CHIMIOMETRIE2019 Montpellier

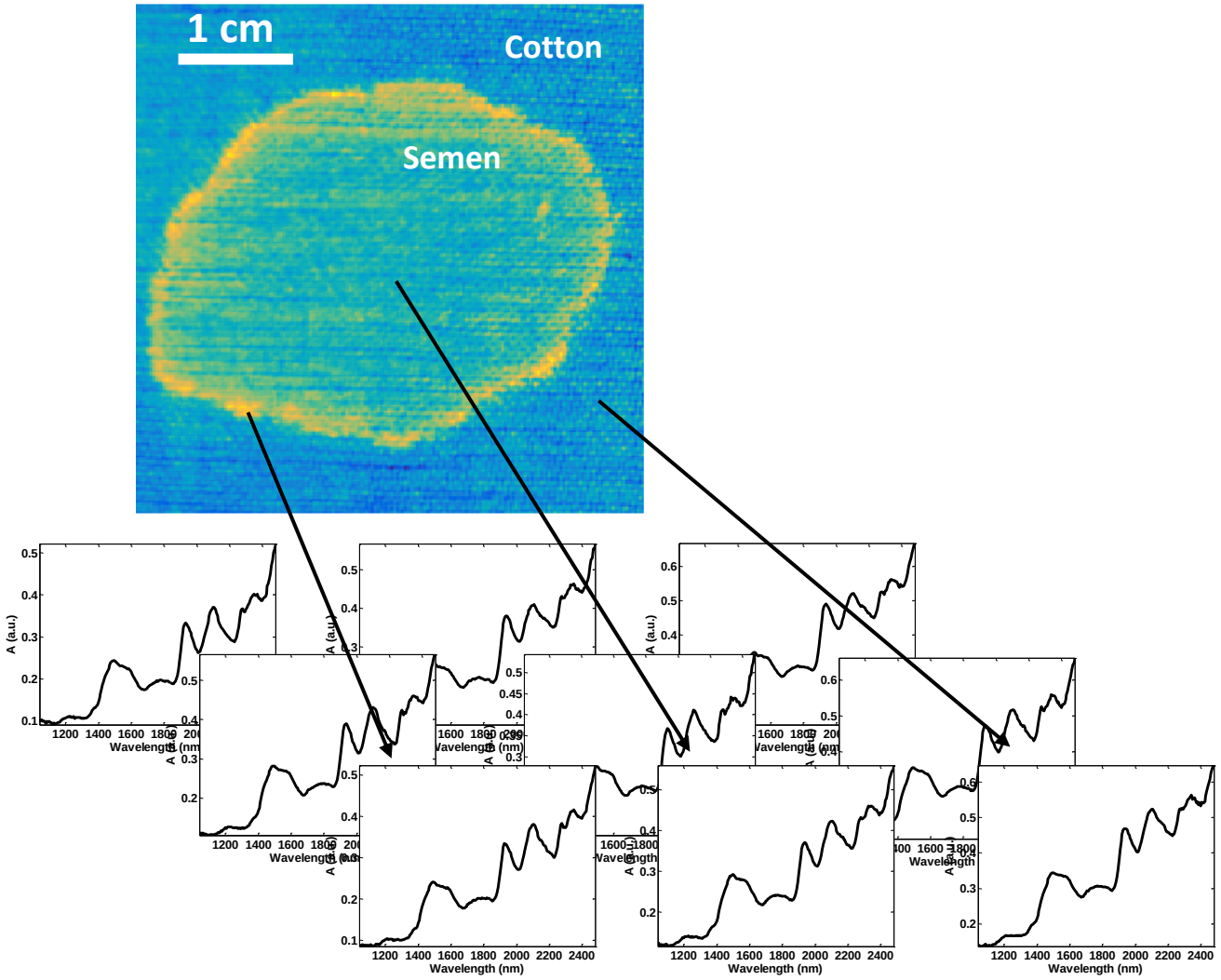
The why and how of image processing constraints in MCR-ALS of hyperspectral imaging data

Cyril Ruckebusch, Siewert Hugelier, Raffaele Vitale, Mahdiyeh Gaffari

DyNaChem LASIR CNRS U LILLE

Hyperspectral imaging

Forensic NIR
Identification of semen on cotton
(Coll J. Amigo & C. Santos)



Chemometrics and Intelligent Laboratory Systems, 5 (1989) 209–220
Elsevier Science Publishers B.V., Amsterdam — Printed in The Netherlands

Principal Component Analysis of Multivariate Images

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(Received 24 April 1988; accepted 25 September 1988)

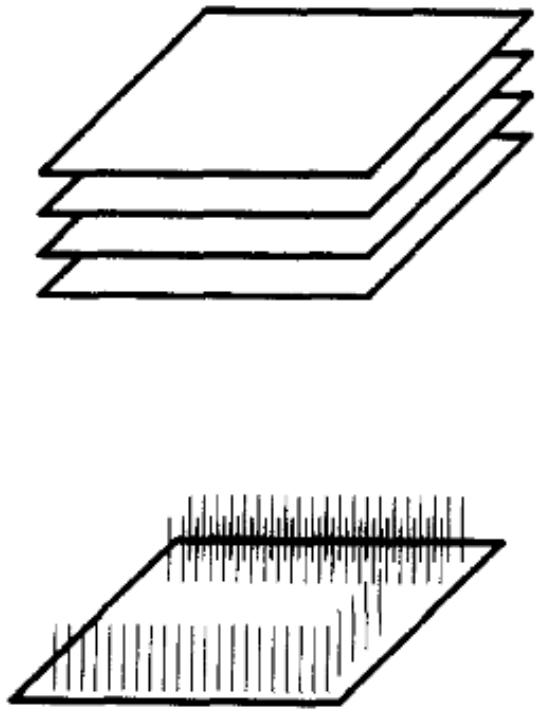
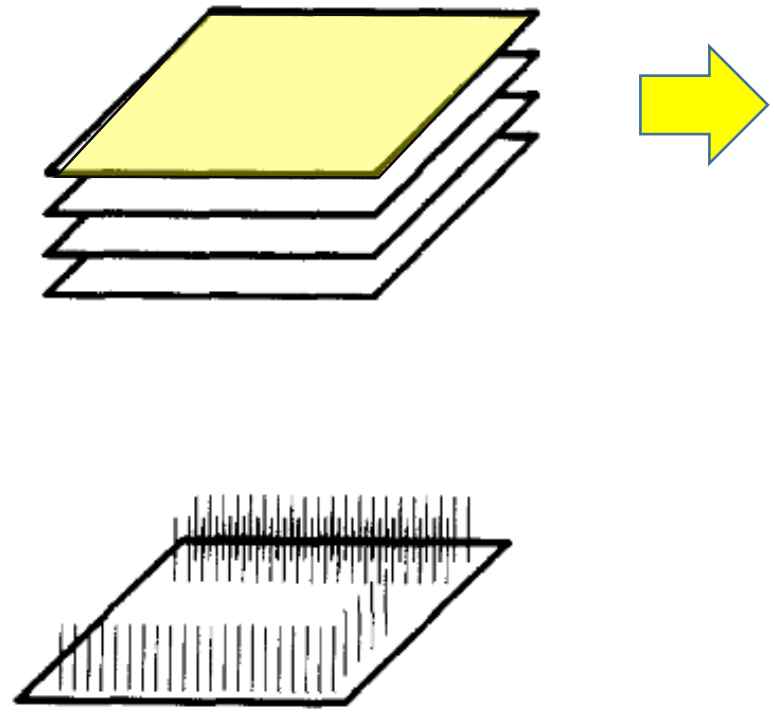


Fig. 8. A multivariate image can be represented as a stack of intensity (univariate) images, one for each wavelength, or as an image where each pixel is a vector of intensity values. For graphical clarity not all vectors are shown.



« Grey level operations »

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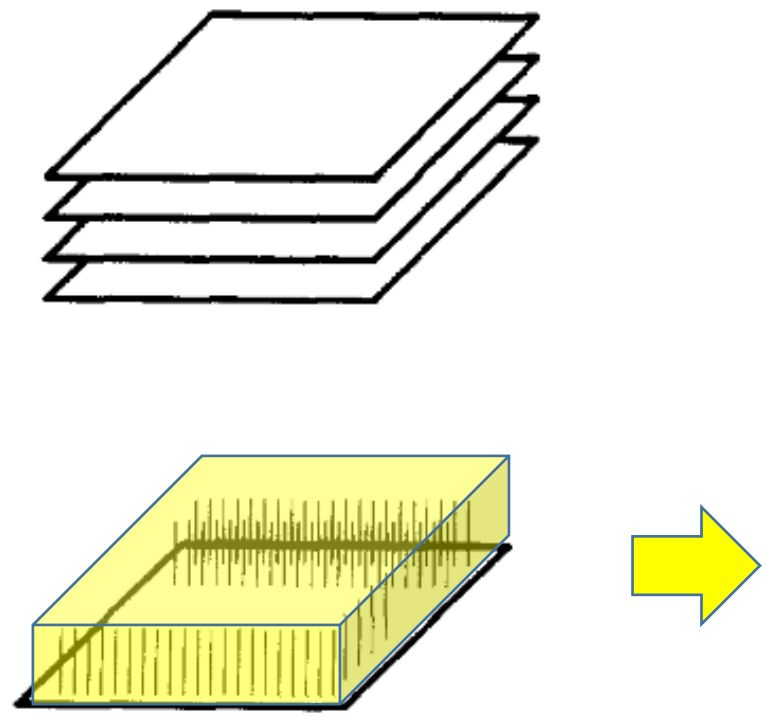

Multivariate image

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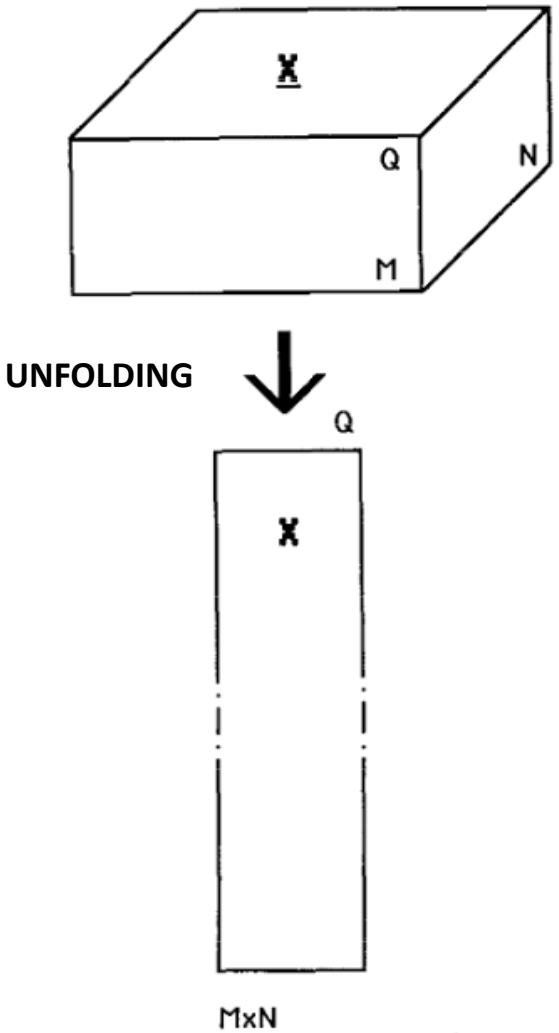
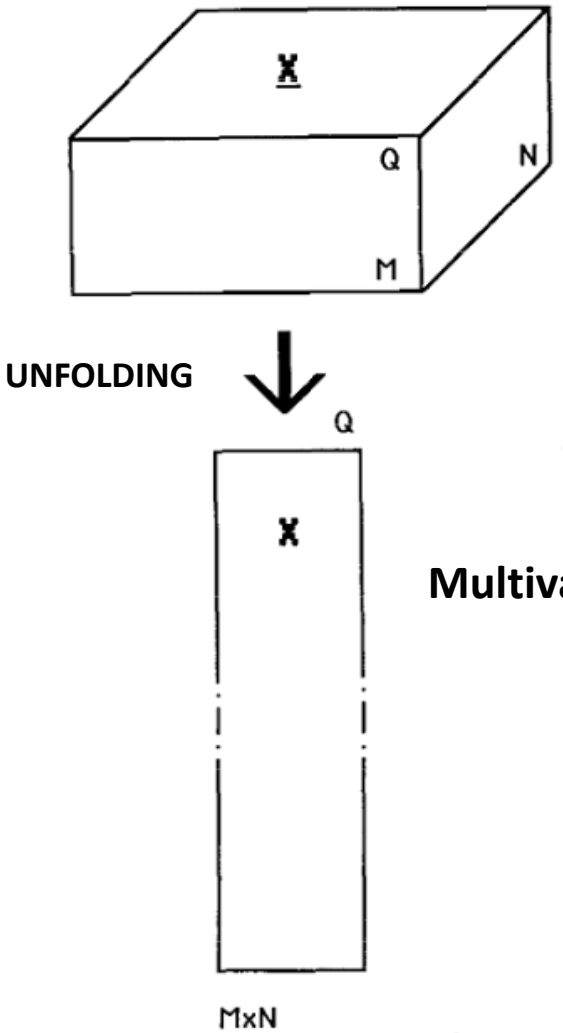


Fig. 4. A multivariate image (or O^2V array) $\underline{\mathbf{X}}$ can be written as a long data matrix $\mathbf{X}$ by unfolding.



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Multivariate Image Analysis

MIA-PCA 1990

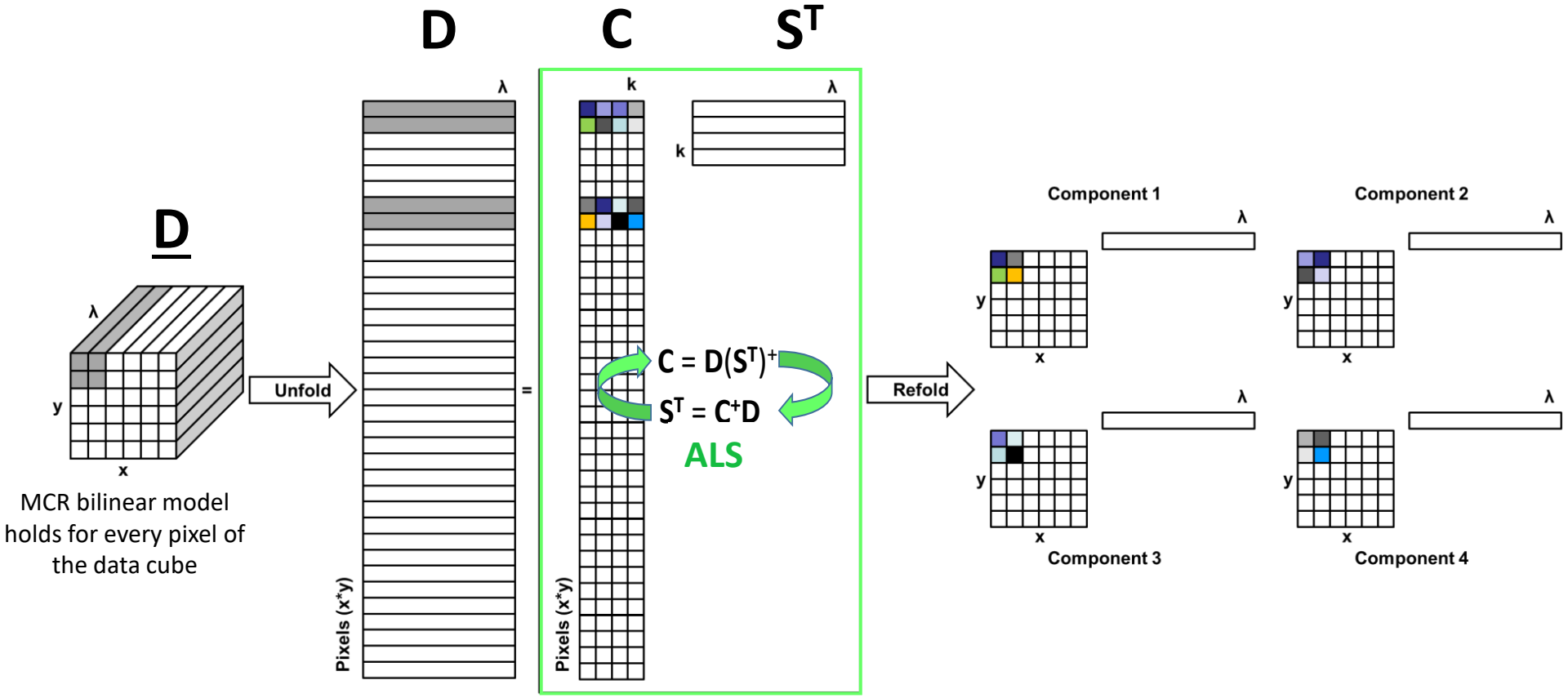
…

MIA-PLS 2000

…

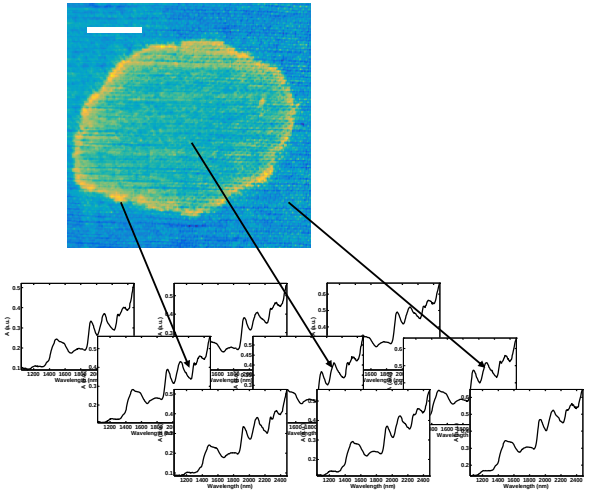
MIA-MCR 2004

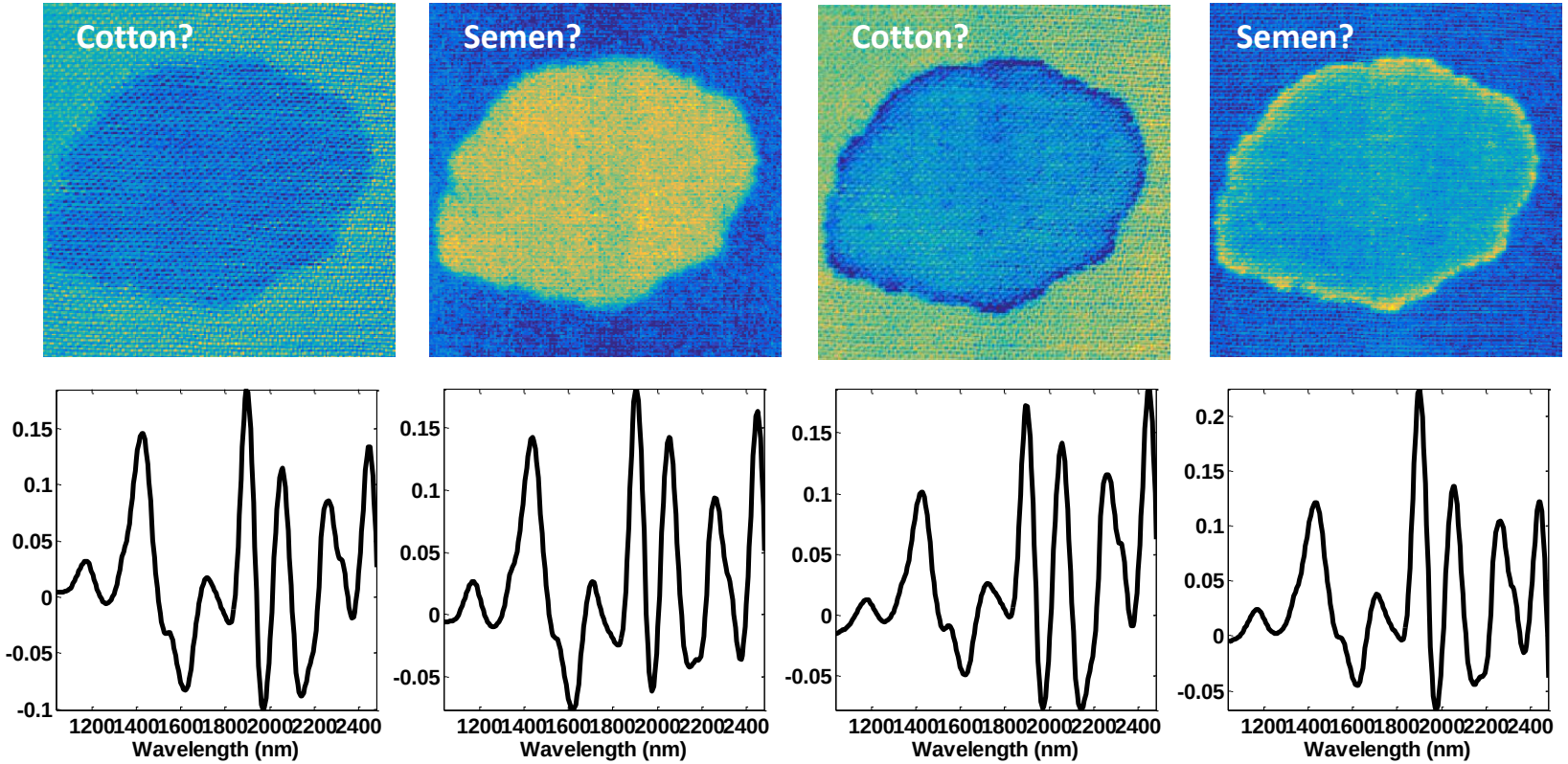
MIA - MCR



MCR-ALS R. Tauler 1995, A. de Juan 2004

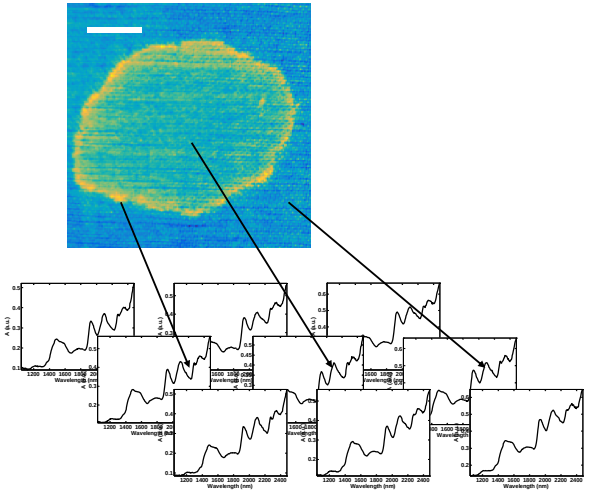
Multivariate curve resolution



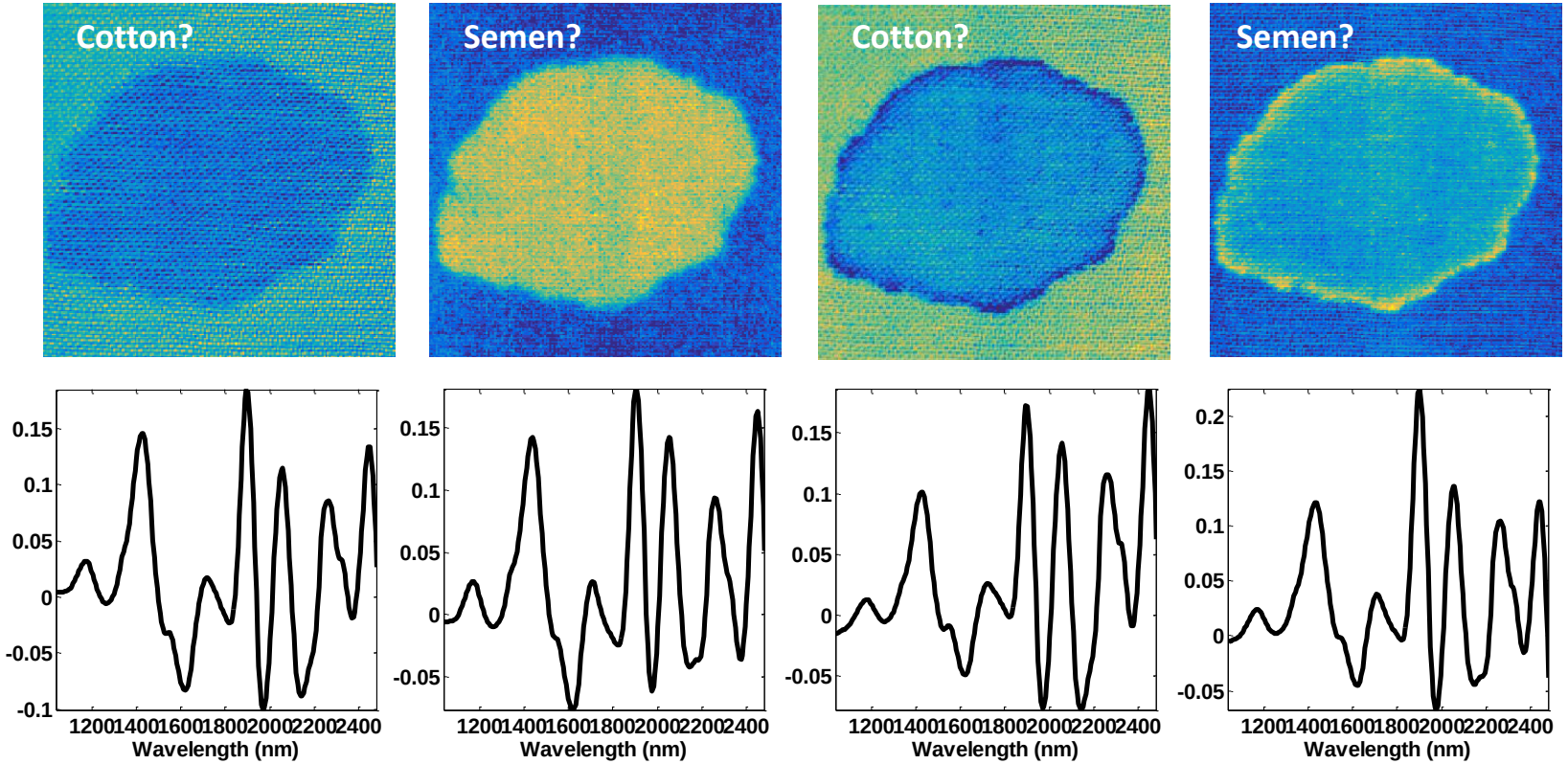


MCR-ALS with non-negativity on **C** (LOF: 4.06 %)

Multivariate curve resolution



NIR reflectance
Heavily mixed spectra
Rank > 2
No pure pixels



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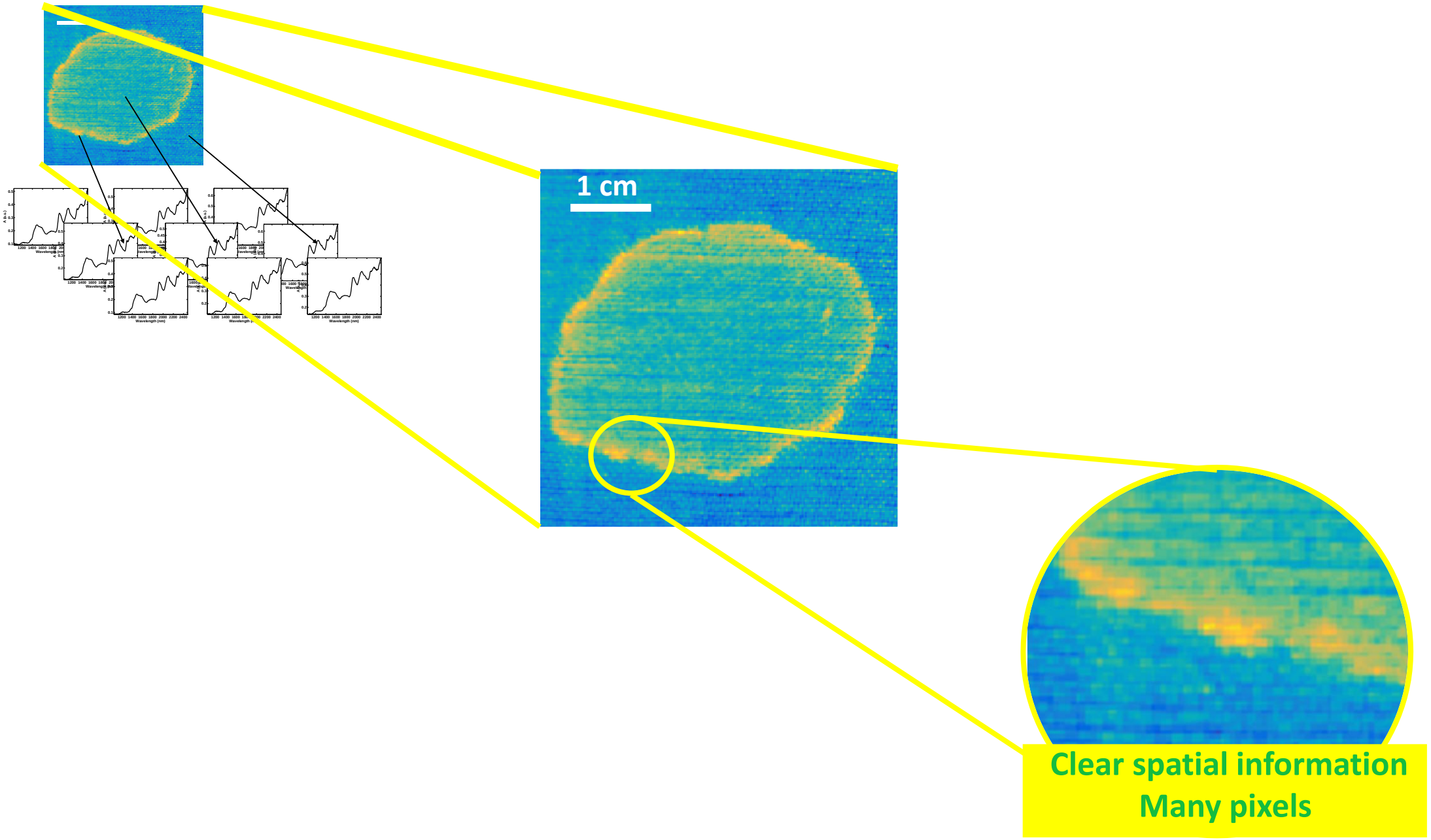
1 cm
Clear spatial information
Many pixels

