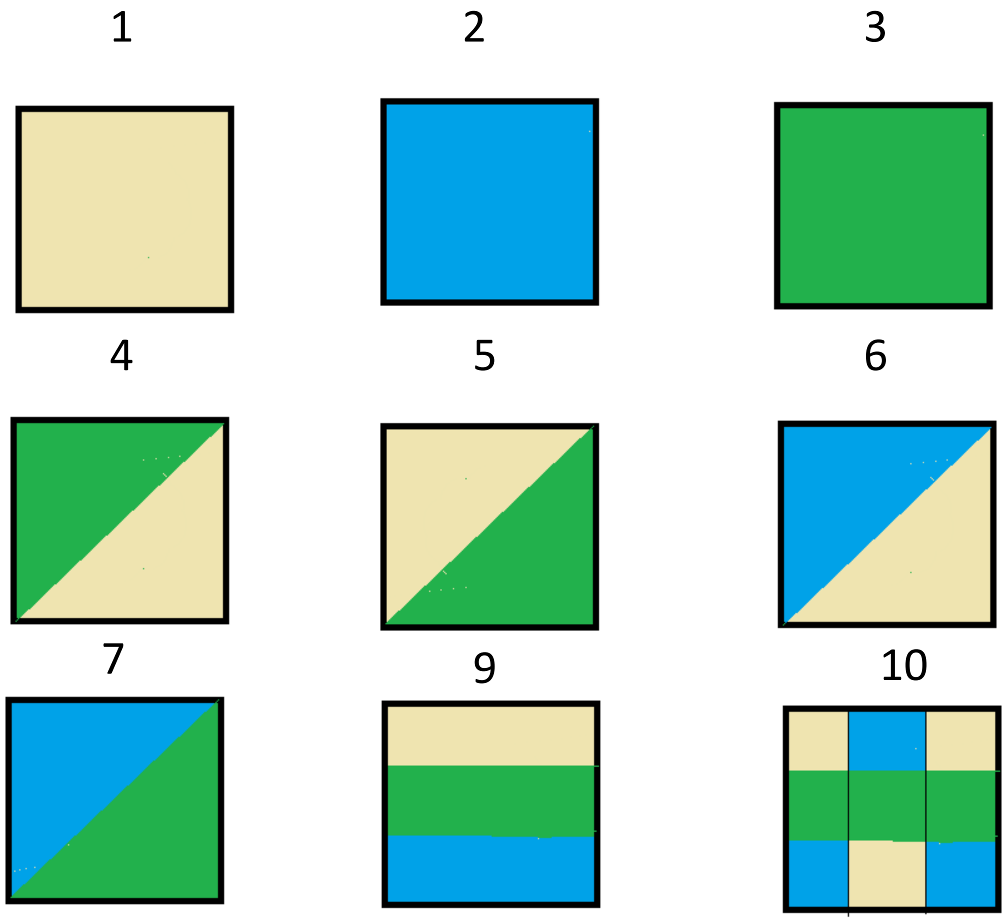
Matrix form

$$\boldsymbol{Y} = \boldsymbol{E}\boldsymbol{A} + \boldsymbol{N} \quad \text{s.t.} \quad \mathbf{1}_r^T \boldsymbol{A} = \mathbf{1}_{\boldsymbol{n}}^{\boldsymbol{T}}, \boldsymbol{A} \geq \mathbf{0}$$

Observed data: $\boldsymbol{Y} \in \mathbb{R}^{p \times n}$
Endmember: $\boldsymbol{E} \in \mathbb{R}^{p \times r}$
Abundances: $\boldsymbol{A} \in \mathbb{R}^{r \times n}$
Noise: $\boldsymbol{N} \in \mathbb{R}^{p \times n}$

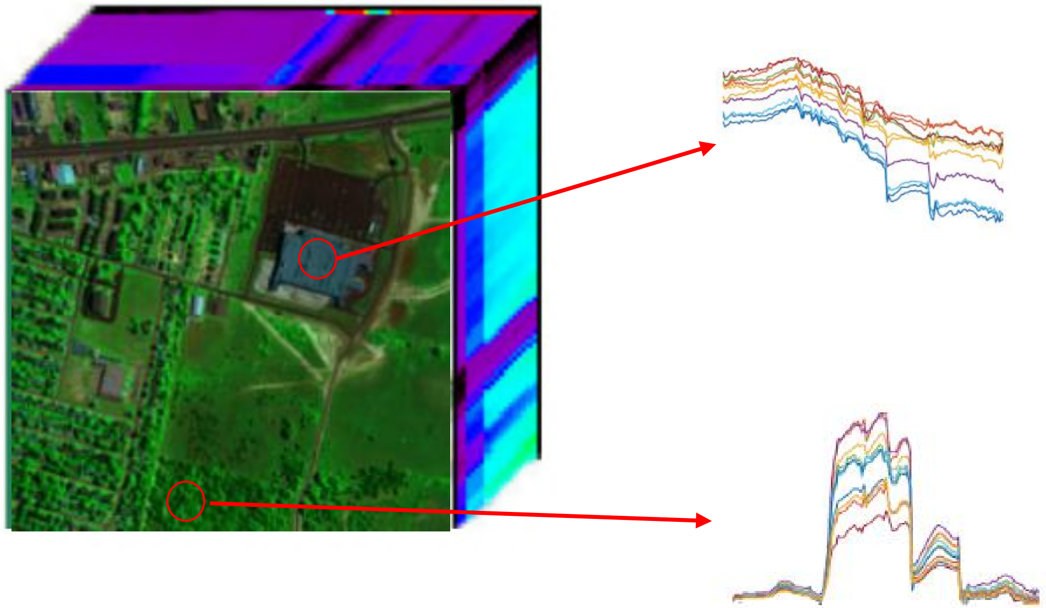
# Pixel Quiz!



# SPECTRAL VARIABILITY

1. Atmospheric effects
2. Illumination variations (Terrain topography, occlusion of the light)
3. The intrinsic variation of materials

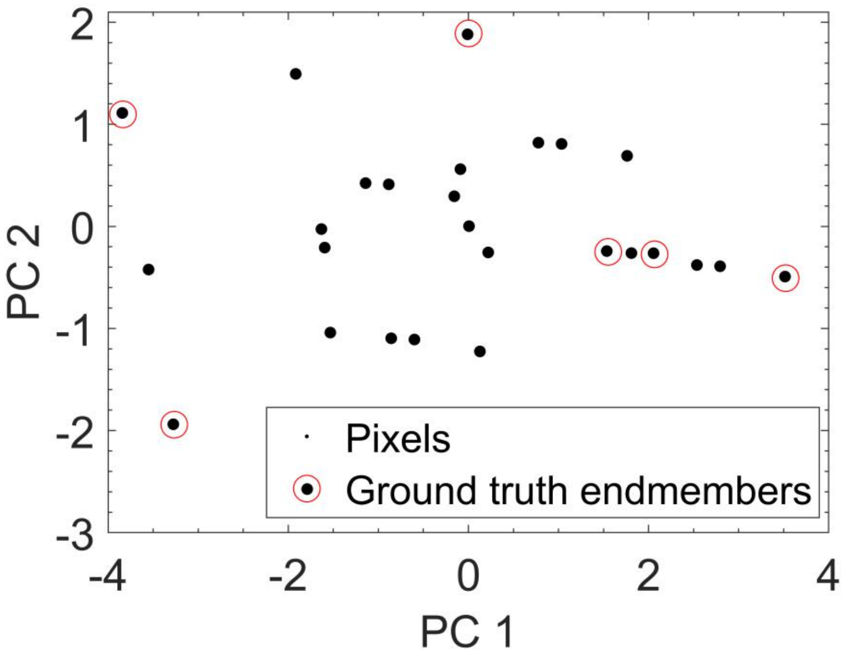


R. A. Borsoi et al., "Spectral Variability in Hyperspectral Data Unmixing: A comprehensive review," in IEEE Geoscience and Remote Sensing Magazine

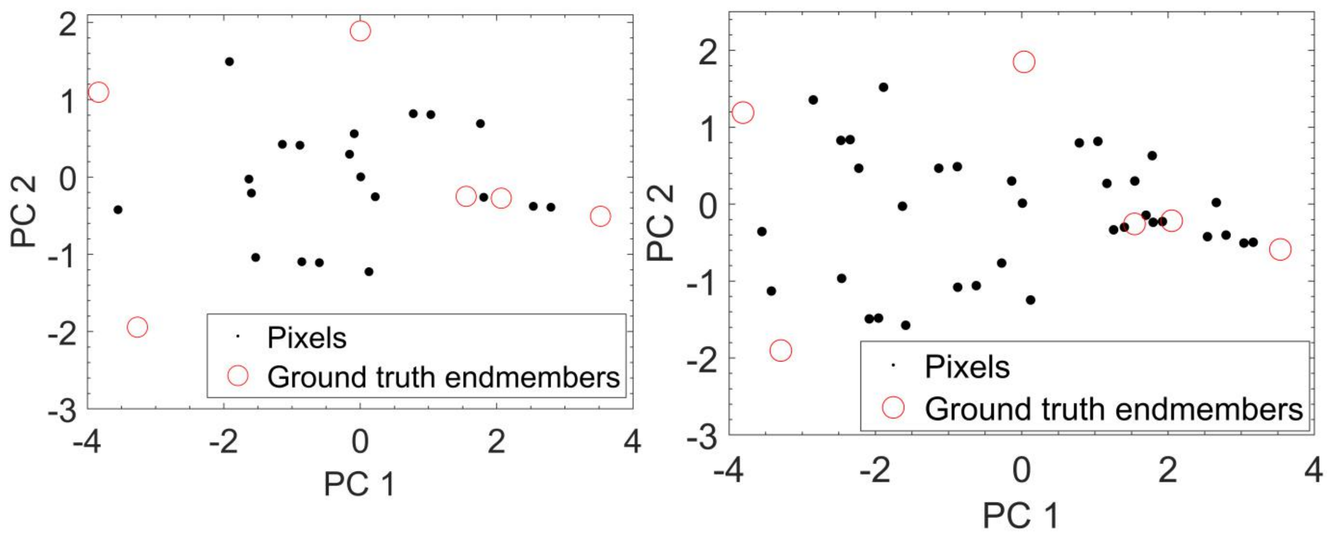
J. Theiler et al., "Spectral Variability of Remotely Sensed Target Materials: Causes, Models, and Strategies for Mitigation and Robust Exploitation," in IEEE Geoscience and Remote Sensing Magazine

