Mineralogical analysis using linear unmixing with group exclusivity constraints

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Goal

- (semi-)supervised automatic detection for near-IR spectroscopy

- Summary (quick look) of the dataset

- Based on advance signal treatment and machine learning

- NO PRECISE QUANTIFICATION
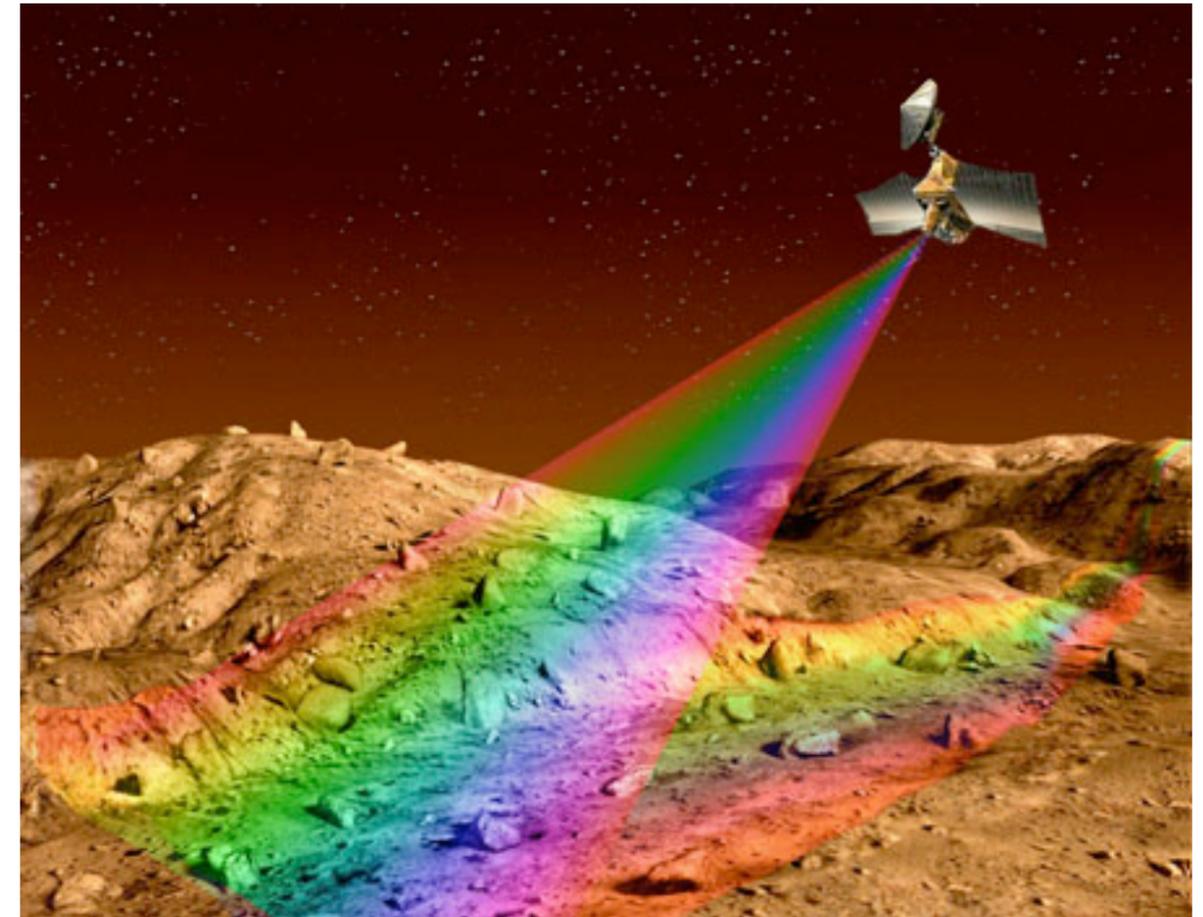
Theory

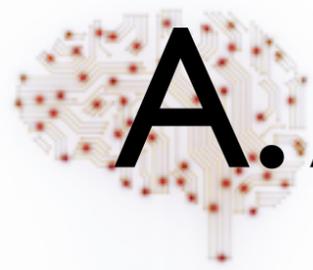- Estimation of endmember spectra (lab) and abundances under constraints:

Observation

Number of endmember

$$\mathbf{Y} = \sum_{i=1}^{N} A_i \cdot \mathbf{S_i}$$

subject to positivity sum-to-one

A. Non-linearities ? grain size ? aerosols ?

B. Large endmember set ?

Theory

- Estimation of endmember spectra (lab) and abundances under constraints:

Number of endmember

Observation

$$Y = \sum_{i=1}^{N} A_i . S_i$$

subject to positivity sum-to-one

A. Non-linearities ? grain size ? aerosols ?

B. Large endmember set ?

A. Approximation of non-linearities

- Simple non-linearity of abundances, under constraints

$$\mathbf{Y} = \sum_{i=1}^{N} A_i . \mathbf{S_i}^{\alpha} + \beta$$
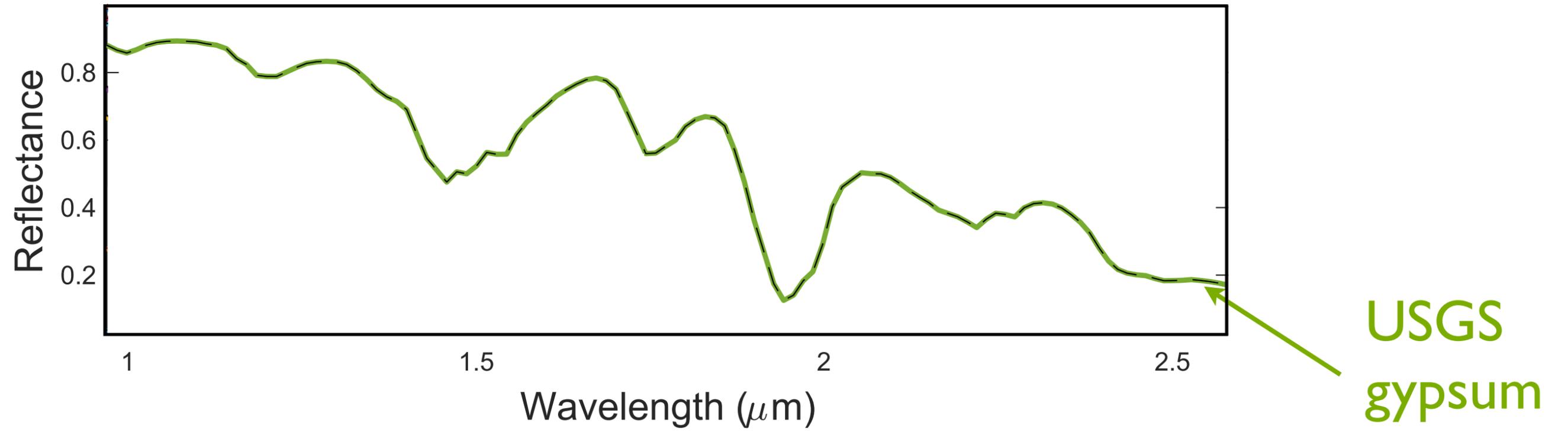
- **Test of radiative transfer ?**
Shkuratov et al., 1999

$$R_b = \frac{\int_0^{2\pi} d\psi \int_0^{\pi/4} d\theta \cdot R_o(n, \theta)}{\int_0^{2\pi} d\psi \int_0^{\pi/2} d\theta \cdot \frac{1}{\cos\theta} \cdot \sin\theta}$$

$$= 2 \int_0^{\pi/4} d\theta \cdot \exp\left(-\frac{4\pi k}{\lambda} \sum_{v=0}^{m} s_v\right) \cdot \prod_{v=0}^{m} R(\theta_v),$$ (9a)

$$I = I_o \cdot T(\theta_{em}) \cdot T(\theta_{in}) \cdot \exp\left(-\frac{4\pi k}{\lambda} \sum_{v=0}^{m} \cdot \frac{1}{\sin\theta}\right) \cdot \prod_{v=0}^{m} R(\theta_v),$$

$$r_b = R_b + \frac{1}{2} T_e T_i R_i \exp(-2\tau)/(1 - R_i \exp(-\tau)),$$

$$= 2 \int_0^{\pi/2} d\theta \cdot R_o(n, \theta) \cdot \frac{1}{\cos\theta} \cdot \sin\theta,$$

$$r_f = R_f + T_e T_i \exp(-\tau) + \frac{1}{2} T_e T_i R_i \exp(-2\tau)/$$

$$(1 - R_i \exp(-\tau)).$$

$$A = \frac{1 + \rho_b^2 - \rho_f^2}{2\rho_b} - \sqrt{\left(\frac{1 + \rho_b^2 - \rho_f^2}{2\rho_b}\right)^2 - 1}.$$ (12)

(6b)

Grain size

USGS gypsum

Grain size

grain size /5

Shkuratov et al., 1999

USGS gypsum

Reflectance

Wavelength (μm)

Reflectance

Grain size

grain size /5

Shkuratov et al., 1999

USGS
gypsum

grain
size

——	fact=1000
——	fact=100
——	fact=10
——	fact=5
——	fact=1
——	fact=1/5
——	fact=1/10
——	fact=1/100
——	fact=1/1000