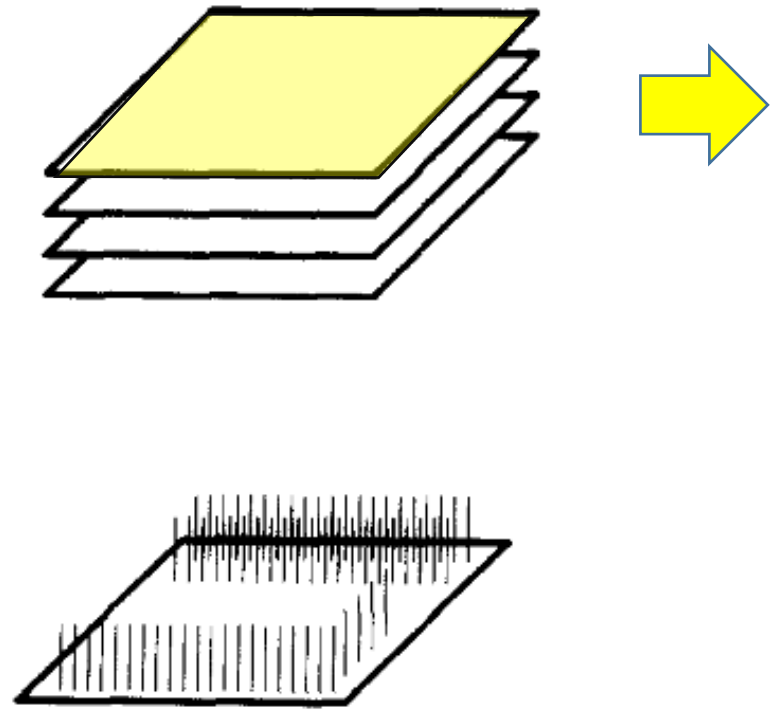

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Image processing

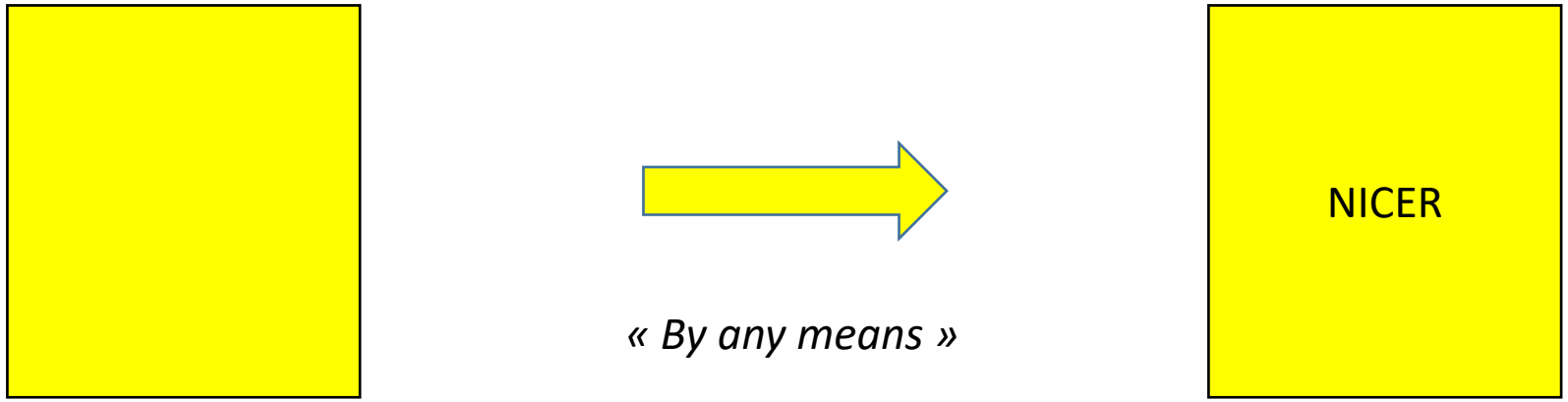


Image processing

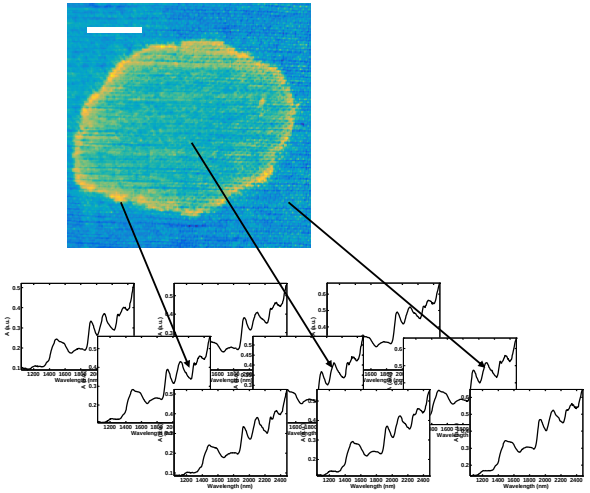
TV

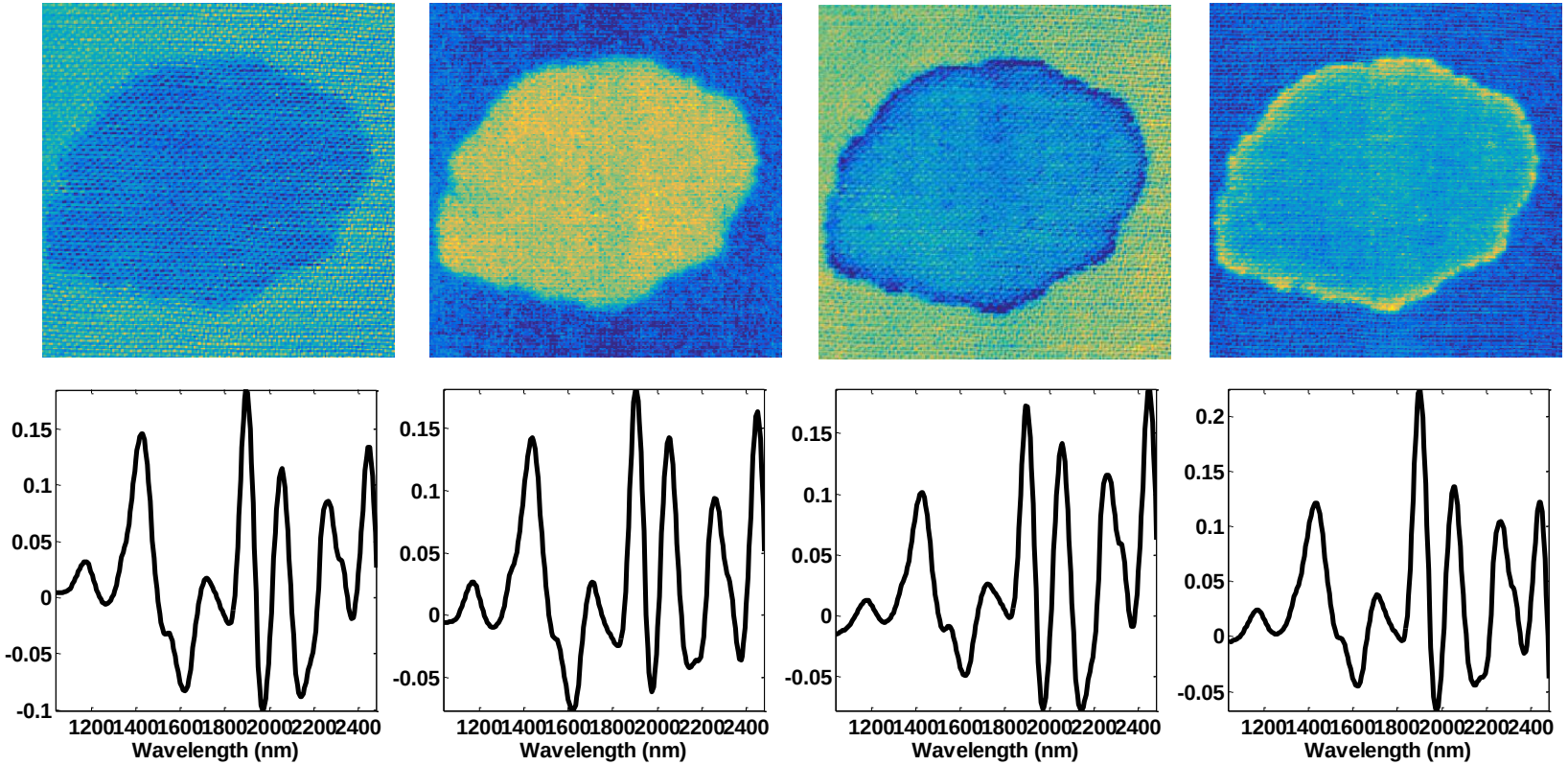
Total variation algorithms
(Rudin *et al.* 92, Xu *et al.* 2012)

$$min\ \|\mathbf{I} - \mathbf{I}_{\boldsymbol{TV}}\|^2 + \lambda \sum_{x,y} \sqrt{\left(i_{x+1,y} - i_{x,y}\right)^2 + \left(i_{x,y+1} - i_{x,y}\right)^2}$$

Segmented smoothing
(Rippe *et al.*, 2012)

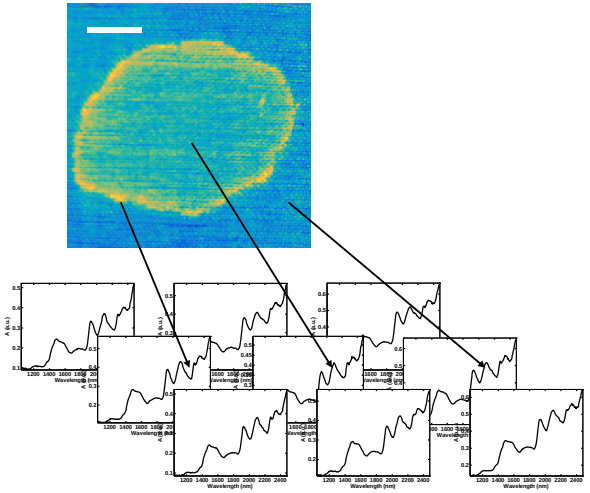
$$min\ \|\mathbf{I} - \mathbf{I}_{\boldsymbol{TV}}\|^2 + \lambda\ \#\ \{p \mid \|\delta_x \mathbf{i}\|_0 + \|\delta_y \mathbf{i}\|_0\ \neq 0\}$$

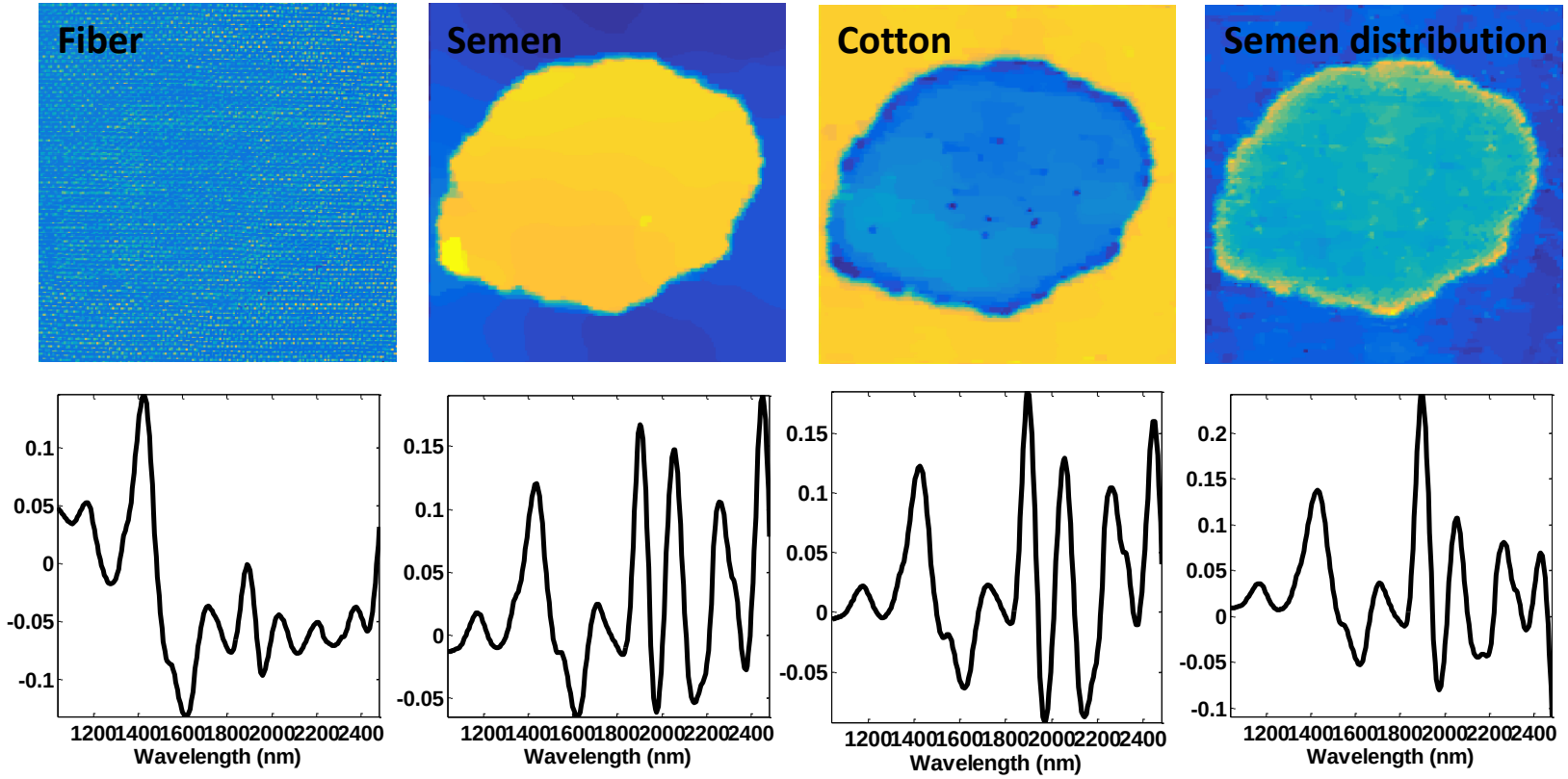




MCR-ALS with non-negativity on **C** (LOF: 4.06 %)

Chimiométrie 2018 Paris

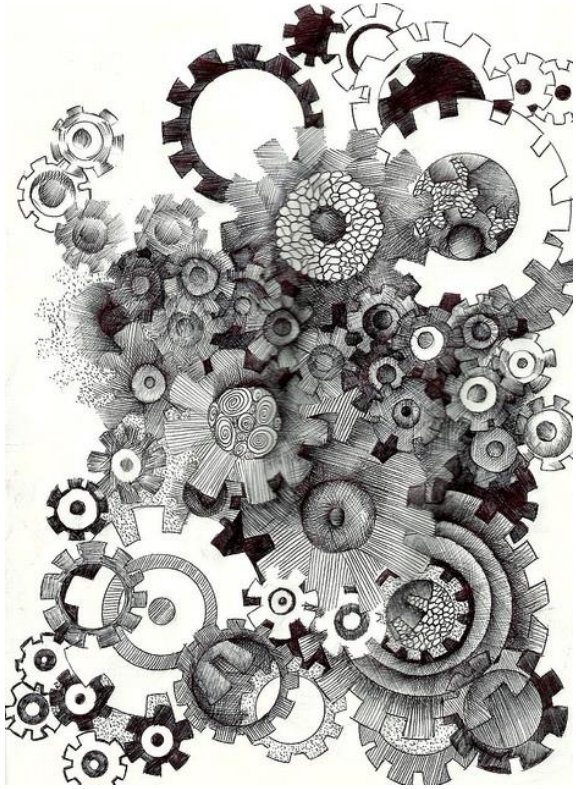




MCR-ALS with **NN** and **TV** constraints on **C** (LOF: 5.46 %)

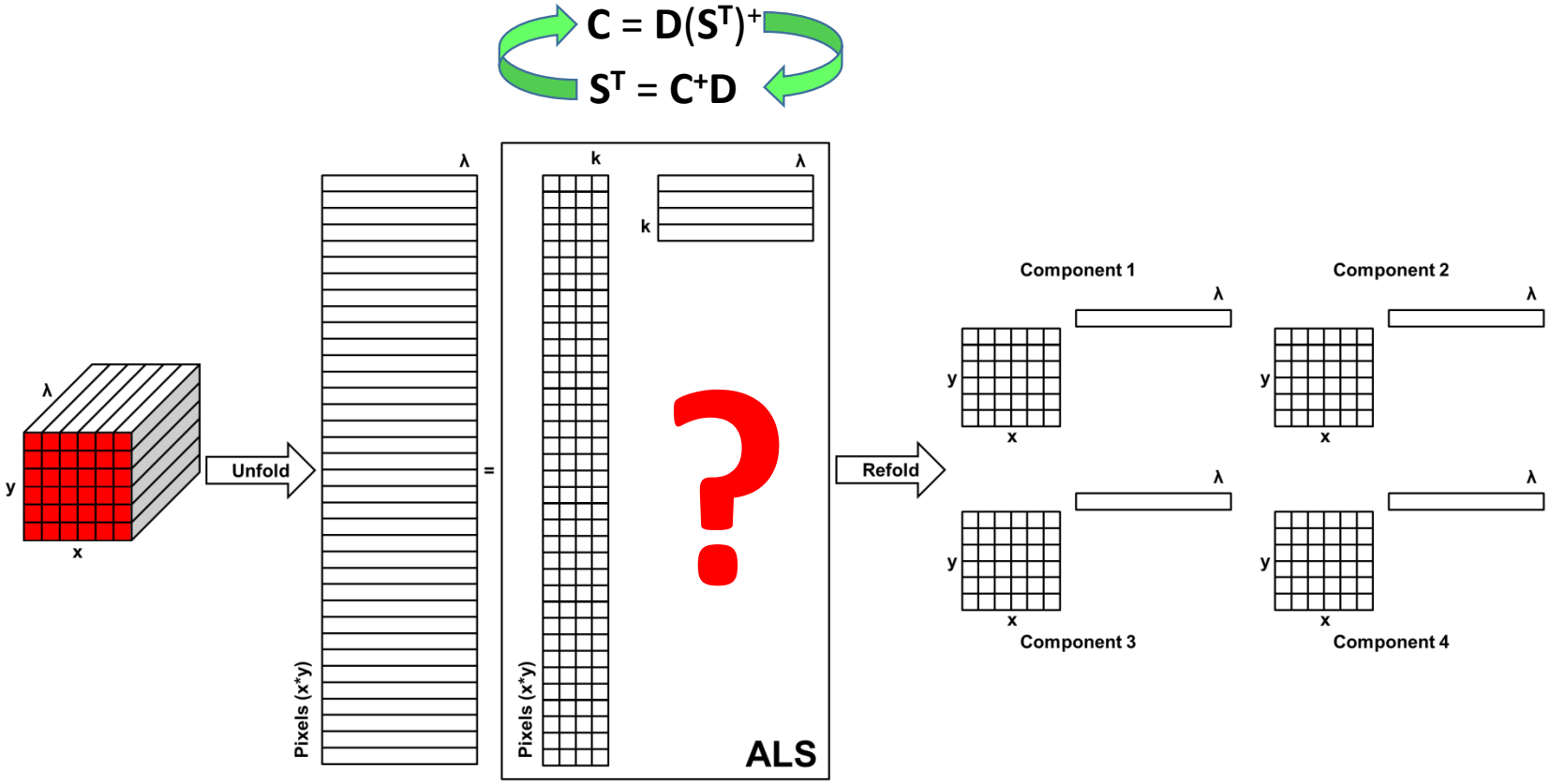
Chimiométrie 2018 Paris

How?



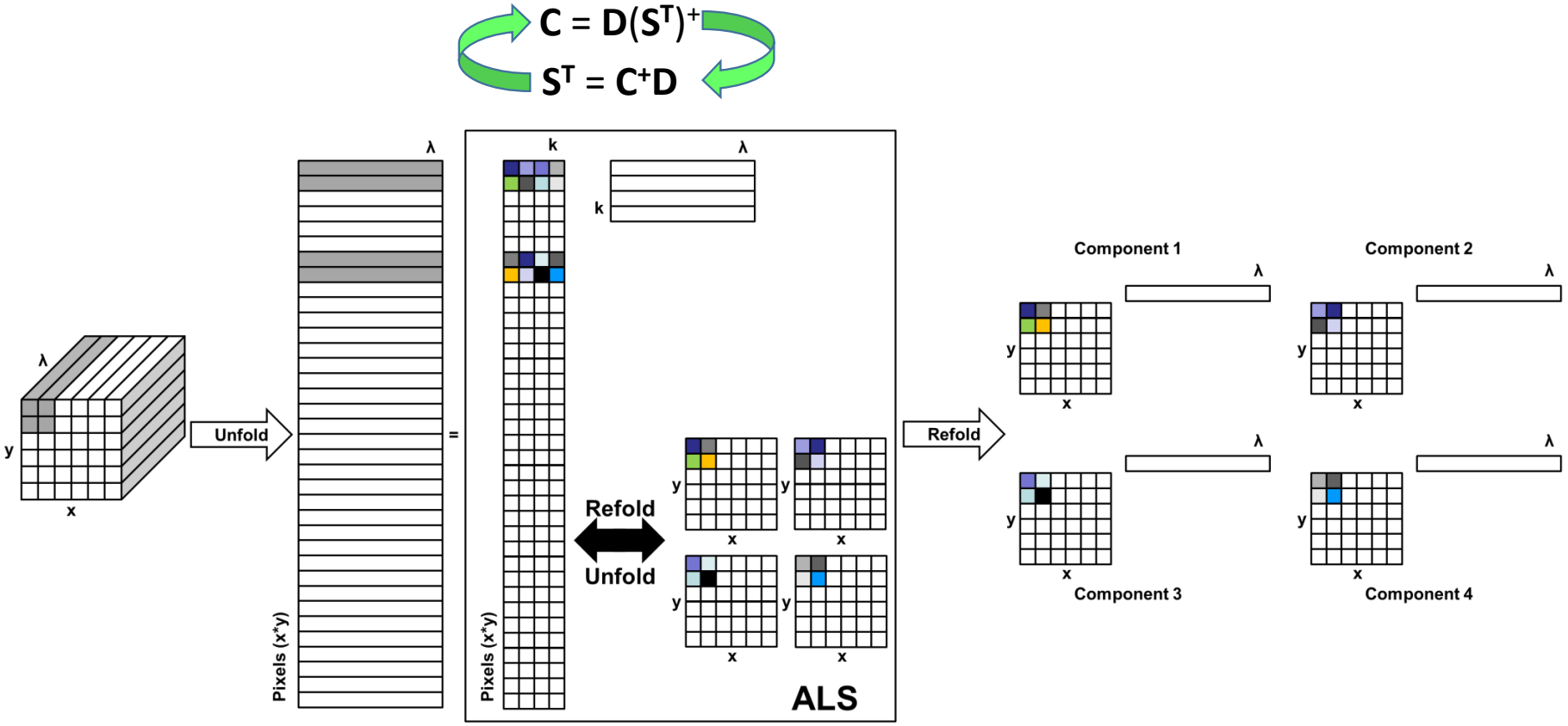
oliviercadic.com

MCR-ALS OF HSI DATA



Spatial information

MCR-ALS OF HSI DATA



Refold / unfold step:

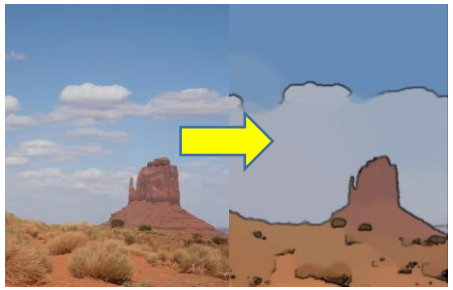
- Spatial information is recovered
- **Image processing constraints** can be applied in a map-wise way and individually for each component

Journal of Chemometrics, 2015

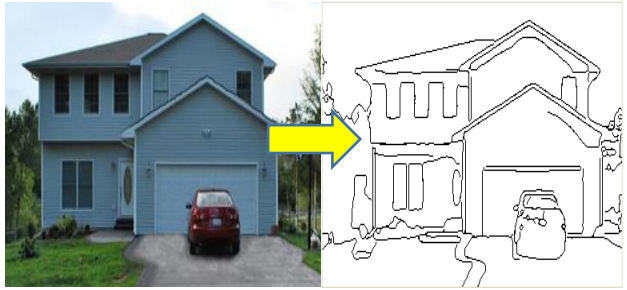
Image processing constraints

- Smoothness
- Sparseness
- Segmentation
- Edge preserving smoothing (TV, RTV)
- …

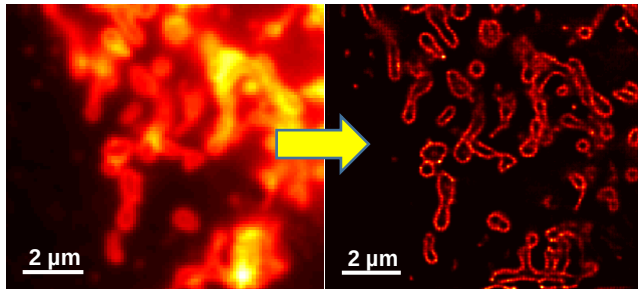
Smoothing



Edge enhancement

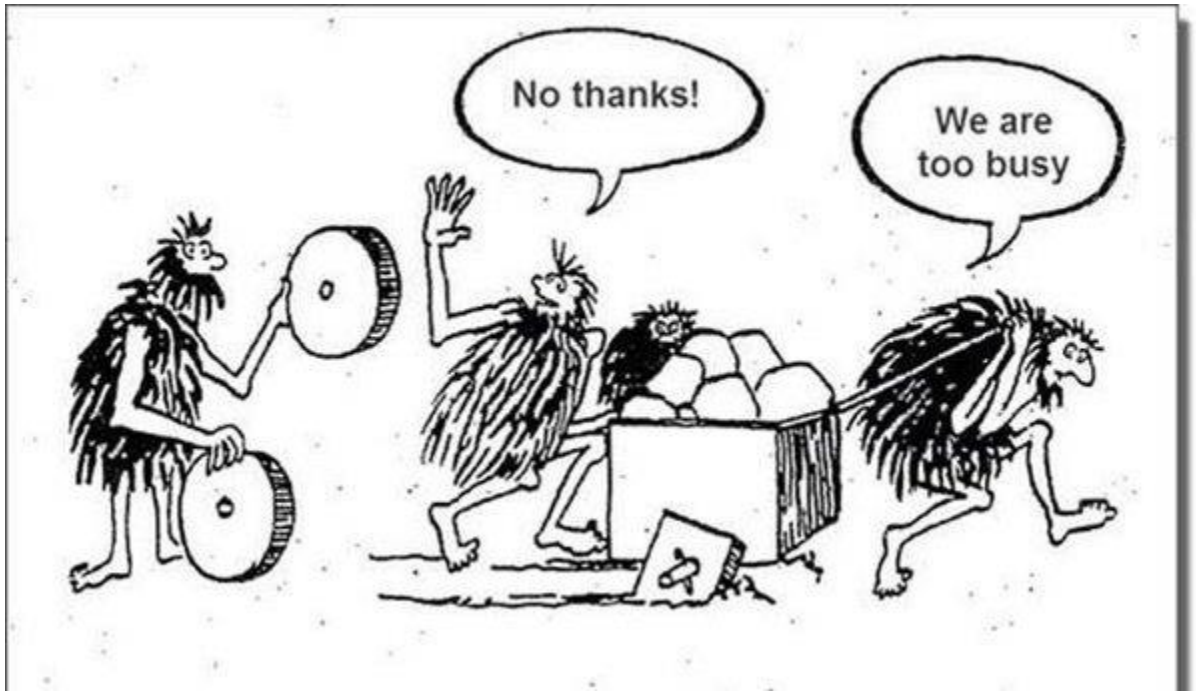


Deconvolution



Journal of Chemometrics, 2016
Applied Spectroscopy, 2018
ACA, 2018

Should we care?