# Pure vs No pure Pixel Scenarios

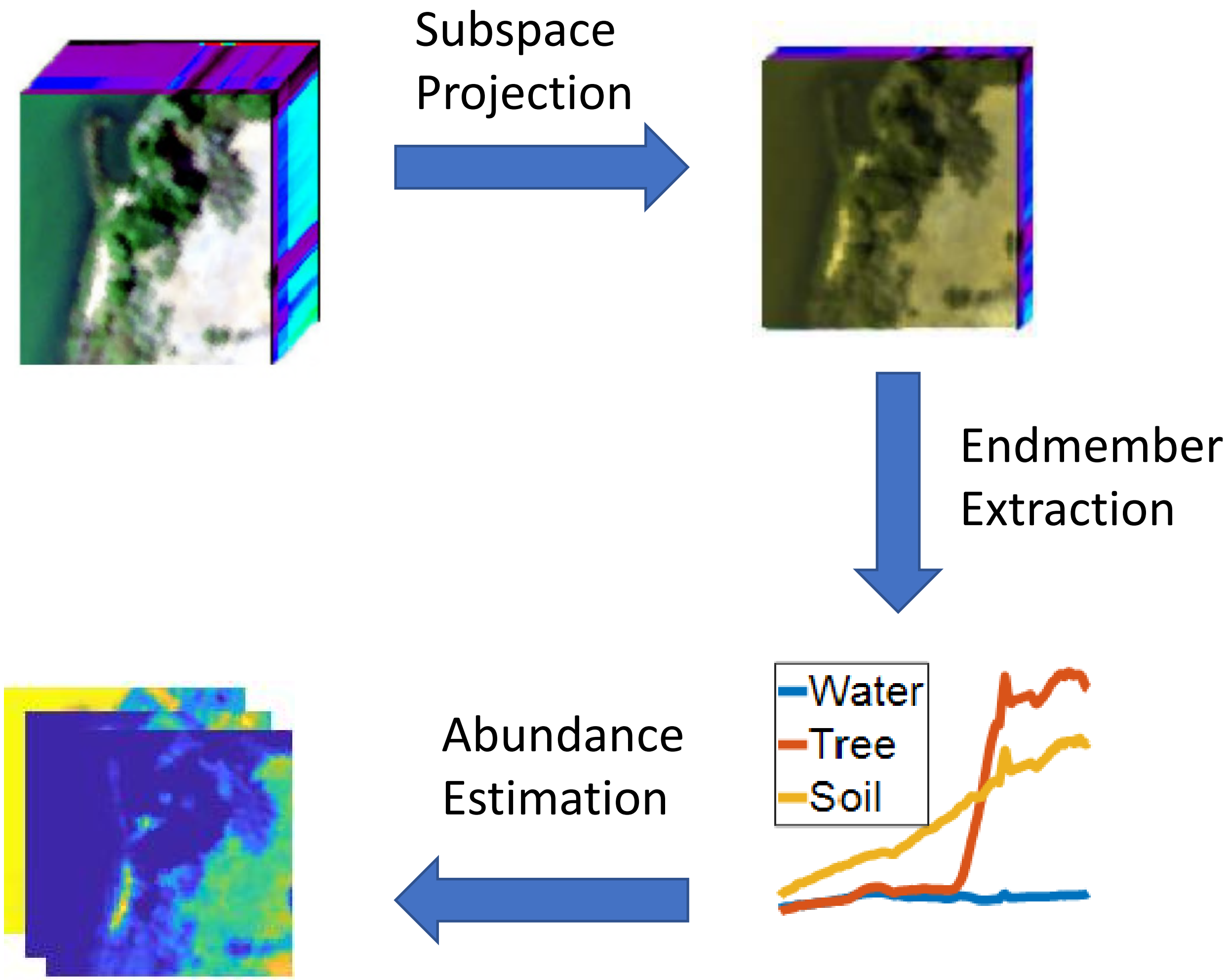
Pure Pixel

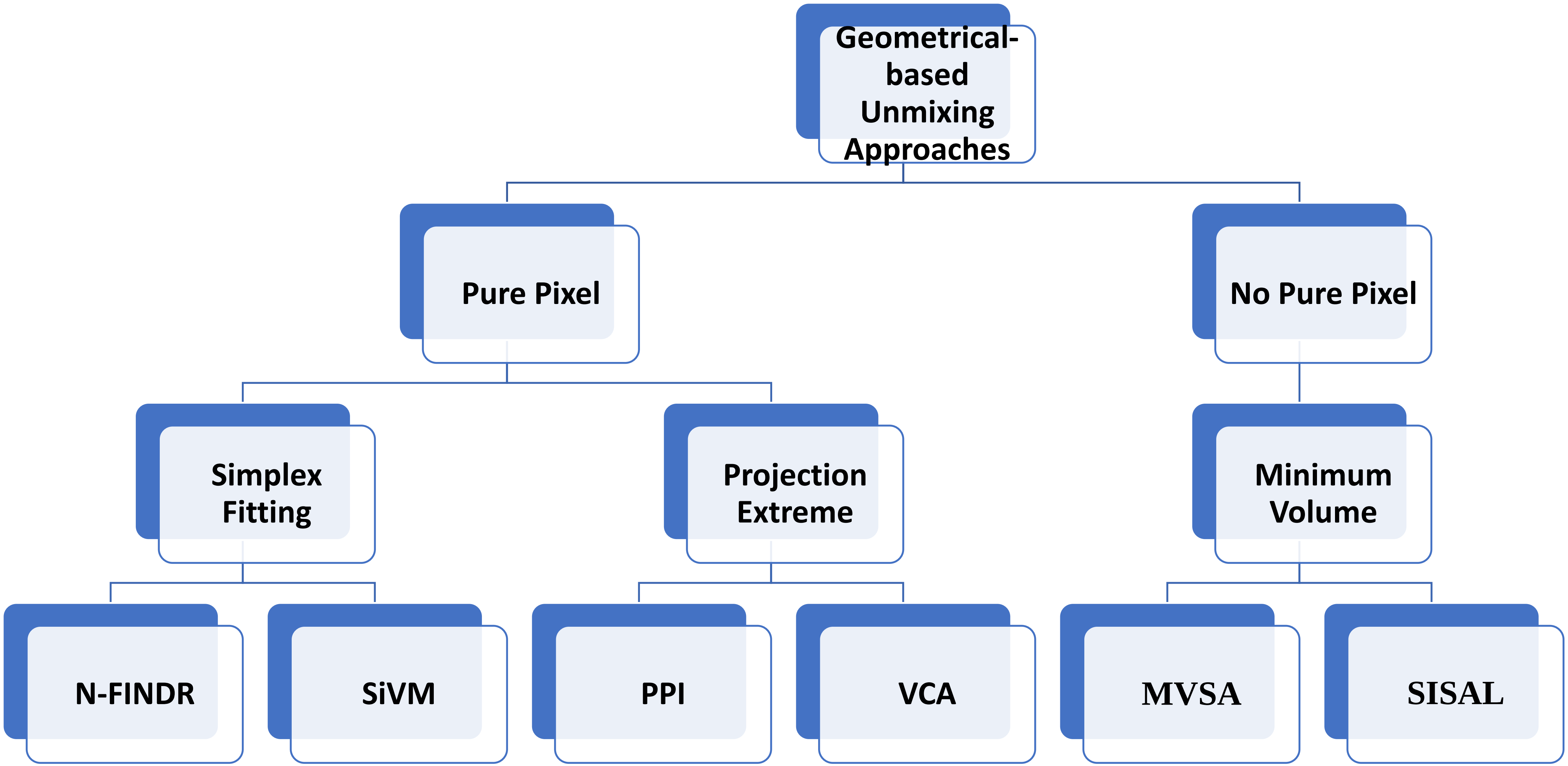



Non-pure Pixel



# Pure Pixel Scenario and Endmember Extraction




Geometrical-based Unmixing Approaches
Pure Pixel
No Pure Pixel
Simplex Fitting
Projection Extreme
Minimum Volume
N-FINDR
SiVM
PPI
VCA
MVSA
SISAL

Unmixing Approaches: In terms of Prior Knowledge of Endmembers

- Supervised Unmixing: Endmembers are known
- Blind Unmixing: Simultaneous Estimation of Endmembers and Abundances
- Semisupervised unmixing (Sparse Unmixing): Prior knowledge of the materials and an endmember library is available

# Norm

- A function which maps a vector space to the nonnegative real numbers
- p-norm of vector $\mathbf{x} \in \mathbb{R}^{\boldsymbol{n}}$

$$\|\mathbf{x}\|_p := \left(\sum_{i=1}^{n} |x_i|^p\right)^{1/p}$$

- $\ell_1$

$$\|\boldsymbol{x}\|_1 := \sum_{i=1}^{n} |x_i|$$

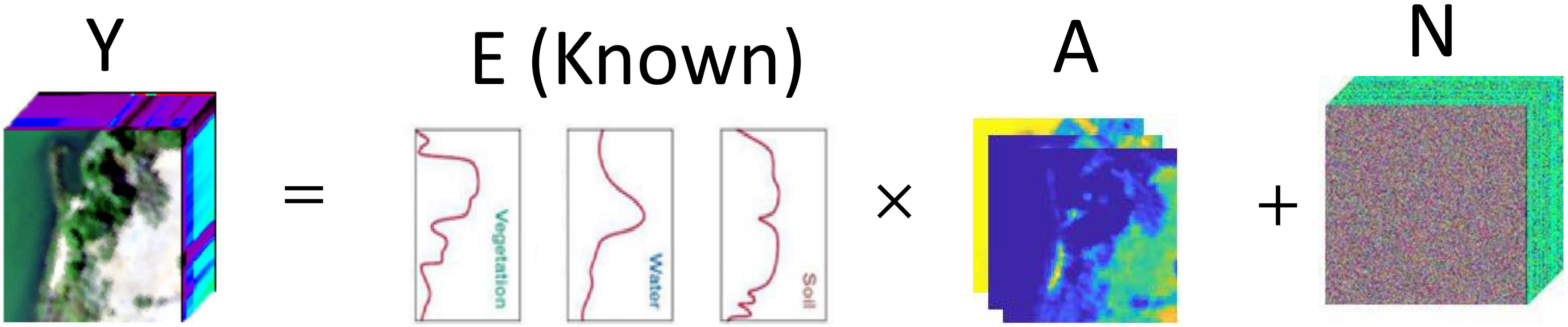
$\ell_2$

$$\|\boldsymbol{x}\|_2 := \sqrt{x_1^2 + \cdots + x_n^2}.$$

# Supervised Unmixing

Endmembers are known

- Extracted using geometrical approaches
- Selected from a Library
- Measured in LAB




- Estimating A

$$(\widehat{\boldsymbol{A}}) = arg\min_{A} \frac{1}{2} ||\boldsymbol{Y} - \boldsymbol{E}\boldsymbol{A}||_F^2 + \lambda\phi(\boldsymbol{A}) \text{ st. } \mathbf{1}_r^T\boldsymbol{A} = \mathbf{1}_{\boldsymbol{n}} \text{ , } \boldsymbol{A} \geq \mathbf{0}$$

# FCLSU: Fully Constrained Least Squares Unmixing

- Endmember extraction (Often using geometrical approaches)
- Then FCLSU

$$\left(\widehat{\boldsymbol{A}}\right) = arg \min_{A} \frac{1}{2} ||\boldsymbol{Y} - \boldsymbol{E}\boldsymbol{A}||_F^2 \text{ st. } \boldsymbol{1}_r^T \boldsymbol{A} = \boldsymbol{1}_{\boldsymbol{n}} \text{ , } \boldsymbol{A} \geq \boldsymbol{0}$$

- Or FCLSU + spatial regularizer $\phi$ (it could be TV, sparsity promoting penalty, or a combination of them)

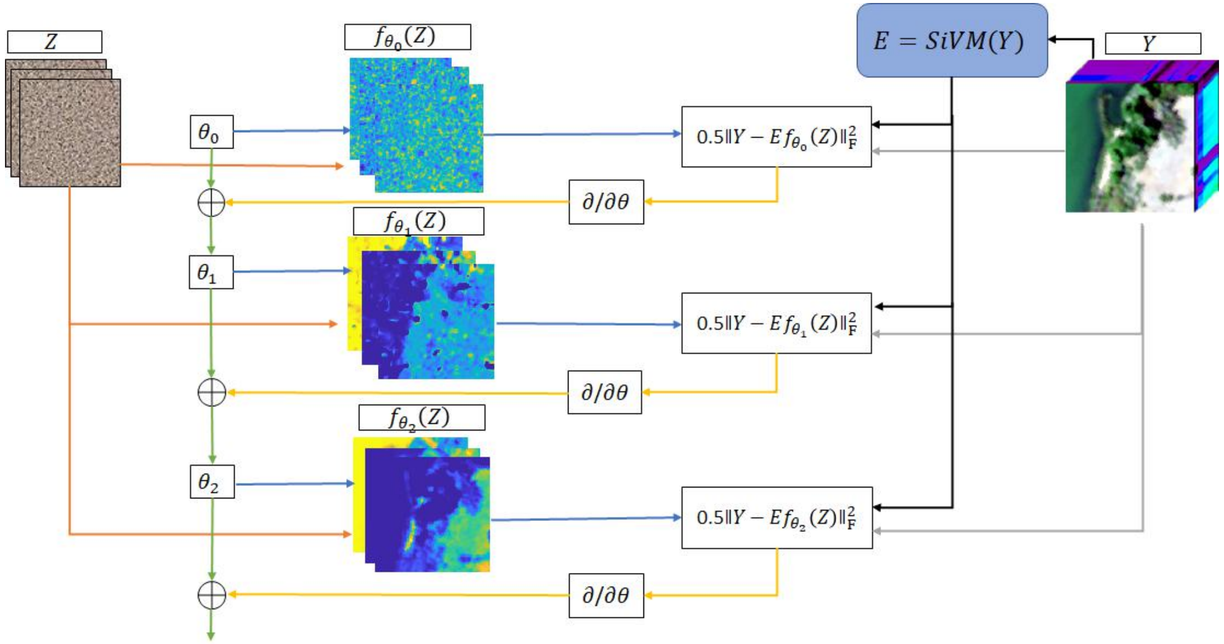
$$\left(\widehat{\boldsymbol{A}}\right) = arg \min_{A} \frac{1}{2} ||\boldsymbol{Y} - \boldsymbol{E}\boldsymbol{A}||_F^2 + \lambda R(\boldsymbol{A}) \text{ st. } \boldsymbol{1}_r^T \boldsymbol{A} = \boldsymbol{1}_{\boldsymbol{n}} \text{ , } \boldsymbol{A} \geq \boldsymbol{0}$$

D. Heinz, C. . -I. Chang and M. L. G. Althouse, "Fully constrained least-squares based linear unmixing [hyperspectral image classification]," *IEEE 1999 International Geoscience and Remote Sensing Symposium. IGARSS'99 (Cat. No.99CH36293)*, 1999, pp. 1401-1403 vol.2, doi: 10.1109/IGARSS.1999.774644.