Reflectance

Wavelength (μm)

Reflectance

Grain size

grain size /5

Shkuratov et al., 1999

USGS gypsum

grain size (decreasing, shown as wedge)
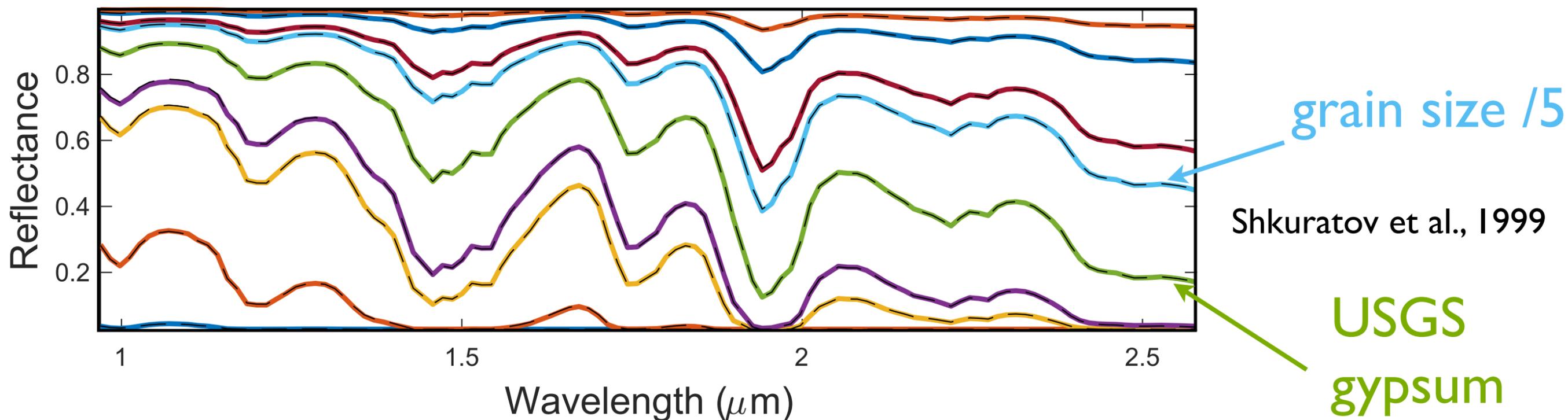
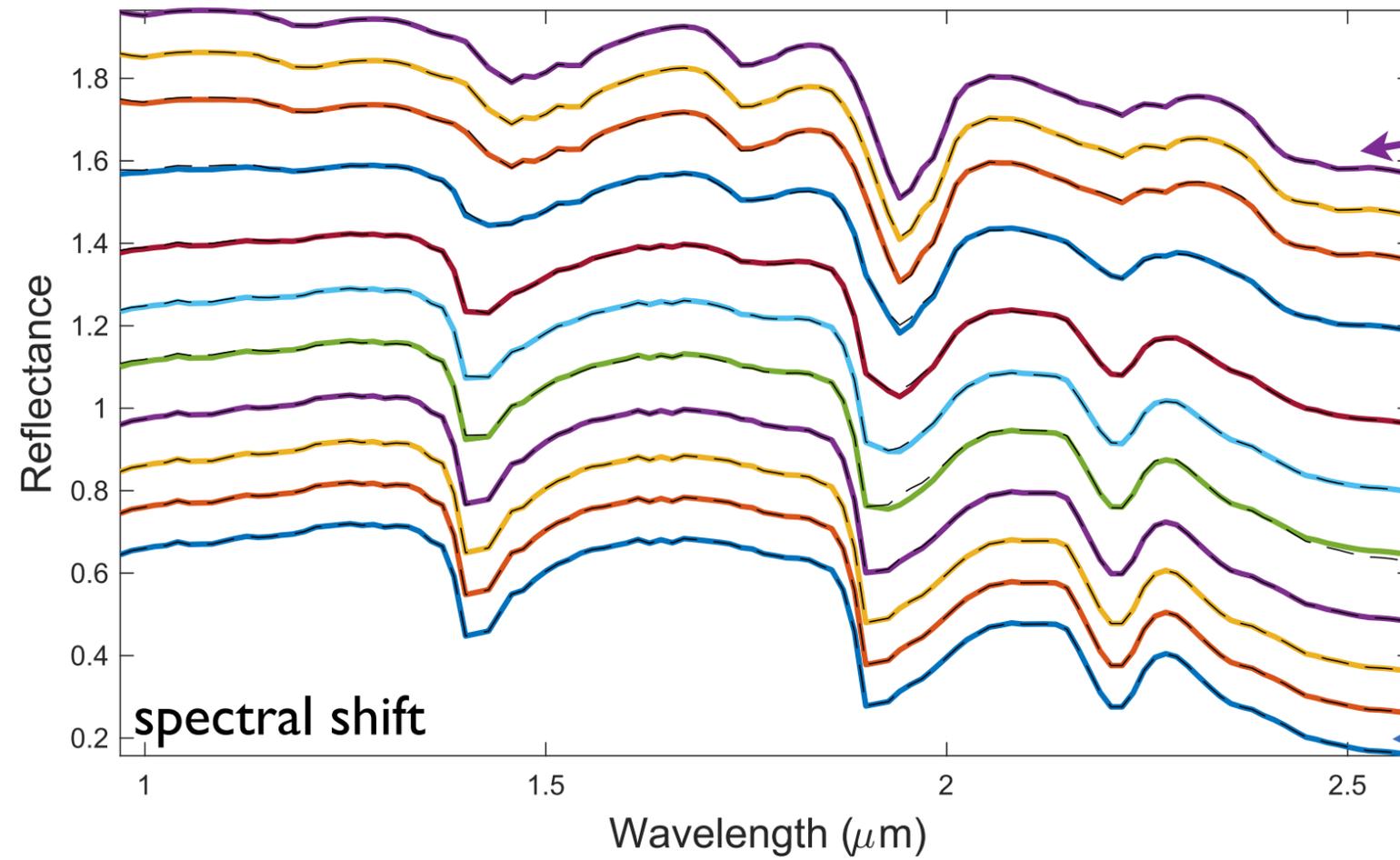|		
fact=1000	:	α=36.69 β=0.03 RMS=2.5e-04
fact=100	:	α=10.78 β=0.03 RMS=1.9e-03
fact=10	:	α=3.38 β=0.02 RMS=2.4e-03
fact=5	:	α=2.36 β=0.02 RMS=3.0e-03
fact=1	:	α=1 β=0 RMS=0.0e+00
fact=1/5	:	α=0.45 β=0 RMS=1.1e-03
fact=1/10	:	α=0.32 β=0 RMS=1.0e-03
fact=1/100	:	α=0.1 β=0 RMS=4.5e-04
fact=1/1000	:	α=0.03 β=0 RMS=1.5e-04

- excellent fit !

$$\mathbf{Y} = \sum_{i=1}^{N} A_i . \mathbf{S_i}^{\alpha} + \beta$$

Granular mixture

USGS pure gypsum X10

USGS pure smectite /10

Shkuratov et al., 1999

spectral shift

Reflectance vs Wavelength (μm)

- prop=1: ab=0.99 α1=3.22 α2=230.25 β=0.01 RMS=8.6e-05
- prop=0.999: ab=0.99 α1=3.22 α2=63.9 β=0.01 RMS=8.7e-05
- prop=0.99: ab=0.99 α1=3.21 α2=40.27 β=0.01 RMS=1.5e-04
- prop=0.9: ab=0.97 α1=3.19 α2=26.28 β=0.03 RMS=1.3e-03
- prop=0.667: ab=0.95 α1=2.25 α2=1.94 β=-0.03 RMS=6.9e-03
- prop=0.5: ab=0.75 α1=3.1 α2=0.22 β=0.01 RMS=2.0e-03
- prop=0.333: ab=0.62 α1=3.05 α2=0.24 β=0.01 RMS=3.0e-03
- prop=0.1: ab=0.3 α1=2.91 α2=0.27 β=0 RMS=4.5e-03
- prop=0.01: ab=-0.15 α1=0 α2=0.26 β=-0.01 RMS=3.3e-03
- prop=0.001: ab=0 α1=1.67 α2=0.32 β=0 RMS=1.1e-03
- prop=0: ab=-0.08 α1=0 α2=0.29 β=0 RMS=2.4e-04

ze

β=0.03 RMS=2.5e-04
β=0.03 RMS=1.9e-03
=0.02 RMS=2.4e-03
=0.02 RMS=3.0e-03
RMS=0.0e+00
=0 RMS=1.1e-03
=0 RMS=1.0e-03
0 RMS=4.5e-04
=0 RMS=1.5e-04

- excellent fit !