http://www.codeops.tech/blog/

THE IMPORTANCE OF CONSTRAINTS IN MCR-ALS

Constraints should

- have a chemical/physical meaning
- help interpretability
- improve reliability
- reduce rotational ambiguity

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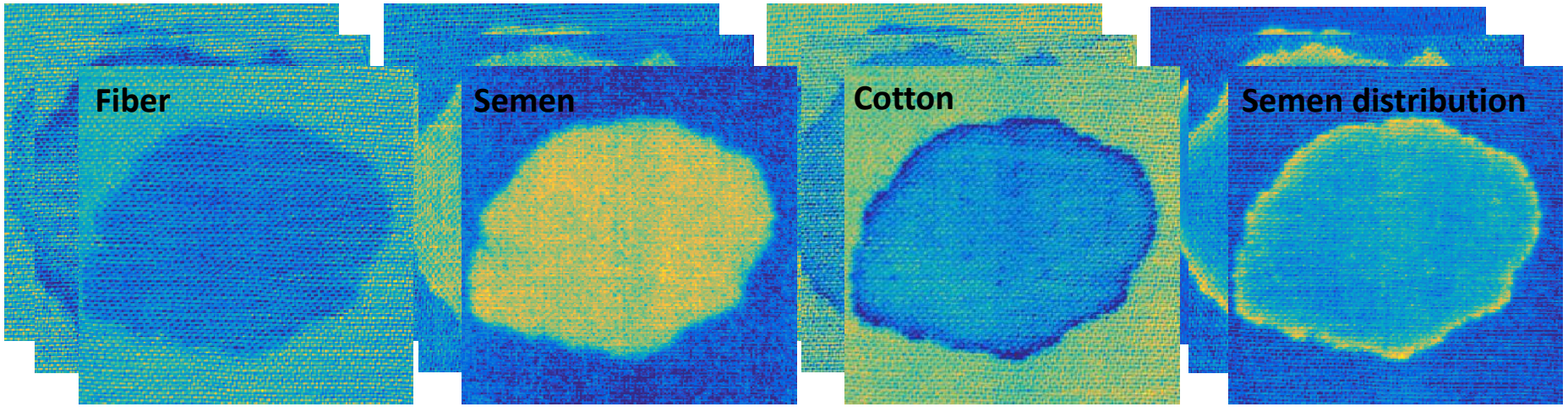
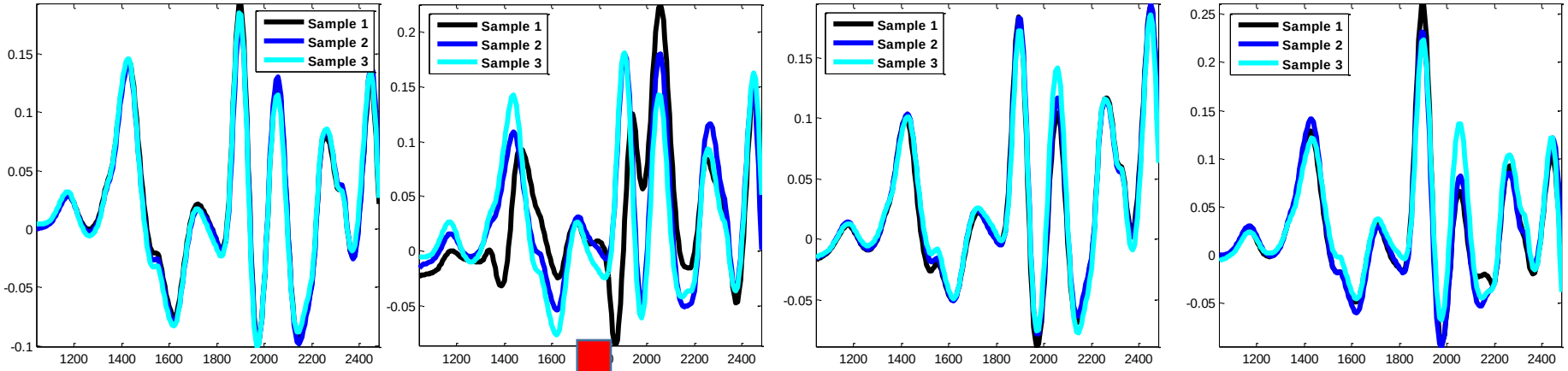
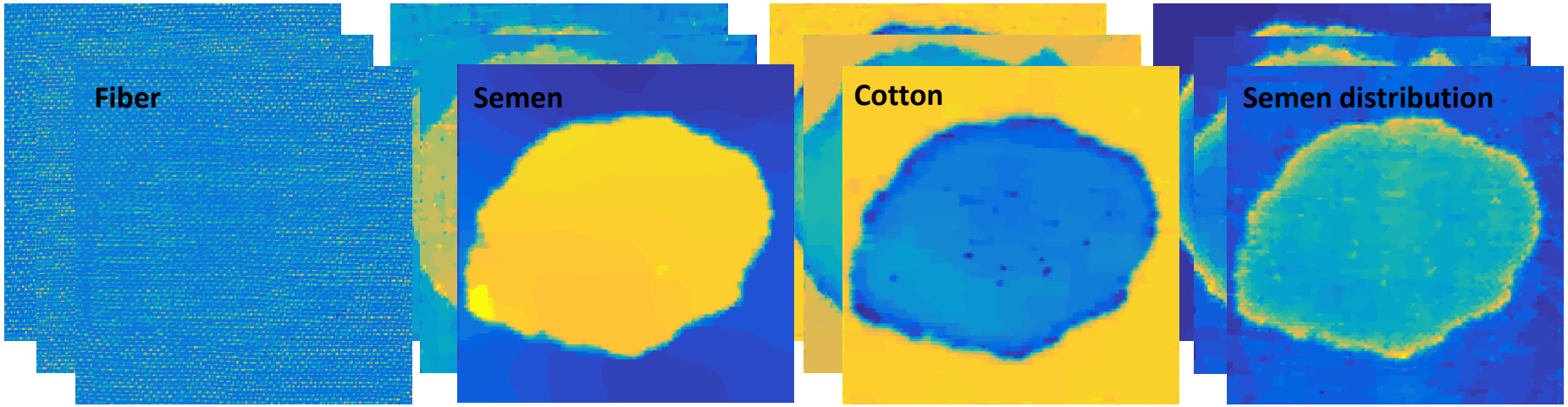
NN MCR-ALS on 3 replicates

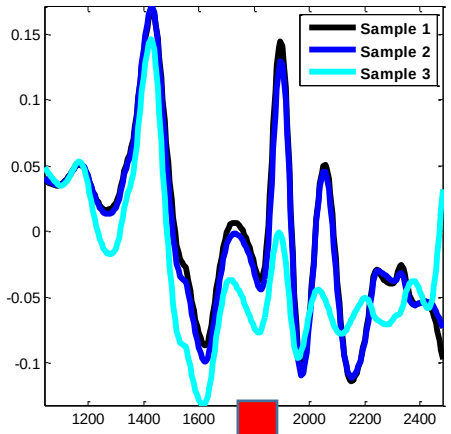


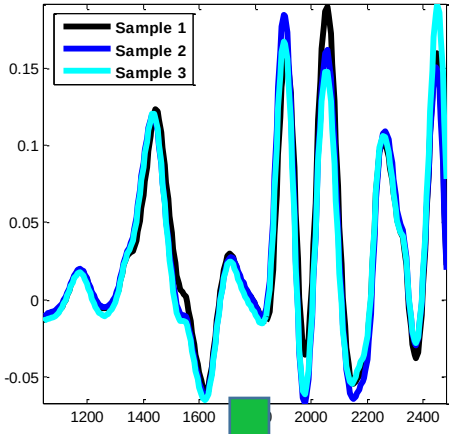


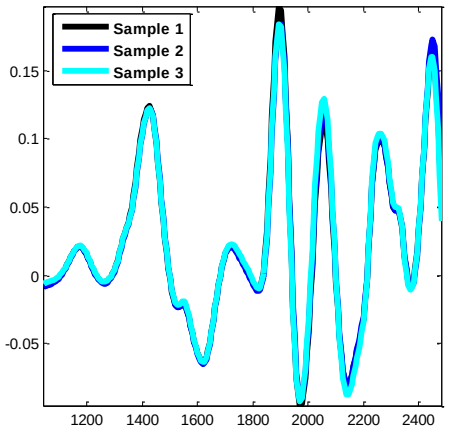
Variability is in the semen component spectrum

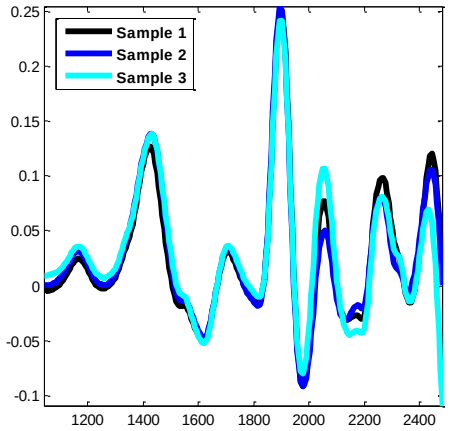
Image processing constraint (RTV) MCR-ALS on 3 replicates











Variability in the texture

Semen spectrum

THE IMPORTANCE OF CONSTRAINTS IN MCR-ALS

Constraints should

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- help interpretability
- improve reliability
- reduce rotational ambiguity

?

ROTATIONAL AMBIGUITY

A major problem in mixture resolution problems, particularly important in the analysis of heavily mixed data (kinetic process, imaging)

$$\mathbf{D} = \mathbf{C}\mathbf{S}^{\mathbf{T}} + \mathbf{E} = (\mathbf{C}\mathbf{R})(\mathbf{R}^{-1}\mathbf{S}^{\mathbf{T}}) + \mathbf{E}$$

The MCR solution is non unique
There is a set of <u>equally feasible solutions</u>

→ How to estimate the set of feasible solutions is still a matter of research

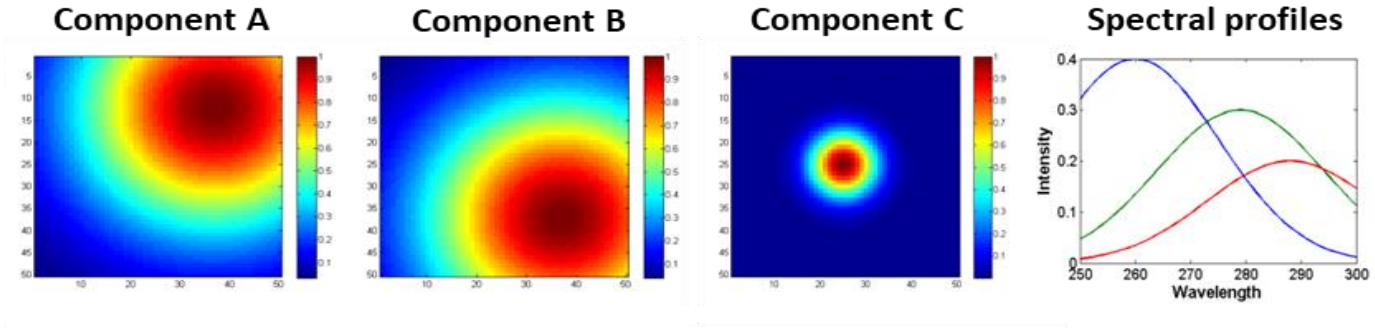
O.S. Borgen, B.R. Kowalski ACA 1985
H. Abdollahi, R. Tauler, Chemolab 2011

THE EFFECT OF IPCs ON THE EXTENT OF ROTATIONAL AMBIGUITY IN MCR-ALS OF HSI

M. Gaffari et al. ACA, 2019

Spatial information

2D-Gaussian components



Heavily mixed spectra

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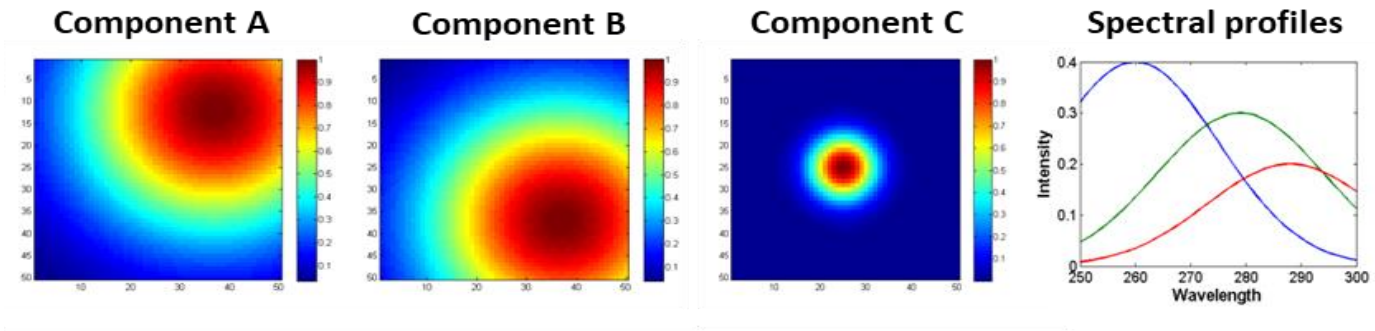
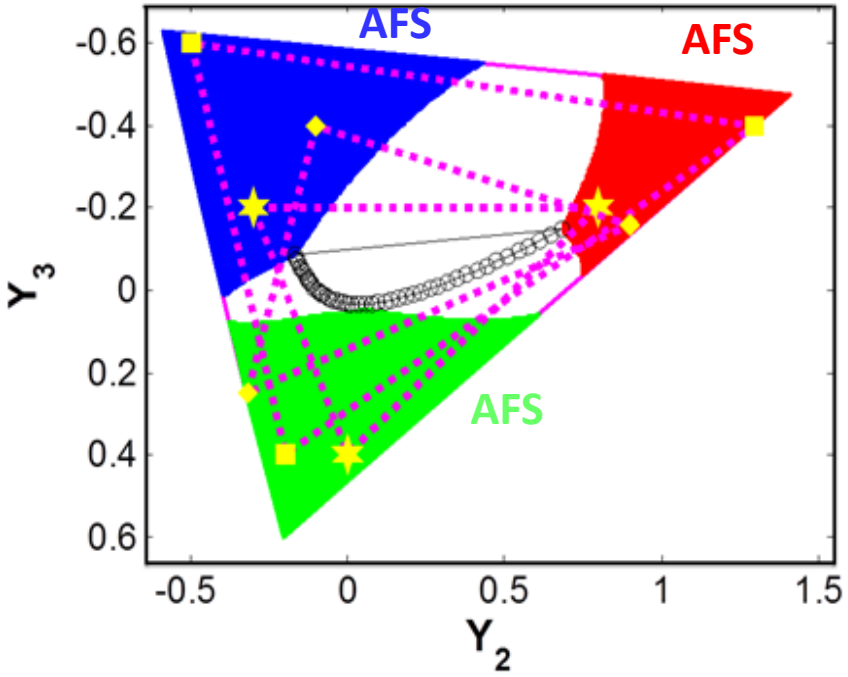
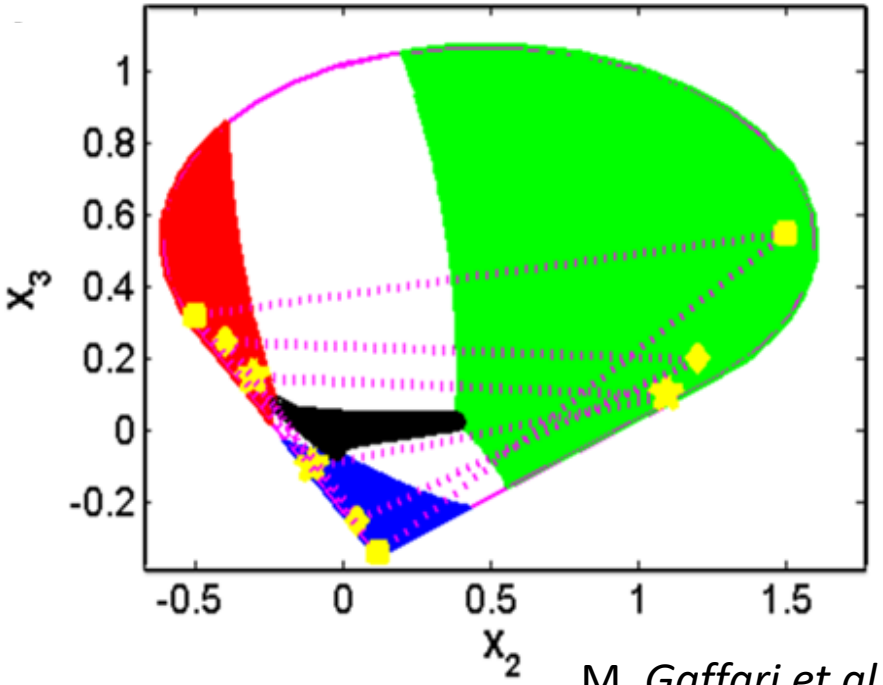


Heavily mixed spectra

$$\mathbf{D} = \mathbf{U}\,\mathbf{S}\,\mathbf{V}^{\mathbf{T}} + \mathbf{E}' = \mathbf{X}\,\mathbf{V}^{\mathbf{T}} + \mathbf{E}' = \mathbf{U}\,\mathbf{Y}^{\mathbf{T}} + \mathbf{E}'$$





M. *Gaffari et al. ACA*, 2019

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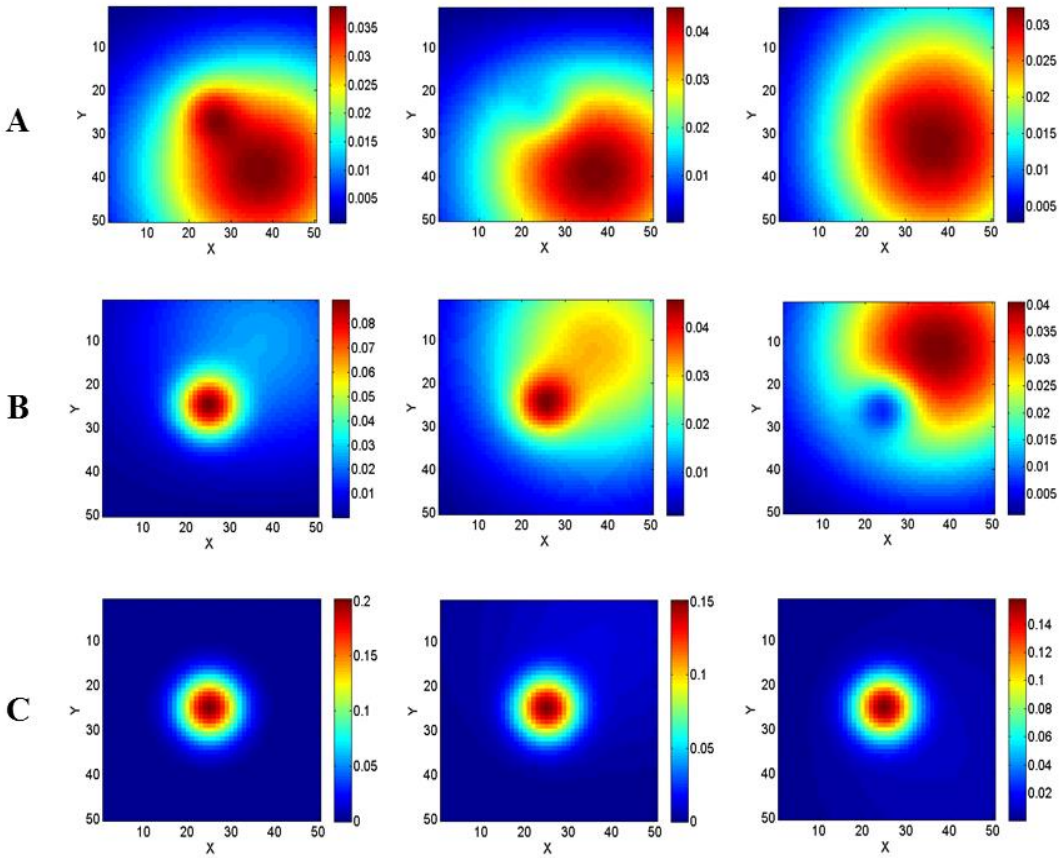

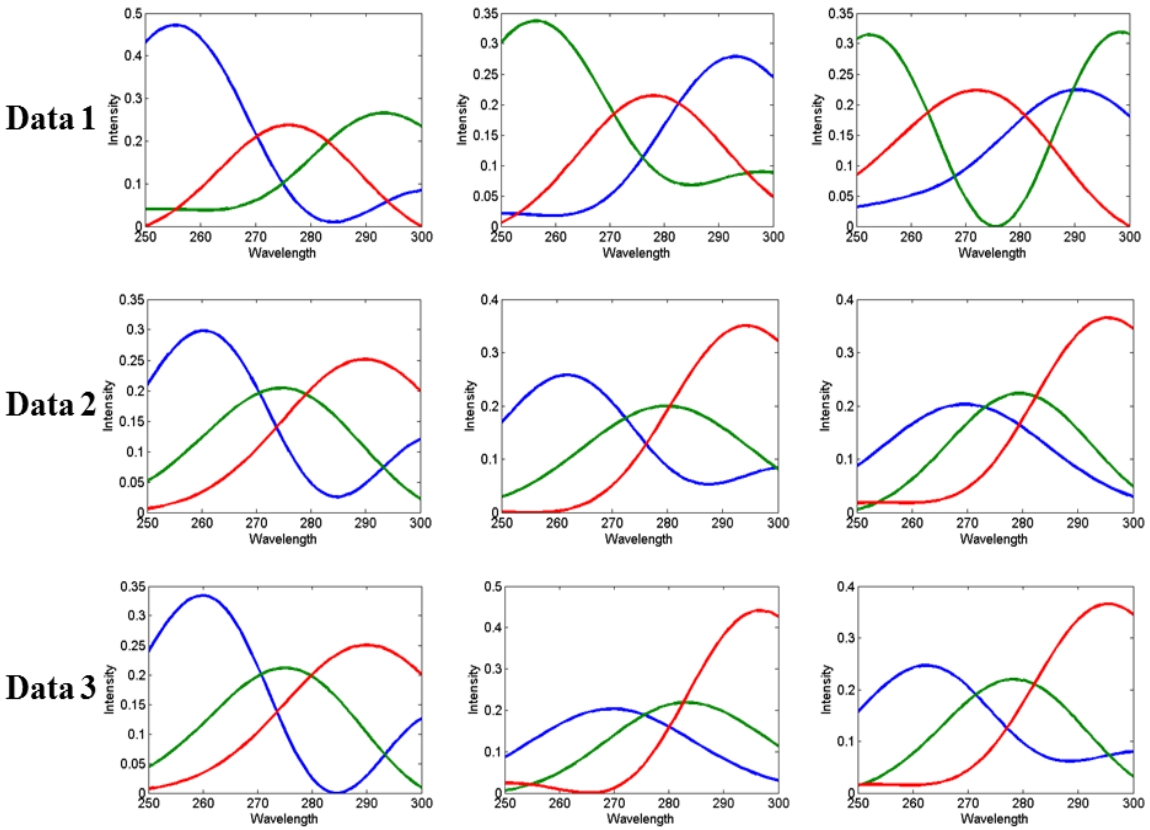

THE EFFECT OF IPCs ON THE EXTENT OF ROTATIONAL AMBIGUITY IN MCR-ALS OF HSI

M. Gaffari et al. ACA, 2019

IPC: 2D-Gaussian hard-model

$$\tilde{\mathbf{C}}_{(:,k)} = A\, e^{-\left(\frac{(x-x_{center})^2}{2\delta_x^2}+\frac{(y-y_{center})^2}{2\delta_y^2}\right)}$$

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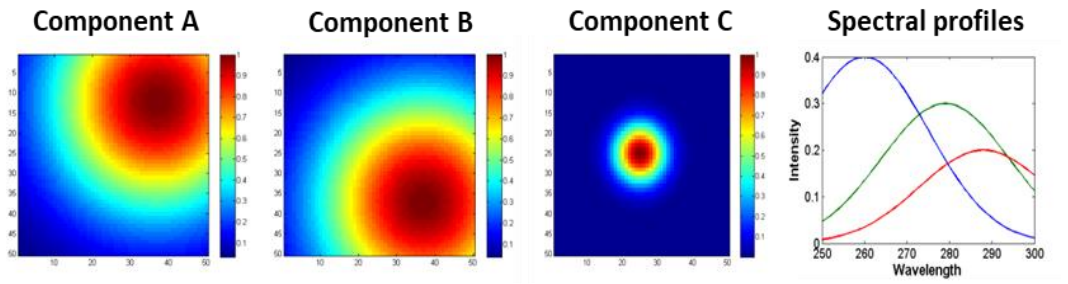

True solution

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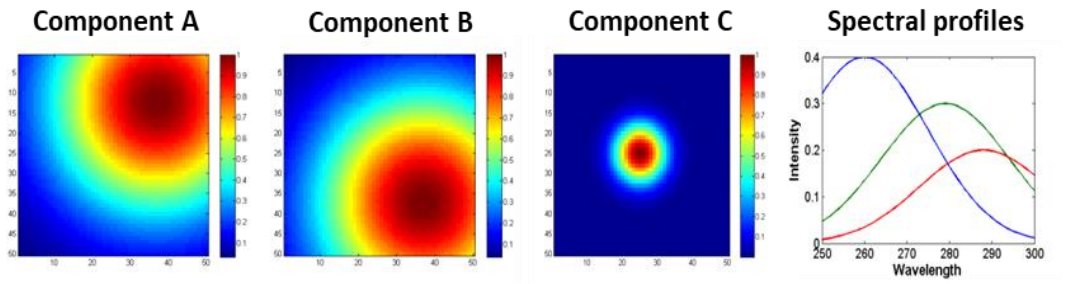

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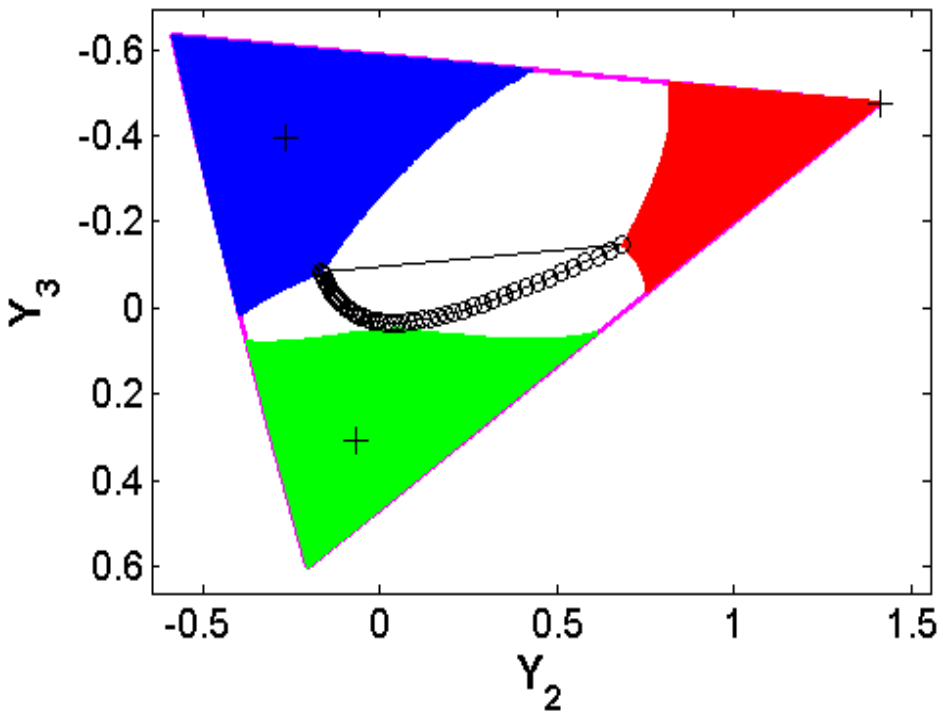

Ambiguity?