# UnDIP: Hyperspectral Unmixing Using Deep Image Prior

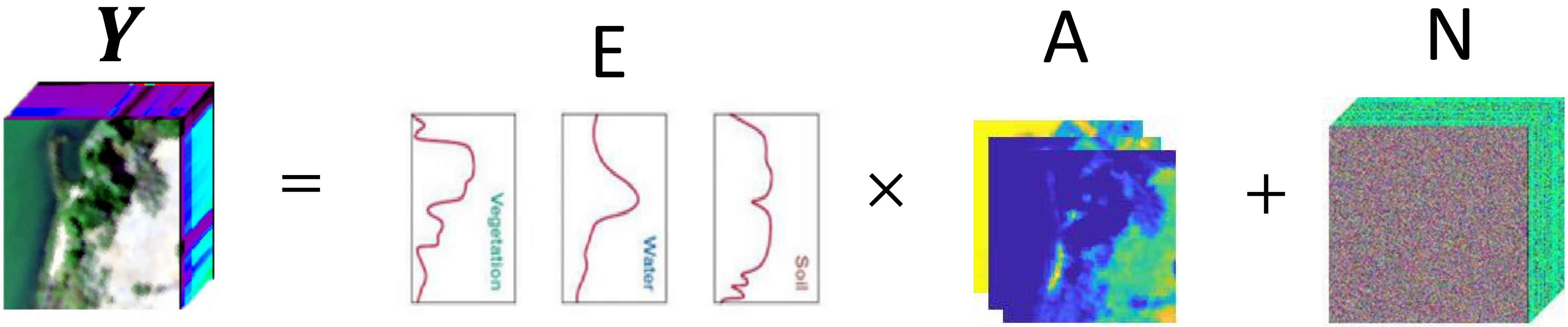
$$(\widehat{\boldsymbol{A}}) = arg\min_{A} \frac{1}{2}||\boldsymbol{Y} - \boldsymbol{E}\boldsymbol{A}||_F^2 + \lambda R(\boldsymbol{A}) \ \text{st.}\ \boldsymbol{1}_r^T \boldsymbol{A} = \boldsymbol{1_n}\ , \boldsymbol{A} \geq \boldsymbol{0}$$

$$(\widehat{\boldsymbol{\theta}}) = arg\min_{\theta} \frac{1}{2}||\boldsymbol{Y} - \boldsymbol{E}f_{\theta}(\boldsymbol{Z})||_F^2 \ \text{st.}\ \widehat{\boldsymbol{A}} = f_{\widehat{\boldsymbol{\theta}}}(\boldsymbol{Z})$$




B. Rasti, B. Koirala, P. Scheunders and P. Ghamisi, "UnDIP: Hyperspectral Unmixing Using Deep Image Prior," in *IEEE Transactions on Geoscience and Remote Sensing*, vol. 60, pp. 1-15, 2022, Art no. 5504615, doi: 10.1109/TGRS.2021.3067802.

# Blind Unmixing




- Estimating E and A

$$(\widehat{\boldsymbol{E}},\widehat{\boldsymbol{A}}) = arg\min_{E,\,A}\frac{1}{2}||\boldsymbol{Y}-\boldsymbol{E}\boldsymbol{A}||_F^2 + \lambda_1\phi_1(\boldsymbol{E}) + \lambda_2\phi_2(\boldsymbol{A})$$
$$\text{st. } \boldsymbol{1}_r^T\boldsymbol{A} = \boldsymbol{1_n}\,,\ \boldsymbol{A} \geq \boldsymbol{0},\ \boldsymbol{0} \leq \boldsymbol{E} \leq 1$$

# No pure pixel scenarios & MV Penalties

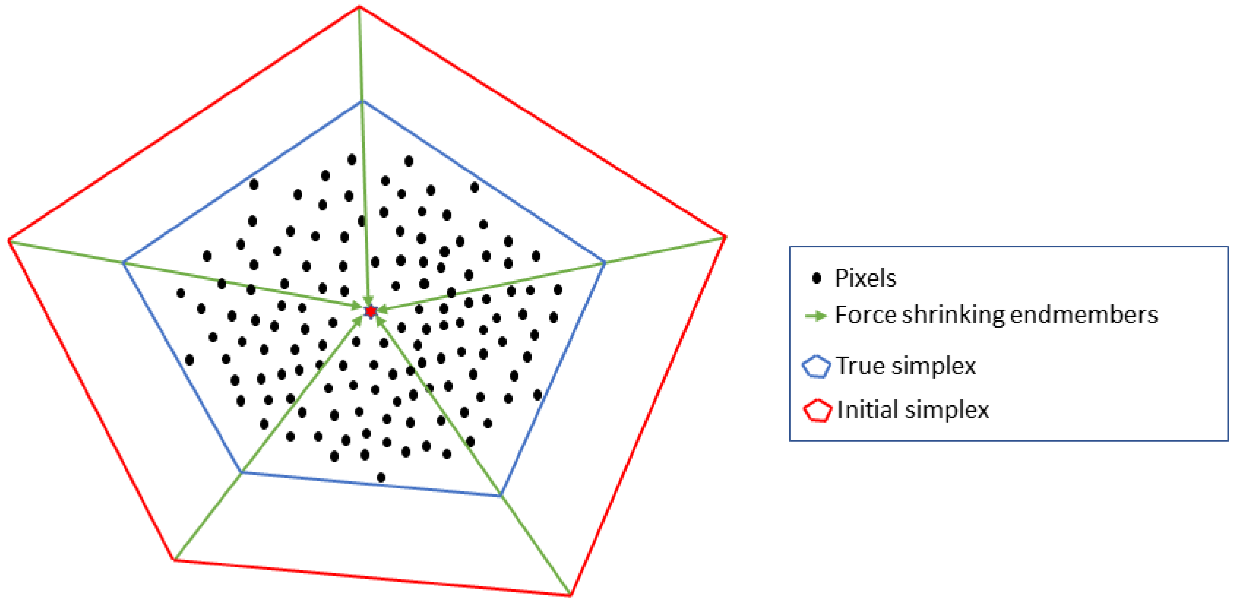
## Quadratic Penalties to promote MV

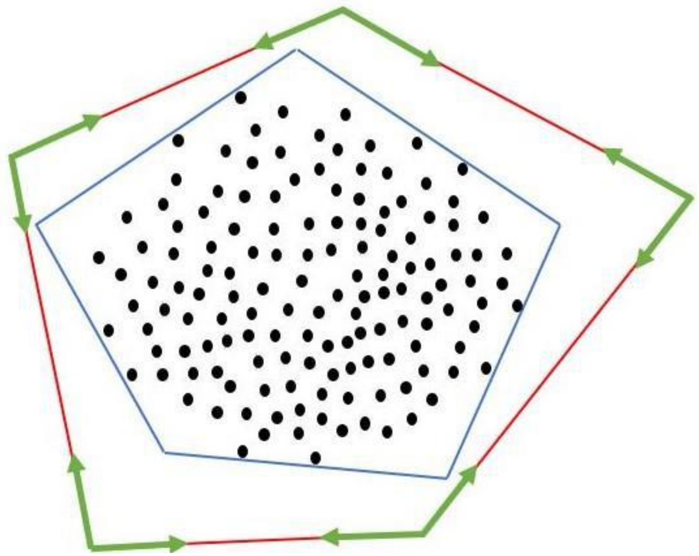
Enforce the endmembers towards the center of the data simplex (m)

$$\phi(\mathbf{E}) = \sum_{i=1}^{r} ||\mathbf{e_i} - \mathbf{m}||_2^2 = ||\mathbf{E} - \mathbf{m}\mathbf{1}_\mathbf{r}^\mathbf{T}||_F^2$$

Enforce the endmembers towards each other

$$\text{TV}(\mathbf{E}) = \sum_{i,j=1}^{r} ||\mathbf{e_i} - \mathbf{e_j}||_2^2 = ||\mathbf{E}(\mathbf{I_r} - \frac{\mathbf{1}}{r}\mathbf{1_r}\mathbf{1}_\mathbf{r}^\mathbf{T})||_F^2$$



# MVC-NMF: Minimum volume constrained nonnegative matrix factorization

- MVC-NMF uses the square of the volume of the simplex defined by the columns of $\boldsymbol{E}$.

$$(\widehat{\boldsymbol{E}}, \widehat{\boldsymbol{A}}) = arg \min_{E,\, A} \frac{1}{2} ||\boldsymbol{Y} - \boldsymbol{E}\boldsymbol{A}||_F^2 + \lambda_1 V^{\boldsymbol{2}}(\boldsymbol{E}) \text{ st. } \boldsymbol{1}_r^T \boldsymbol{A} = \boldsymbol{1}_{\boldsymbol{n}} \,, \boldsymbol{A} \geq \boldsymbol{0}, \boldsymbol{E} \geq \boldsymbol{0}$$

- Where $\boldsymbol{E} = [\boldsymbol{e}_{(i)}]$ and

$$V(\mathbf{E}) = \frac{\mathbf{1}}{(\mathbf{r}-\mathbf{1})!} \left| \det \begin{bmatrix} 1 & \dots & 1 \\ \mathbf{e}_{(1)} & \dots & \mathbf{e}_{(\mathbf{r})} \end{bmatrix} \right|$$

- A Python implementation

https://github.com/bm424/mvcnmf/blob/master/mvcnmf.py

L. Miao and H. Qi, "Endmember Extraction From Highly Mixed Data Using Minimum Volume Constrained Nonnegative Matrix Factorization," in *IEEE Transactions on Geoscience and Remote Sensing*, vol. 45, no. 3, pp. 765-777, March 2007, doi: 10.1109/TGRS.2006.888466.

# CoNMF: Collaborative nonnegative matrix factorization for remotely sensed hyperspectral unmixing

- Promoting sparsity on abundances and MV on the simplex

$$\left(\widehat{\boldsymbol{E}}, \widehat{\boldsymbol{A}}\right) = arg \min_{E,\, A} \frac{1}{2} ||\boldsymbol{Y} - \boldsymbol{E}\boldsymbol{A}||_F^2 + \lambda_1 ||\boldsymbol{E} - \boldsymbol{m}\mathbf{1}_r^T||_F^2 + \lambda_2 \sum_{i=1}^{r} ||a_{(i)}||_2^q$$

$$\text{st. } \mathbf{1}_r^T \boldsymbol{A} = \mathbf{1}_{\boldsymbol{n}} \text{ , } \boldsymbol{A} \geq \mathbf{0} \text{ , } 0 < q \leq 1$$

- Selecting the tuning parameter is challenging.