$$\mathbf{Y} = \sum_{i=1}^{N} A_i . \mathbf{S_i}^{\alpha} + \beta$$

Approximation

$$Y = \sum_{i=1}^{N} A_i . S_i^{\alpha} + \beta$$
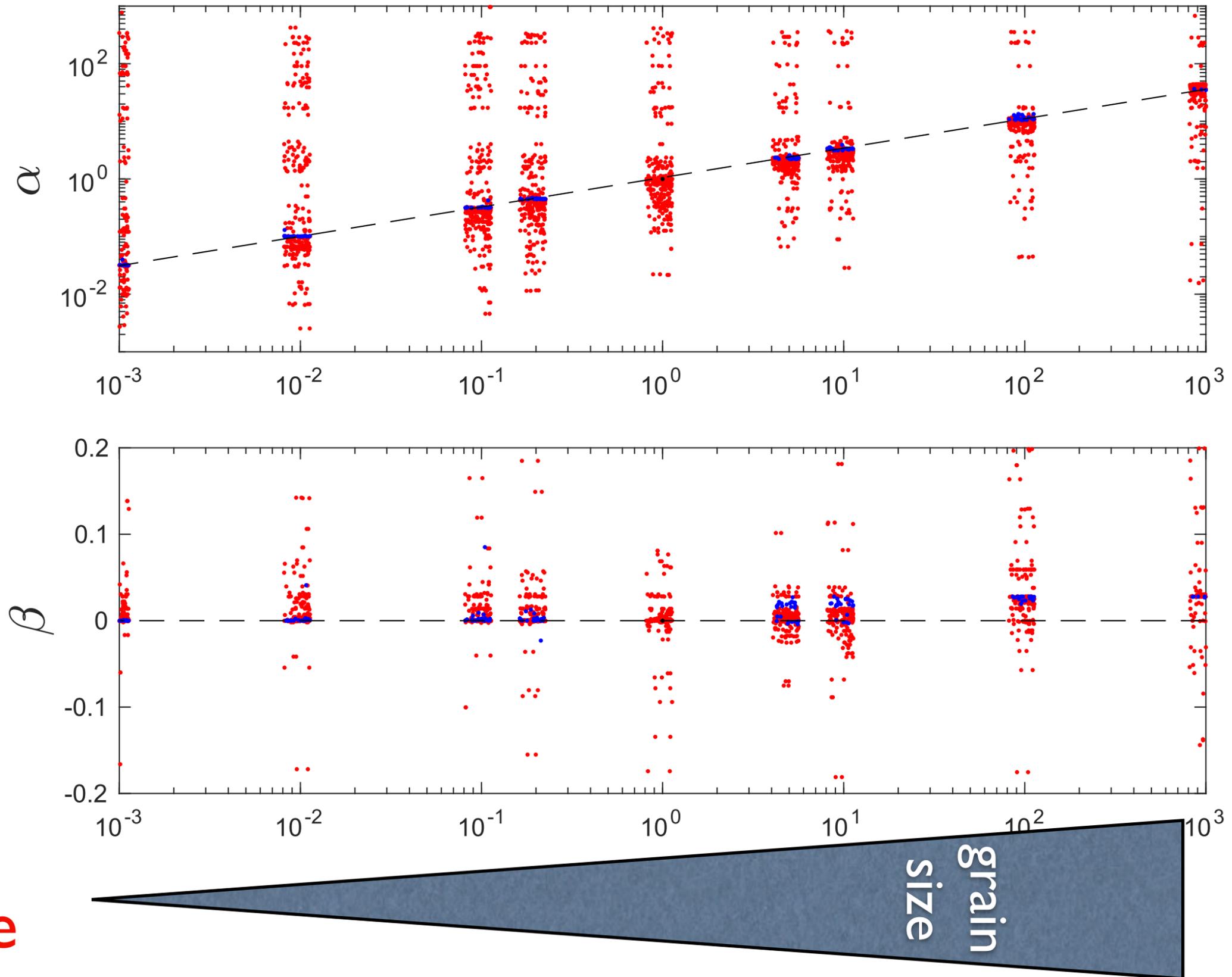
- ## 26 minerals

Schmidt, F.; Legendre, M. & Le Mouëlic, S. Minerals detection for hyperspectral images using adapted linear unmixing: LinMin *Icarus*, **2014**, *237*, 61-74, http://dx.doi.org/10.1016/j.icarus.2014.03.044

- ## Excellent fit (98% RMS < 10⁻²)

- Clear trend for grain size
- No trend for granular mixture

Approximation

- Simple non-linearity of abundances, under constraints

$$\mathbf{Y} = \sum_{i=1}^{N} A_i . \mathbf{S_i}^{\alpha} + \beta$$

- **Test of Martian aerosols effect ?**

Aerosols Vincendon et al., 2007;

DISORT Stamnes et al., 1988
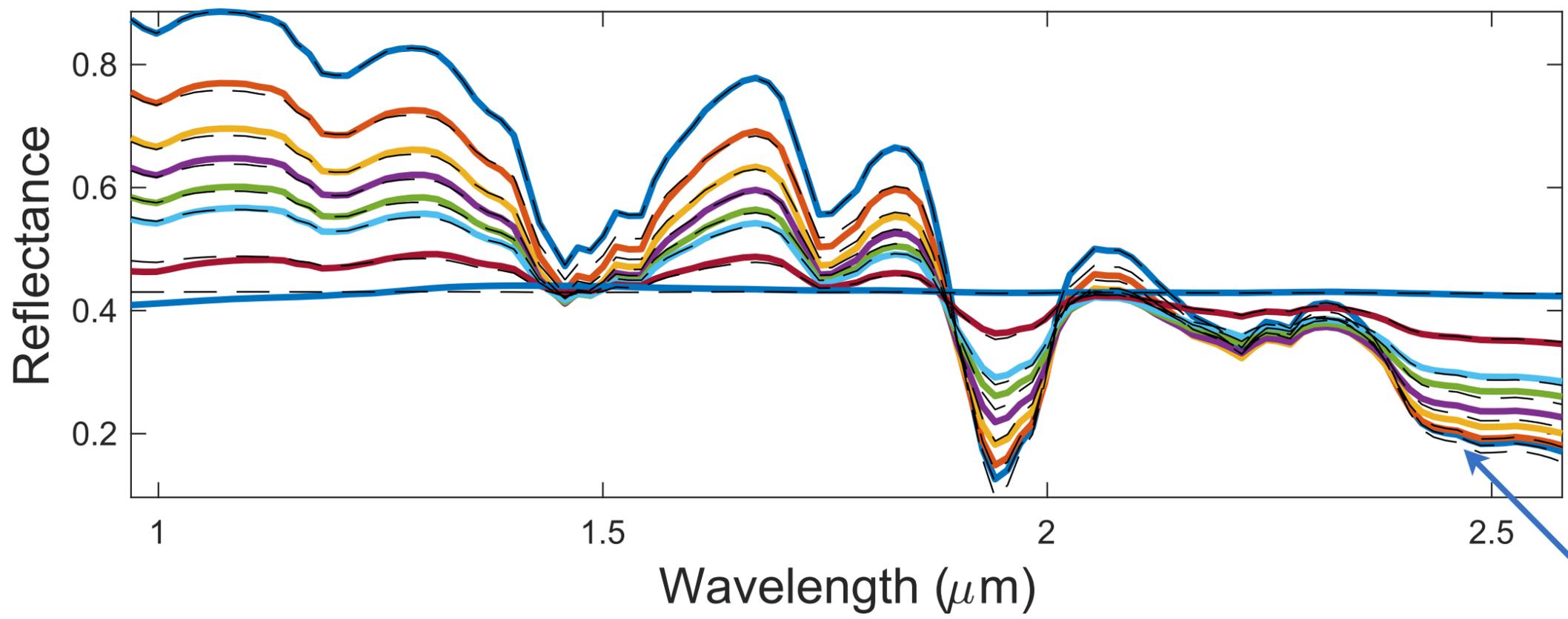
$$I = I_{\rm o} \cdot T(\theta_{\rm em}) \cdot T(\theta_{\rm in}) \cdot \exp\left(-\frac{4\pi k}{\lambda} \cdot \sum_{v=0}^{m} s_v\right) \cdot \prod_{v=0}^{m} R(\theta_v),$$ (9a)

$$R_b = \frac{\int_0^{2\pi} d\psi \int_0^{\pi/4} d\theta \cdot R_{\rm o}(n, \theta)}{\int_0^{2\pi} d\psi \int_0^{\pi/2} d\theta} = 2\int_0^{\pi/4} d\theta \cdot \frac{R_{\rm o}(n, \theta)}{\cos\theta \cdot \sin\theta}$$

$$r_b = R_b + \frac{1}{2} T_e T_i R_i \exp(-2\tau)/(1 - R_i \exp(-\tau)),$$

$$= 2\int_0^{\pi/2} \frac{d\psi \int_0^{\pi/4} d\theta \cdot R_{\rm o}(n, \theta)}{\cos\theta \cdot \sin\theta}$$

$$r_b = R_b + T_e T_i \exp(-\tau) + \frac{1}{2} T_e T_i R_i \exp(-2\tau)/$$

$$(1 - R_i \exp(-\tau)).$$ (12)

$$A = \frac{1 + \rho_b^2 - \rho_f^2}{2\rho_b} - \sqrt{\left(\frac{1 + \rho_b^2 - \rho_f^2}{2\rho_b}\right)^2 - 1}.$$ (6b)