AFS- NNMCR

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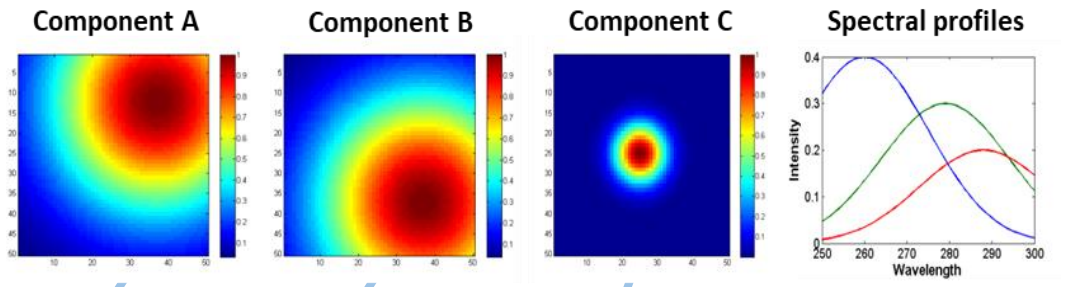

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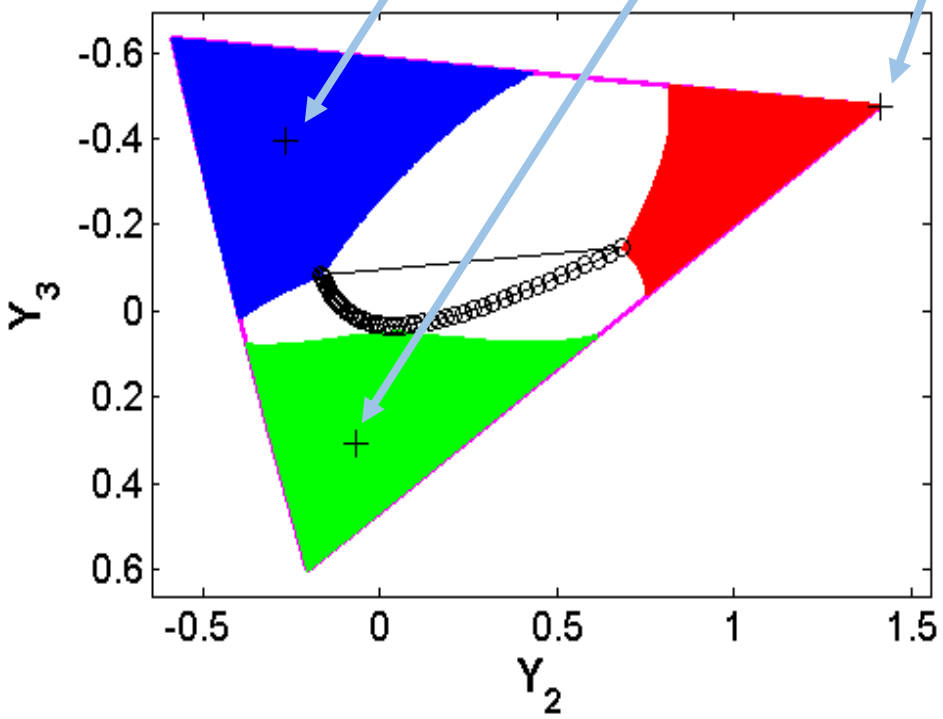

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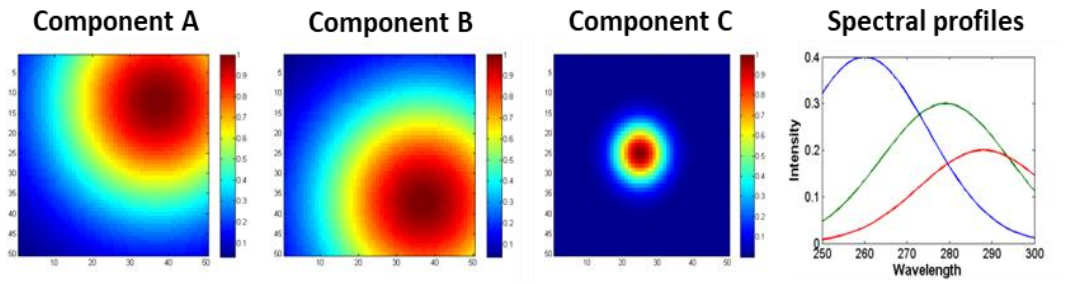
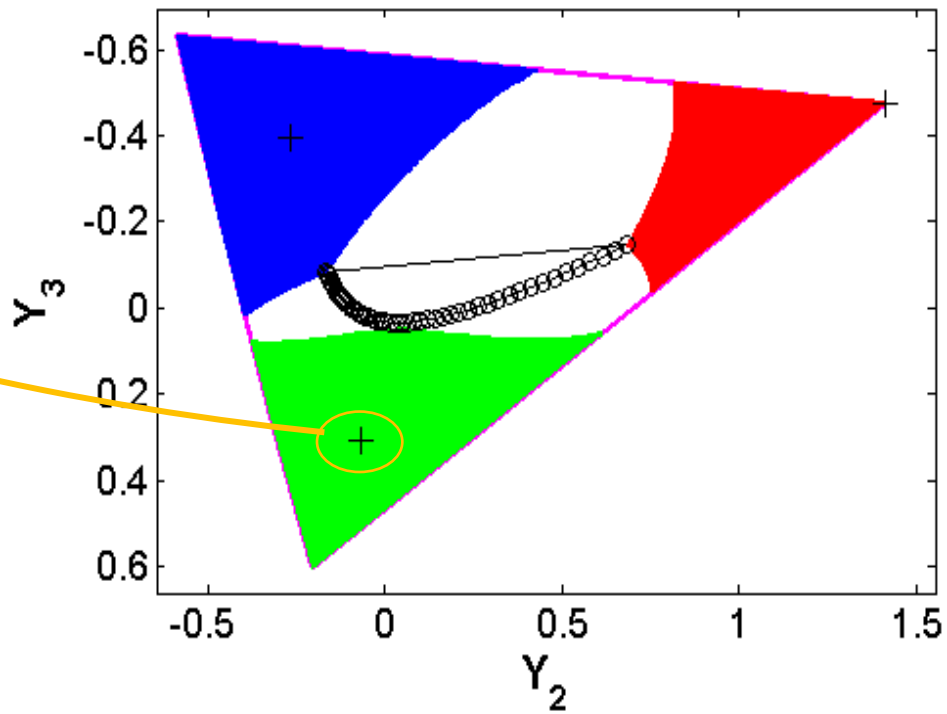


True solution

$\mathbf{c}_{(:,k)}$



Ambiguity?

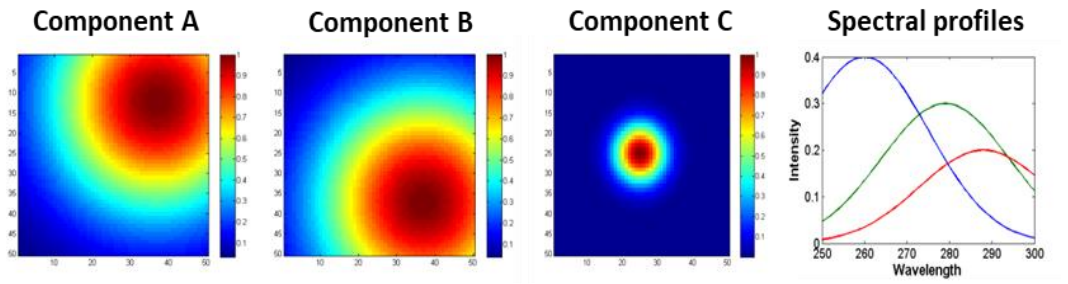
AFS- NNMCR

THE EFFECT OF IPCs ON THE EXTENT OF ROTATIONAL AMBIGUITY IN MCR-ALS OF HSI

M. Gaffari et al. ACA, 2019

IPC: 2D-Gaussian hard-model

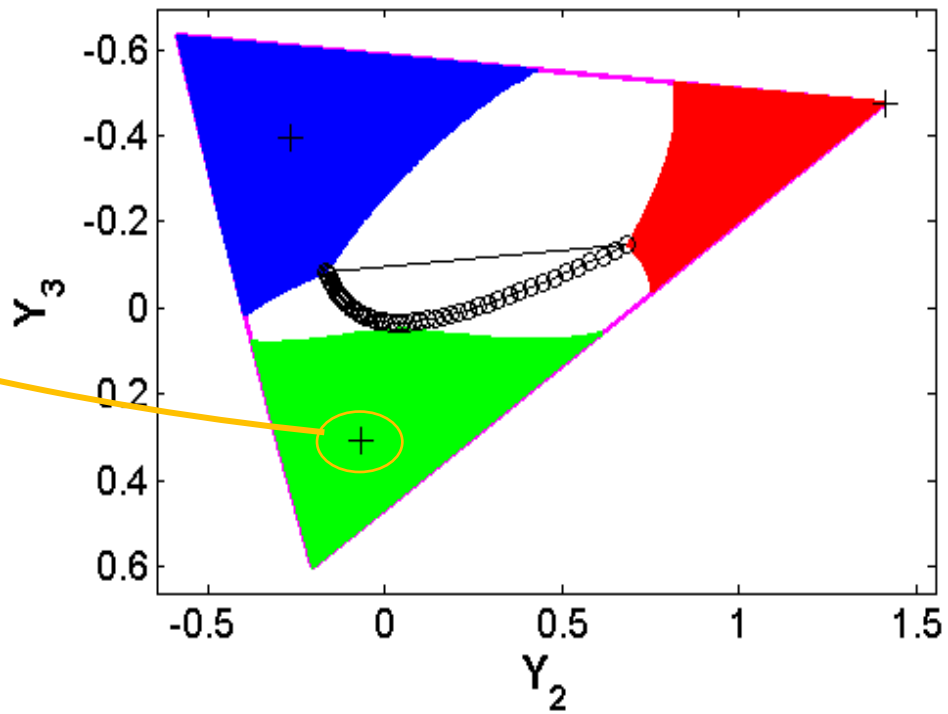
$$\tilde{\mathbf{C}}_{(:,k)} = A\, e^{-\left(\frac{(x-x_{center})^2}{2\delta_x^2}+\frac{(y-y_{center})^2}{2\delta_y^2}\right)}$$



True solution

$$\mathbf{r} = \mathbf{C}_{(:,k)} - \tilde{\mathbf{C}}_{(:,k)}$$

$$\mathbf{C}_{(:,k)}$$



Ambiguity?

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THE EFFECT OF IPCs ON THE EXTENT OF ROTATIONAL AMBIGUITY IN MCR-ALS OF HSI

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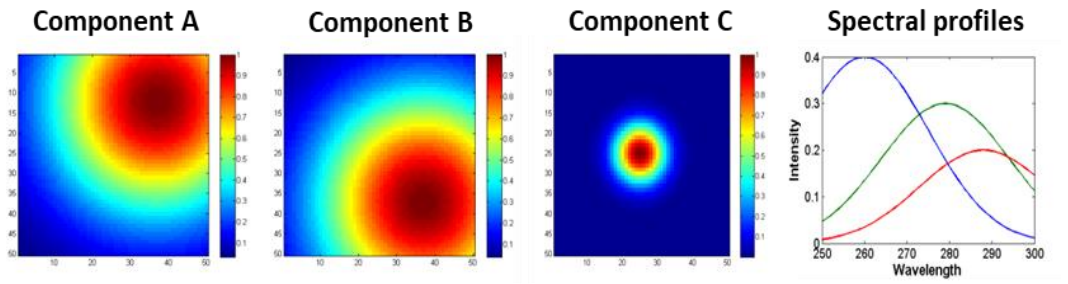
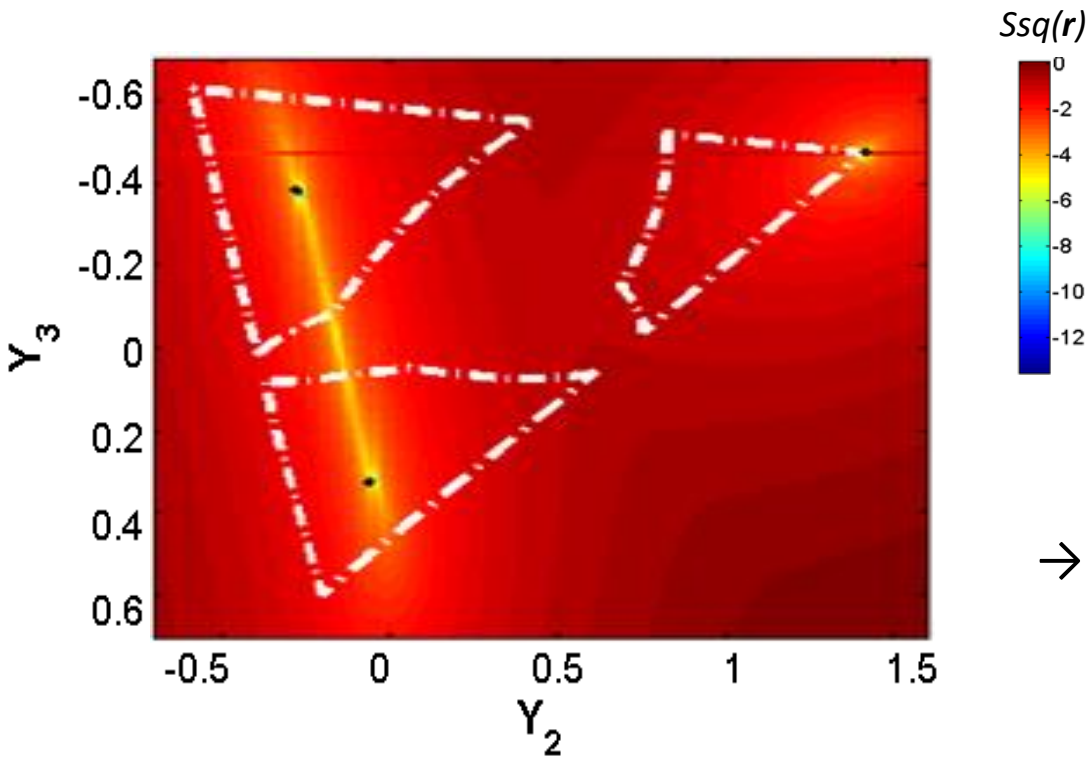


True solution

$$\mathbf{r} = \mathbf{C}_{(:,k)} - \tilde{\mathbf{C}}_{(:,k)}$$



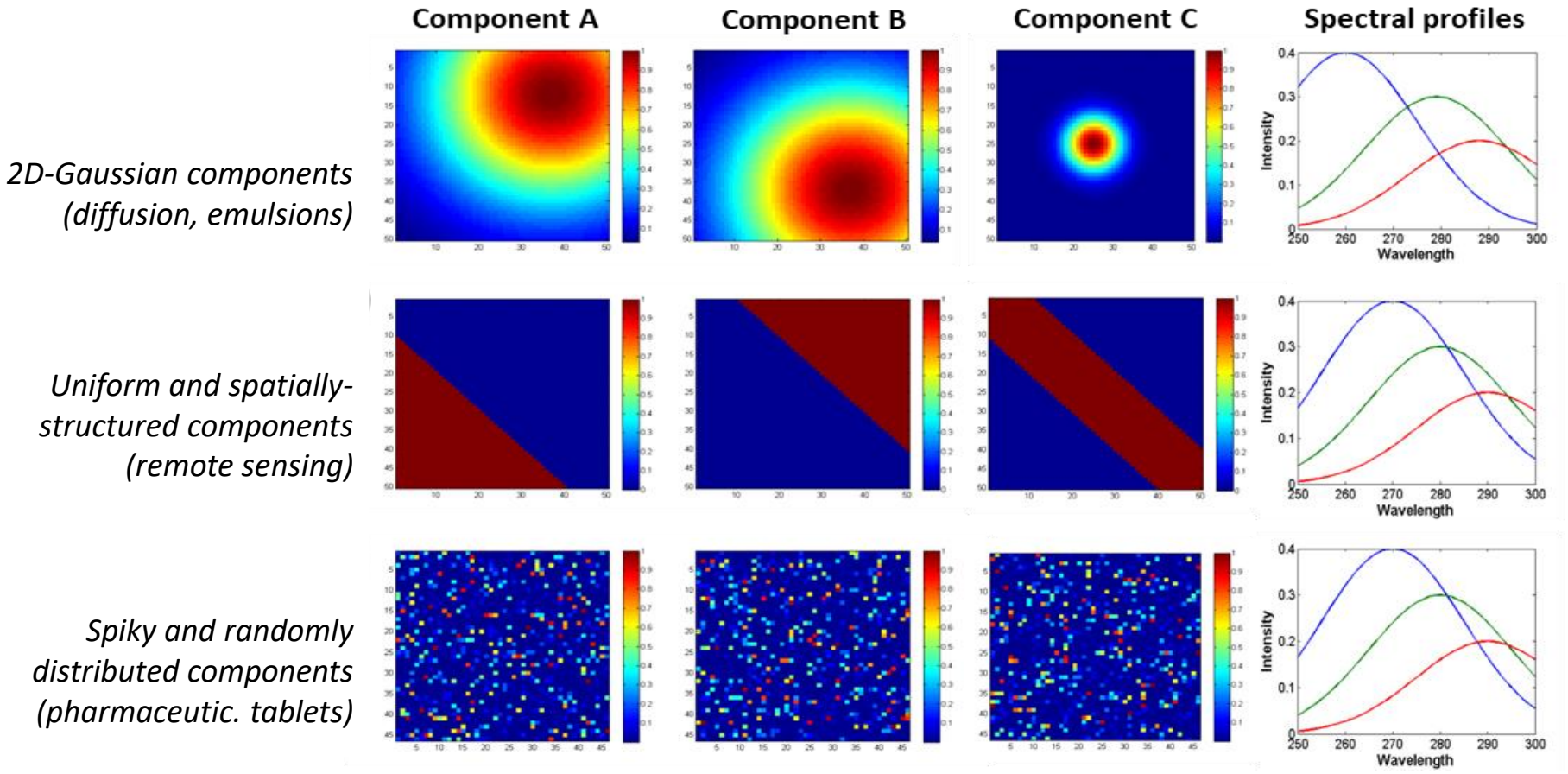
Ambiguity

→ the solution is unique

AFS- NNMCR

THE EFFECT OF IPCs ON THE EXTENT OF ROTATIONAL AMBIGUITY IN MCR-ALS OF HSI

M. Gaffari et al. ACA, 2019

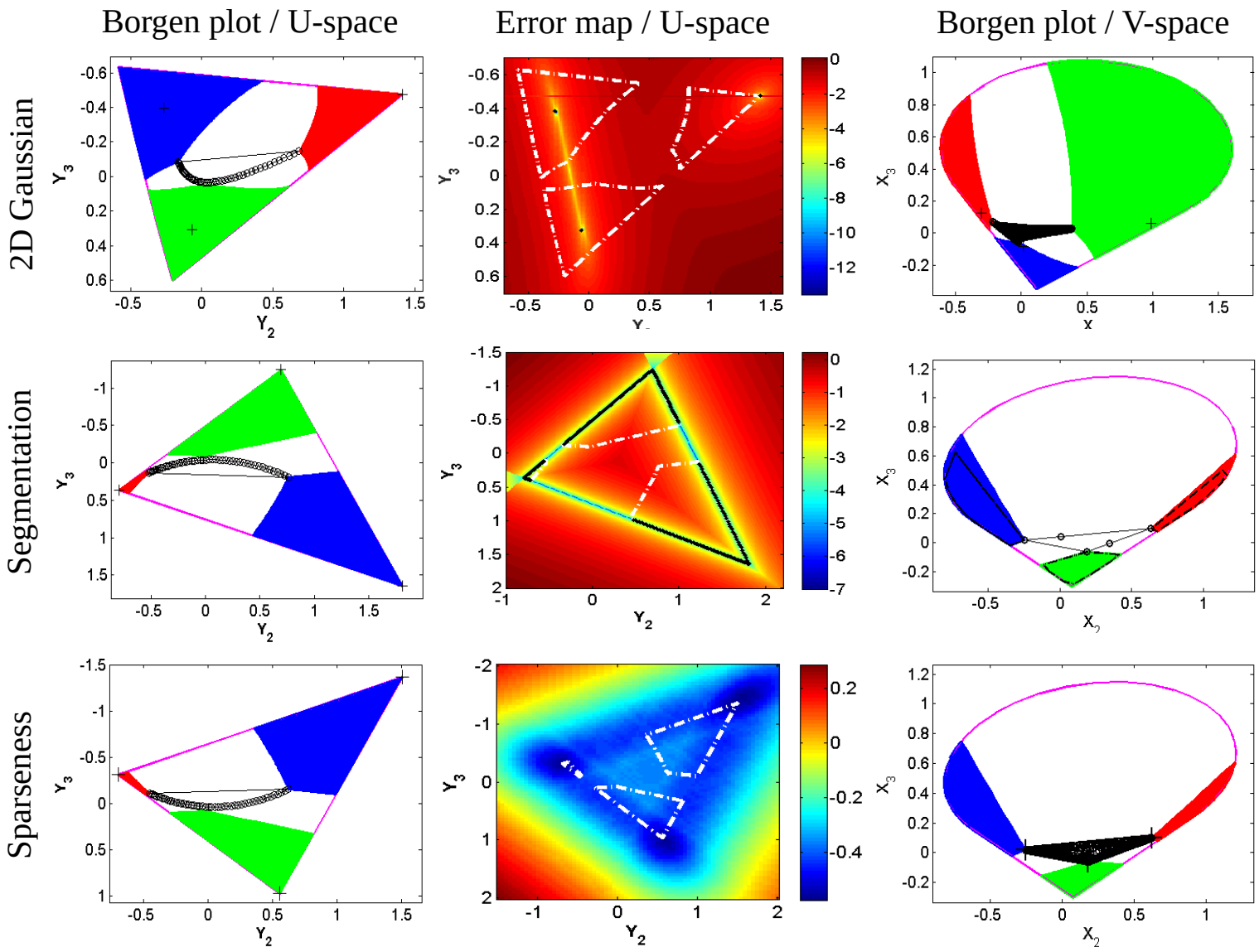


Heavily mixed spectra but clear spatial information

M. *Gaffari et al*. *ACA*, 2019

THE EFFECT OF IPCs ON THE EXTENT OF ROTATIONAL AMBIGUITY IN MCR-ALS OF HSI

M. Gaffari et al. ACA, 2019



In MCR-ALS of HSIs,
When they hold,
And have a physical meaning,

Image Processing Constraints do

- help interpretability
- improve reliability
- reduce rotational ambiguity
- provide a solution colser to the true one

References

Structure/texture constraint for MCR-ALS of hyperspectral images
D. Cevoli, R. Vitale, S. Hugelier,, C. Ruckebusch, tbp 2019

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M. Gaffari, S. Hugelier, L.Duponchel, H. Abdollahi, C. Ruckebusch, ACA 2019

MCR-ALS of hyperspectral images with spatio-spectral fuzzy clustering constraint
P. Firmani, S. Hugelier, F. Marini, C. Ruckebusch, Chemolab 2018

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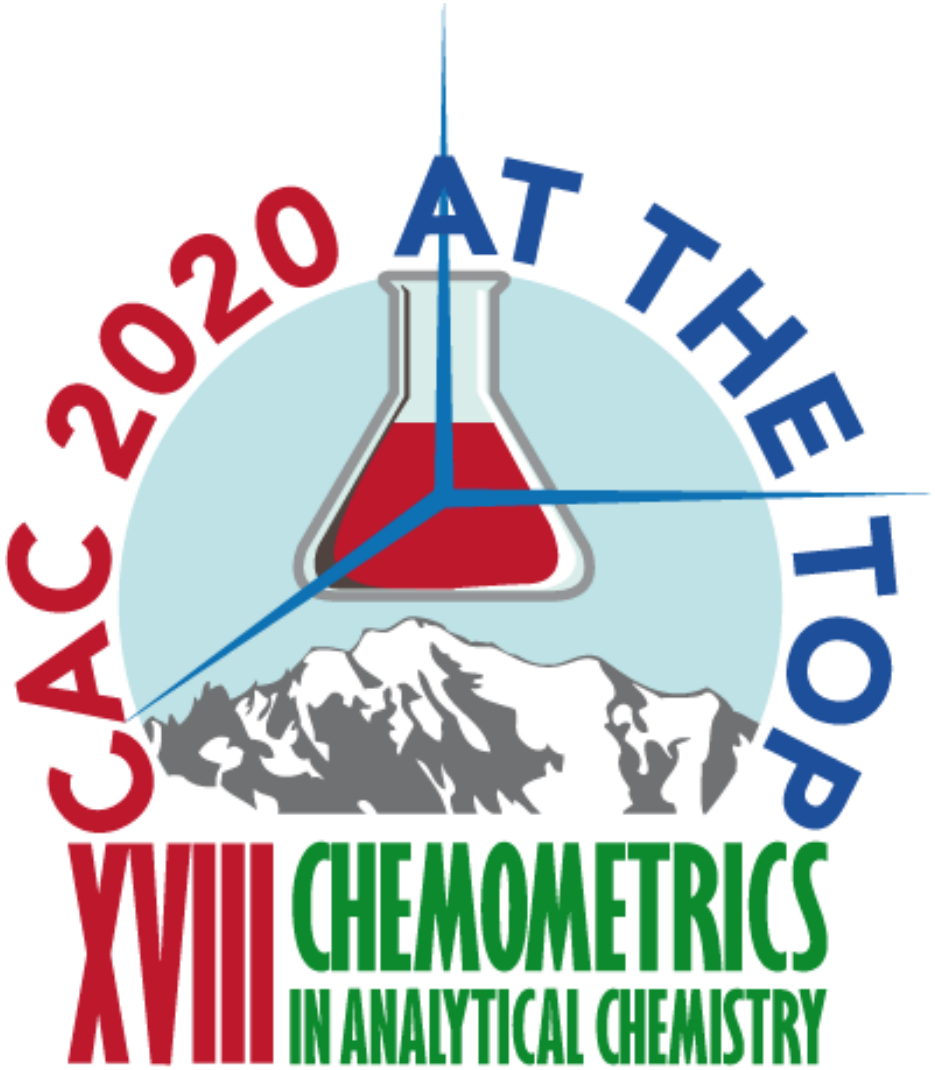
S. Hugelier, R. Vitale, C. Ruckebusch, Applied Spectroscopy 2018

Application of a sparseness constraint in multivariate curve resolution – Alternating least squares
S. Hugelier, S. Piqueras, A. de Juan, C. Ruckebusch, Analytica Chimica Acta 2018

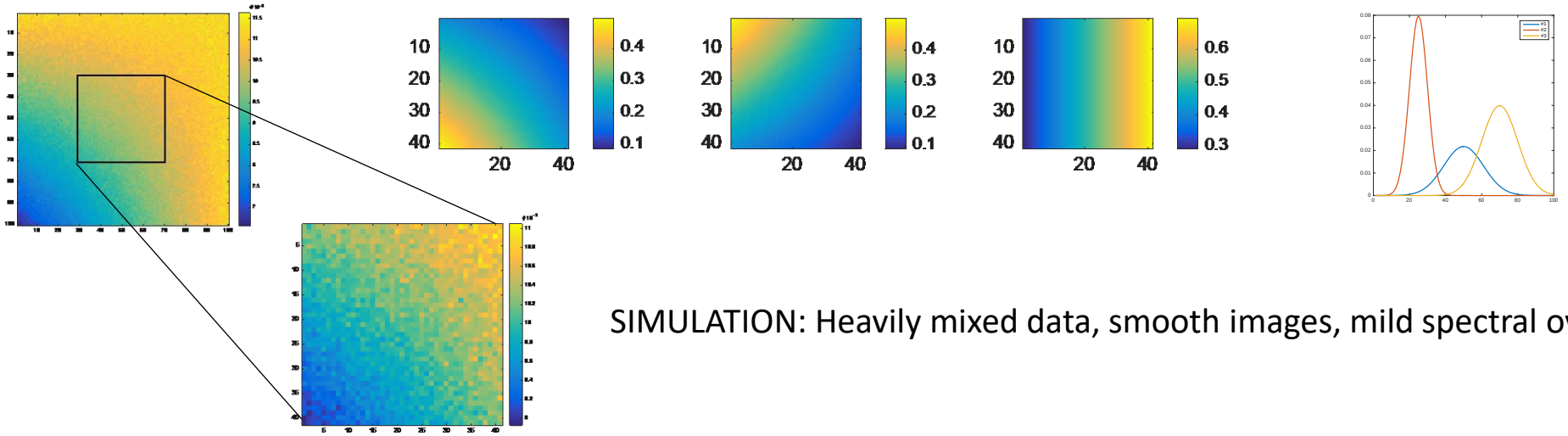
Constraining shape smoothness in multivariate curve resolution-alternating least squares
S. Hugelier, O. Devos, C. Ruckebusch, Journal of Chemometrics 2015