J. Li, J. M. Bioucas-Dias and A. Plaza, "Collaborative nonnegative matrix factorization for remotely sensed hyperspectral unmixing," *2012 IEEE International Geoscience and Remote Sensing Symposium*, 2012, pp. 3078-3081, doi: 10.1109/IGARSS.2012.6350775.

# NMF-QMV: Nonnegative Matrix Factorization-Quadratic Minimum Volume

- Quadratic MV penalties and no spatial regularization

$$\left(\widehat{\boldsymbol{E}}, \widehat{\boldsymbol{A}}\right) = arg \min_{E,\, A} \frac{1}{2} ||\boldsymbol{Y} - \boldsymbol{E}\boldsymbol{A}||_F^2 + \lambda ||\boldsymbol{E}\boldsymbol{B} - \boldsymbol{O}||_F^2 \quad \text{st. } \boldsymbol{A} \in \Theta_{r-1}^{r} \;\; \mathbf{1}_r^T \boldsymbol{A} = \mathbf{1}_{\boldsymbol{n}} \,, \boldsymbol{A} \geq \mathbf{0}$$

| QMV | Center | TV | Boundary |
|---|---|---|---|
| $\boldsymbol{B}$ | $\boldsymbol{I_r}$ | $\boldsymbol{I_r} - \mathbf{1}/\boldsymbol{r}(\mathbf{1}_{\mathbf{r}}\mathbf{1}_{\mathbf{r}}^{\mathbf{T}})$ | $\boldsymbol{I_r}$ |
| $\boldsymbol{O}$ | $\boldsymbol{m}\mathbf{1}_r^T$ | $\mathbf{0}$ | Extremes (VCA) |

- Parameter selection

$$\lambda_{opt} = \text{arg}\min_{\lambda} D(G, \widehat{E_\lambda})$$

- $D \triangleq \frac{1}{n}\sum_{j=1}^{n} dist(g_j, \widehat{E_\lambda})$,
- $G \triangleq \{g_1, \dots, g_n\}$ (the set of vertices of the convex hull of the observations projected into a subspace)

L. Zhuang, C. -H. Lin, M. A. T. Figueiredo and J. M. Bioucas-Dias, "Regularization Parameter Selection in Minimum Volume Hyperspectral Unmixing," in *IEEE Transactions on Geoscience and Remote Sensing*, vol. 57, no. 12, pp. 9858-9877, Dec. 2019, doi: 10.1109/TGRS.2019.2929776.

# Estimating in Subspace

- The unmixing problem can be solved in a subspace

$$(\widehat{\boldsymbol{E}}, \widehat{\boldsymbol{A}}) = arg \min_{E,\,A} \frac{1}{2} ||\boldsymbol{Y} - \boldsymbol{EA}||_F^2 + \lambda_1 ||\boldsymbol{EB} - \boldsymbol{O}||_F^2 \quad \text{st. } \boldsymbol{1}_r^T \boldsymbol{A} = \boldsymbol{1_n} \text{ , } \boldsymbol{A} \geq \boldsymbol{0}$$

- Instead, we solve

$$(\widehat{\boldsymbol{E}}, \widehat{\boldsymbol{A}}) = arg \min_{E,\,A} \frac{1}{2} ||\boldsymbol{V^T}(\boldsymbol{Y} - \boldsymbol{EA})||_F^2 + \lambda_1 ||\boldsymbol{V^T}(\boldsymbol{EB} - \boldsymbol{O})||_F^2 \quad \text{st. } \boldsymbol{1}_r^T \boldsymbol{A} = \boldsymbol{1_n} \text{ , } \boldsymbol{A} \geq \boldsymbol{0}$$

- Where $\boldsymbol{V^T V} = \boldsymbol{I_r}$ and can be obtained by SVD or PCA.
- Pros: Computationally efficient and more robust to noise
- Cons: Estimating negative values for $\boldsymbol{E}$

# Entropic Descent Archetypal Analysis for Blind Hyperspectral Unmixing

- The blind unmixing problem

$$(\widehat{\boldsymbol{E}}, \widehat{\boldsymbol{A}}) = arg \min_{E,\, A} \frac{1}{2} ||\boldsymbol{Y} - \boldsymbol{E}\boldsymbol{A}||_F^2 \quad \text{st. } \boldsymbol{1}_r^T \boldsymbol{A} = \boldsymbol{1}_{\boldsymbol{n}} \,, \boldsymbol{A} \geq \boldsymbol{0}, \boldsymbol{0} \leq \boldsymbol{E} \leq 1$$

- Note that columns of $\boldsymbol{A} = [\boldsymbol{a}_1, \ldots, \boldsymbol{a}_n]$ belong to the simplex

$$\Delta_r \triangleq \{\boldsymbol{a} \in \mathbb{R}^r | \boldsymbol{a} \geq \boldsymbol{0}, \sum_{i=1}^{r} a_i = 1\}$$

- We can rewrite the blind unmixing problem

$$(\widehat{\boldsymbol{E}}, \widehat{\boldsymbol{A}}) = arg \min_{E,\, A} \frac{1}{2} ||\boldsymbol{Y} - \boldsymbol{E}\boldsymbol{A}||_F^2 \quad \text{st.} \quad \boldsymbol{a}_{(\boldsymbol{i})} \in \Delta_r \text{ for } 1 \leq i \leq n, \boldsymbol{0} \leq \boldsymbol{E} \leq 1$$

Alexandre Zouaoui, Gedeon Muhawenayo, Behnood Rasti, Jocelyn Chanussot, Julien Mairal , "Entropic Descent Archetypal Analysis for Blind Hyperspectral Unmixing," Submitted in *IEEE Transactions on Image Processing*.

# Entropic Descent Archetypal Analysis for Blind Hyperspectral Unmixing

- The archetypal analysis formulation was used to enforce the endmembers to be convex combinations of the pixels

$$\left(\widehat{\boldsymbol{E}},\widehat{\boldsymbol{B}}\right)=arg\min_{E,\,B}\frac{1}{2}||\boldsymbol{Y}-\boldsymbol{YBA}||_F^2 \text{ st. } \quad \boldsymbol{a}_{(\boldsymbol{i})}\in\Delta_r \text{ for } 1\leq i\leq n$$

$$\boldsymbol{b}_{(\boldsymbol{j})}\in\Delta_n \text{ for } 1\leq j\leq r$$

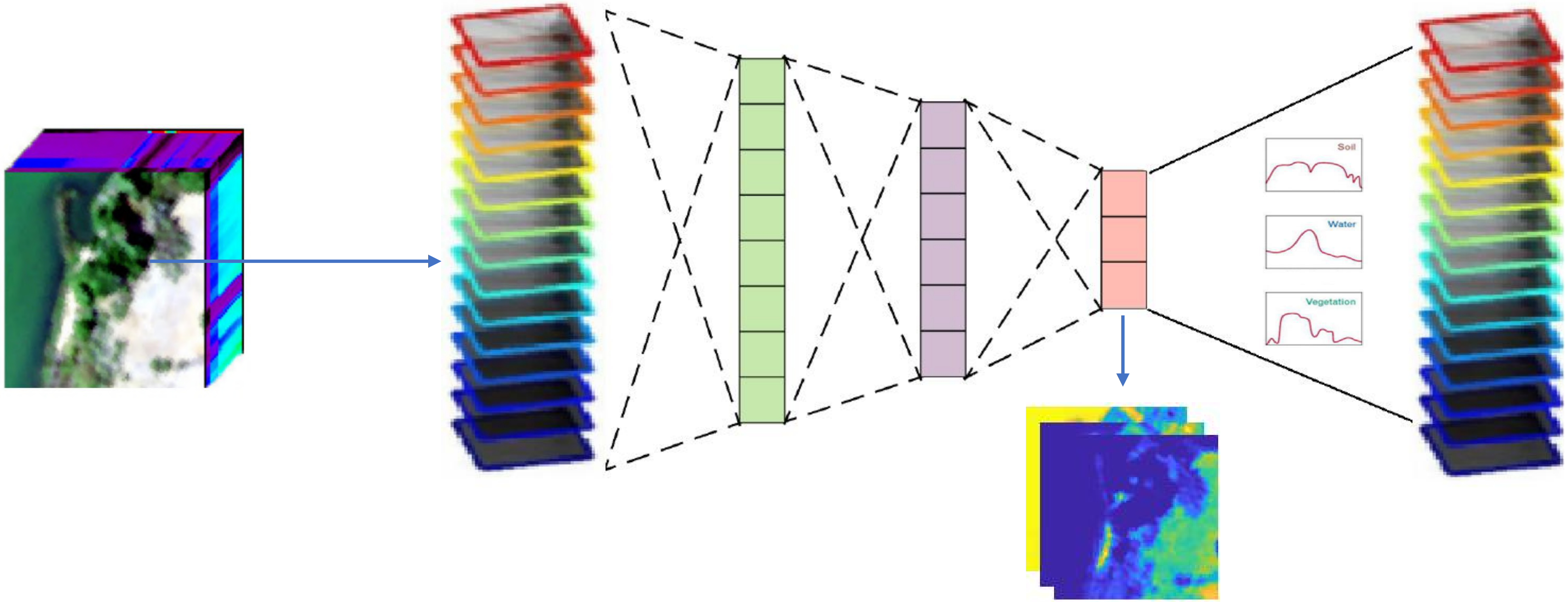
- Where $\boldsymbol{B}\in\mathbb{R}^{n\times r}$ and therefore the columns of $\boldsymbol{B}=[\boldsymbol{b}_1,\ldots,\boldsymbol{b}_r]$ belong to the simplex $\Delta_n$.
- The problem is solved using an Entropic descent algorithm (EDA).
- The solution is sensitive to the initialization of $\boldsymbol{B}$ and therefore a model selection technique suggested where the coherence $\mu=\max_{i\neq j}<\widehat{\boldsymbol{e}}_{\boldsymbol{i}},\widehat{\boldsymbol{e}}_{\boldsymbol{j}}>$ and $\ell_1$residual $||Y-\widehat{\boldsymbol{E}}\widehat{\boldsymbol{A}}||_1$are minimized.

Alexandre Zouaoui, Gedeon Muhawenayo, Behnood Rasti, Jocelyn Chanussot, Julien Mairal , "Entropic Descent Archetypal Analysis for Blind Hyperspectral Unmixing," Submitted in *IEEE Transactions on Image Processing*.