Martian aerosols

Vincendon et al., 2007
Stamnes et al., 1988

USGS pure gypsum

• Excellent fit
(96% RMS < 10⁻²)

dust
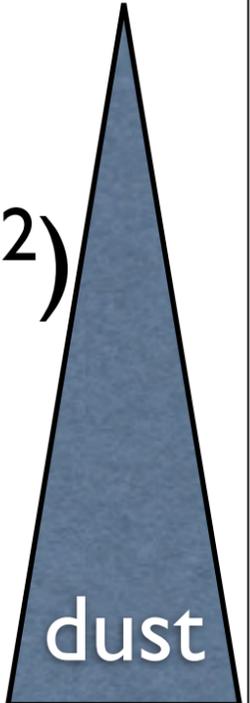
aot=0.01:	α=0.98	β=-0.01 RMS=1.3e-03
aot=0.22:	α=0.64	β=-0.17 RMS=1.4e-02
aot=0.51:	α=0.63	β=-0.16 RMS=1.2e-02
aot=0.92:	α=0.62	β=-0.16 RMS=9.8e-03
aot=1.61:	α=0.55	β=-0.19 RMS=7.3e-03
aot=2.3:	α=0.58	β=-0.18 RMS=4.0e-03
aot=5:	α=0.26	β=-0.38 RMS=5.5e-03
aot=20:	α=0.01	β=-0.56 RMS=6.7e-03

Approximation

- Simple non-linearity of abundances, under constraints

$$Y = \sum_{i=1}^{N} A_i . S_i^{\alpha} + \beta$$

- **Test of radiative transfer** ✅
- **Test of Martian aerosols effect** ✅

$$R_b = \frac{\int_0^{2\pi} d\psi \int_0^{\pi/4} d\theta \cdot R_o(n,\theta)}{\int_0^{2\pi} d\psi \int_0^{\pi/2} d\theta \cdot R_o(n,\theta)}$$

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$$I = I_o \cdot T(\theta_{em}) \cdot T(\theta_{in}) \cdot \exp\left(-\frac{4\pi\kappa}{\lambda} \cdot \sum_{v=0}^{m} S_v\right) \cdot \prod_{v=0}^{m} R(\theta_v),$$

$$r_b = R_b + \frac{1}{2} T_e T_i R_i \exp(-2\tau)/(1 - R_i \exp(-\tau)), \quad (9a)$$

$$= 2\int_{\pi/4}^{\pi/2} d\theta \cdot R_o(n,\theta) \cdot \cos\theta \cdot \sin\theta,$$

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$$(1 - R_i \exp(-\tau)).$$

$$A = \frac{1 + \rho_b^2 - \rho_f^2}{2\rho_b} - \sqrt{\left(\frac{1 + \rho_b^2 - \rho_f^2}{2\rho_b}\right)^2 - 1}. \quad (12)$$

$$(6b)$$

NO QUANTIFICATION !

Schmidt, F. Approximation of Radiative Transfer for Surface Spectral Features *IEEE Geoscience and Remote Sensing Letters, Institute of Electrical and Electronics Engineers (IEEE)*, **2023**, *20*, 1-3, http://dx.doi.org/10.1109/lgrs.2023.3263356

Gurgurewicz, J., et al., **2022**. Megashears and hydrothermalism at the Martian crustal dichotomy in Valles Marineris. *Nature Communications Earth and Environment*, 3(1).

Theory

- Estimation of endmember spectra (lab) and abundances under constraints:

Number of endmember

Observation

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subject to
positivity
sum-to-one

A. Non-linearities ? grain size ? aerosols ?

B. **Large endmember set ?**

Algorithms

$$y(\lambda) = \sum_{i=1}^{N_s} S_i(\lambda).a_i$$

$$\min \|\mathbf{y} - S\mathbf{a}\|, a_i > 0, \sum_{i=1}^{N_s} a_i = 1$$

- **FCLS**

  Heinz, D. & I-Chang, C., TGRS, **2001**, *39*, 529-545,

- **MELSUM**

  Combe, J.-P.; et al., Analysis of OMEGA/Mars Express data hyperspectral data using a Multiple-Endmember Linear Spectral Unmixing Model (MELSUM): Methodology and first results *Planetary and Space Science*, **2008**, *56*, 951-975, http://dx.doi.org/10.1016/j.pss.2007.12.007

- **Primal-dual interior-point**

  Chouzenoux, E.; Legendre, M.; Moussaoui, S. & Idier, J. Fast Constrained Least Squares Spectral Unmixing Using Primal-Dual Interior-Point Optimization *Selected Topics in Applied Earth Observations and Remote Sensing, IEEE Journal of*, **2014**, *7*, 59-69, http://dx.doi.org/10.1109/JSTARS.2013.2266732

- **GPU implementation**

  Legendre, M.; Capriotti, L.; Schmidt, F.; Moussaoui, S. & Schmidt, A. GPU implementation issues for fast unmixing of hyperspectral images *EGU General Assembly Conference Abstracts*, **2013**, *15*, 11686,

- **LIMITATIONS : 50 endmembers << 100 wavelengths**

  How to deal with large spectral database (500 spectra) ?

Spectral database

- Selection of ~500 spectra from USGS

Clark, R. N.; Swayze, G. A.; Wise, R.; Livo, K. E.; Hoefen, T. M.; Kokaly, R. F. & Sutley, S. J. USGS Digital Spectral Library splib05a *U.S. Geological Survey, U.S. Geological Survey,* **2003** http://speclab.cr.usgs.gov/spectral-lib.html