On the implementation of spatial constraints in multivariate curve resolution alternating least squares for hyperspectral image analysis
C. Ruckebusch, S. Hugelier, Journal of Chemometrics 2015

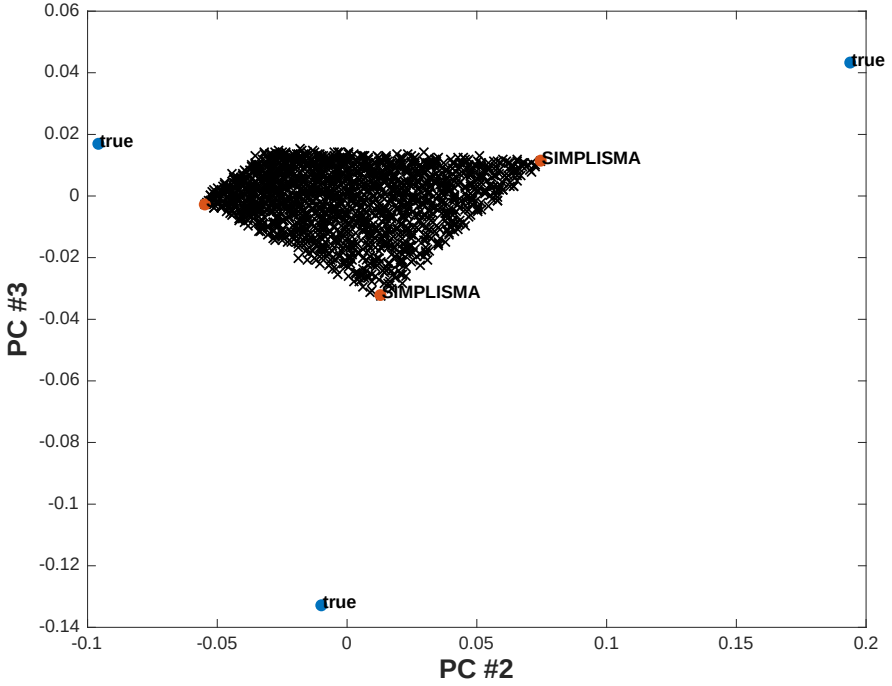


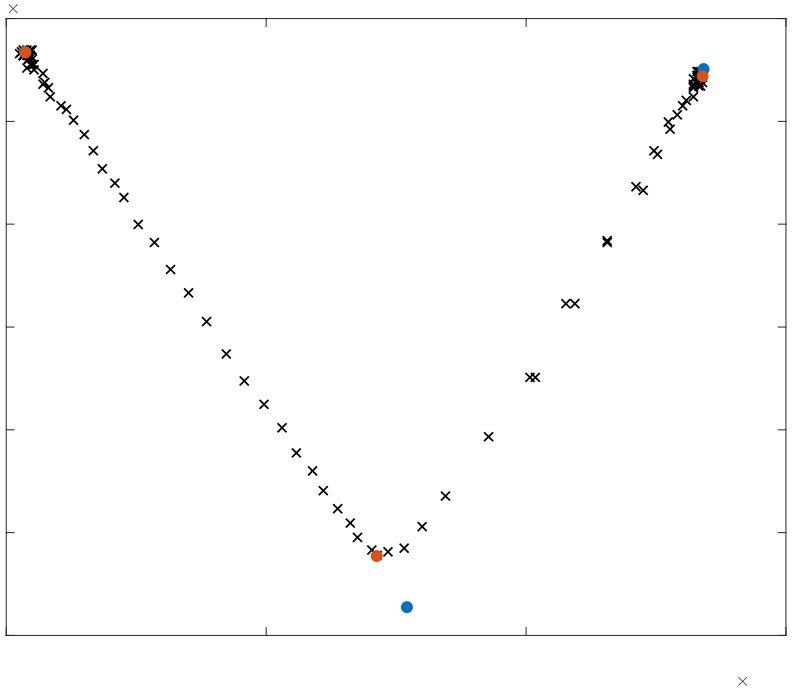
Courmayeur - Italy
Chamonix - France
June 18 - 20, 2020

• Interplay between spatial constraints and spectral unmixing

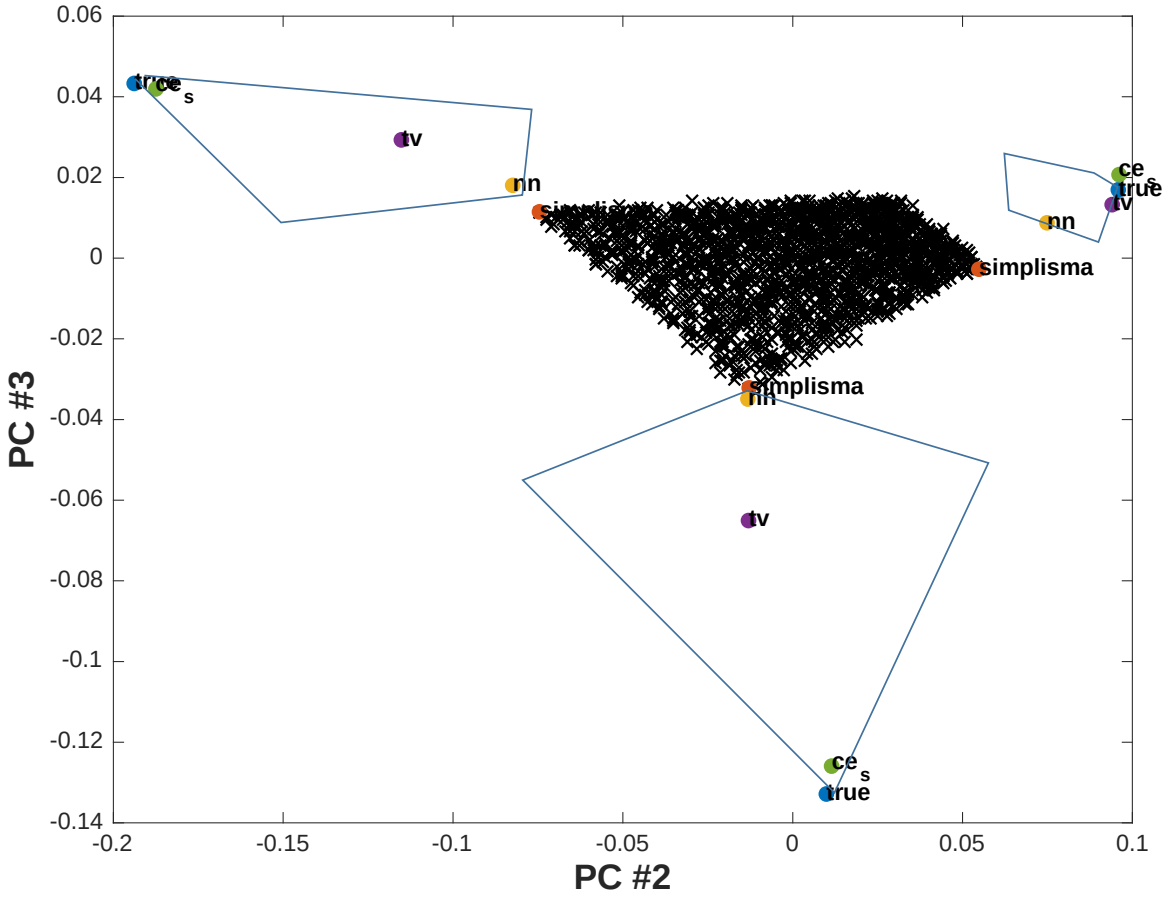


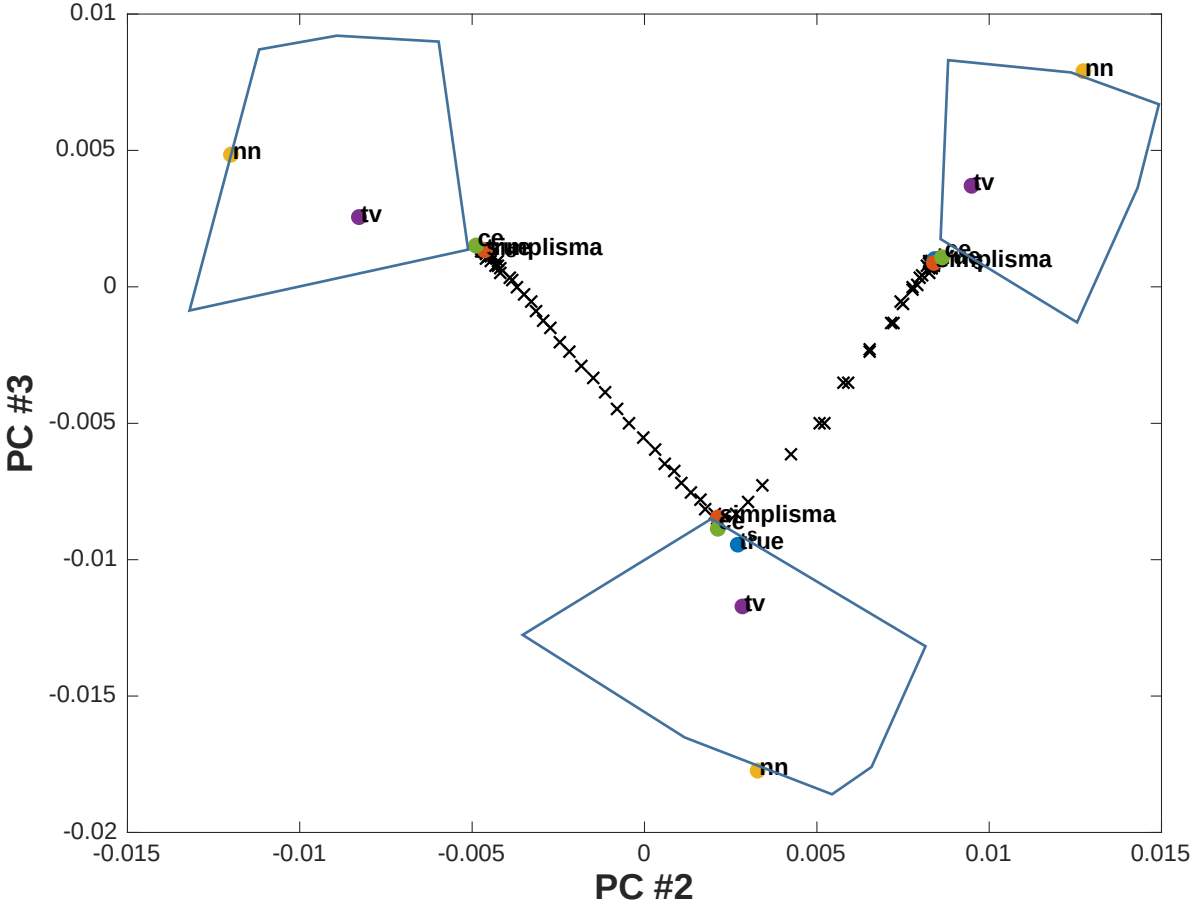
SIMULATION: Heavily mixed data, smooth images, mild spectral overlap



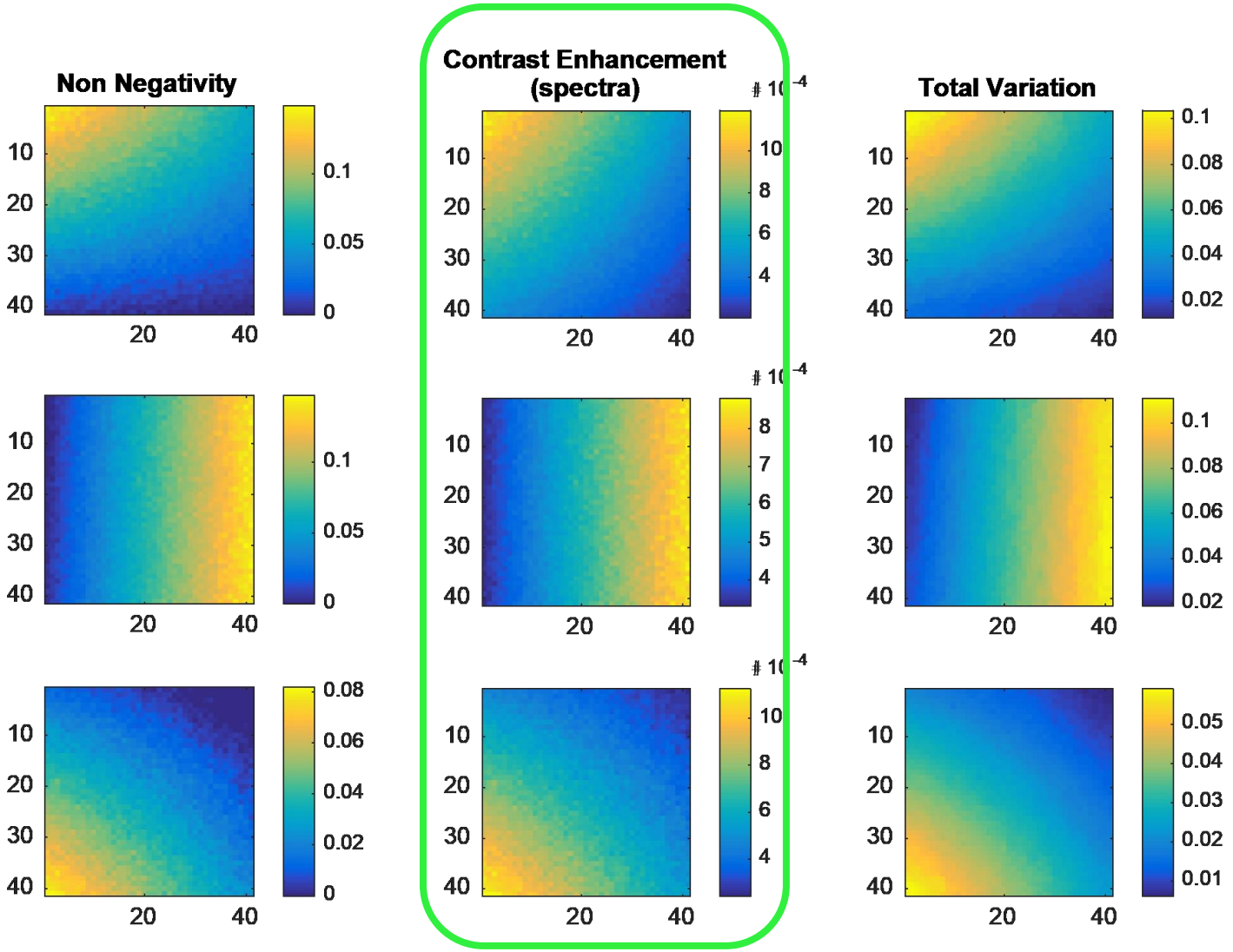


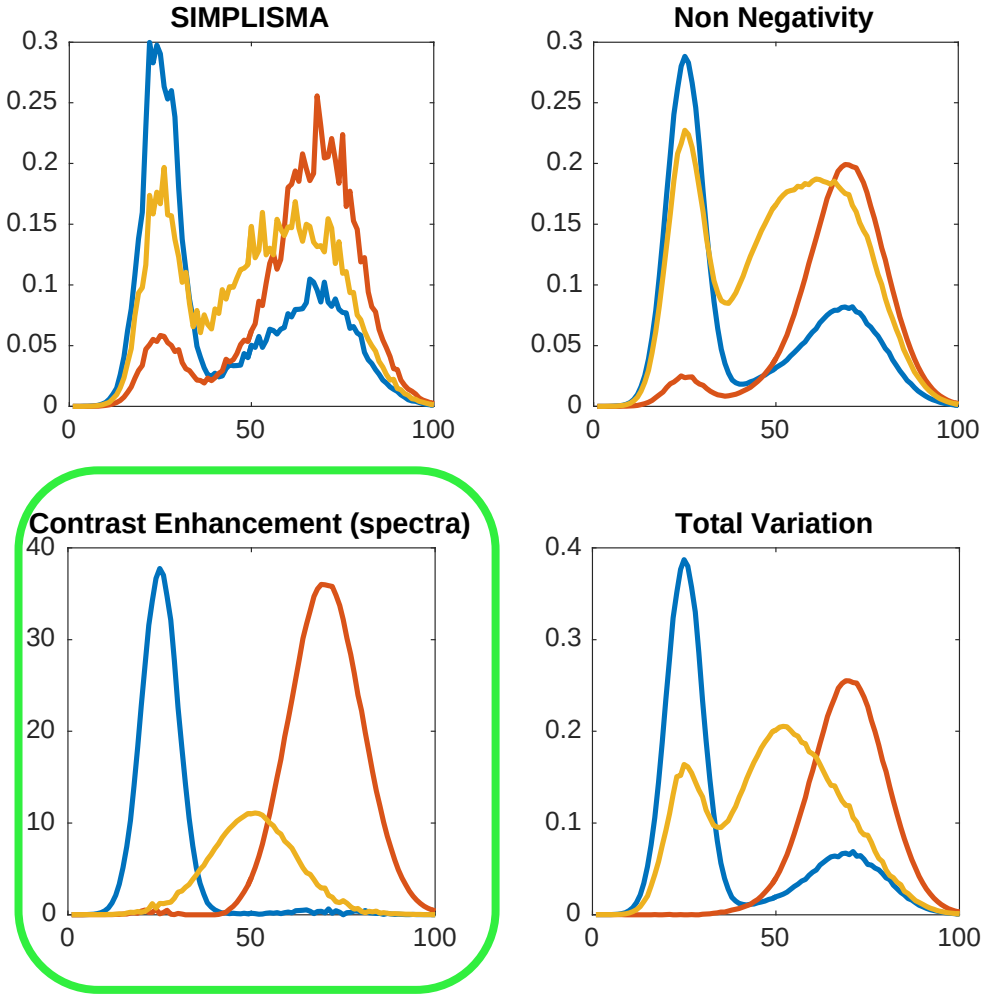
● Interplay between spatial constraints and spectral unmixing



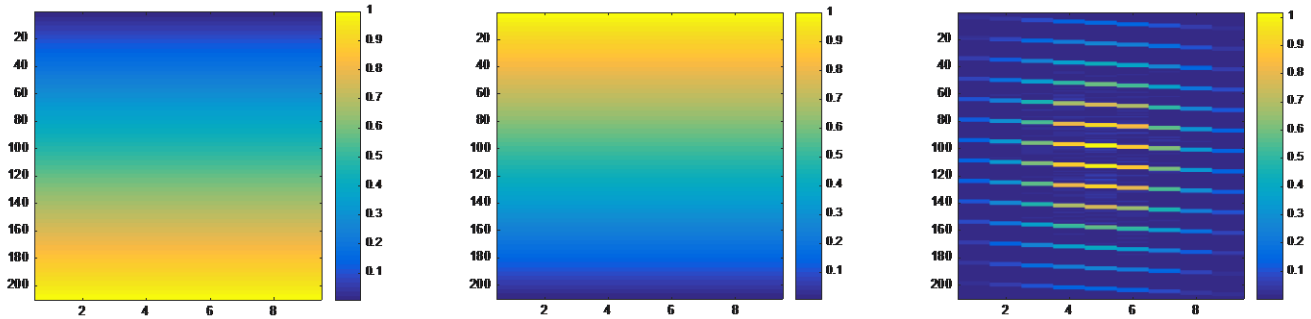


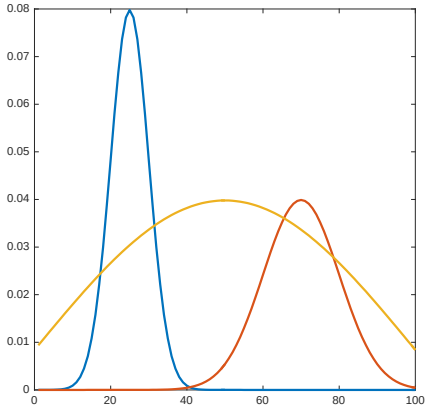
• Interplay between spatial constraints and spectral unmixing



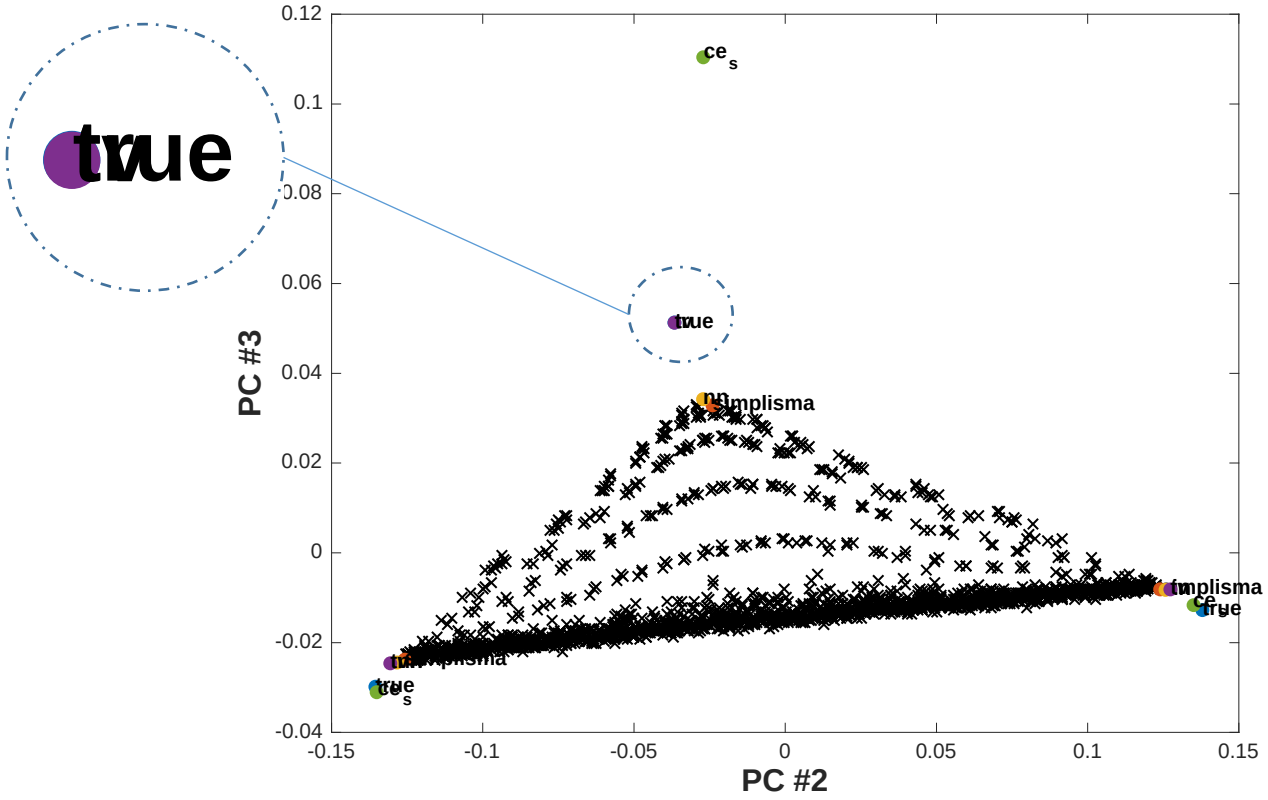


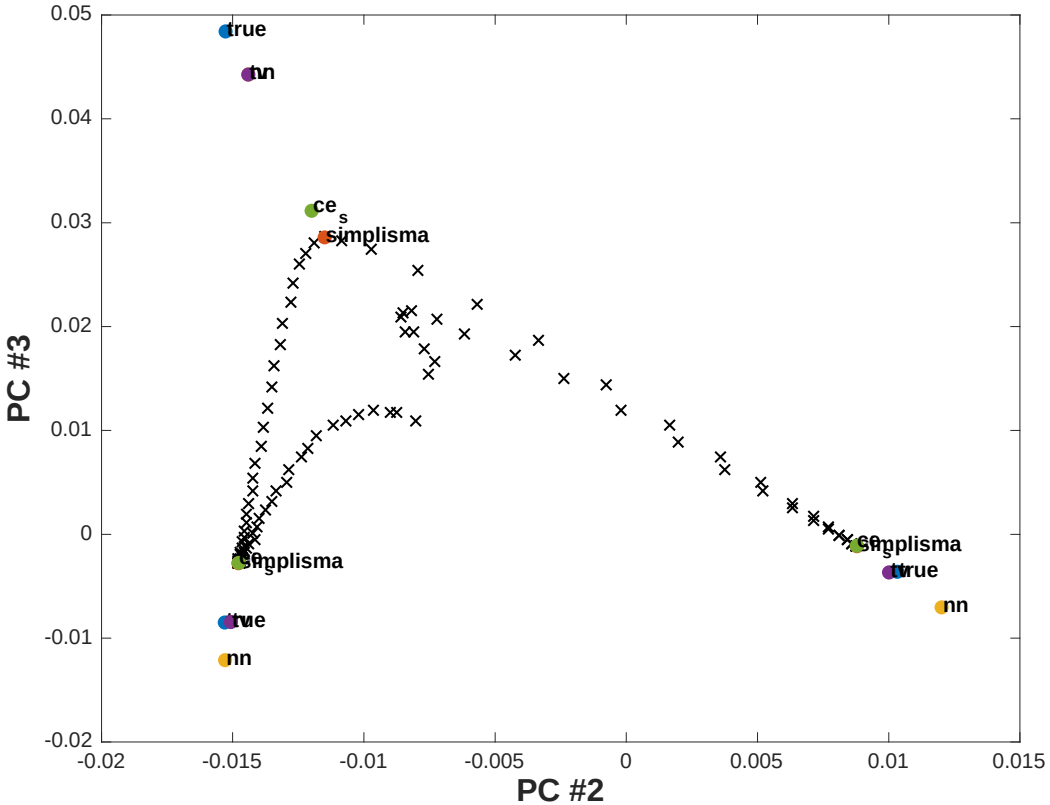
• Applicability of TV image processing constraints