# Blind Unmixing Using Autoencoders

- Encoder encodes an input into abundances: $\boldsymbol{a} = \boldsymbol{\sigma}(\boldsymbol{W}_{en}(\boldsymbol{y}))$
- Decoder reconstruct the signal: $\widehat{\boldsymbol{y}}$= $\boldsymbol{\sigma}(\boldsymbol{W}_{de}(\boldsymbol{a}))$
- Endmembers: the weights of the decoders
- Often deep encoder, shallow decoder

$$L_{reg} = L(\boldsymbol{y}, \widehat{\boldsymbol{y}}) + \lambda J(\boldsymbol{a}, \boldsymbol{W}_{de}, \boldsymbol{W}_{en})$$



# Realization of ASC and ANC

1. Applying Nonnegative activation function such as ReLU and Normalization for ASC

$$a = \frac{a}{\sum_{i=1}^{r} a_i}$$

2. Or

$$a = \frac{|a|}{\sum_{i=1}^{r} |a_i|}$$

3. Softmax

$$Softmax(a) = \frac{e^a}{\sum_{i=1}^{r} e^{a_i}}$$

4. Adding a penalty term to the loss function

# Common Loss Functions

- $L_{reg} = L(\boldsymbol{y}, \widehat{\boldsymbol{y}}) + \lambda J(\boldsymbol{a}, \boldsymbol{W}_{de}, \boldsymbol{W}_{en})$
- $L$ is often $\ell_2$ norm (or MSE)

$$L_{\ell_2}(\boldsymbol{y}, \widehat{\boldsymbol{y}}) = ||\boldsymbol{y} - \widehat{\boldsymbol{y}}||_2^2$$

- or SAD

$$L_{SAD}(\boldsymbol{y}, \widehat{\boldsymbol{y}}) = \arccos\left(\frac{\boldsymbol{y}^T \widehat{\boldsymbol{y}}}{||\boldsymbol{y}||_2 ||\widehat{\boldsymbol{y}}||_2}\right)$$

- The regularization term $J$ is often a Minimum Volume Penalty

$$J = MV(E) = MV(\boldsymbol{W}_{de})$$

# ENDNET: SPARSE AUTOENCODER NETWORK FOR ENDMEMBER EXTRACTION AND HYPERSPECTRAL UNMIXING

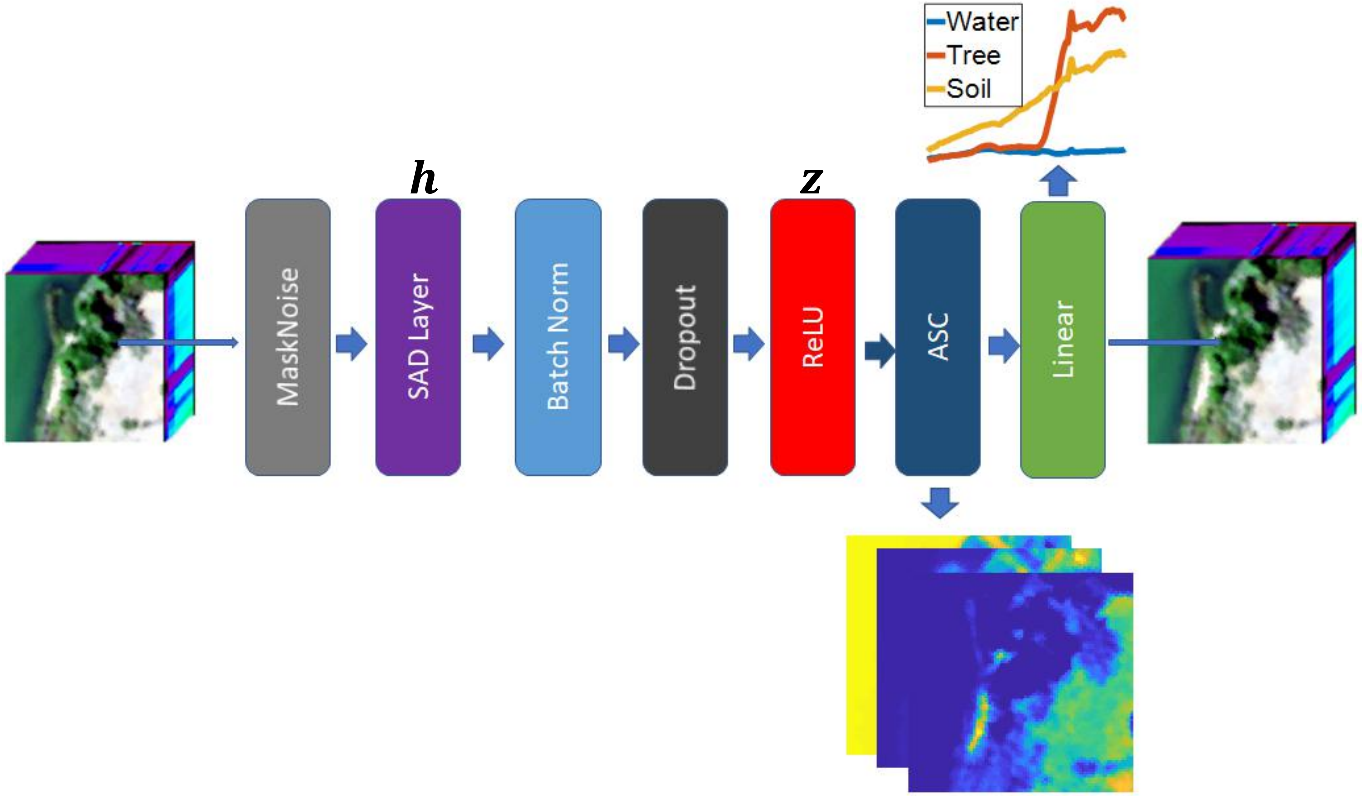
$$L_{\ell_2}(\boldsymbol{y}, \widehat{\boldsymbol{y}}) = \frac{\lambda_0}{2} ||\boldsymbol{y} - \widehat{\boldsymbol{y}}||_2^2 - \lambda_1 D_{KL}(1.0||C(\boldsymbol{y}, \widehat{\boldsymbol{y}})) + \lambda_2 ||\boldsymbol{z}||_1 + \lambda_3 ||\boldsymbol{W}_{en}||_F + \lambda_4 ||\boldsymbol{W}_{de}||_F + \lambda_5 ||\boldsymbol{\rho}||_2$$

$$C(\boldsymbol{y_i}, \boldsymbol{y_j}) = \mathbf{1.0} - \frac{\boldsymbol{SAD}(\boldsymbol{y_i}, \boldsymbol{y_j})}{\boldsymbol{\pi}}$$

$$BN(\boldsymbol{h}) = \frac{\boldsymbol{h} - \mu}{\sqrt{\sigma^2 + \epsilon}} + \boldsymbol{\rho}$$

$$ASC(\boldsymbol{z}^*) = \frac{\boldsymbol{z}^*}{||\boldsymbol{z}^*||_{\mathbf{1}} + \boldsymbol{\epsilon}}$$

$\boldsymbol{z}^*$ contains the n highest activations $\boldsymbol{z}$



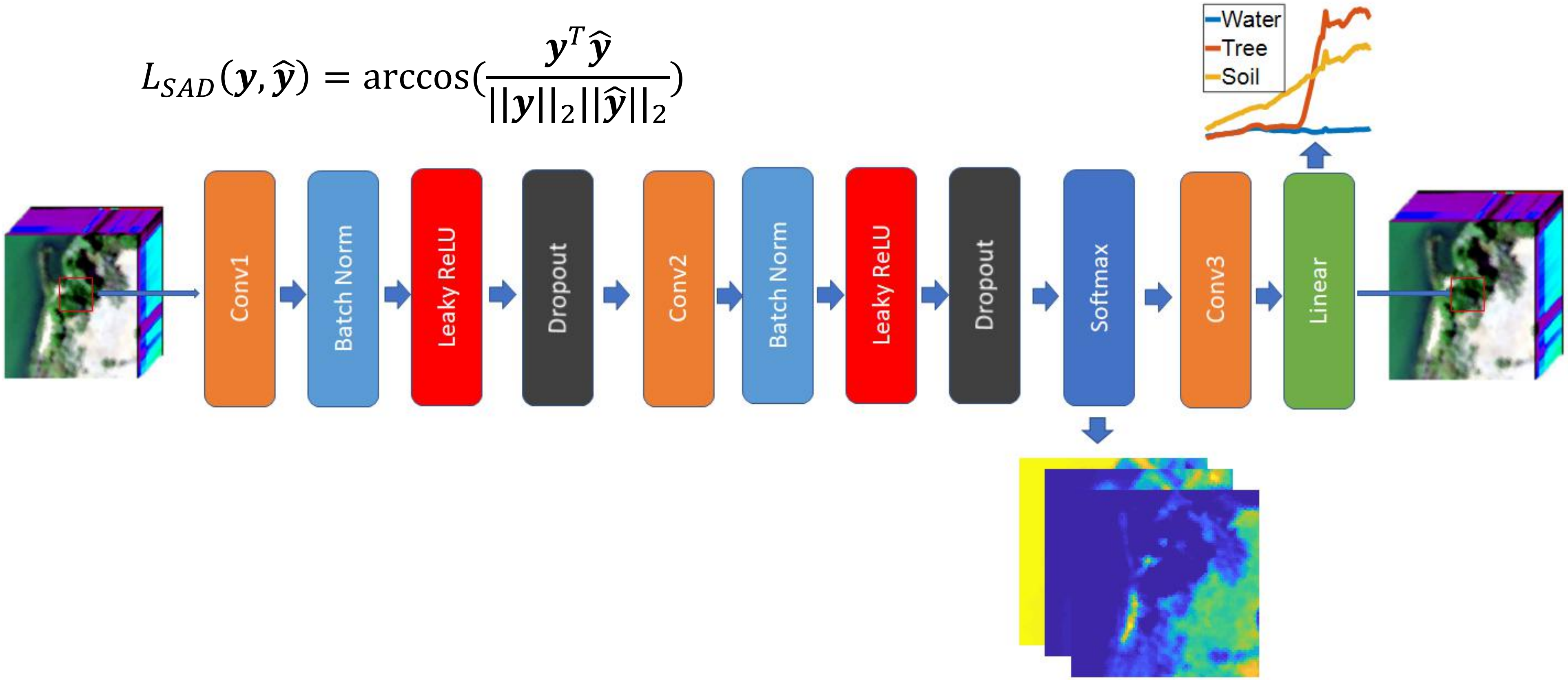

S. Ozkan, B. Kaya and G. B. Akar, "EndNet: Sparse AutoEncoder Network for Endmember Extraction and Hyperspectral Unmixing," in *IEEE Transactions on Geoscience and Remote Sensing*, vol. 57, no. 1, pp. 482-496, Jan. 2019, doi: 10.1109/TGRS.2018.2856929.

B. Palsson, J. R. Sveinsson and M. O. Ulfarsson, "Blind Hyperspectral Unmixing Using Autoencoders: A Critical Comparison," in *IEEE Journal of Selected Topics in Applied Earth Observations and Remote Sensing*, vol. 15, pp. 1340-1372, 2022, doi: 10.1109/JSTARS.2021.3140154.

# CNNAEU: Convolutional autoencoder for Unmixing

## Loss Function: SAD

$$L_{SAD}(\boldsymbol{y}, \widehat{\boldsymbol{y}}) = \arccos\left(\frac{\boldsymbol{y}^T \widehat{\boldsymbol{y}}}{||\boldsymbol{y}||_2 ||\widehat{\boldsymbol{y}}||_2}\right)$$



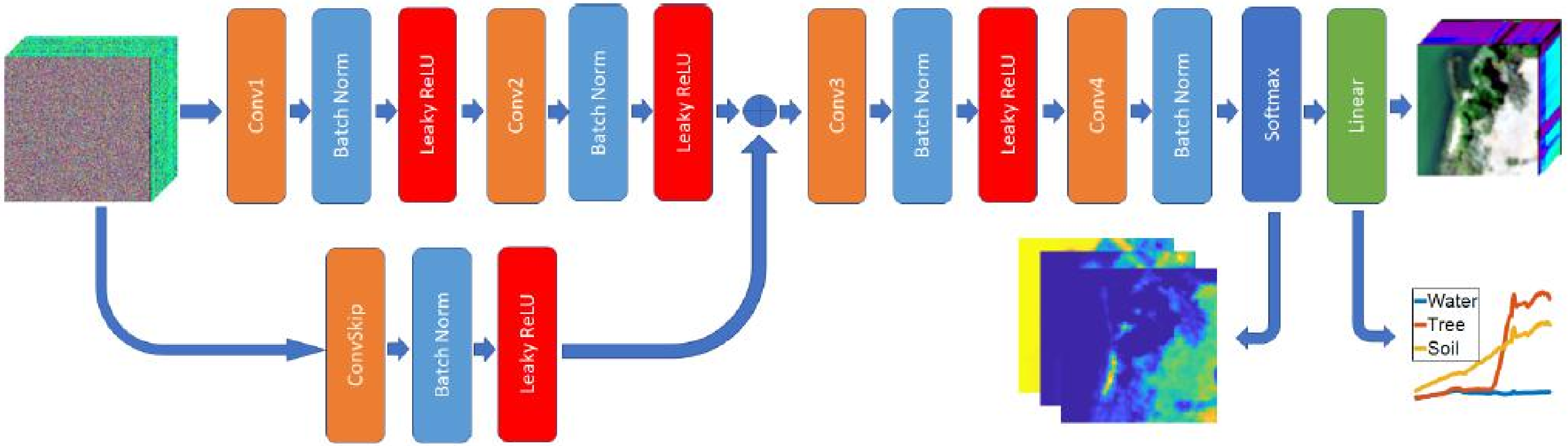

B. Palsson, M. O. Ulfarsson and J. R. Sveinsson, "Convolutional Autoencoder for Spectral–Spatial Hyperspectral Unmixing," in *IEEE Transactions on Geoscience and Remote Sensing*, vol. 59, no. 1, pp. 535-549, Jan. 2021, doi: 10.1109/TGRS.2020.2992743.