Spectra in the library

	Family name	Minerals
Tectosilicates	Plagioclases	Andesine Anorthite Bytownite Labradorite Oligoclase
	Feldspars	Adularia Buddingtonite Celsian
	Zeolites	Analcime Chabazite Clinoptilolite Heulandite
		Laumontite Mordenite Natrolite Scolecite Stilbite
	Others	Dipyre Lazurite Marialite Mizzonite Nepheline
Cyclosilicates		Axinite Beryl Cordierite Elbaite Tourmaline
Inosilicates	Pyroxenes	Acmite Augite Bronzite Diopside Enstatite Fassaite
		Hedenbergite Hypersthene Jadeite Pigeonite Pyroxene Spodumene
	Amphiboles	Actinolite Amphibole Anthophyllite Cummingtonite
		Glaucophane Holmquistite Hornblende Hornblende_Fe
		Hornblende_Mg Richterite Riebeckite
		Smaragdite Tremolite Uralite
	Others	Pectolite Rhodonite
Nesosilicates	Olivines	Monticellite Olivine Tephroite
	Garnets	Almandine Andradite Grossular
		Hydrogrossular Spessartine Uvarovite
	Others	Andalusite Datolite Dumortierite Sillimanite
		Sphene Staurolite Topaz Zircon
Phyllosilicates	Chlorites	Chlorite Clinochlore Clinochlore_Fe Cookeite
		Corrensite Prochlorite Thuringite
	Biotites	Annite Biotite Siderophyllite
	Micas	Illite Lepidolite Margarite Muscovite Paragonite
		Phlogopite Rectorite Roscoelite
	Clays	Ammonio-Illite/Smec Ammonio-Smectite Endellite Halloysite
		Hectorite Kaolinite Montmorillonite Nacrite Nontronite
		Palygorskite Pyrophyllite Saponite Sauconite
		Sepiolite Talc Vermiculite
	Serpentines	Antigorite Chrysotile Cronstedtite Dickite Lizardite Serpentine
Sorosilicates		Allanite Clinozoisite Epidote Vesuvianite Zoisite
Oxides	Iron oxides	Chromite Ferrihydrite Goethite Hematite Ilmenite
		Lepidocrosite Maghemite Magnetite
	Others	Brookite Brucite Cassiterite Chalcedony Corundum
		Cuprite Diaspore Europium_Oxide Gibbsite Manganite
		Neodymium_Oxide Niter Praseodymium_Oxide
		Psilomelane Rutile Samarium_Oxide
Sulfides		Arsenopyrite Chalcopyrite Covellite Galena
		Pyrite Pyrrhotite Sphalerite
Sulfates		Alunite Ammonio-jarosite Ammonioalunite Barite Bassanite
		Bloedite Butlerite Copiapite Coquimbite Epsomite Eugsterite
		Gypsum Jarosite Kainite Mascagnite Mirabilite
		Polyhalite Syngenite
Carbonates		Calcite Dolomite Rhodochrosite Siderite Strontianite Witherite
	Na - rich	Gaylussite Trona
	Cu - rich	Azurite Malachite
Halides		Ammonium_Chloride Carnallite
Phosphates		Hydroxyl-Apatite Monazite
Borates		Colemanite Howlite Pinnoite Rivadavite Tincalconite Ulexite
Others		Opal
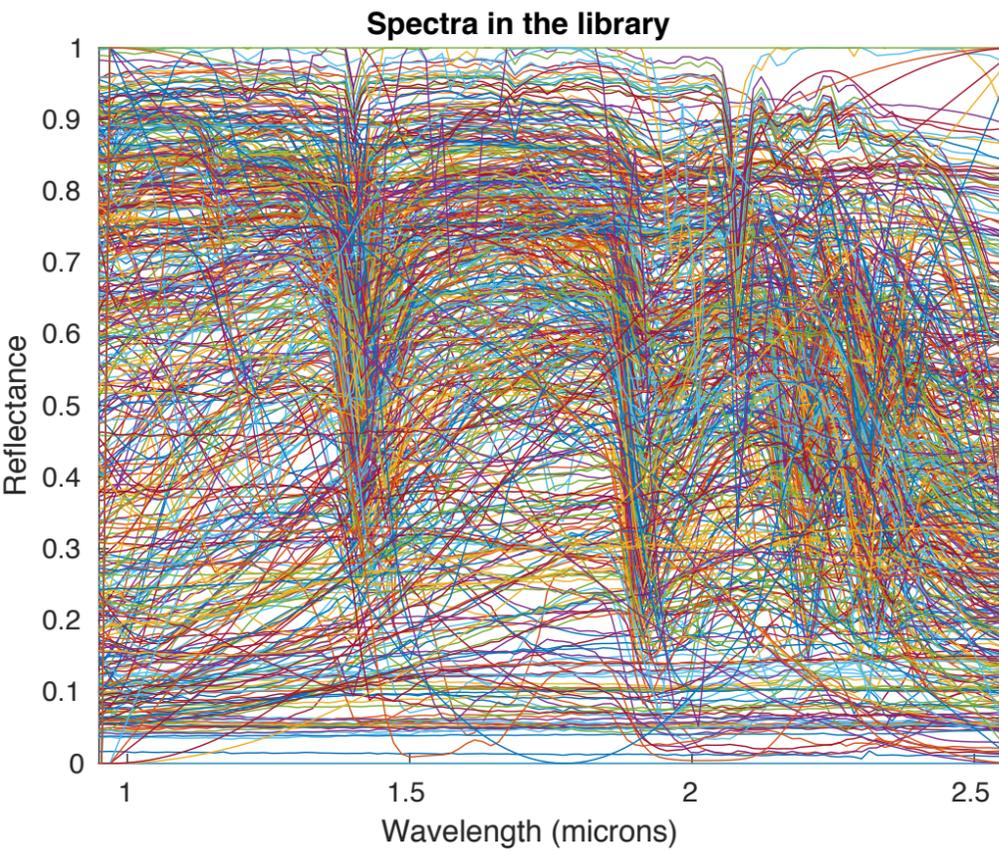
Spectra in the defined families (from 1 to 2.5 microns)
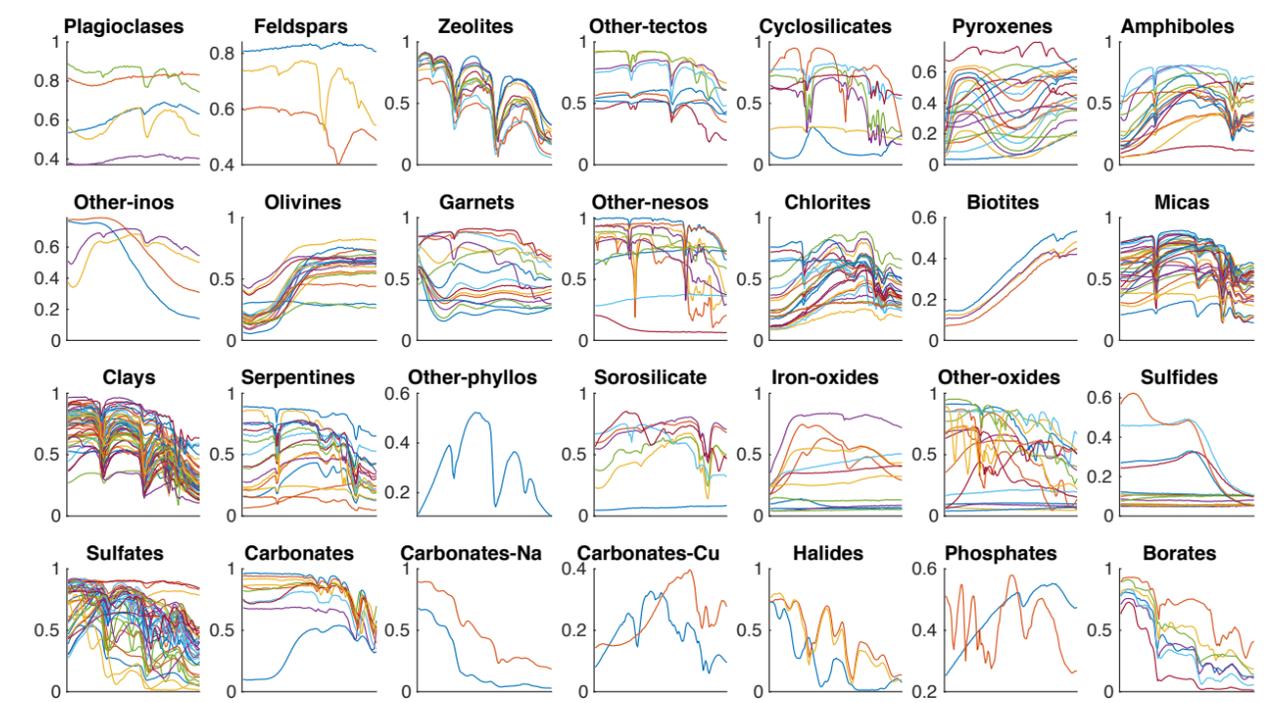
- 27 families of minerals

- 216 groups of minerals

If 3 endmembers, 500x499x498 = 10^8 combinations to test !!!

Algorithms: Mixed Integer Programming

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

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

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

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

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

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

- Sparsity: most abundances are zero [Iordache et al., 2011]
- Structuration of the dictionary into groups [Meyer et al., 2016, Drumetz et al., 2019]
- Minimum values on the nonzero coefficients [never seen ...]
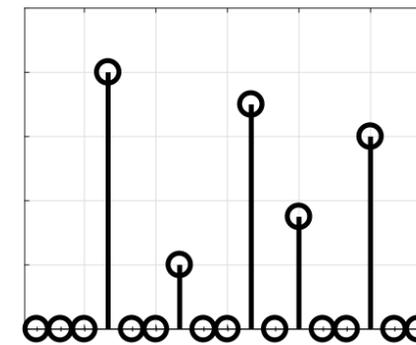
S. Bourguignon, J. Ninin, H. Carfantan, and M. Mongeau, "Exact sparse approximation problems via mixed-integer programming : Formulations and computational performance," IEEE Trans. Signal Process., vol. 64, no. 6, Mars 2016.

Exact ℓ_0-norm sparsity

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

Mixed Integer Programming
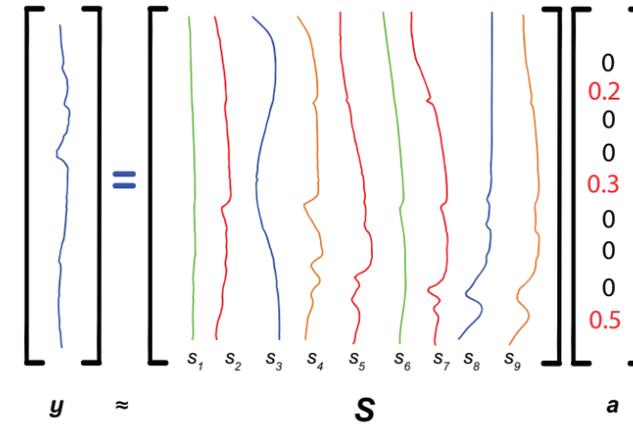
$\rightarrow$ $\boldsymbol{a}$ must be sparse:

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

- Standard sparse methods perform poorly (ℓ_1-norm, greedy algorithms)
- ⤳ **Exact ℓ_0-norm constraint:**