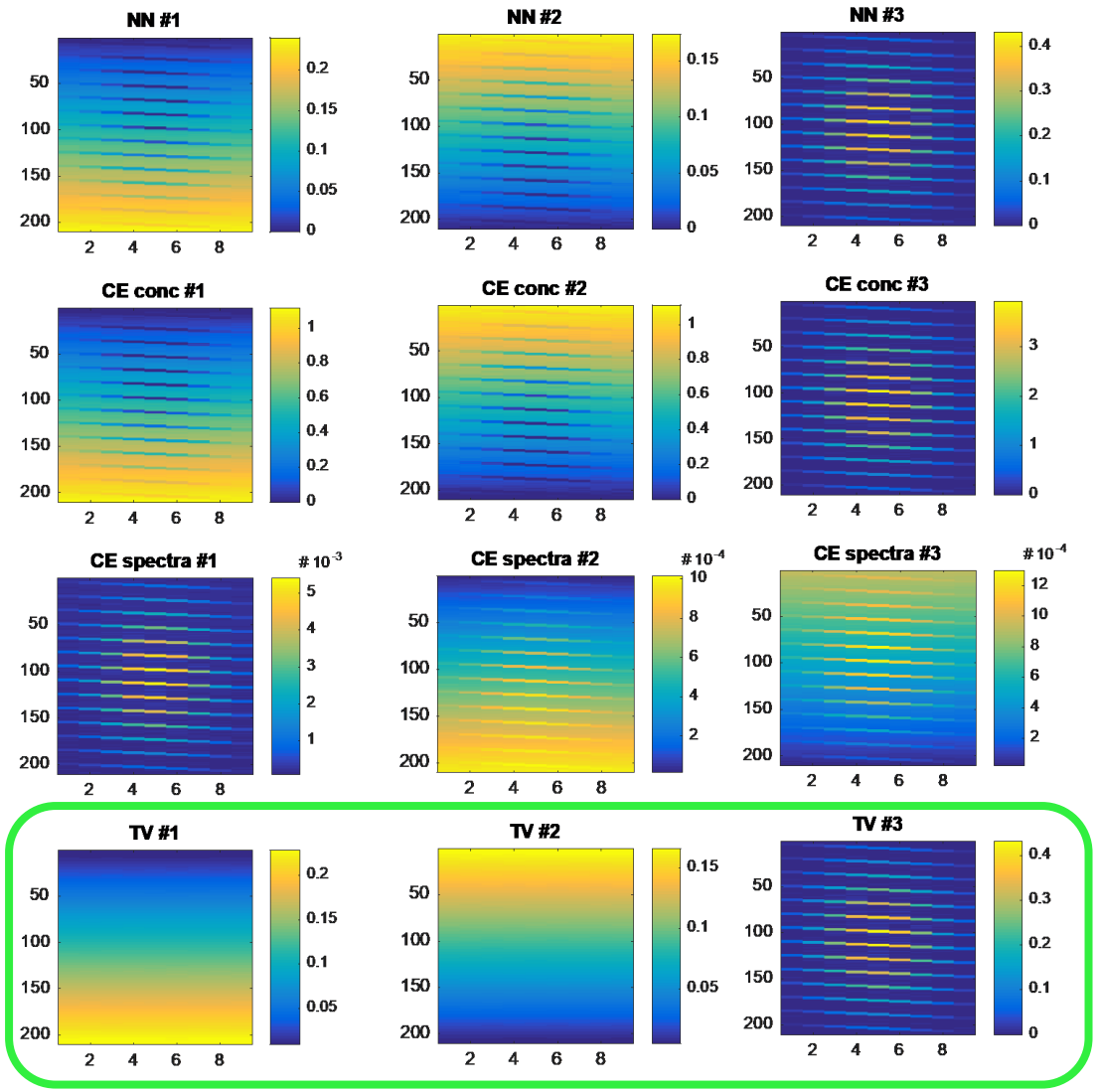


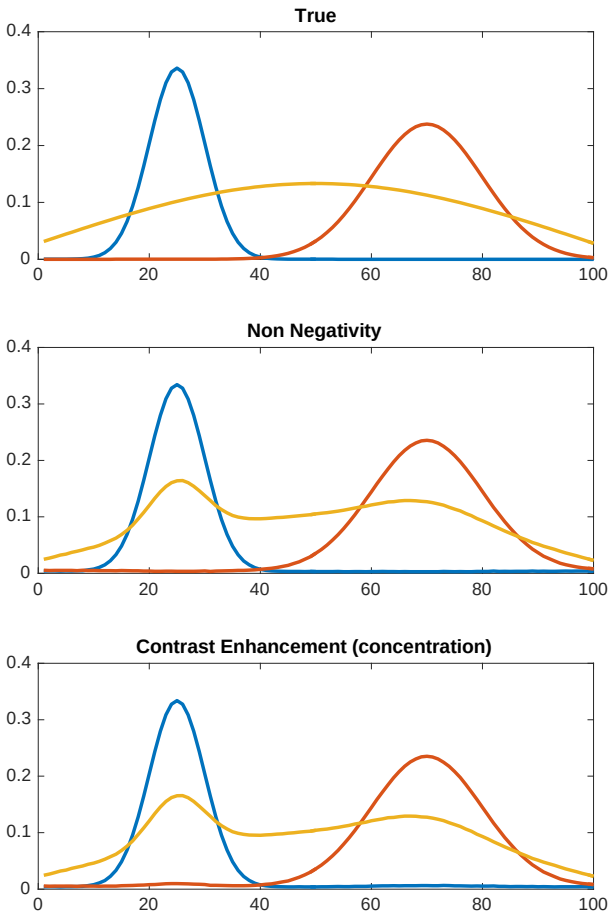
SIMULATION : A texture like component with background spectrum

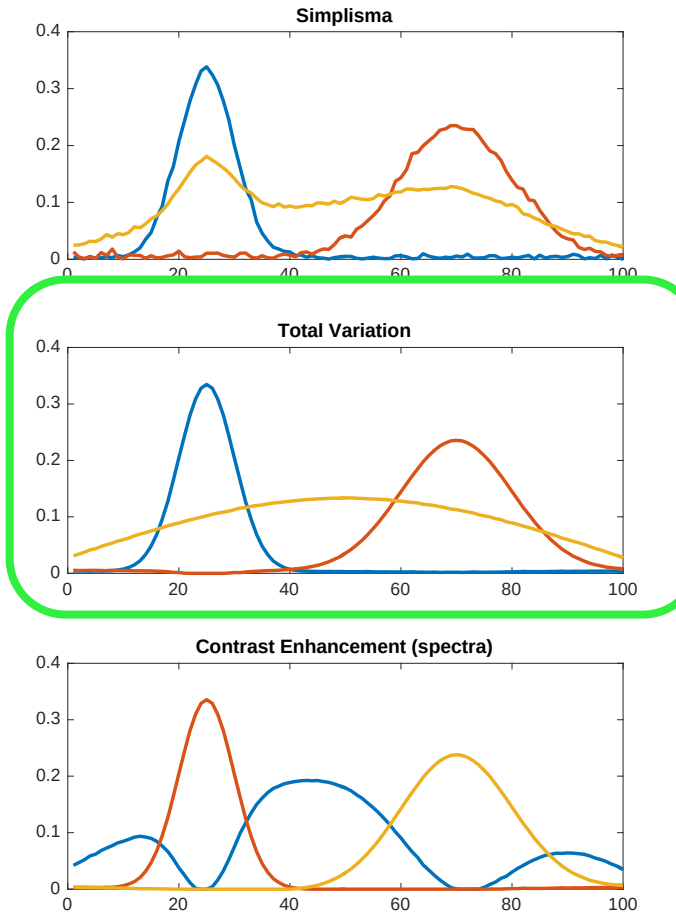




• Applicability of TV image processing constraint





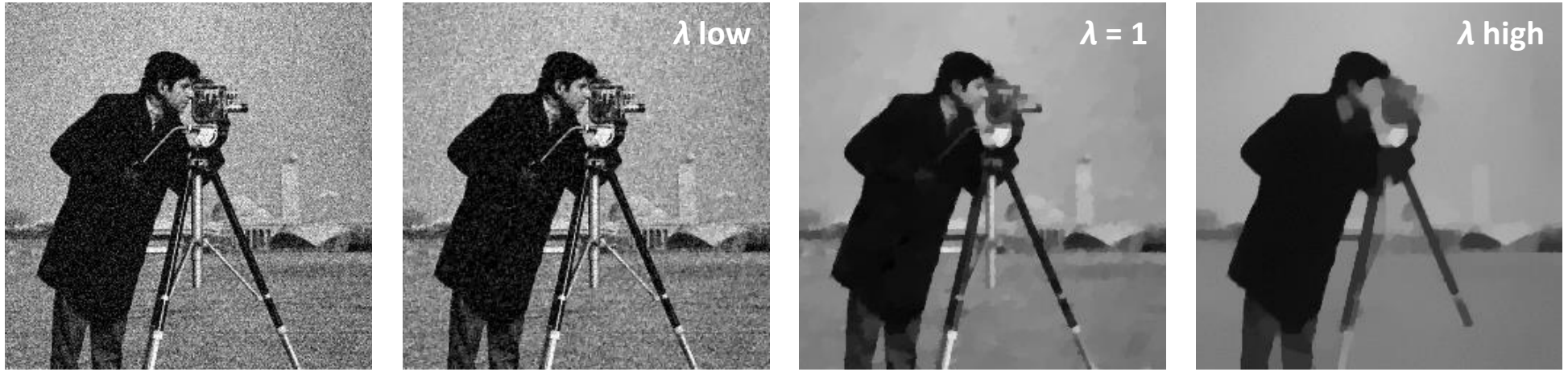


Spatial constraints to circumvent spectral preprocessing (scattering)?

Edge preserving smoothing

$$min\ \|\mathbf{I} - \mathbf{I}_{\boldsymbol{TV}}\|^2 + \lambda \sum_{x,y} \sqrt{\left(i_{x+1,y} - i_{x,y}\right)^2 + \left(i_{x,y+1} - i_{x,y}\right)^2}$$

$$min\ \|\mathbf{I} - \mathbf{I}_{\boldsymbol{TV}}\|^2 + \lambda\ \#\ \{p \mid \|\delta_{\mathrm{x}}\mathbf{i}\|_0 + \|\delta_{\mathrm{y}}\mathbf{i}\|_0\ \neq 0\}$$



Total variation algorithms (Rudin *et al.* 92, Xu *et al.* 2012)
Segmented smoothing (Rippe *et al.*, 2012)

Calculating all feasible solutions in bilinear decomposition of hyperspectral image data clearly help us to visualize the accuracy of the results. All feasible solutions have the same worth and MCR-ALS just calculate one of them. Actually the later solution is in the range of all feasible ones and logically we should report our results and the related conclusions as an feasible interval. This interval practically is more meaningful than any individual solution which can be obtained from MCR-ALS or any other similar methods. i think this issue is very important for further discussion.

Incorporating of any information in multivariate curve resolution of hyperspectral image data can affect on the range of feasible solutions. So, a systematic investigation on any constraint in spatial or spectral modes of data matrix can be monitored via calculation all feasible solutions and interpretation of obtained results. This issue is alsa can be discussed further in our email grou

MCR-ALS under constraints

- Constraints improve reliability of the solution (rotational ambiguity)

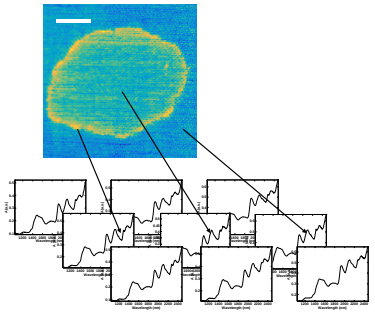
- Constraints improve interpretability, physical/chemical meaning of the solution (unimodality, kinetic hard-modelling)

- Constraints are very few in MCR-ALS of HSI

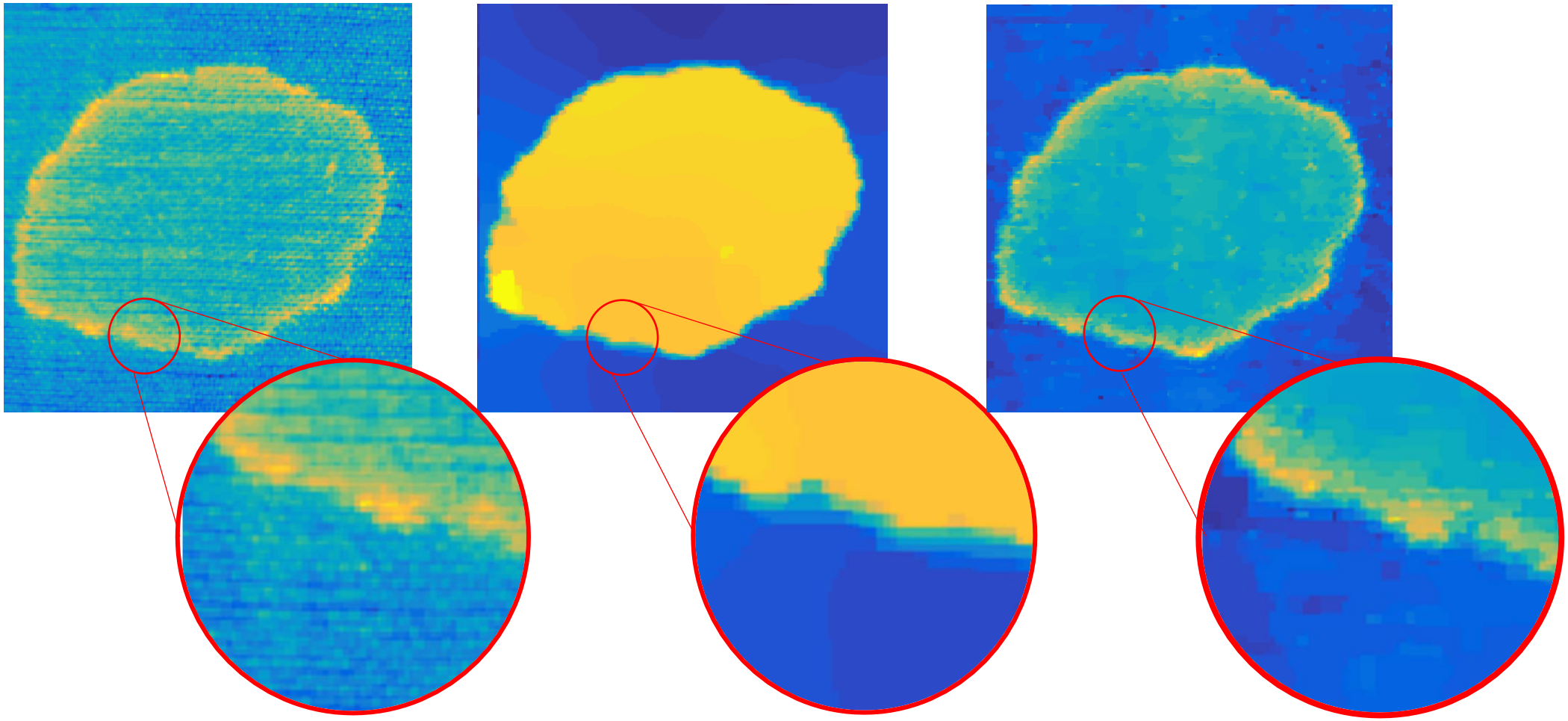
→ Spatial information should be input as constraint whenever possible and in particular when spectral information is highly mixed

In mathematical optimization, **constrained optimization** (in some contexts called **constraint optimization**) is the process of optimizing an objective function with respect to some variables in the presence of constraints on those variables. The objective function is either a cost function or energy function, which is to be minimized, or a reward function or utility function, which is to be maximized. Constraints can be either **hard constraints**, which set conditions for the variables that are required to be satisfied, or **soft constraints**, which have some variable values that are penalized in the objective function if, and based on the extent that, the conditions on the variables are not satisfied.

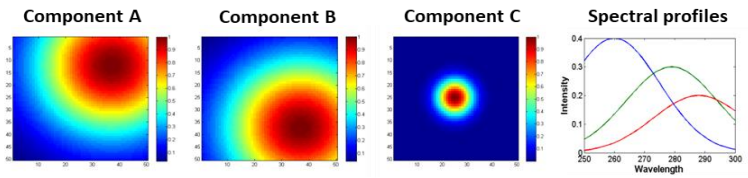
Edge preserving smoothing (RTV)



Forensic NIR Identification of semen on cotton (Coll J. Amigo & C. Santos)

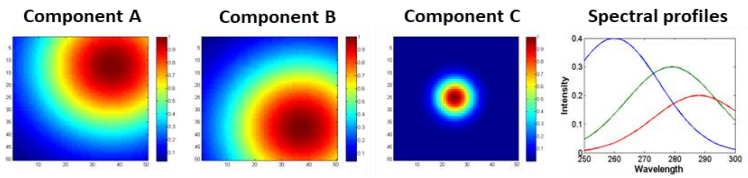


Effect of IPC on rotational ambiguity of the MCR solution



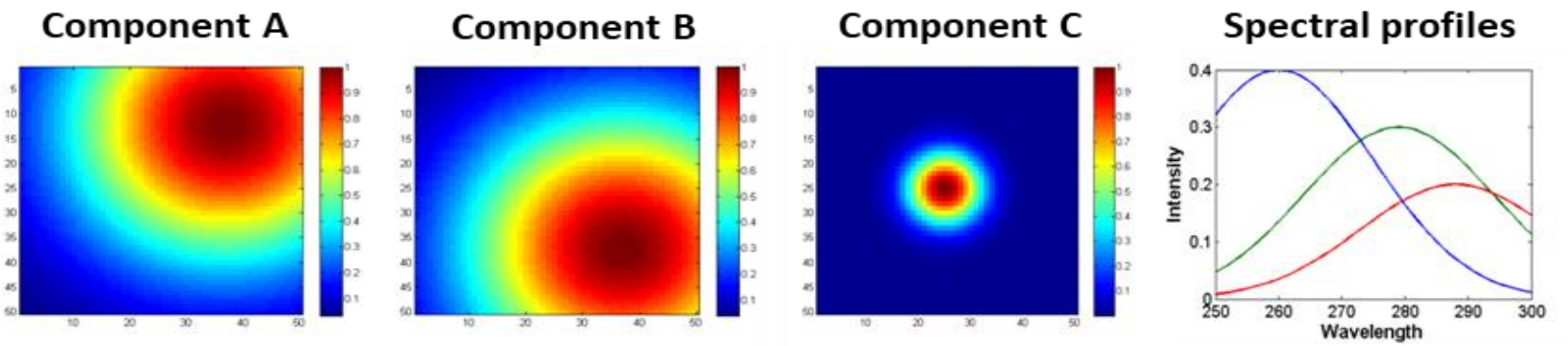
MCR-ALS with NN +
Gaussian shape constraint

Effect of IPC on rotational ambiguity of the MCR solution



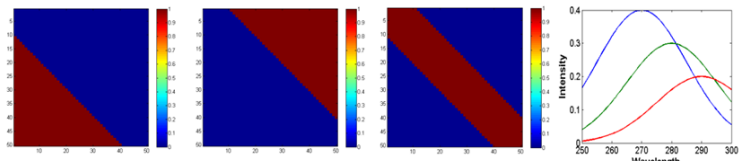
MCR-ALS with NN + ***Gaussian shape constraint***

$$\tilde{\mathbf{C}}_{(:,k)} = A\, e^{-\left(\frac{(x-x_{center})^2}{2\delta_x^2}+\frac{(y-y_{center})^2}{2\delta_y^2}\right)}$$

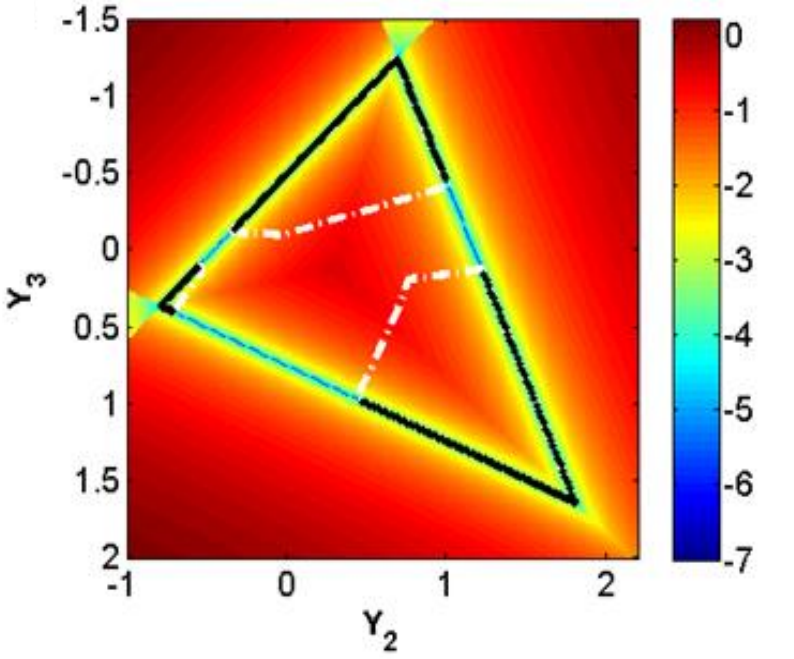


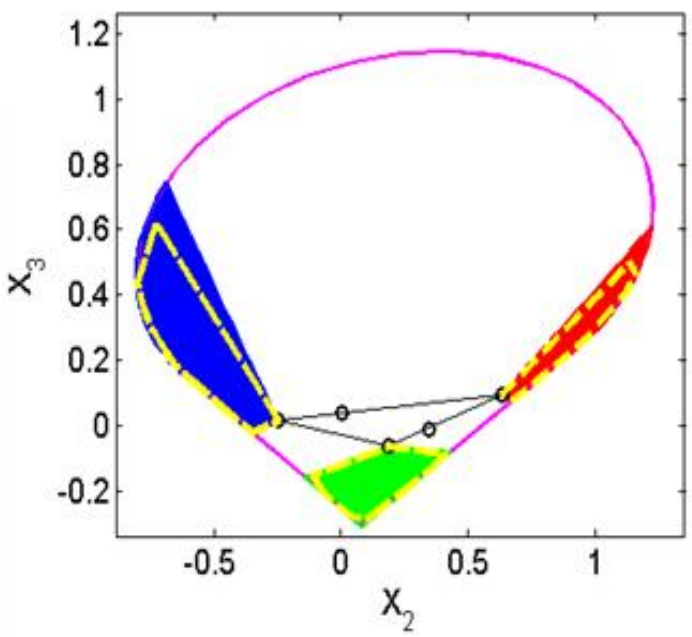
MCR results looks « perfect »!

Effect of IPC on rotational ambiguity of the MCR solution



*MCR-ALS with NN + **segmentation constraint***

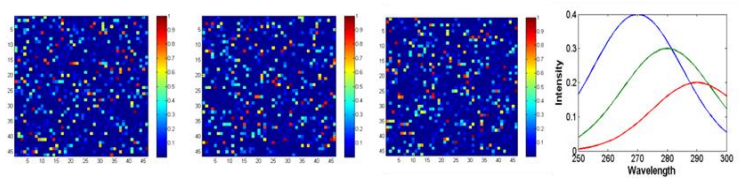




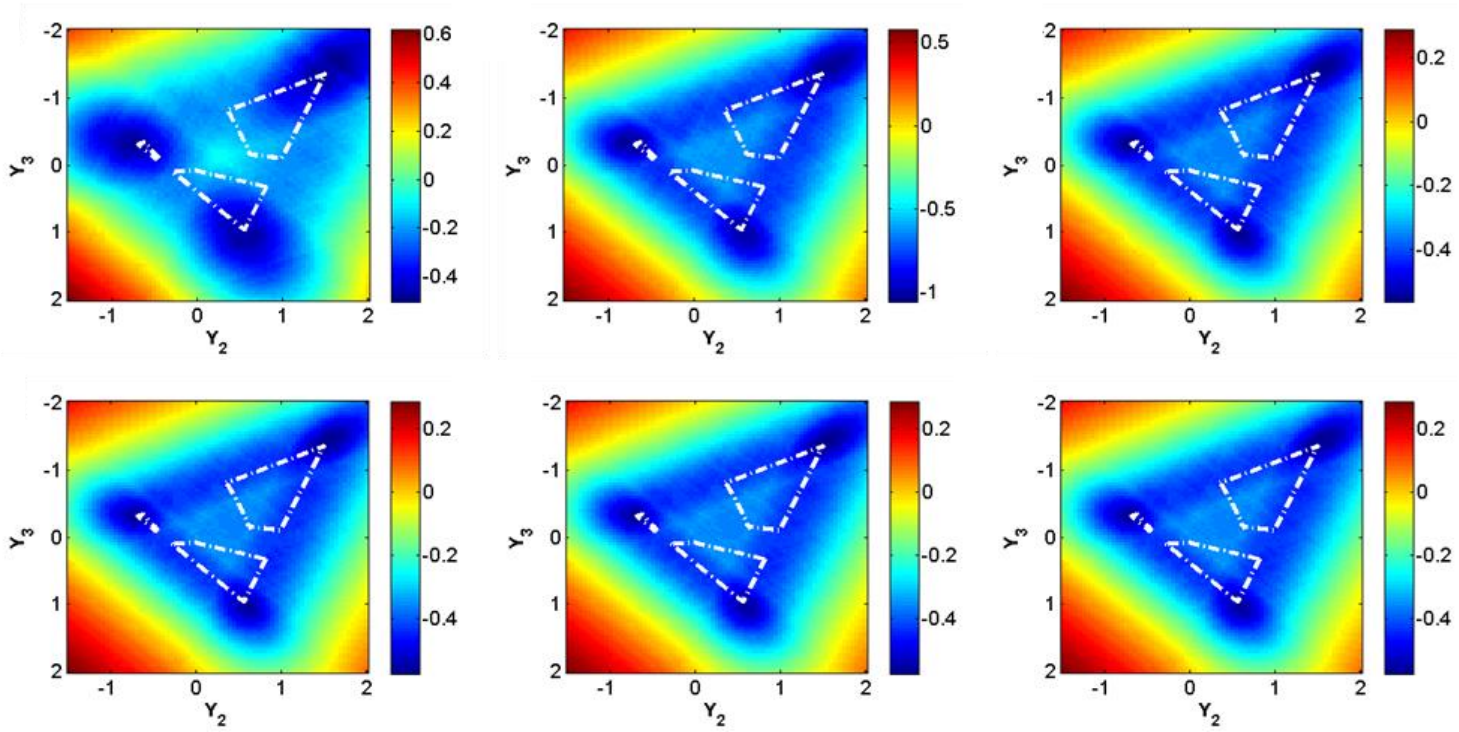
Amiguity highly reduced

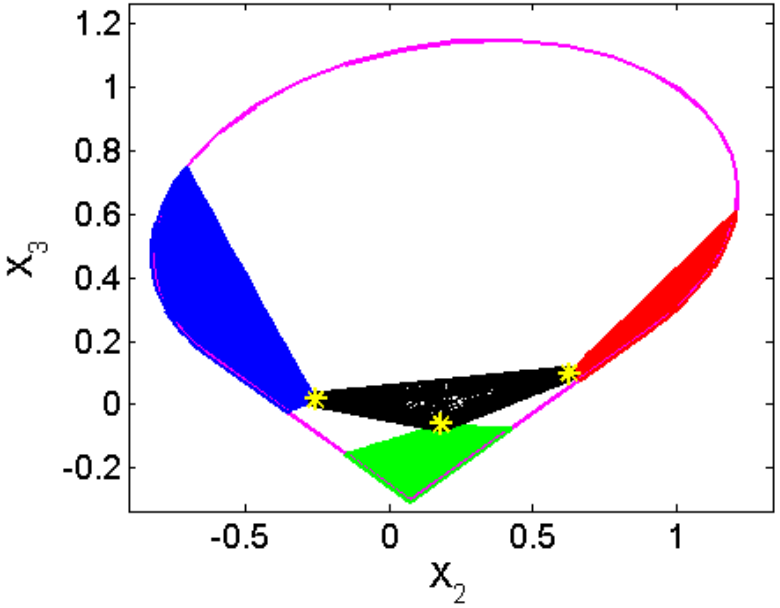
M. Ghaffari *et al. 2019*

Effect of IPC on rotational ambiguity of the MCR solution



*MCR-ALS with NN + **sparseness constraint***





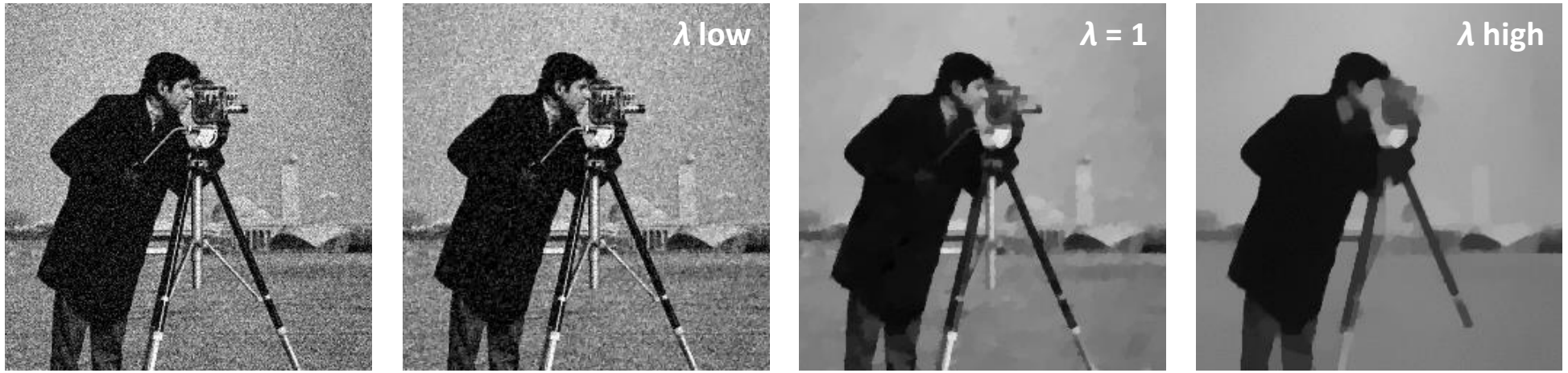
M. Ghaffari *et al. 2019*

Acknowledgement

Edge preserving smoothing

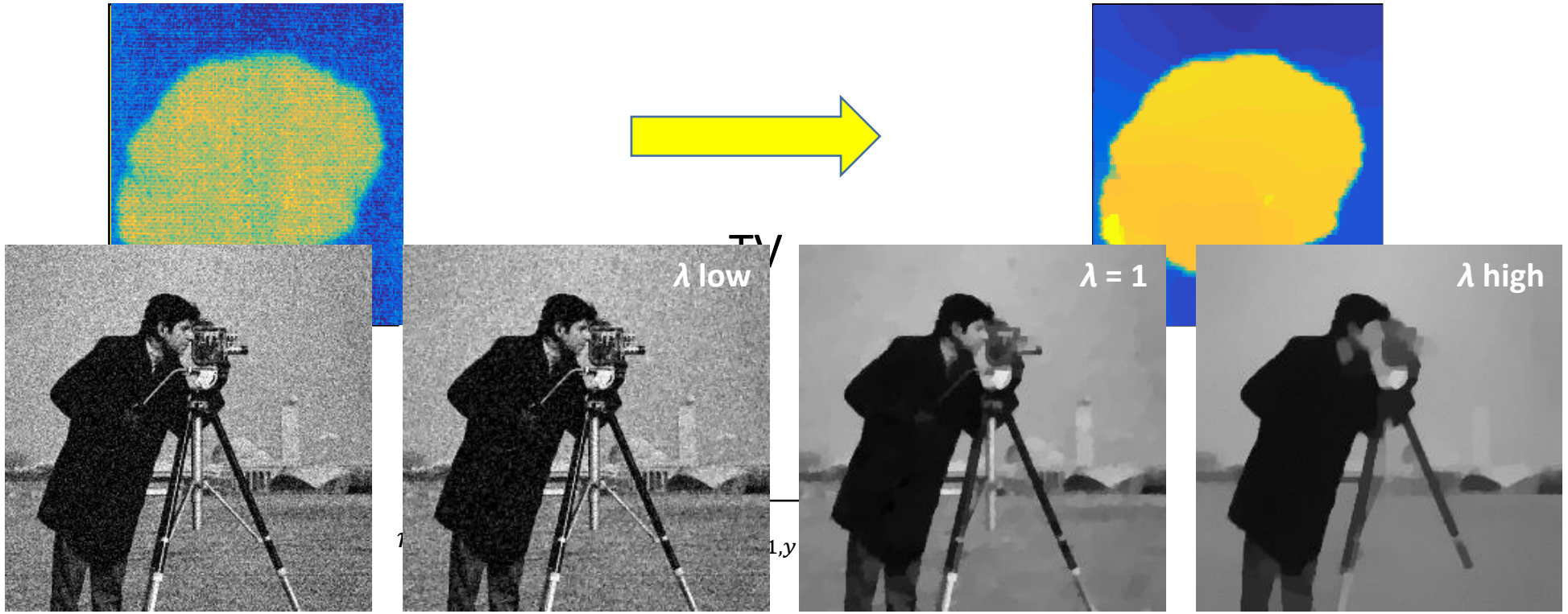
$$min\ \|\mathbf{I} - \mathbf{I}_{\boldsymbol{TV}}\|^2 + \lambda \sum_{x,y} \sqrt{\left(i_{x+1,y} - i_{x,y}\right)^2 + \left(i_{x,y+1} - i_{x,y}\right)^2}$$

$$min\ \|\mathbf{I} - \mathbf{I}_{\boldsymbol{TV}}\|^2 + \lambda\ \#\ \{p \mid \|\delta_{\mathrm{x}}\mathbf{i}\|_0 + \|\delta_{\mathrm{y}}\mathbf{i}\|_0\ \neq 0\}$$