# MiSiCNet: Minimum Simplex Convolutional Network for Deep Hyperspectral Unmixing

$$\left(\widehat{\boldsymbol{E}},\widehat{\boldsymbol{A}}\right) = arg\min_{E,\,A}\frac{1}{2}||\boldsymbol{Y}-\boldsymbol{EA}||_F^2+\lambda_1||\boldsymbol{E}-\boldsymbol{m}\boldsymbol{1}_r^T||_F^2+\lambda_2 R(\boldsymbol{A})$$

$$\text{st. } \boldsymbol{1}_r^T\boldsymbol{A}=\boldsymbol{1_n}\,,\ \boldsymbol{A}\geq\boldsymbol{0}\,,\ 0\leq\boldsymbol{E}\leq 1$$

$$L\left(\boldsymbol{Y},\widehat{\boldsymbol{Y}},\widehat{\boldsymbol{\theta_2}},\boldsymbol{m}\right)=\frac{1}{2}||\boldsymbol{Y}-\widehat{\boldsymbol{Y}}||_F^2+\lambda_1||\widehat{\boldsymbol{\theta_2}}-\boldsymbol{m}\boldsymbol{1}_r^T||_F^2$$




B. Rasti, B. Koirala, P. Scheunders and J. Chanussot, "MiSiCNet: Minimum Simplex Convolutional Network for Deep Hyperspectral Unmixing," in *IEEE Transactions on Geoscience and Remote Sensing*, vol. 60, pp. 1-15, 2022, Art no. 5522815, doi: 10.1109/TGRS.2022.3146904.

# Metrics for Quantitative Measurements

- RMSE: the root mean squared error (RMSE) in percentage between the estimated and ground truth abundance fractions

$$\mathrm{RMSE}(\hat{\mathbf{A}}, \mathbf{A}) = 100 \times \sqrt{\frac{1}{rn} \sum_{i=1}^{r} \sum_{j=1}^{n} \left( \hat{\mathbf{A}}_{ij} - \mathbf{A}_{ij} \right)^2},$$

- SAD: The mean of the spectral angle distance (SAD) in degree between the estimated and ground truth endmembers:

$$\mathrm{SAD}(\mathbf{E}, \hat{\mathbf{E}}) = \frac{1}{r} \sum_{i=1}^{r} \arccos \left( \frac{\langle \mathbf{e}_{(i)}, \hat{\mathbf{e}}_{(i)} \rangle}{\left\| \mathbf{e}_{(i)} \right\|_2 \left\| \hat{\mathbf{e}}_{(i)} \right\|_2} \right) \frac{180}{\pi},$$

- SRE: Signal to reconstruction error (SRE) between the estimated and ground truth abundance fractions

$$SRE(A, \hat{A}) = 10log_{10}(\frac{||A||_F}{||A - \hat{A}||_F})$$

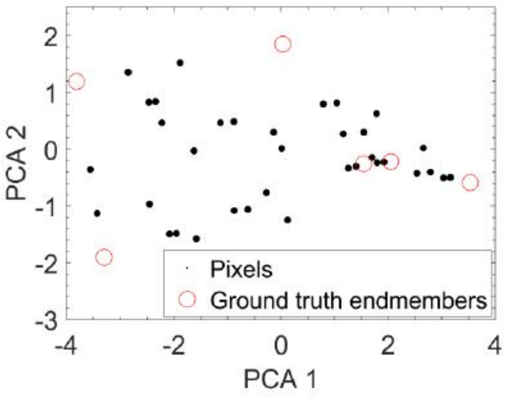



TABLE II
RMSE (SIMULATED 1). THE BEST PERFORMANCES ARE SHOWN IN BOLD.

| | FCLSU | UnDIP | uDAS | CyCUNet | Collab. | NMF-QMV | MiSiCNet |
|---|---|---|---|---|---|---|---|
| 20dB | 11.13±1.93 | 8.75±0.56 | 9.40±1.73 | 17.97±2.93 | 10.69±1.53 | **3.81±0.20** | 3.90±0.08 |
| 30dB | 12.28±3.44 | 7.19±0.87 | 9.40±1.91 | 17.83±4.73 | 11.22±2.29 | 1.81±0.42 | **1.80±0.04** |
| 40dB | 12.29±2.49 | 7.73±0.87 | 9.36±2.03 | 17.97±7.02 | 10.07±1.68 | 1.70±0.90 | **1.23±0.05** |
| 50dB | 11.15±2.72 | 7.36±0.88 | 8.46±2.04 | 16.07±0.76 | 10.35±2.02 | 3.71±0.74 | **1.21±0.08** |

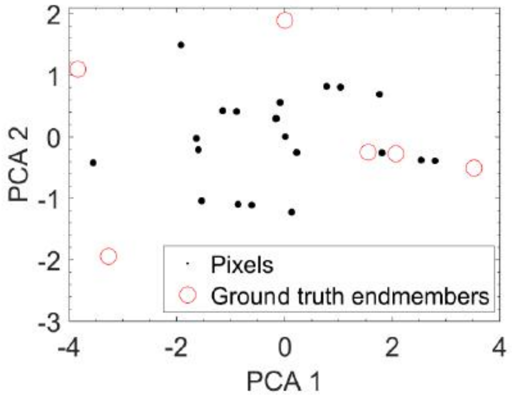



TABLE III
RMSE (SIMULATED 2). THE BEST PERFORMANCES ARE SHOWN IN BOLD.

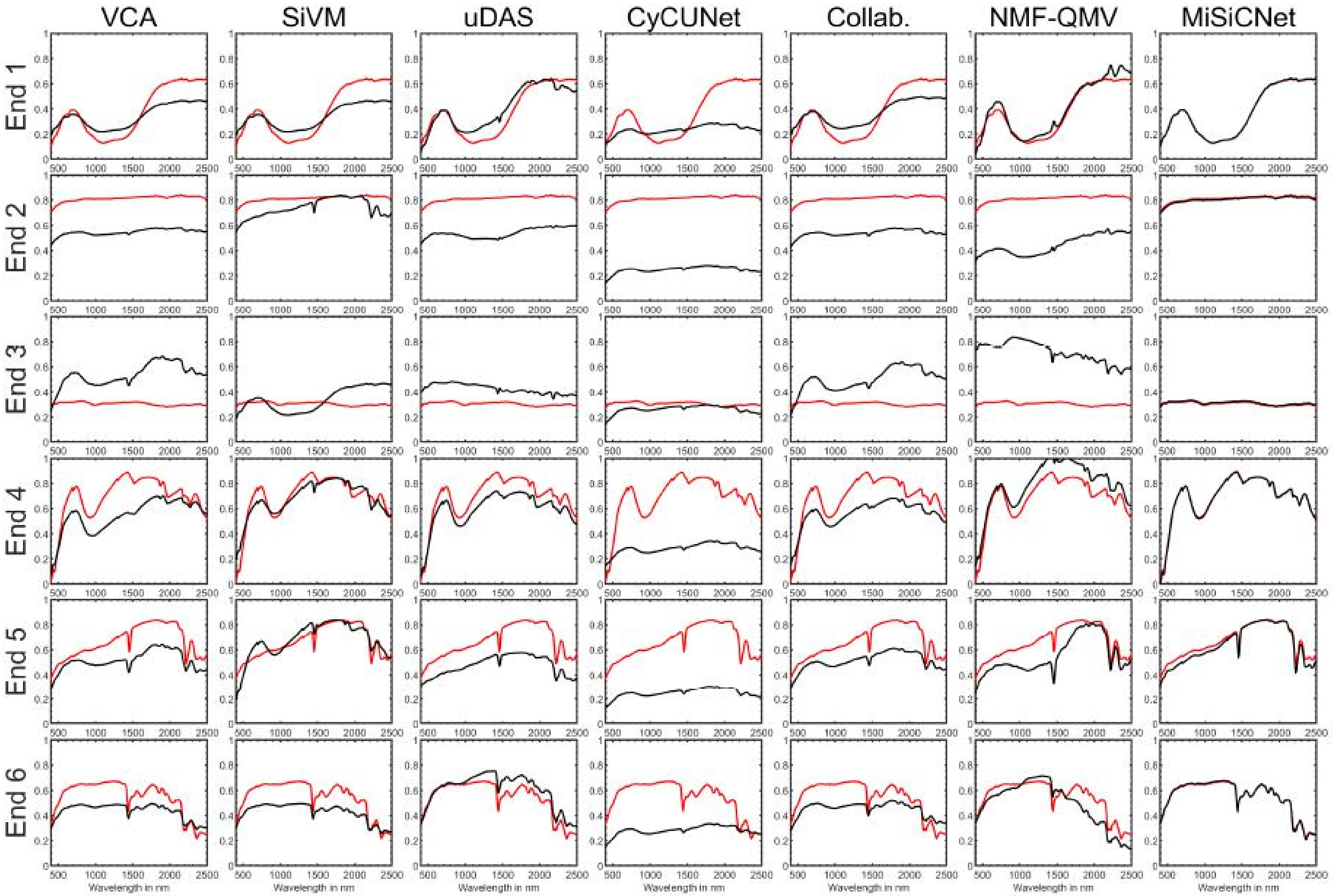
| | FCLSU | UnDIP | uDAS | CyCUNet | Collab. | NMF-QMV | MiSiCNet |
|---|---|---|---|---|---|---|---|
| 20dB | 12.55±1.89 | 12.15±1.04 | 11.43±2.69 | 19.51±5.89 | 12.05±0.61 | 4.03±0.54 | **3.96±0.04** |
| 30dB | 21.45±2.49 | 10.49±0.21 | 12.57±5.11 | 15.87±2.71 | 13.83±1.94 | 3.79±2.33 | **2.45±0.02** |
| 40dB | 21.6±4.11 | 10.52±0.22 | 10.84±4.29 | 14.57±1.3 | 14.11±1.93 | 7.37±1.13 | **2.15±0.03** |
| 50dB | 22.89±2.71 | 10.37±0.17 | 10.76±4.24 | 15.96±2.02 | 14.14±1.18 | 6.91±1.17 | **2.12±0.03** |