$$\min_{\boldsymbol{a}\in[0,1]^N,\ \boldsymbol{b}\in\{0,1\}^N} \frac{1}{2}\|\boldsymbol{y}-\mathbf{S}\boldsymbol{a}\|^2 \text{ s.t.} \begin{cases} \mathbf{0} \leq \boldsymbol{a} \leq \boldsymbol{b} \\ \sum_{n=1}^N b_n \leq K \\ \sum_{n=1}^N a_n = 1 \end{cases}$$
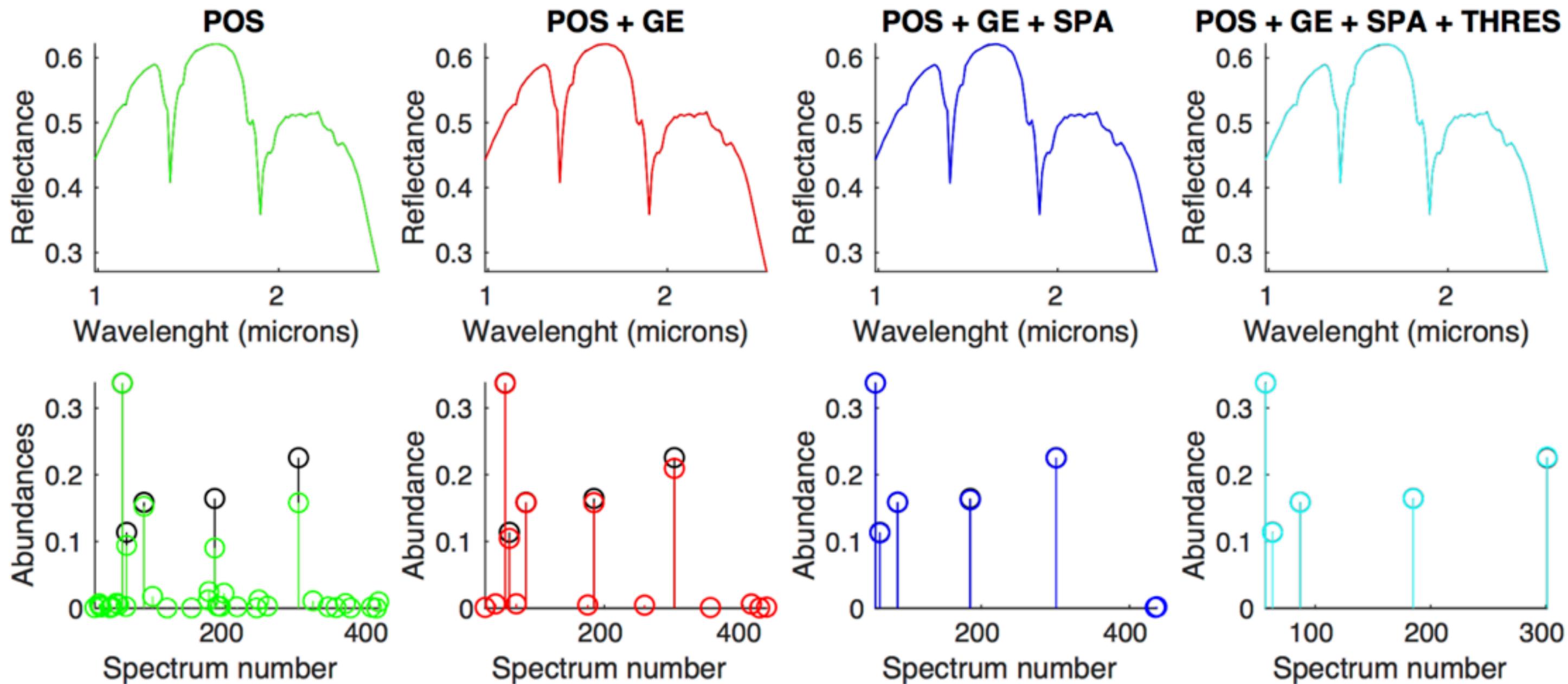
Mhenni, R. B., Bourguignon, S., & Ninin, J. (2019). Global optimization for sparse solution of least squares problems.

Constraints in Mixed Integer Programming

- ℓ_0-norm sparsity

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

- Group Exclusivity **GE**

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

- Significant Abundances **SA**

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

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

$\rightarrow$ These constraints can be mixed

Ben Mhenni, R.; Bourguignon, S.; Ninin, J. & Schmidt, F. Spectral Unmixing with Sparsity and Structuring Constraints *Workshop on Hyperspectral Image and Signal Processing: Evolution in Remote Sensing (WHISPERS), 2018 9th Workshop, held 23-26 September 2018, Amsterdam, The Netherlands,* **2018**, 1-4

Results

$$y_{simul} = Sa$$

Results

$$\mathbf{y_{simul}} = S\mathbf{a}$$

$$\min_{x,x_1} \frac{1}{2} \|\mathbf{Y} - (\mathbf{Sx} + \mathbf{S_1 x_1})\|_2^2$$

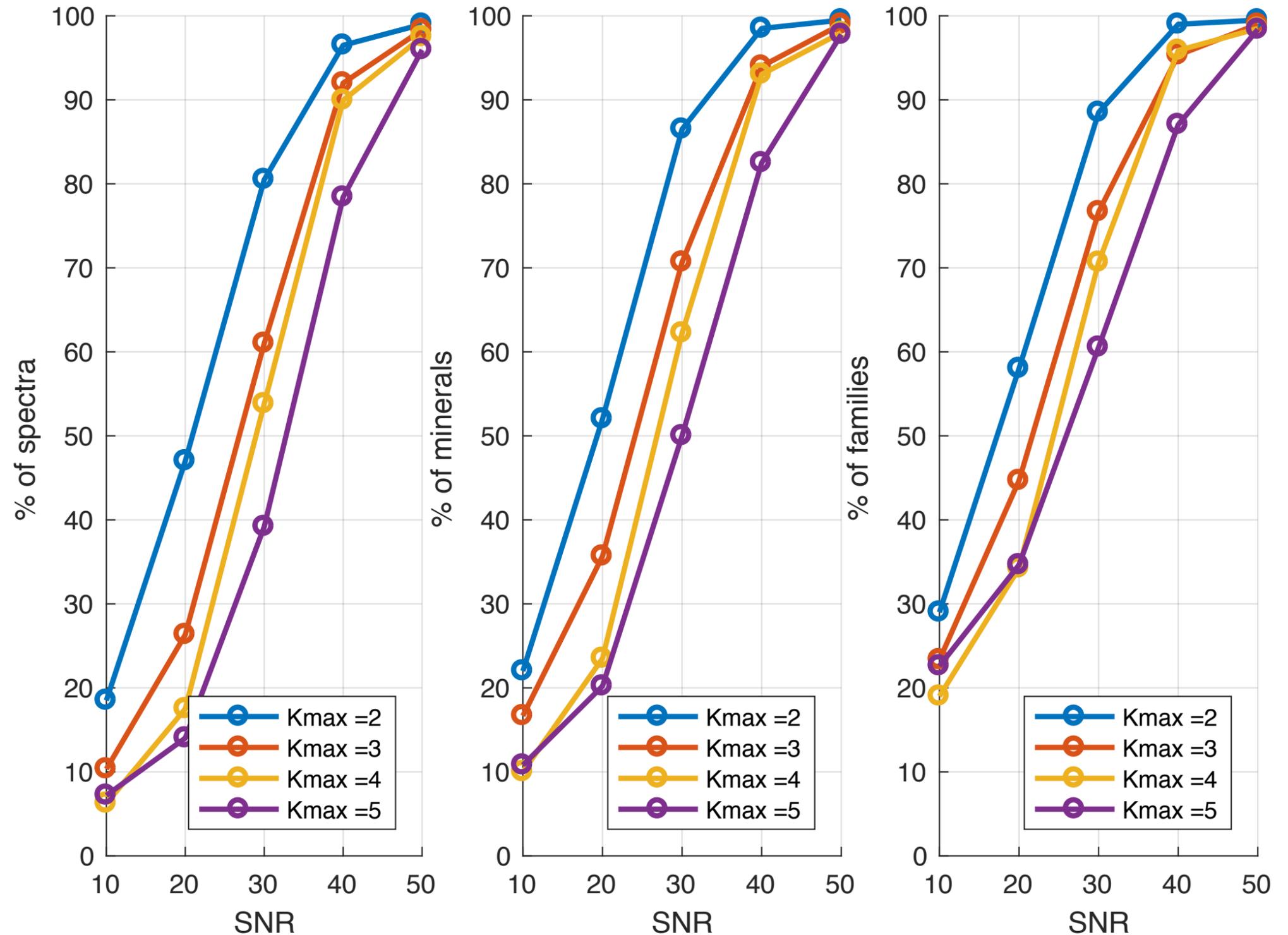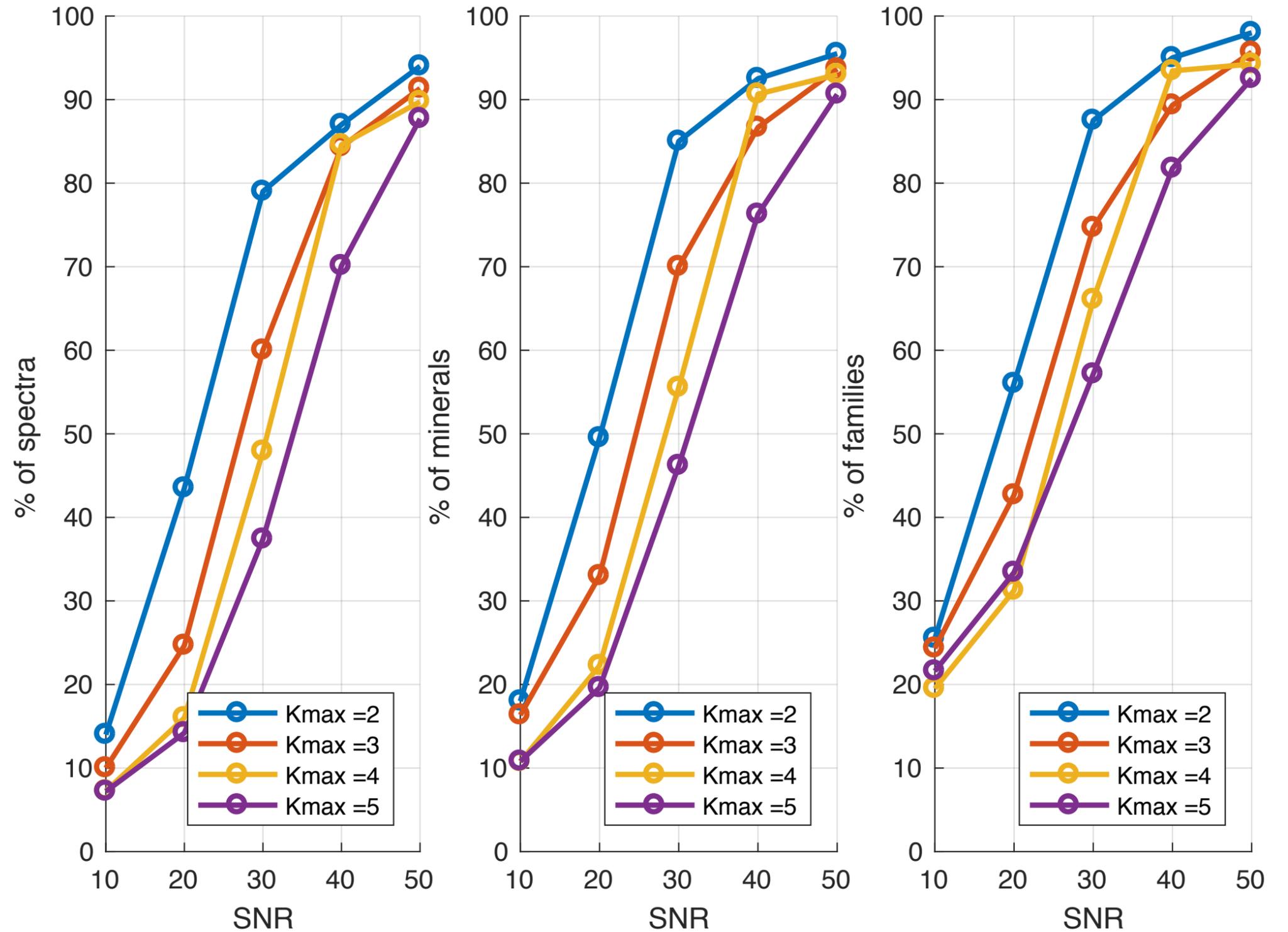$$s.t. \|x\|_0 \leq K_{max}$$