Total variation algorithms (Rudin *et al.* 92, Xu *et al.* 2012)
Segmented smoothing (Rippe *et al.*, 2012)

Imaging processing



$$min\ \|\mathbf{I} - \mathbf{I}_{\boldsymbol{TV}}\|^2 + \lambda\ \#\ \{p \mid \|\delta_x \mathbf{i}\|_0 + \|\delta_y \mathbf{i}\|_0 \neq 0\}$$

Total variation algorithms (Rudin *et al.* 92, Xu *et al.* 2012)
Segmented smoothing (Rippe *et al.*, 2012)

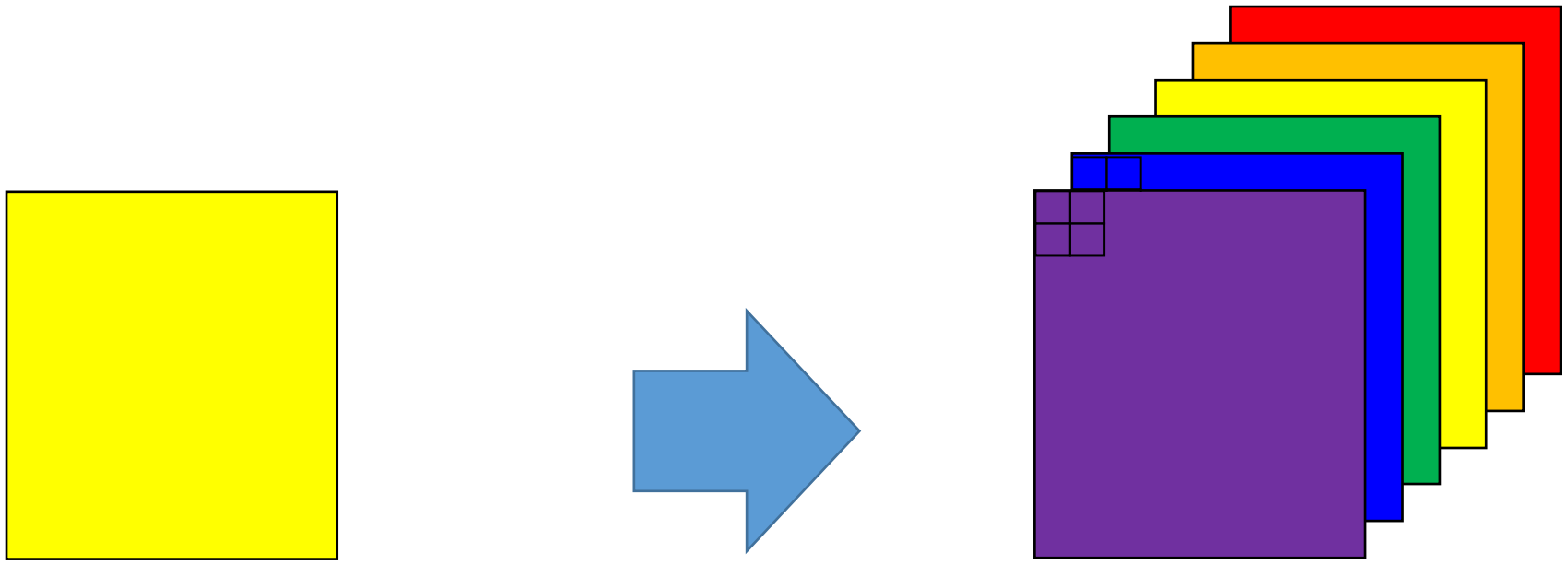
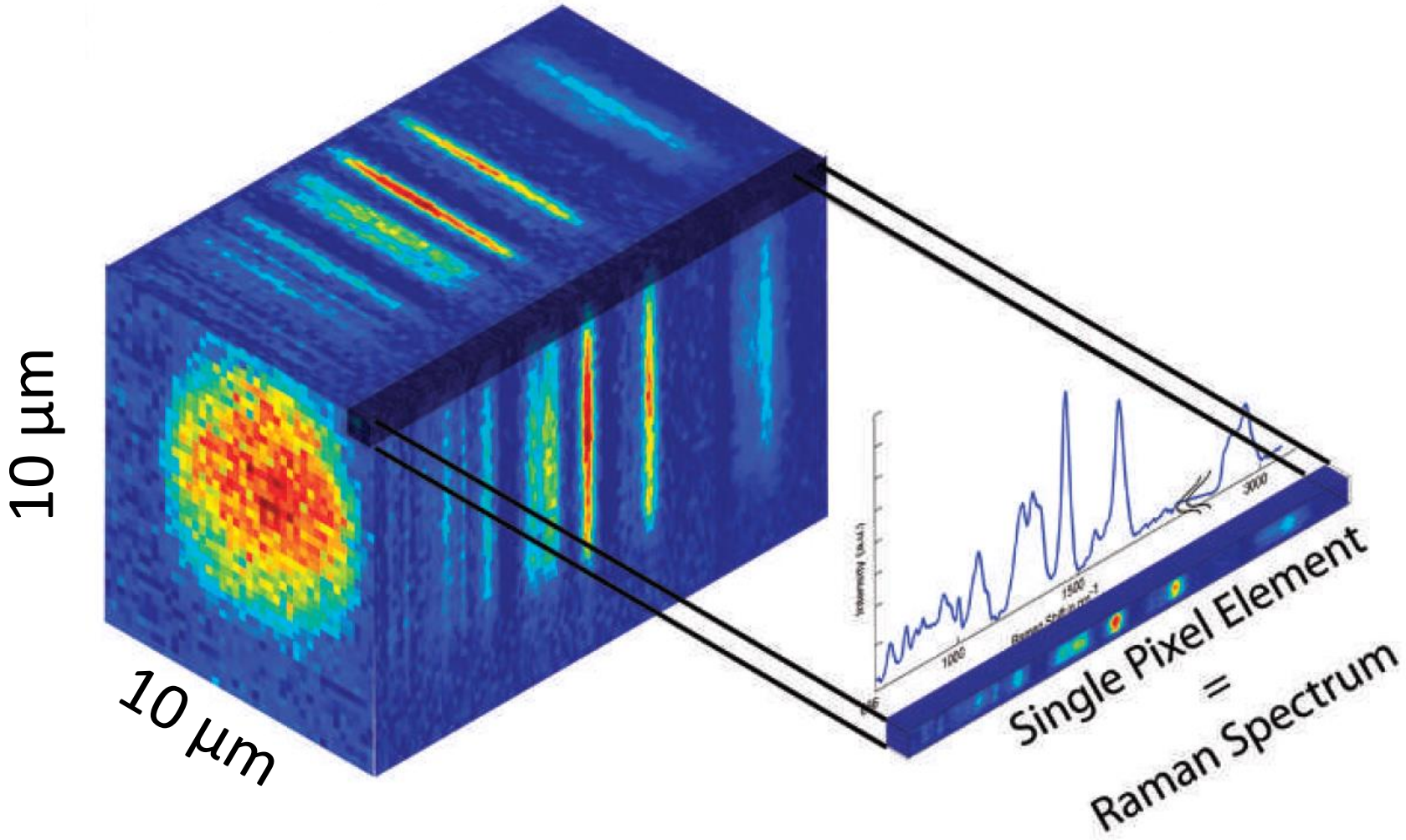


IMAGE PROCESSING **MULTIVARIATE IMAGE ANALYSIS**

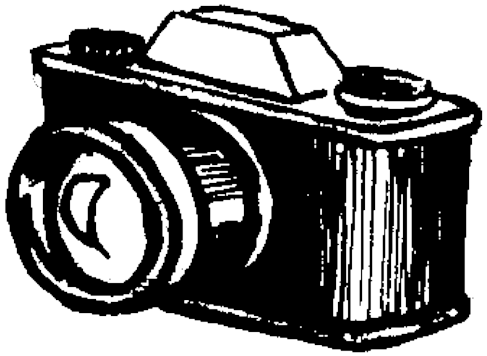
Spatial constraints in MCR-ALS

(Hyper)spectral imaging data



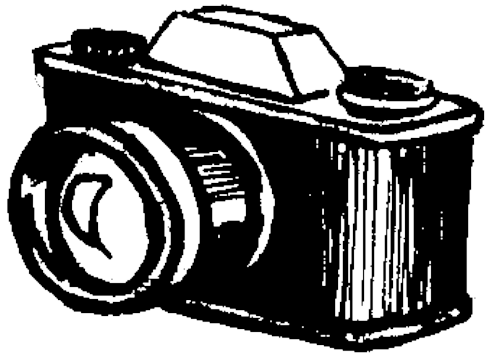
References

Scene, Object
(True latent Image)



Camera, Microscope
(Blurring operator)

Image
(Blurred and noisy)



Camera, Microscope
(Blurring operator)

Image
(Blurred and noisy)

Scene, Object
(True latent Image)

Image processing

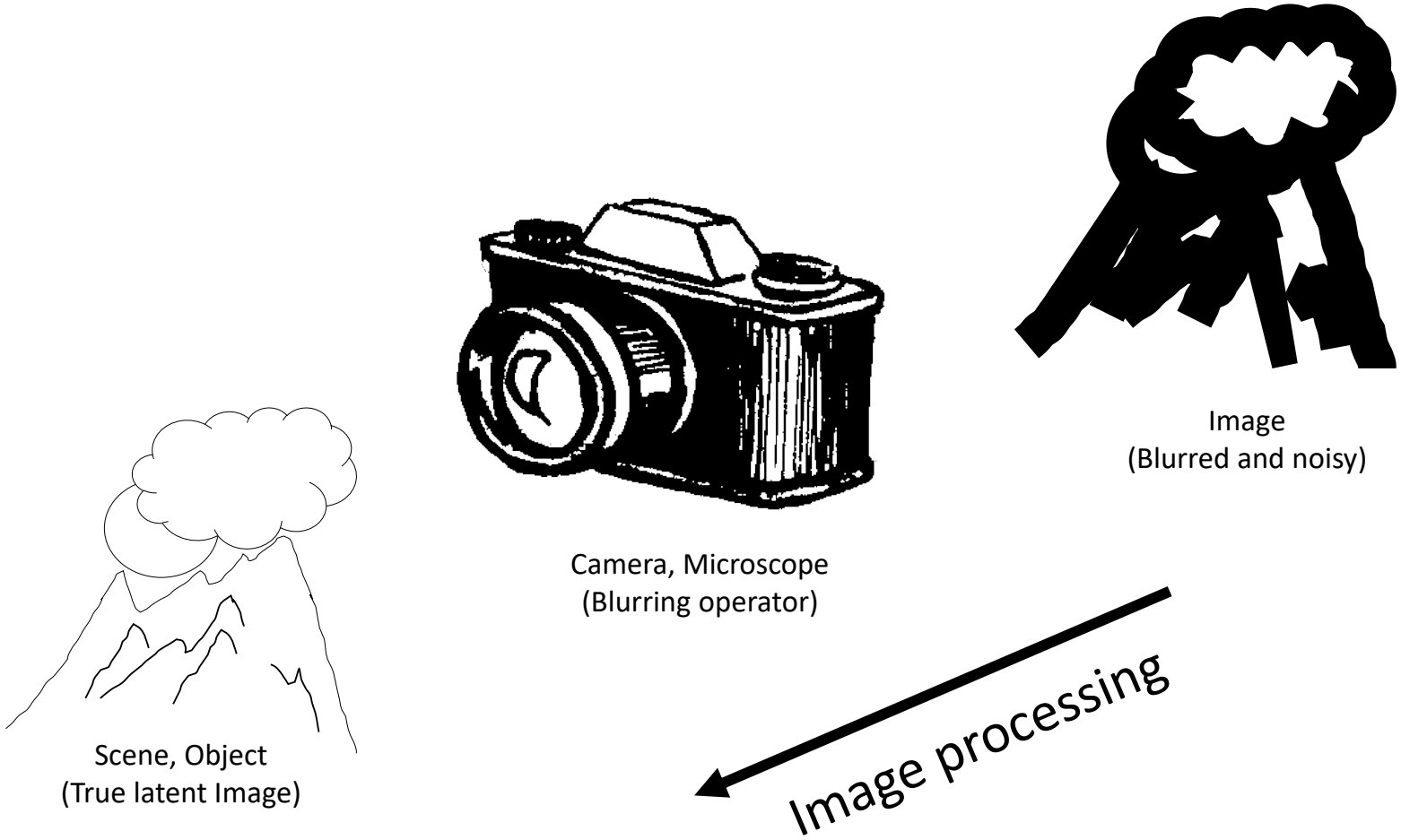
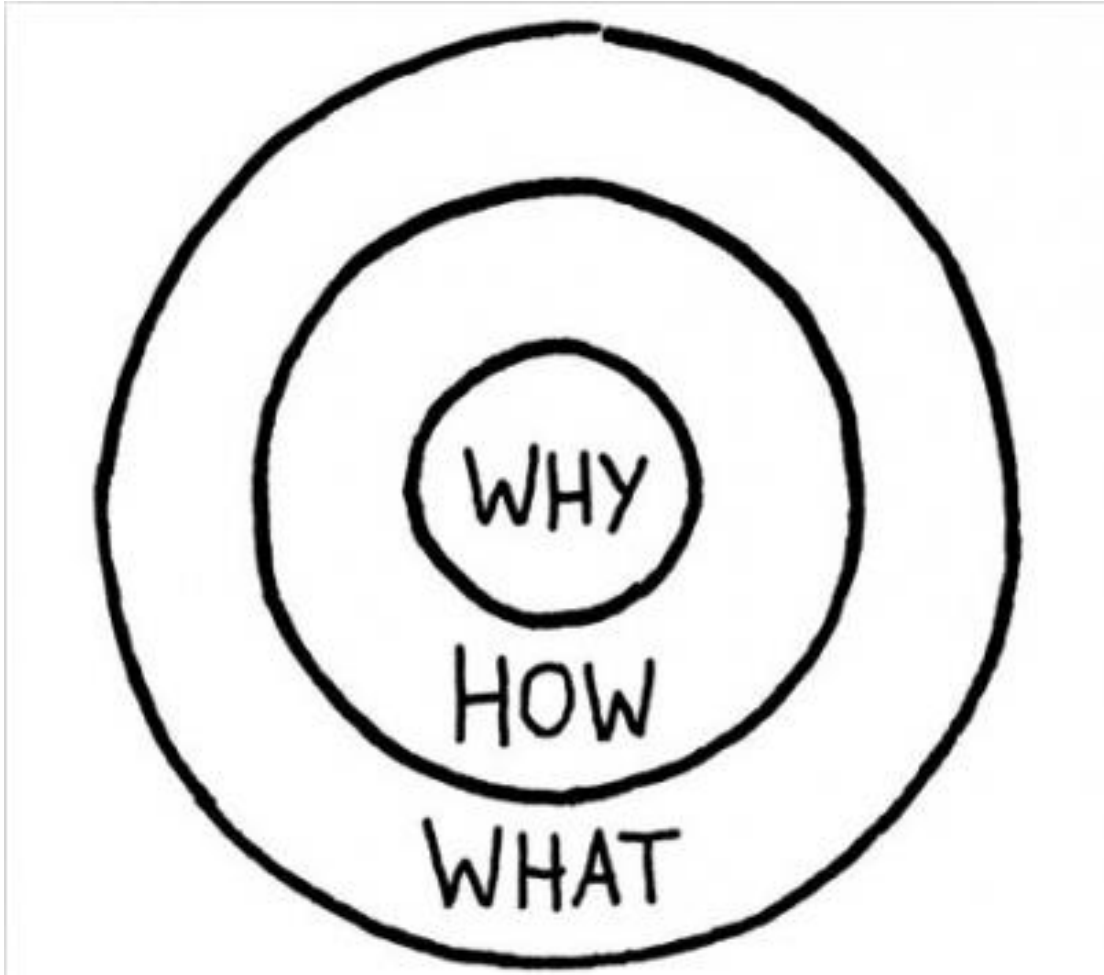
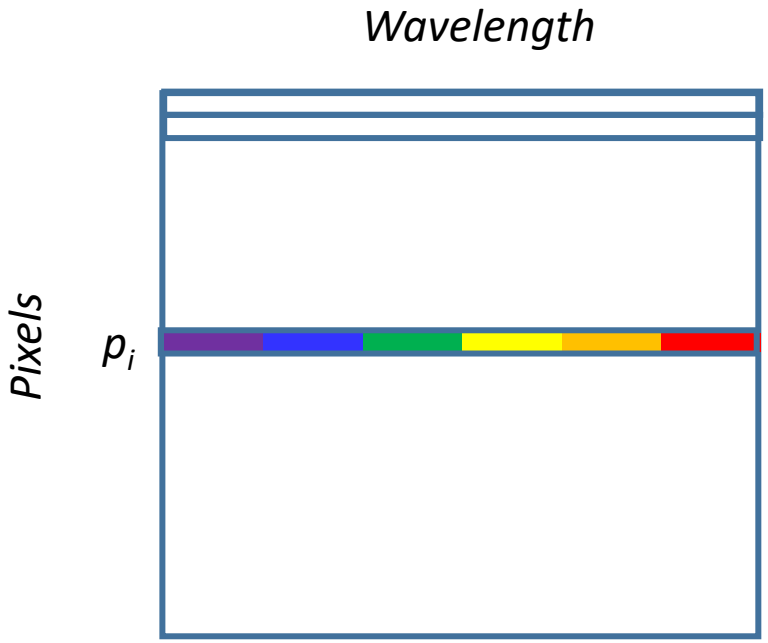


Image
(Blurred and noisy)
Camera, Microscope
(Blurring operator)
Scene, Object
(True latent Image)
Image processing



The why wheel (C. Fitness)

(Hyper)spectral imaging data
Unfolding



Multivariate image analysis

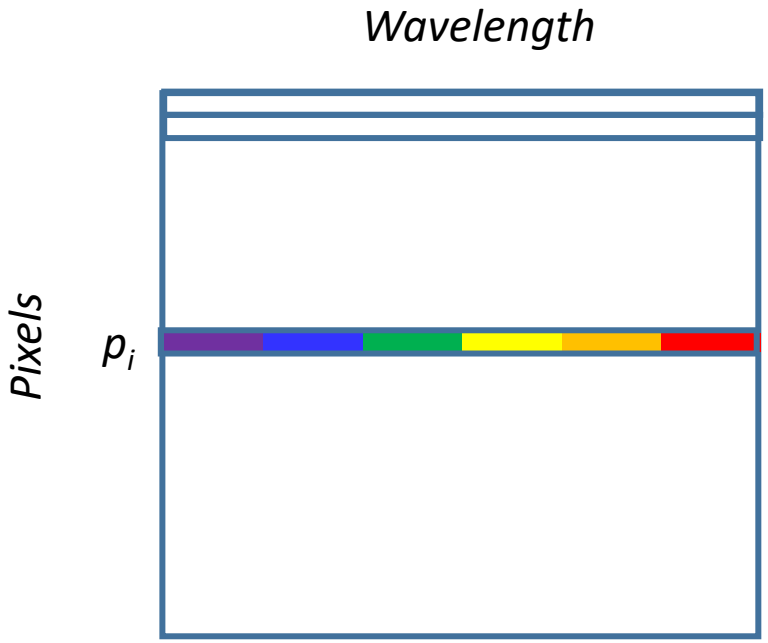
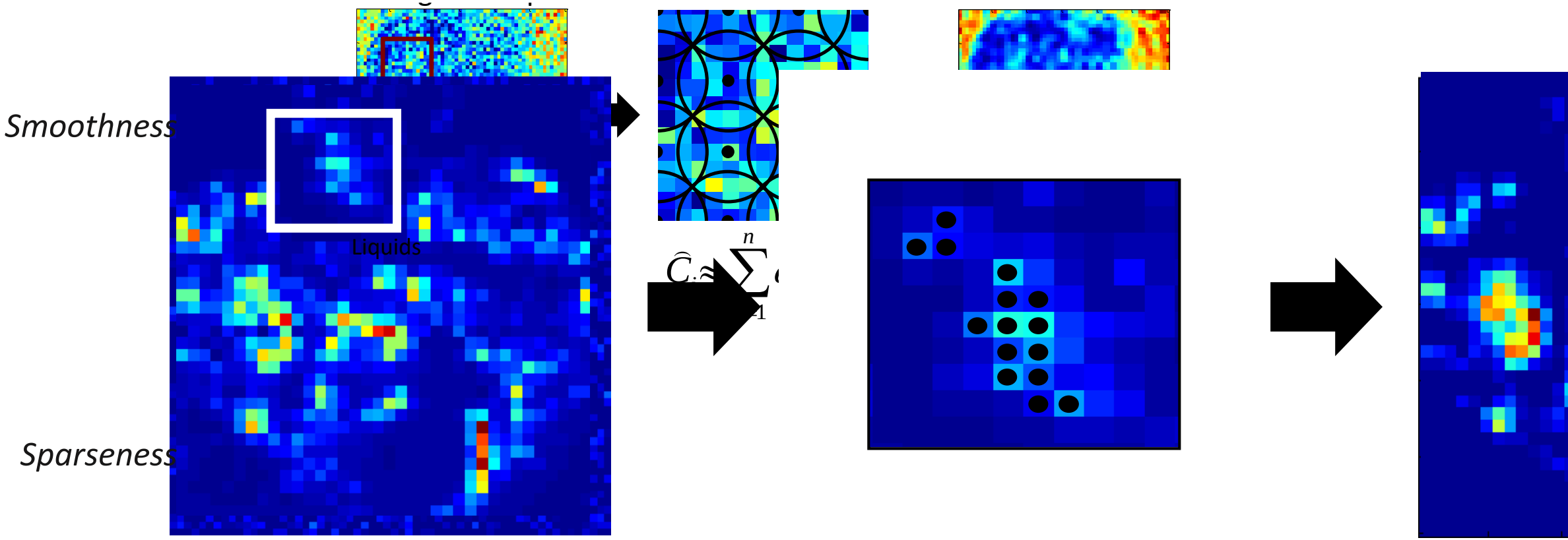


Image processing constraints



Tablets, minoritary compounds

$$\hat{\mathbf{c}} = (\mathbf{I}'\mathbf{I} + \lambda\mathbf{W})^{-1}\mathbf{I}'\mathbf{c}$$


DEPT 59
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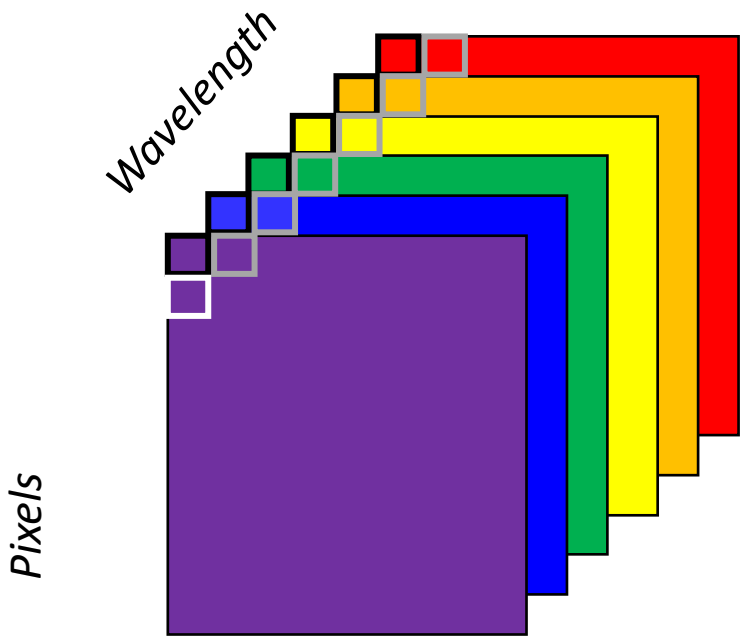
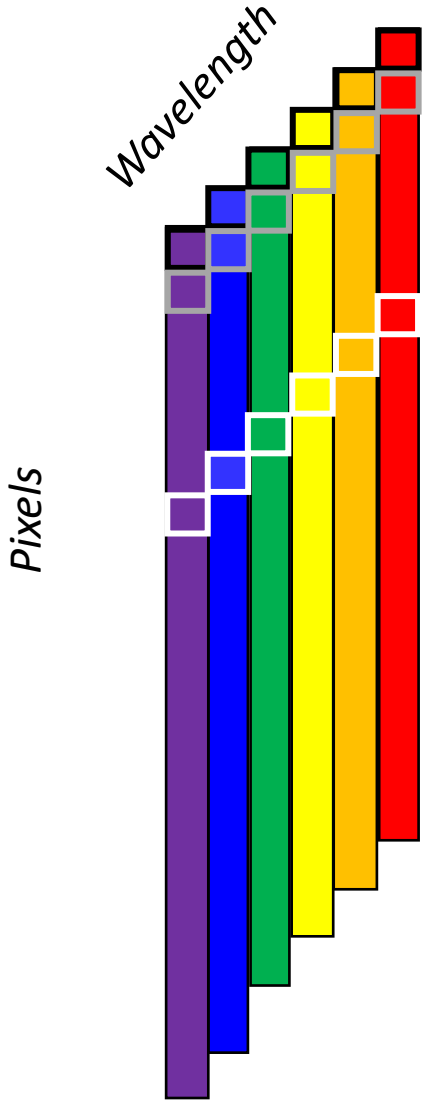
Préfet du Nord
de bureau délégué
Signature du titulaire