# Experimental Results

# Experimental Results

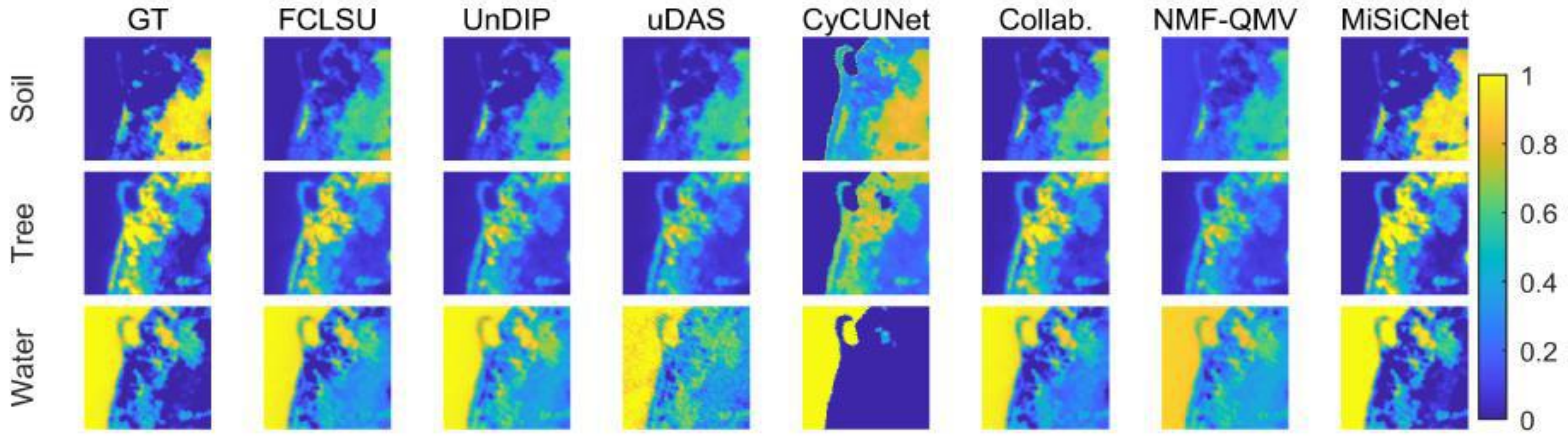
SAD (SIMULATED 2). THE BEST PERFORMANCES ARE SHOWN IN BOLD.

| | VCA | SiVM | uDAS | CyCUNet | Collab. | NMF-QMV | MiSiCNet |
|---|---|---|---|---|---|---|---|
| 20dB | 7.83±0.88 | 8.03±0.08 | 11.77±3.62 | 9.41±0.63 | 8.36±0.63 | 2.47±0.48 | **1.76±0.03** |
| 30dB | 7.72±1.29 | 7.83±0.02 | 14.68±4.42 | 9.73±0.5 | 7.21±0.57 | 8.45±7.73 | **0.83±0.02** |
| 40dB | 8.24±1.02 | 7.85±0.01 | 13.95±5.97 | 9.96±0.6 | 7.82±1.2 | 22.95±2.75 | **0.64±0.02** |
| 50dB | 7.73±1.23 | 7.86±0.01 | 14.47±5.77 | 10.57±0.23 | 7.65±0.28 | 24.13±1.26 | **0.62±0.02** |




40 dB

# Experimental Results

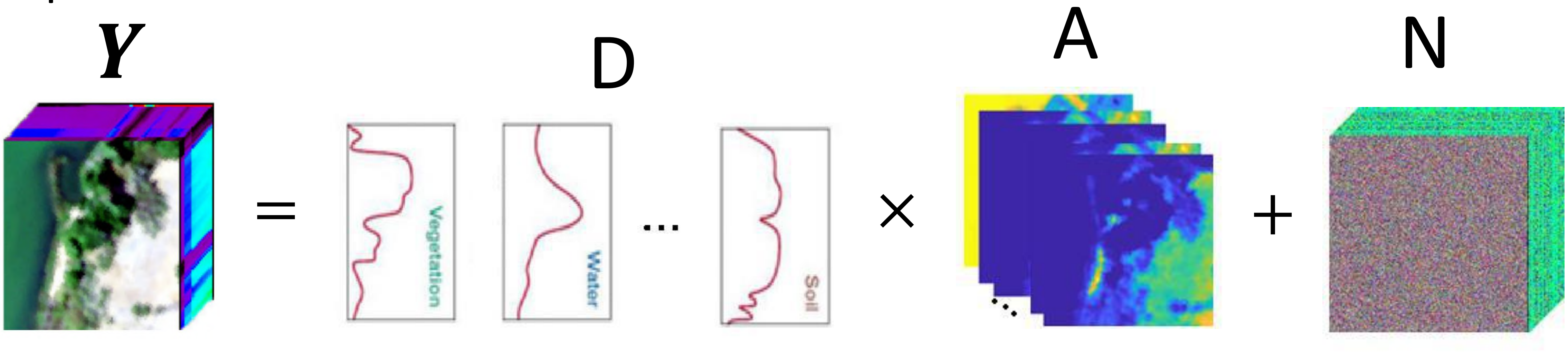



RMSE (SAMSON DATASET). THE BEST PERFORMANCES ARE SHOWN IN BOLD.

| | FCLSU | UnDIP | uDAS | CyCUNet | Collab. | NMF-QMV | MiSiCNet |
|---|---|---|---|---|---|---|---|
| Soil | 17.66 | 17.78 | 17.99 | 24.17 | 15.06 | 52.35 | **2.76** |
| Tree | 6.53 | 13.30 | 13.83 | 13.86 | 6.07 | 39.90 | **2.44** |
| Water | 14.92 | 20.96 | 23.03 | 26.54 | 11.81 | 45.98 | **2.07** |
| Overall | 13.87 | 17.63 | 18.67 | 22.21 | 11.59 | 46.36 | **2.44** |

# Sparse Unmixing (José M. Bioucas Dias)

- Only a few endmembers can reconstruct the mixed hyperspectral pixel




- Estimating A

$$(\widehat{\boldsymbol{A}}) = arg\min_{A} \frac{1}{2}||\boldsymbol{Y} - \boldsymbol{DA}||_F^2 + \lambda_1 \sum_{i=1}^{n} ||\boldsymbol{a}_{(\boldsymbol{i})}||_q$$

Observed data: $\boldsymbol{Y} \in \mathbb{R}^{p\times n}$
Endmember: **D**$\in \mathbb{R}^{p\times m}$
Abundances: $\boldsymbol{A} \in \mathbb{R}^{m\times n}$
Noise: $\boldsymbol{N} \in \mathbb{R}^{p\times n}$

# Sparse unmixing by variable splitting and augmented Lagrangian

- SUnSAL :

$$\left(\widehat{\boldsymbol{A}}\right) = arg\min_{A} \frac{1}{2} ||\boldsymbol{Y} - \boldsymbol{D}\boldsymbol{A}||_F^2 + \lambda_1 \sum_{\mathrm{i}=1}^{n} ||\boldsymbol{a}_{(\boldsymbol{i})}||_{\boldsymbol{1}} \text{ st. } \boldsymbol{1}_r^T\boldsymbol{A} = \boldsymbol{1}_{\boldsymbol{n}} \text{ , } \boldsymbol{A} \geq \boldsymbol{0}$$

- SUnSAL-TV:

$$\left(\widehat{\boldsymbol{A}}\right) = arg\min_{A} \frac{1}{2} ||\boldsymbol{Y} - \boldsymbol{D}\boldsymbol{A}||_F^2 + \lambda_1 \sum_{\mathrm{i}=1}^{n} ||\boldsymbol{a}_{(\boldsymbol{i})}||_{\boldsymbol{1}} + \lambda_2 TV(\boldsymbol{A}) \text{ st. } \boldsymbol{A} \geq \boldsymbol{0}$$

- Using the nonisotropic TV

$$TV(\boldsymbol{A}) = ||\boldsymbol{R}\boldsymbol{A}||_1 \text{ , } \boldsymbol{R}\boldsymbol{A} = \begin{bmatrix} \boldsymbol{D_h}\boldsymbol{A} \\ \boldsymbol{D_v}\boldsymbol{A} \end{bmatrix}$$

J. M. Bioucas-Dias and M. A. T. Figueiredo, "Alternating direction algorithms for constrained sparse regression: Application to hyperspectral unmixing," *2010 2nd Workshop on Hyperspectral Image and Signal Processing: Evolution in Remote Sensing*, 2010, pp. 1-4, doi: 10.1109/WHISPERS.2010.5594963.

M. -D. Iordache, J. M. Bioucas-Dias and A. Plaza, "Total Variation Spatial Regularization for Sparse Hyperspectral Unmixing," in *IEEE Transactions on Geoscience and Remote Sensing*, vol. 50, no. 11, pp. 4484-4502, Nov. 2012, doi: 10.1109/TGRS.2012.2191590.

# Sparse unmixing by variable splitting and augmented Lagrangian

- Collaborative sparse unmixing

$$(\widehat{\boldsymbol{A}}) = arg \min_{A} \frac{1}{2} ||\boldsymbol{Y} - \boldsymbol{D}\boldsymbol{A}||_F^2 + \lambda_1 \sum_{\mathbf{j}=1}^{m} ||\boldsymbol{a}_{\boldsymbol{j}}||_{\mathbf{2}} \text{ st., } \boldsymbol{A} \geq \mathbf{0}$$


M. -D. Iordache, J. M. Bioucas-Dias and A. Plaza, "Collaborative Sparse Regression for Hyperspectral Unmixing," in *IEEE Transactions on Geoscience and Remote Sensing*, vol. 52, no. 1, pp. 341-354, Jan. 2014, doi: 10.1109/TGRS.2013.2240001.

L. Drumetz, T. R. Meyer, J. Chanussot, A. L. Bertozzi and C. Jutten, "Hyperspectral Image Unmixing With Endmember Bundles and Group Sparsity Inducing Mixed Norms," in *IEEE Transactions on Image Processing*, vol. 28, no. 7, pp. 3435-3450, July 2019, doi: 10.1109/TIP.2019.2897254.

# SUnCNN: Sparse Unmixing Using Unsupervised Convolutional Neural Network

$$(\hat{\boldsymbol{A}}) = arg\min_{A} \frac{1}{2}||\boldsymbol{Y} - \boldsymbol{D}\boldsymbol{A}||_F^2 + \lambda_1 \sum_{\mathrm{i}=1}^{n} ||\boldsymbol{A}_{(\boldsymbol{i})}||_q \text{st. } \mathbf{1}_m^T\boldsymbol{A} = \mathbf{1}_{\boldsymbol{n}}\ ,\ \boldsymbol{A} \geq \mathbf{0}$$

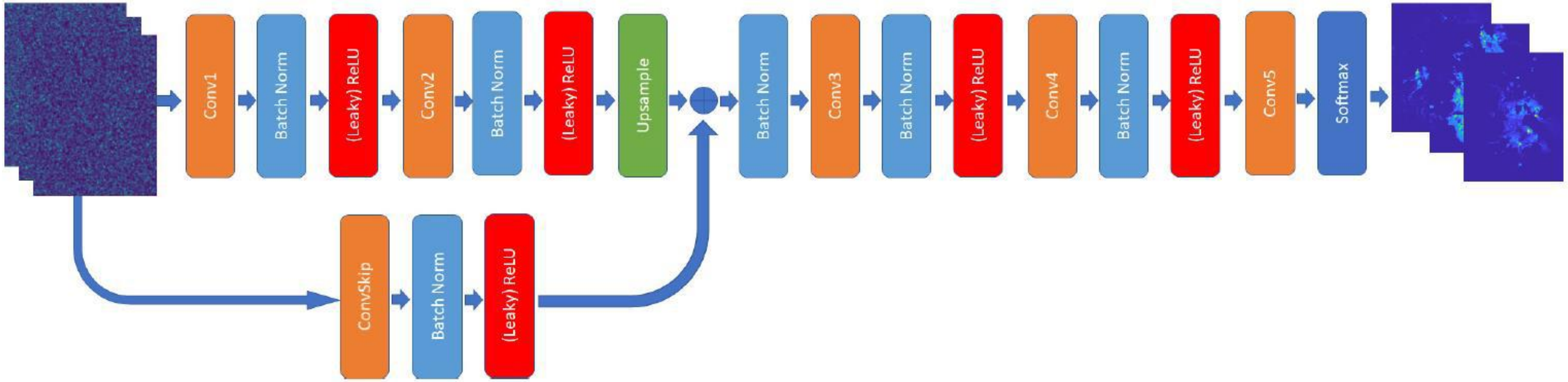
Image Prior

$$(\hat{\boldsymbol{A}}) = arg\min_{A} \frac{1}{2}||\boldsymbol{Y} - \boldsymbol{D}\boldsymbol{A}||_F^2 + \lambda_1 R(\boldsymbol{A}) \text{ st. } \mathbf{1}_m^T\boldsymbol{A} = \mathbf{1}_{\boldsymbol{n}}\ ,\ \boldsymbol{A} \geq \mathbf{0}$$