$$s.t. x \geq T$$

$$s.t. \sum x = 1$$

$$s.t. group\ exclusivity$$

- Average of 100 runs

- High rate of correct families

Results

Proportion of correct endmembers/minerals/families identified

$$\mathbf{y_{simul}} = S\mathbf{a}$$

(0.9)

$$\min_{x, x_1} \frac{1}{2} \|\mathbf{Y} - (\mathbf{S}\mathbf{x} + \mathbf{S_1}\mathbf{x_1})\|_2^2$$
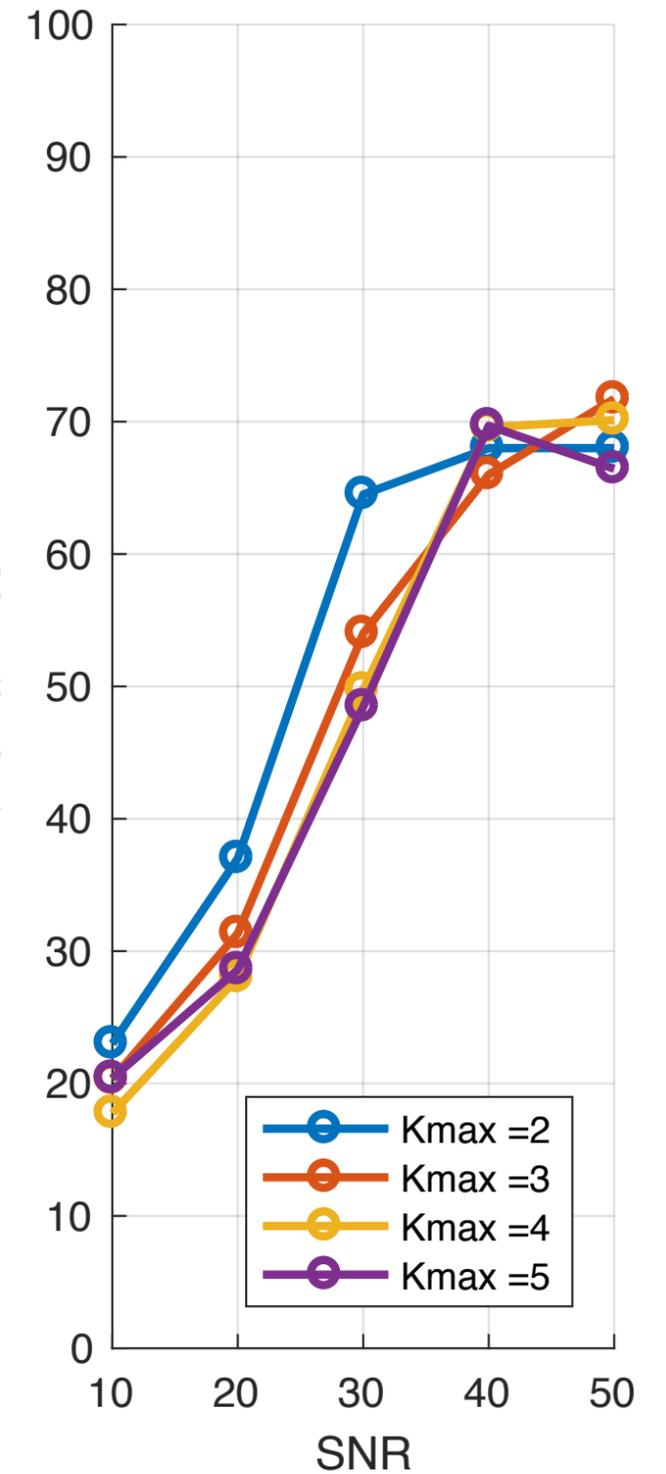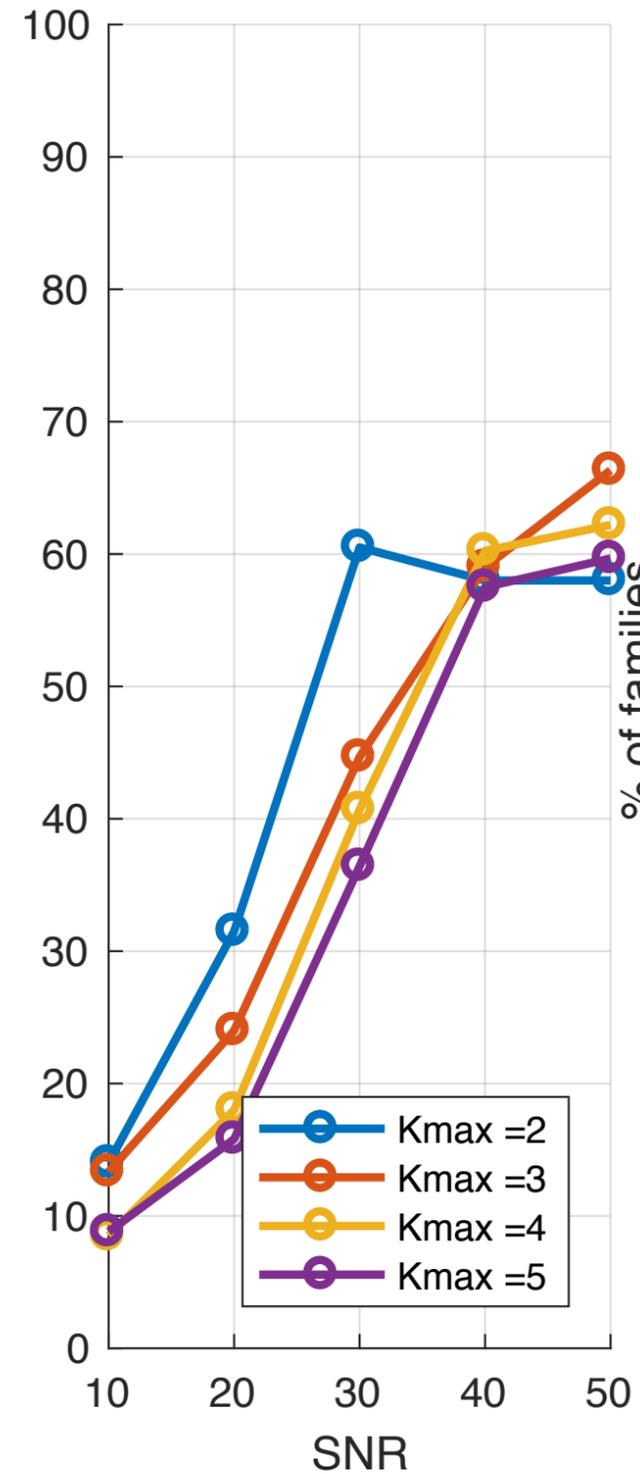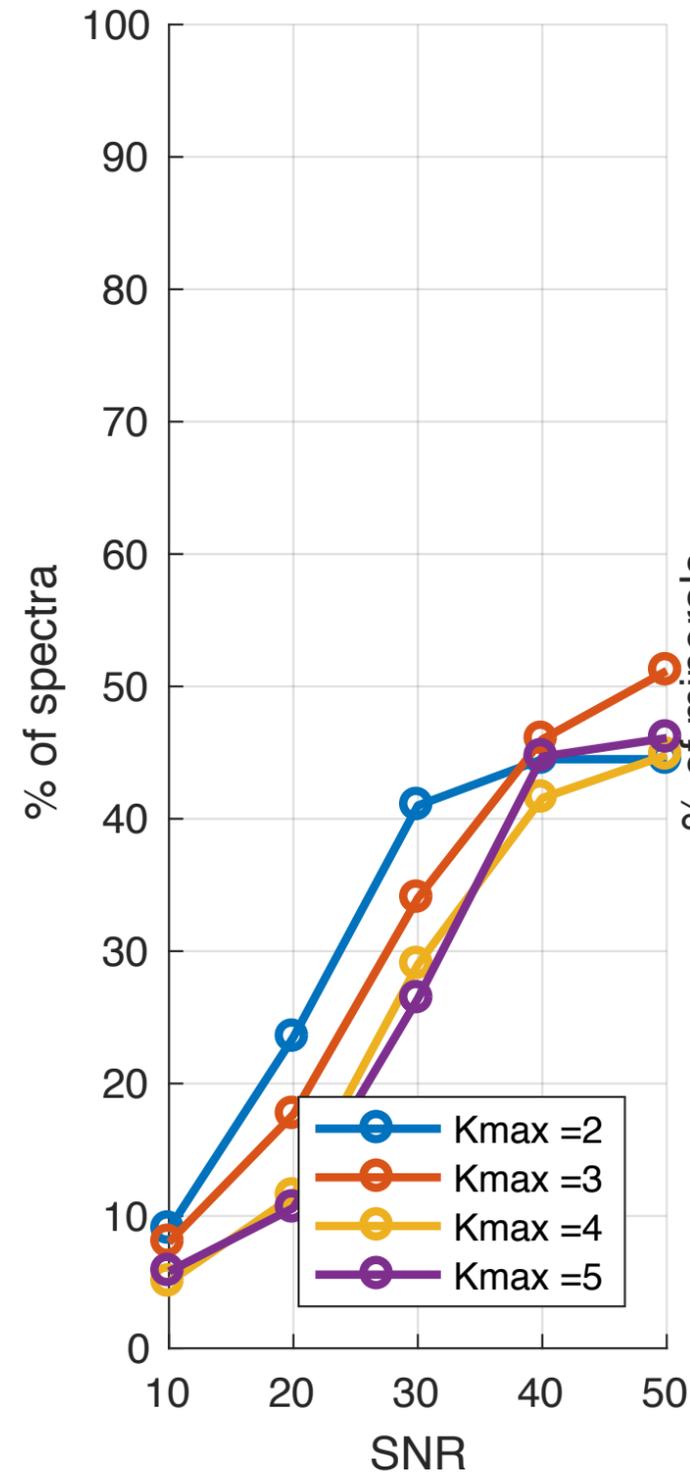
$$s.t. \|x\|_0 \leq K_{max}$$