GDZ 7685

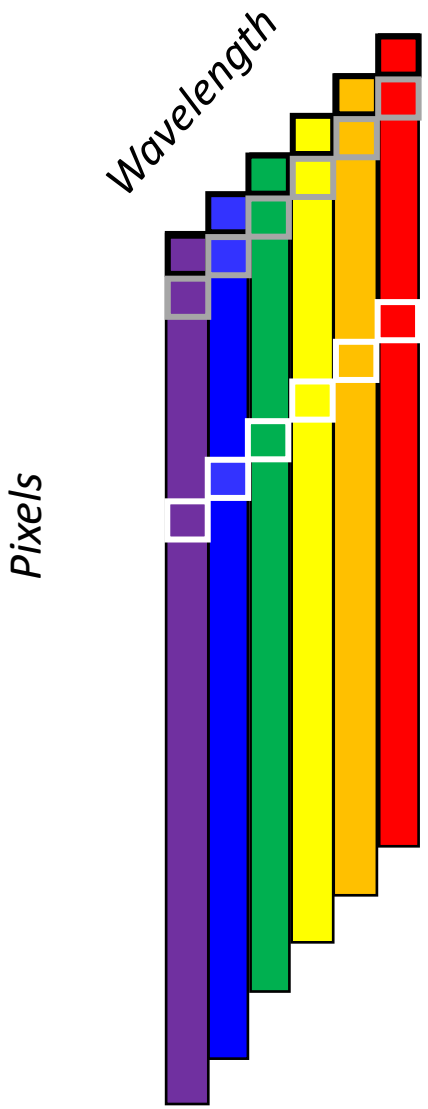
Hyperspectral imaging data



Hyperspectral imaging data
Unfolding



Hyperspectral imaging data
Unfolding



Multivariate Image Analysis

Classification (Class membership *p*)
Curve resolution (**C** and **S**)
…

Hyperspectral imaging data

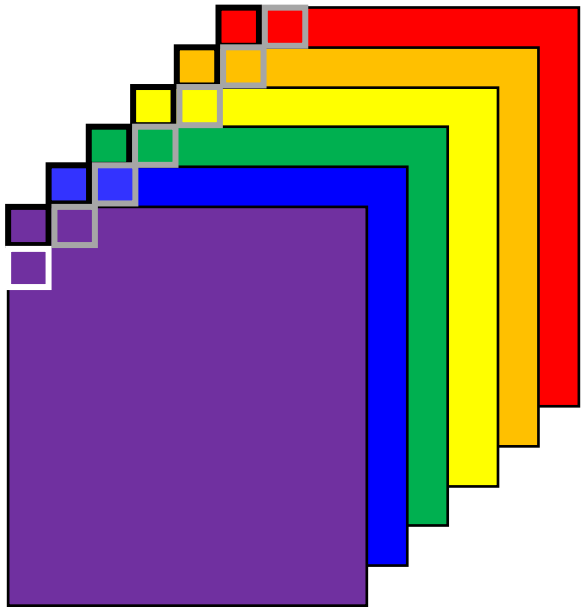
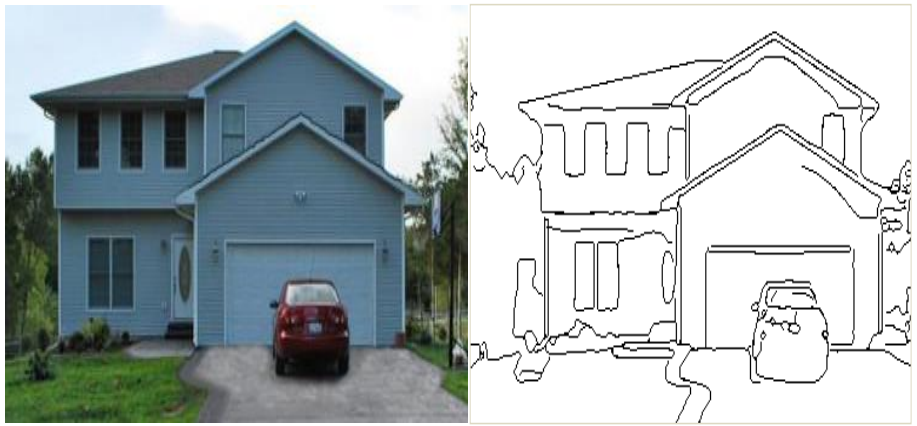


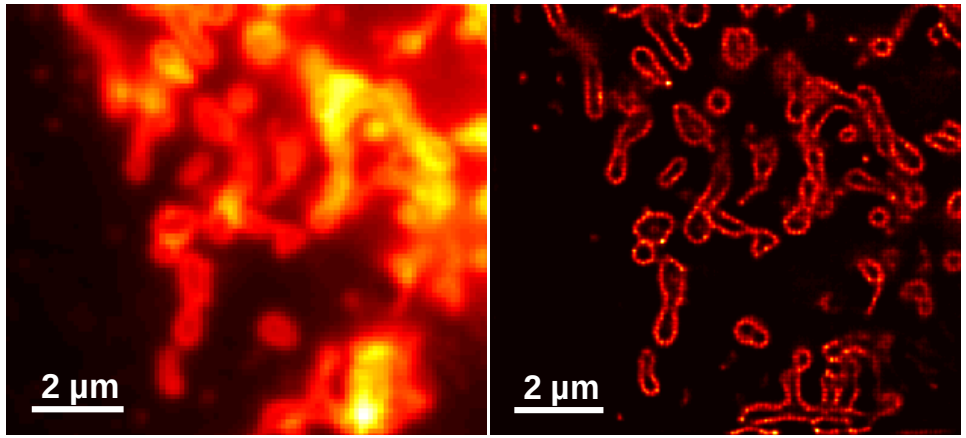
Image processing

Smoothing

Edge enhancement



Deconvolution



Imaging processing

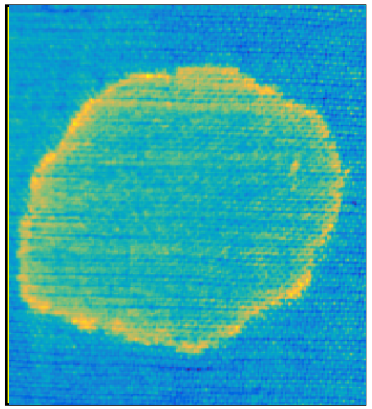
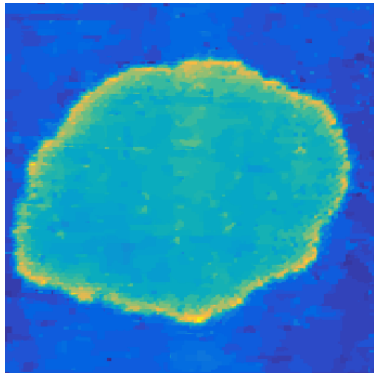
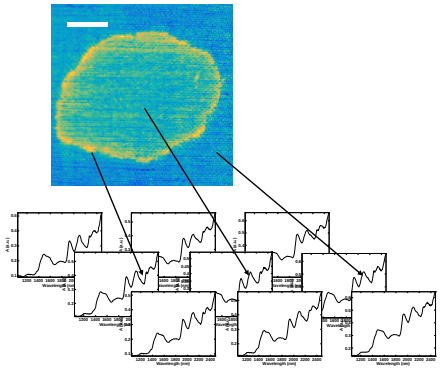


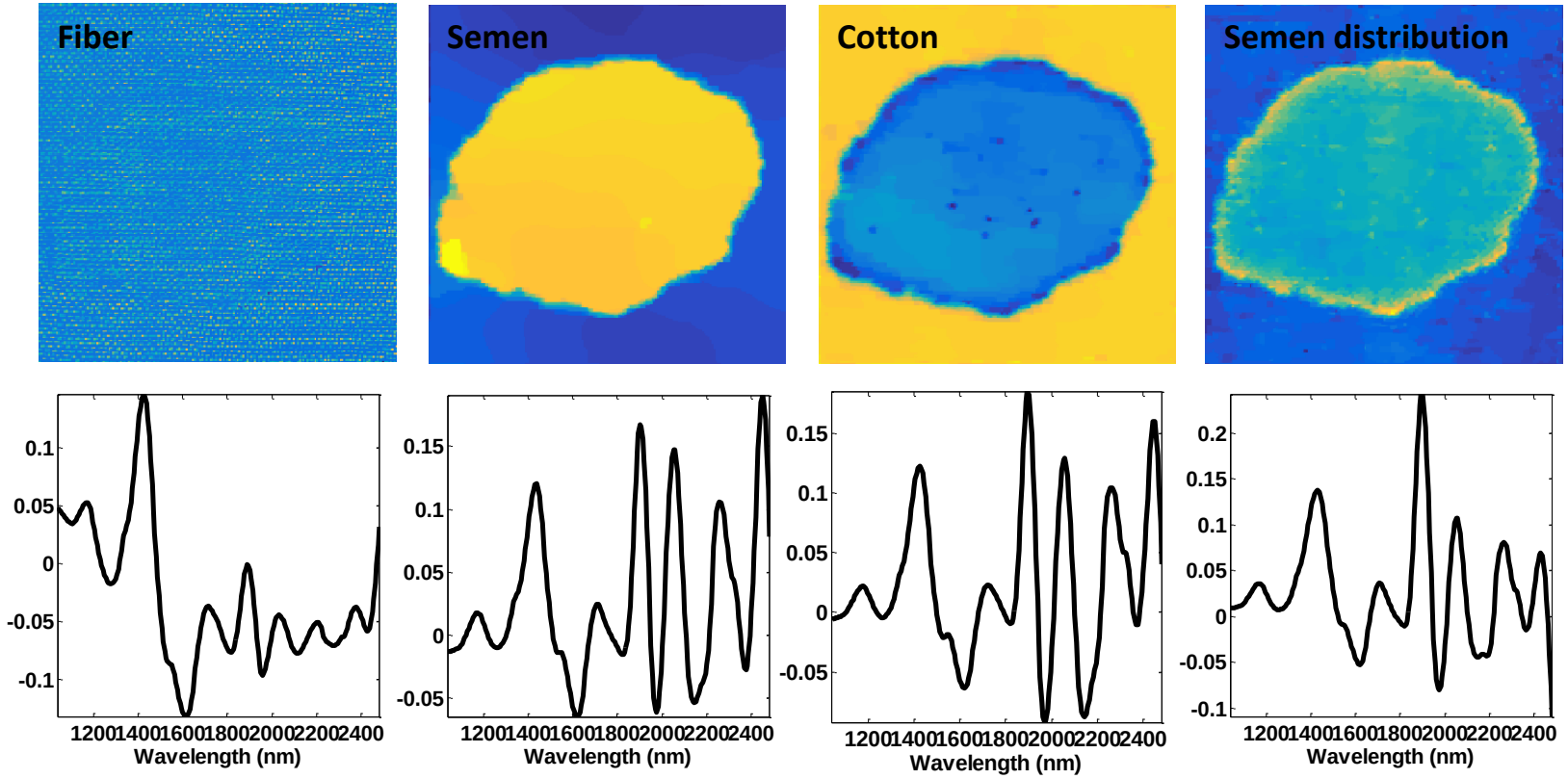
Image Processing



Multivariate curve resolution

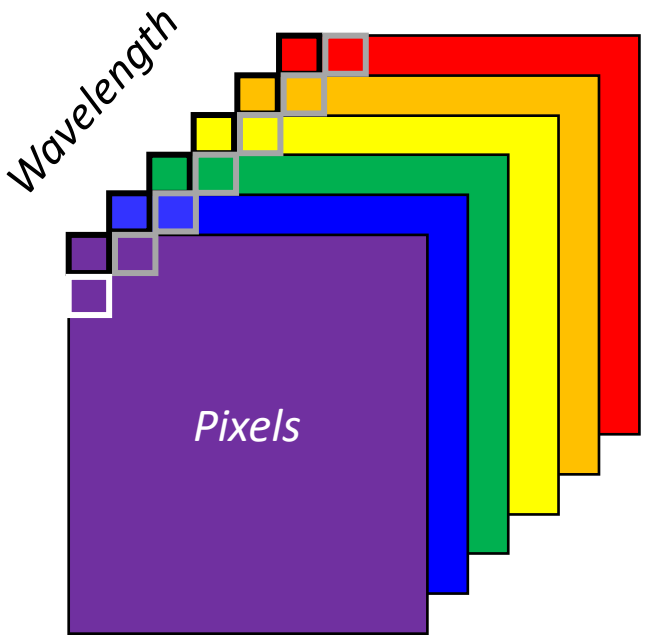


Forensic NIR Identification of semen on cotton (Coll J. Amigo & C. Santos)

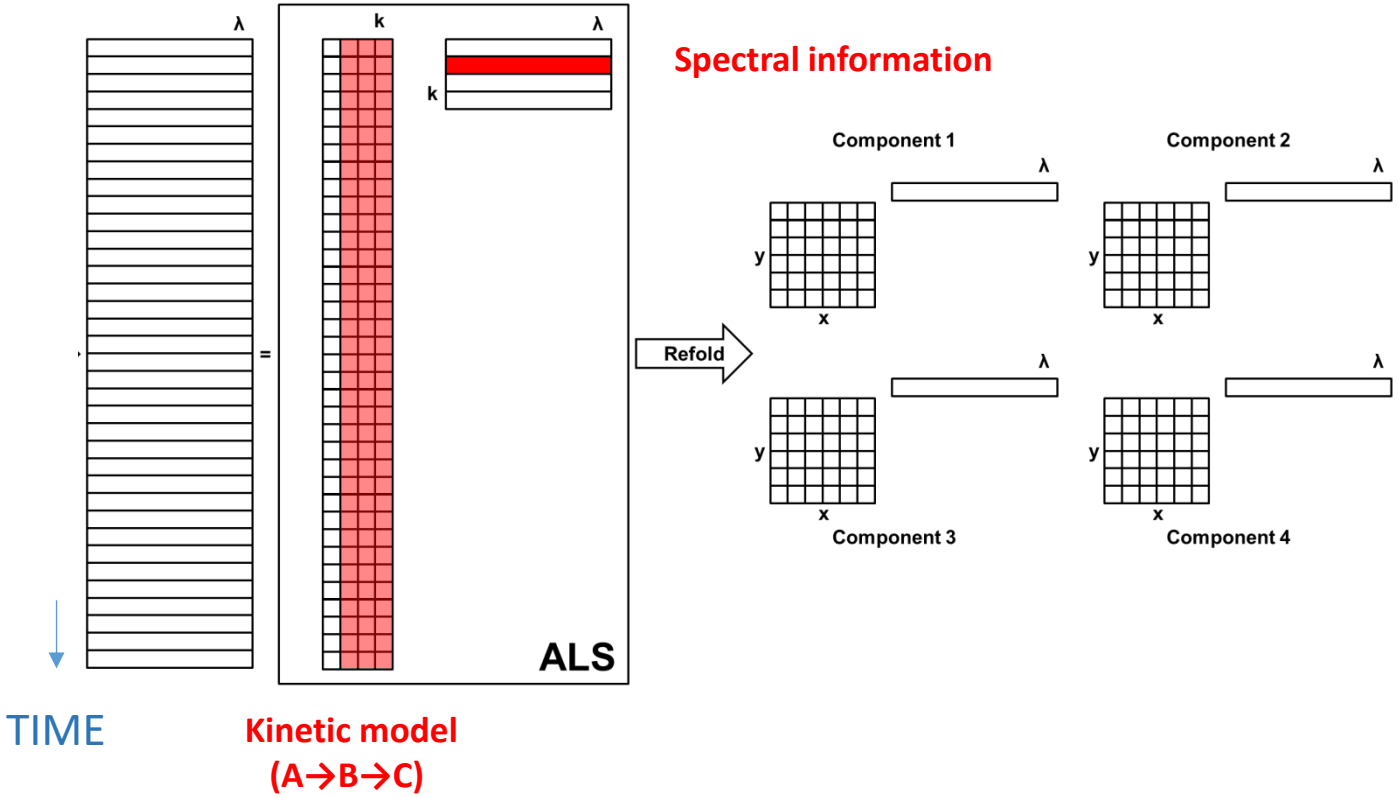


MCR-ALS with **NN** and **image processing (TV)** constraint on **C** (LOF: 5.46 %)

Hyperspectral imaging data



MCR-ALS OF PROCESS SPECTROSCOPY DATA



*Constraints set conditions on **C** and **S** within ALS

MCR

$$D = CS^T$$

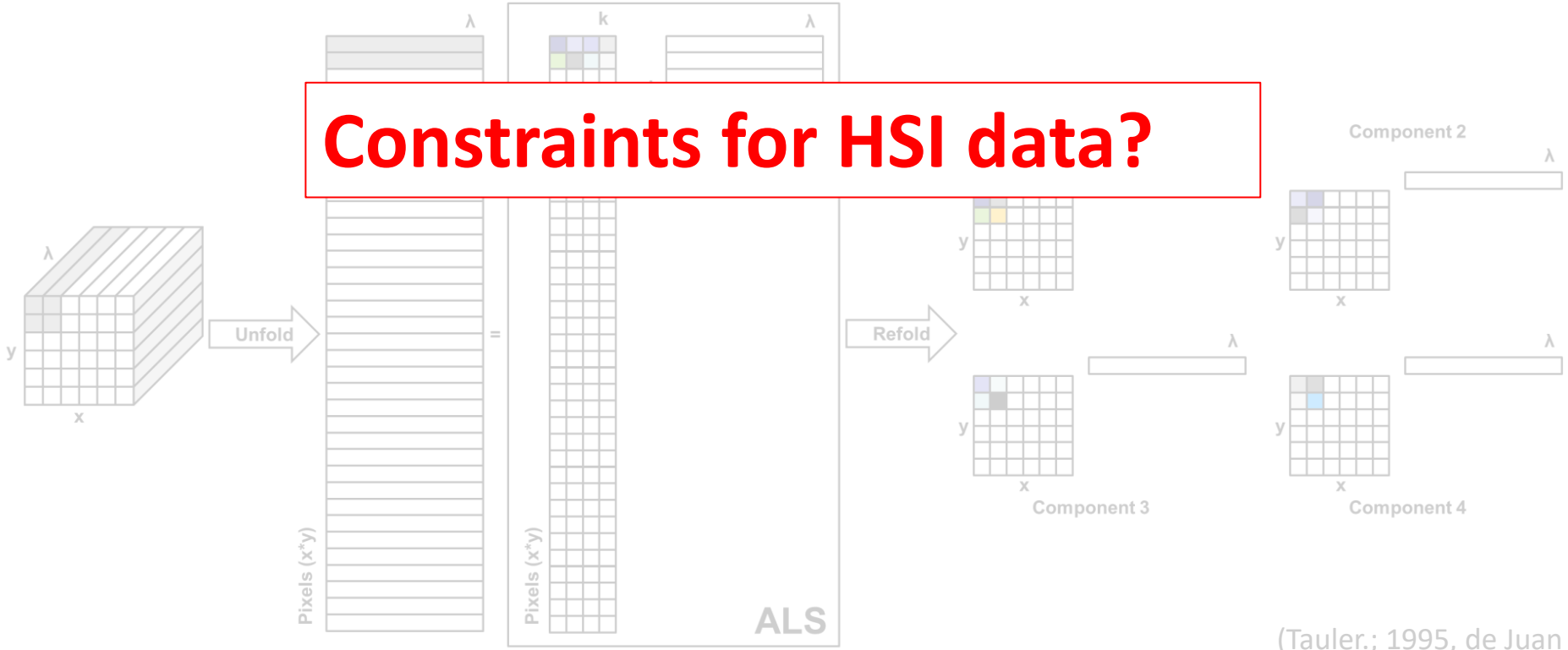
$$D=(CR)(R^{-1}S^T)$$

$$C = D(S^T)^+$$

$$S^T = C^+D$$

Constraints on C and S

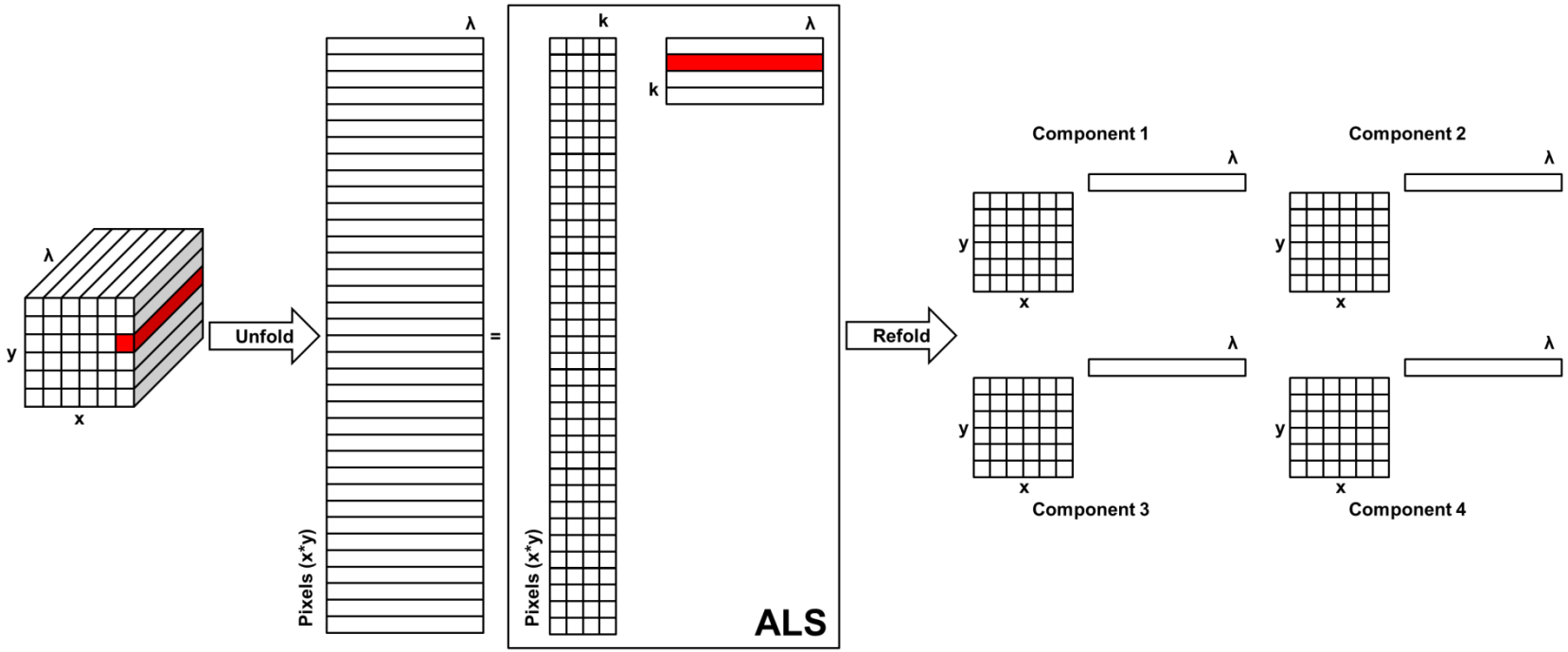
Constraints for HSI data?



(Tauler.; 1995, de Juan et al.; 2004)

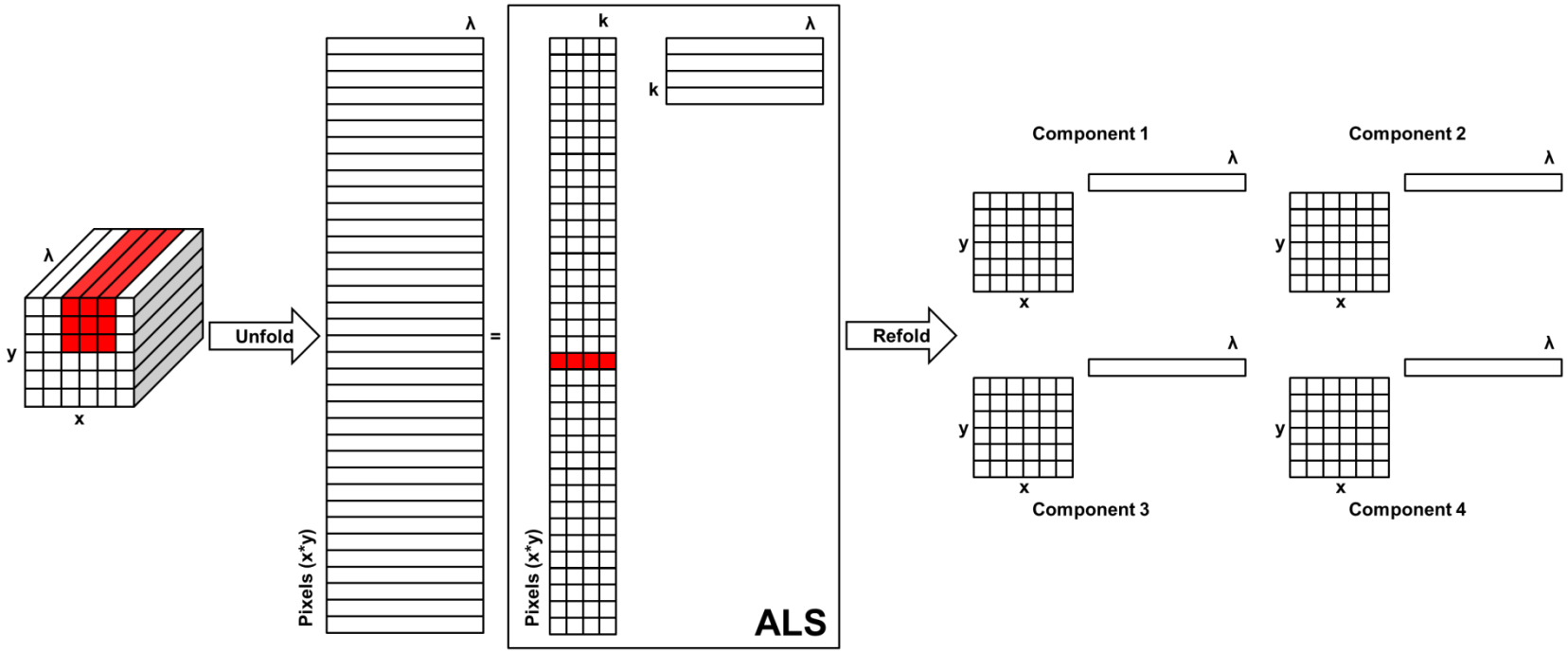
-> The MCR bilinear model holds for every pixel of the data cube

MCR-ALS OF HSI DATA



Spectral information

MCR-ALS OF HSI DATA

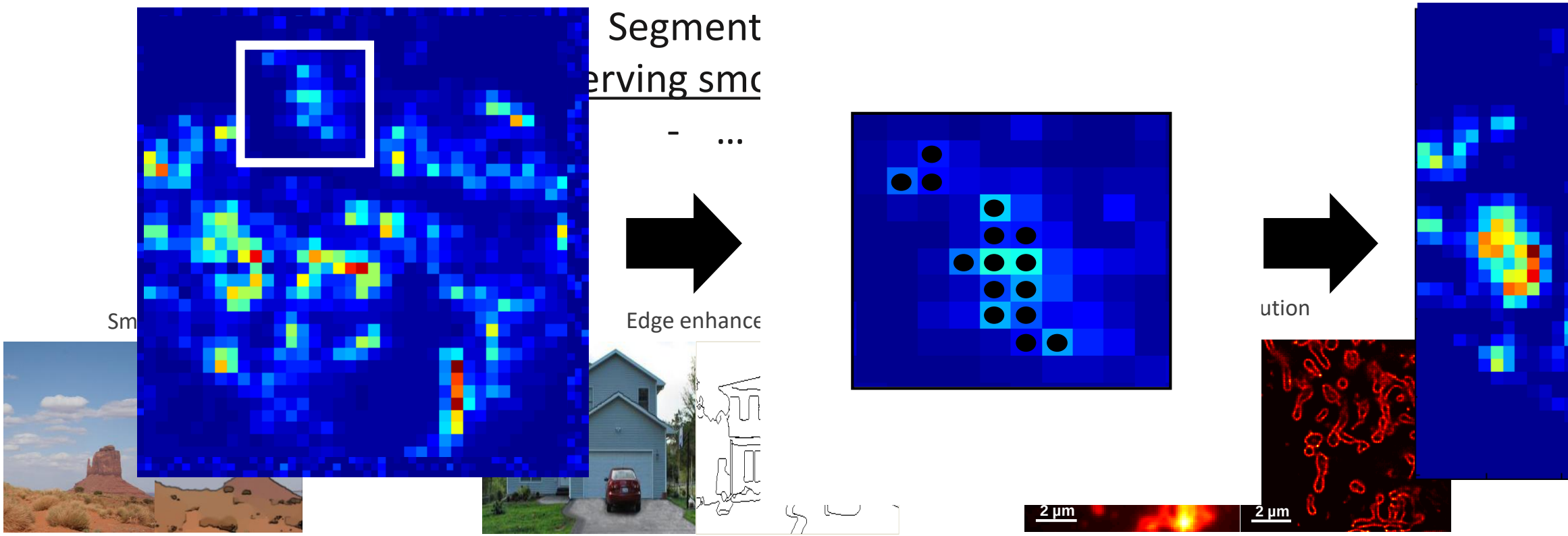


Spatial-spectral information

(Local rank, de Juan et al.; 2005)

Image processing constraints

- Smoothness
- Sparseness
- Segment
- erving smo
- ...



Journal of Chemometrics, 2016
Applied Spectroscopy, 2018
ACA, 2018