Deep Image Prior

$$(\hat{\boldsymbol{\theta}}) = arg\min_{\boldsymbol{\theta}} \frac{1}{2}||\boldsymbol{Y} - \boldsymbol{D}f_\theta(\boldsymbol{Z})||_F^2 \text{ st. } \hat{\boldsymbol{A}} = f_\theta(\boldsymbol{Z})$$

Holding the ANC and ASC Using a final softmax layer

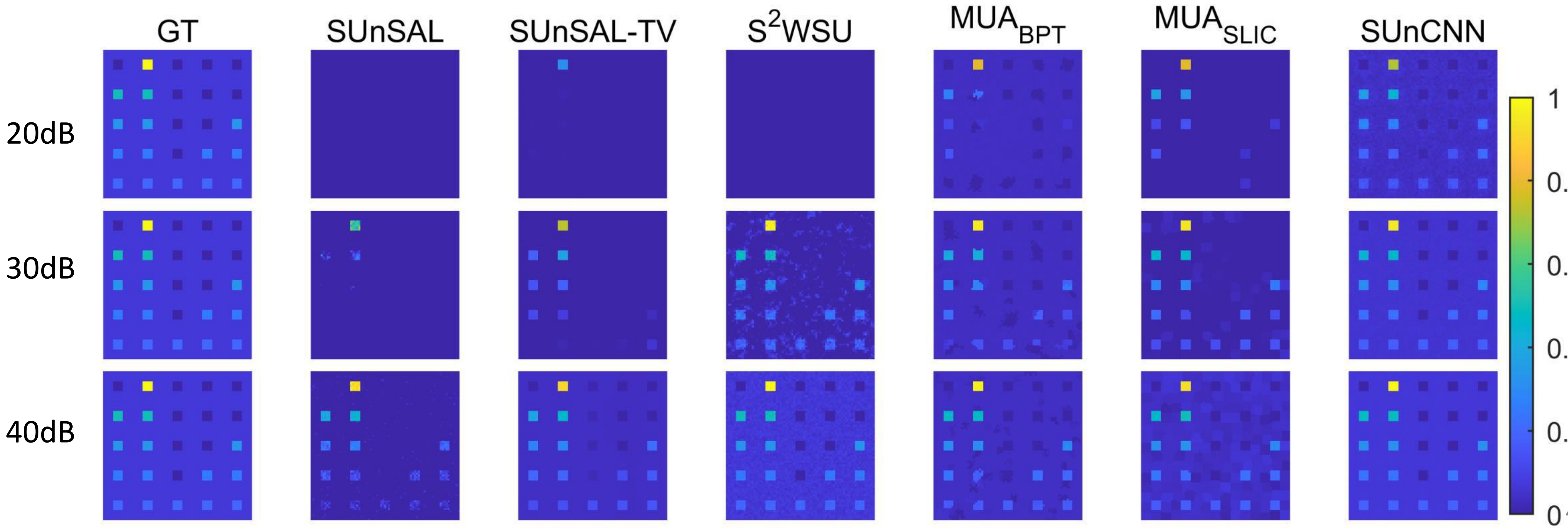



B. Rasti and B. Koirala, "SUnCNN: Sparse Unmixing Using Unsupervised Convolutional Neural Network," in *IEEE Geoscience and Remote Sensing Letters*, vol. 19, pp. 1-5, 2022, Art no. 5508205, doi: 10.1109/LGRS.2021.3100992.

# Experimental Results

## Signal to reconstruction error (SRE)

| SNR | SUnSAL | SUnSAL-TV | $S^2$WSU | $MUA_{BPT}$ | $MUA_{SLIC}$ | SUnCNN |
|---|---|---|---|---|---|---|
| 20 dB | 2.27 | 4.71 | 3.85 | **6.70** | 5.67 | 5.71 |
| 30 dB | 4.46 | 7.22 | 7.74 | 9.13 | 7.87 | **10.25** |
| 40 dB | 6.89 | 11.05 | 14.12 | 10.72 | 11.17 | **15.20** |



# Further Study

- Estimation of number of endmembers (Subspace Identification)

J. M. Bioucas-Dias and J. M. P. Nascimento, "Hyperspectral Subspace Identification," in *IEEE Transactions on Geoscience and Remote Sensing*, vol. 46, no. 8, pp. 2435-2445, Aug. 2008, doi: 10.1109/TGRS.2008.918089.

B. Rasti, M. O. Ulfarsson and J. R. Sveinsson, "Hyperspectral Subspace Identification Using SURE," in *IEEE Geoscience and Remote Sensing Letters*, vol. 12, no. 12, pp. 2481-2485, Dec. 2015, doi: 10.1109/LGRS.2015.2485999.

Chein-I Chang and Qian Du, "Estimation of number of spectrally distinct signal sources in hyperspectral imagery," in *IEEE Transactions on Geoscience and Remote Sensing*, vol. 42, no. 3, pp. 608-619, March 2004, doi: 10.1109/TGRS.2003.819189.

A. Ambikapathi, T. -H. Chan, C. -Y. Chi and K. Keizer, "Hyperspectral Data Geometry-Based Estimation of Number of Endmembers Using p-Norm-Based Pure Pixel Identification Algorithm," in *IEEE Transactions on Geoscience and Remote Sensing*, vol. 51, no. 5, pp. 2753-2769, May 2013, doi: 10.1109/TGRS.2012.2213261.

- Spectral Variability, endmember variabilities

R. A. Borsoi et al., "Spectral Variability in Hyperspectral Data Unmixing: A comprehensive review," in IEEE Geoscience and Remote Sensing Magazine

J. Theiler et al., "Spectral Variability of Remotely Sensed Target Materials: Causes, Models, and Strategies for Mitigation and Robust Exploitation," in IEEE Geoscience and Remote Sensing Magazine

- Nonlinear Unmixing

R. Heylen, M. Parente and P. Gader, "A Review of Nonlinear Hyperspectral Unmixing Methods," in *IEEE Journal of Selected Topics in Applied Earth Observations and Remote Sensing*, vol. 7, no. 6, pp. 1844-1868, June 2014, doi: 10.1109/JSTARS.2014.2320576.

B. Rasti, B. Koirala and P. Scheunders, "HapkeCNN: Blind Nonlinear Unmixing for Intimate Mixtures Using Hapke Model and Convolutional Neural Network," in *IEEE Transactions on Geoscience and Remote Sensing*, vol. 60, pp. 1-15, 2022, Art no. 5536315, doi: 10.1109/TGRS.2022.3202490.

- Comparison of Autoencoders for Blind Unmixing

B. Palsson, J. R. Sveinsson and M. O. Ulfarsson, "Blind Hyperspectral Unmixing Using Autoencoders: A Critical Comparison," in *IEEE Journal of Selected Topics in Applied Earth Observations and Remote Sensing*, vol. 15, pp. 1340-1372, 2022, doi: 10.1109/JSTARS.2021.3140154.

# Make sure you are ready to come all the way with us

- Check out the GitHub repository https://github.com/BehnoodRasti/Unmixing_Tutorial_IEEE_IADF
- If you don't have a GPU, then Make sure that you signed up for a google account so you can work with google colab.
- If you have a GPU of your own, then follow the instruction on the GitHub page and install the dependencies.
- Prerequisite: Basic concepts of deep/machine learning such as gradient descent, convolution, and autoencoder.

# Rules of the Game

- Here is the link to the GitHub repository for the IEEE IADF Summer School https://github.com/BehnoodRasti/Unmixing_Tutorial_IEEE_IADF
- Those who are experienced in programming should go ahead and do all the exercises.
- Those who are not experienced python programmers should use the colab button on the top of each method. Before running, make sure that you change the runtime and select GPU for your runtime. When switching between the notebooks, make sure you disconnect and delete runtime.
- Only for those who want to run the codes on their GPU: Read the instruction of the Readme file of the GitHub repository and follow the steps to install the requirements.
- We help everyone to run the codes and get the results, even those who don't know python and don't have GPU.
- Answering all the questions takes time, be patient and try to solve the problem yourself while we get to you. We try to answer in the chat for future reference.
- Please check the already asked question before writing your query. We might have already answered your question there.
- Upload the questions in chat, and we go one by one in order.

# Exercises for Blind and Supervised Unmixing

1. Run the supervised and blind unmixing approaches from the package and fill out the tables below.

| aRMSE | FCLSU | UnDIP | EDAA | EndNet | CNNAE | MiSiCNet |
|---|---|---|---|---|---|---|
| Road | | | | | | |
| Tree | | | | | | |
| Roof | | | | | | |
| Water | | | | | | |
| Overall | | | | | | |

| SAD | FCLSU | UnDIP | EDAA | EndNet | CNNAE | MiSiCNet |
|---|---|---|---|---|---|---|
| Road | | | | | | |
| Tree | | | | | | |
| Roof | | | | | | |
| Water | | | | | | |
| Overall | | | | | | |

# Exercises for Blind and Supervised Unmixing

2. Change the Endmember initialization for FCLSU and compare the results

| FCLSU | True Endmember | Random Pixel | VCA |
| --- | --- | --- | --- |
| aRMSE | | | |
| SAD | | | |

3. Change LR for the MiSiCNet approach and fill out the table below.

| MiSiCNet | LR=0.01 | LR=0.001 | LR=0.0001 |
| --- | --- | --- | --- |
| aRMSE | | | |
| SAD | | | |

4. Change lambMV for the MiSiCNet approach and fill out the table below.

| MiSiCNet | lambMV=1 | lambMV=10 | lambMV=100 |
| --- | --- | --- | --- |
| aRMSE | | | |
| SAD | | | |

# Exercises for Blind and Supervised Unmixing

4. Change nf for the MiSiCNet approach and fill out the table below.

| MiSiCNet | nf=64 | nf=128 | nf=256 |
|---|---|---|---|
| aRMSE | | | |
| SAD | | | |

5. Change num_iter1 for the MiSiCNet approach and fill out the table below.

| MiSiCNet | num_iter1 =4000 | num_iter1 =6000 | num_iter1 =8000 |
|---|---|---|---|
| aRMSE | | | |
| SAD | | | |

6. Apply the unmixing approach to the other datasets such as Samson and Jasper. Change the number of endmembers accordingly.

# Exercises for Sparse Unmixing

1. Run the SUnCNN.ipynb from the package and fill out the table below. This corresponds to the SNR=20dB.
2. Change the setup (as explained in the code) for DC2 and repeat exercise 1.
3. If you want to run the code for all the SNRs, then set the variable “tol1=npar.shape[1]” to fill out the rest of the table below. You should do that for DC1 and DC2 separately. This will take time.
4. Change the network hyperparameters such as the number of filters, the size of filters, and the number of iterations and see if you can fine-tune the network to get better results.
5. Set the PLOT flag to True and see how abundances change over the iterations compared to the GT abundances. This is a color image of three abundances. Plot all abundances and compare them with GT. Change the SNRs and compare the results for 40dB.
6. Comment out `plt.plot(out_LR_np.reshape(LibS,nr1*nc1))` to see the value of the abundance changes over the iterations. What do you observe and what is the reason for that?

Note that for reproducing the results in the manuscript, you should run the code 10 times and compute the mean. You can do that by setting tol2=10. This takes time.

| SRE | SNR=20dB | SNR=30dB | SNR=40dB |
|---|---|---|---|
| DC1 | ? | | |
| DC2 | ? | | |

# Appreciation

- Alexandre Zouaoui
- Dr. Bikram Koirala
- Prof. Paul Scheunders
- Prof. Julien Mairal
- Prof. Jocelyn Chanussot