$$s.t. x \geq T$$

$$s.t. \sum x = 1$$

$$s.t. group\ exclusivity$$

- Average of 100 runs

- High rate of correct families

Results

Proportion of correct endmembers/minerals/families identified

$$\mathbf{y_{simul}} = S\mathbf{a}^{0.5}$$

$$\min_{x,x_1} \frac{1}{2} \|\mathbf{Y} - (\mathbf{Sx} + \mathbf{S_1x_1})\|_2^2$$

$$s.t. \|x\|_0 \leq K_{max}$$

$$s.t. x \geq T$$

$$s.t. \sum x = 1$$

$$s.t. group\ exclusivity$$

- Average of 100 runs

- High rate of correct families

Figure: Three line plots of % of spectra, % of minerals, and % of families versus SNR, each showing curves for Kmax =2, Kmax =3, Kmax =4, Kmax =5.

Conclusion

- New constraints from Mixed Integer Programming (group exclusivity)

- Can handle mineral but also family ✅

- Family significantly improves the detectability even for ~500 spectra in the database ✅

- Strong non-linearity still difficult to handle

- Future work : application on real data


Mob Programming
A Whole Team Approach

Schmidt, F. et al. *IEEE Transaction in Geoscience and Remote Sensing, Institute of Electrical and Electronics Engineers (IEEE),* **2023** *submitted soon :-)*

Results

$$\mathbf{y_{simul}} = S\mathbf{a}$$

$$\min_x \frac{1}{2}||\mathbf{Y} - \mathbf{Sx}||_2^2$$
$$s.t.||x||_0 \leq K_{max}$$
$$s.t. x \geq T$$
$$s.t. \sum x = 1$$
$$s.t. group\ exclusivity$$

- Average of 100 runs

- High rate of correct families

Proportions of good endmembers/minerals/families identified in the mixture
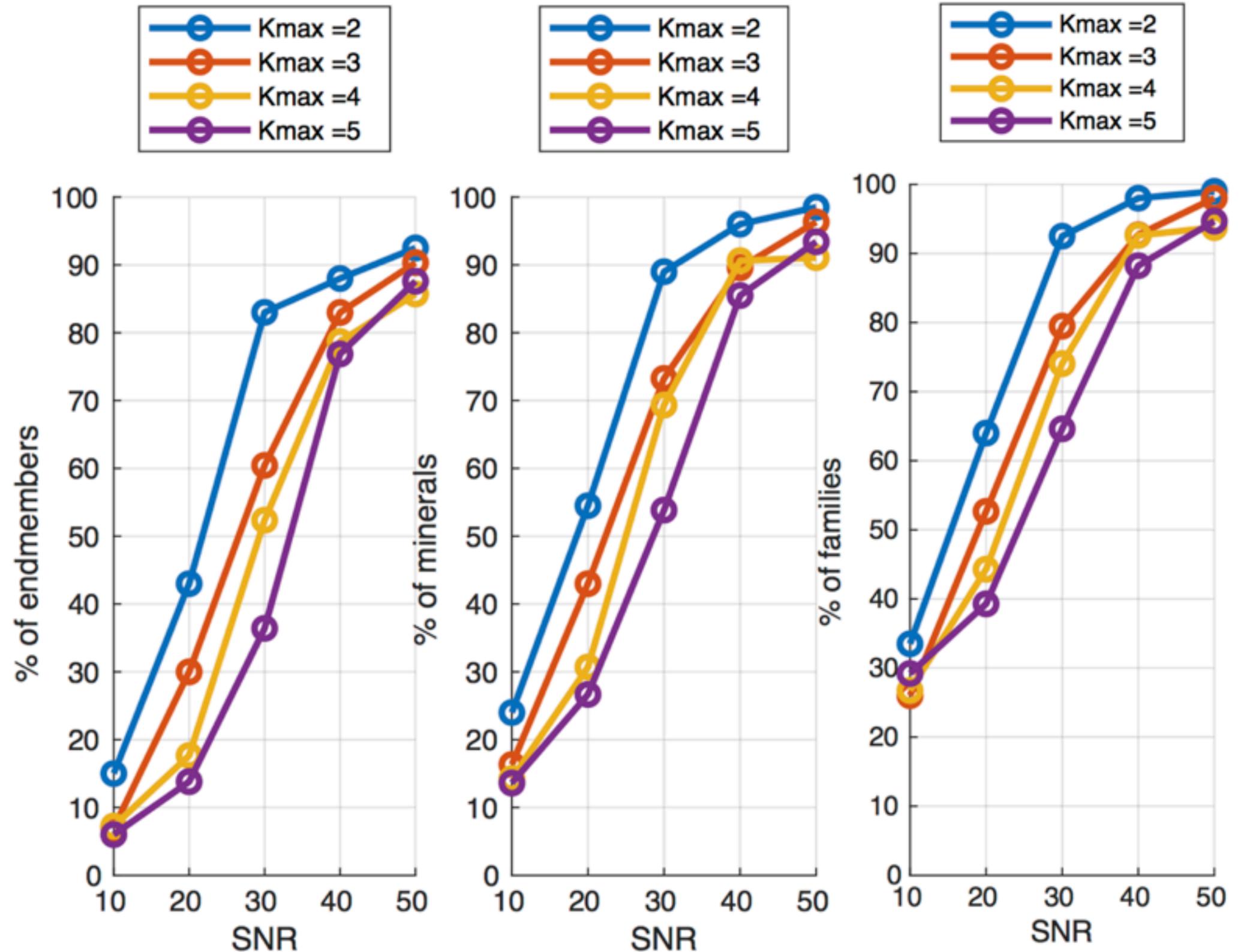
Results

$$\mathbf{y_{simul}} = S\mathbf{a} + 0.1$$

LEVEL CHANGE

$$\min_x \frac{1}{2}\|\mathbf{Y} - \mathbf{Sx}\|_2^2$$
$$s.t.\|x\|_0 \leq K_{max}$$
$$s.t.\, x \geq T$$
$$s.t. \sum x = 1$$
$$s.t.\, group\ exclusivity$$

- Average of 100 runs

- Middle rate of correct families

Proportions of good endmembers/minerals/families identified in the mixture