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

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DyNaChem LASIR CNRS U LILLE
Forensic NIR
Identification of semen on cotton (Coll J. Amigo & C. Santos)
Principal Component Analysis of Multivariate Images

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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.
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Fig. 4. A multivariate image (or $O^3$ array) $X$ can be written as a long data matrix $X$ by unfolding.
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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

MCR-ALS with non-negativity on C (LOF: 4.06 %)
Forensic NIR Identification of semen on cotton (Coll J. Amigo & C. Santos)

Clear spatial information
Many pixels
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.
Image processing

« By any means »

NICER
Image processing

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

Segmented smoothing
(Rippe et al., 2012)

$$
\min ||I - I_{TV}||^2 + \lambda \sum_{x,y} \sqrt{(i_{x+1,y} - i_{x,y})^2 + (i_{x,y+1} - i_{x,y})^2}
$$

$$
\min ||I - I_{TV}||^2 + \lambda \# \{p \mid ||\delta_x i||_0 + ||\delta_y i||_0 \neq 0\}
$$
MCR-ALS with non-negativity on C (LOF: 4.06 %)
Forensic NIR Identification of semen on cotton (Coll J. Amigo & C. Santos)

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

Chimiométrie 2018 Paris
How?
MCR-ALS OF HSI DATA

\[ C = D(S^T)^+ \]
\[ S^T = C + D \]

Spatial information
Refold / unfold step:
- Spatial information is recovered
- Image processing constraints can be applied in a map-wise way and individually for each component
Image processing constraints

- Smoothness
- Sparseness
- Segmentation
- Edge preserving smoothing (TV, RTV)
  - ...
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
THE IMPORTANCE OF CONSTRAINTS IN MCR-ALS

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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

Fiber  
Semen  
Cotton  
Semen distribution

Variability in the texture  
Semen spectrum
THE IMPORTANCE OF CONSTRAINTS IN MCR-ALS

Constraints should

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ROTATIONAL AMBIGUITY

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

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

The MCR solution is non unique
There is a set of equally feasible solutions

→ 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

Component A
Component B
Component C

Spectral profiles

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

M. Gaffari et al. ACA, 2019

\[ D = U S V^T + E' = X V^T + E' = U Y^T + E' \]
THE EFFECT OF IPCs ON THE EXTENT OF ROTATIONAL AMBIGUITY IN MCR-ALS OF HSI

M. Gaffari et al. ACA, 2019

A

B

C

Data 1

Data 2

Data 3
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
\[ \tilde{C}_{(i,k)} = \lambda \left( \frac{(x-x_{\text{center}})^2}{2\delta_x^2} \right) \left( \frac{(y-y_{\text{center}})^2}{2\delta_y^2} \right) \]
IPC: 2D-Gaussian hard-model

\[ \tilde{C}_{(i,k)} = A e^{-\frac{(x-x_{\text{center}})^2}{2\delta_x^2} - \frac{(y-y_{\text{center}})^2}{2\delta_y^2}} \]

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

M. Gaffari et al. ACA, 2019
THE EFFECT OF IPCs ON THE EXTENT OF ROTATIONAL AMBIGUITY IN MCR-ALS OF HSI

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IPC: 2D-Gaussian hard-model

\[ \tilde{C}_{(i,j)} = A e^{-\left(\frac{(x-x_{\text{center}})^2}{2\delta_x^2} + \frac{(y-y_{\text{center}})^2}{2\delta_y^2}\right)} \]
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\[ \tilde{C}_{(i,k)} = A e^{-\frac{(x-x_{\text{center}})^2}{2\delta_x^2} - \frac{(y-y_{\text{center}})^2}{2\delta_y^2}} \]

\[ C_{(i,k)} \]

Ambiguity?

TRUE SOLUTION
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
\( \mathbf{\tilde{C}}_{(i,k)} = A e^{-\frac{(x-x_{\text{center}})^2}{2\delta_x^2} + \frac{(y-y_{\text{center}})^2}{2\delta_y^2}} \)

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

\( \mathbf{C}_{(i,k)} \)

Ambiguity?

True solution
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
\( \tilde{C}_{(:,k)} = A e^{\frac{(x-x_{\text{center}})^2}{2\delta_x^2} + \frac{(y-y_{\text{center}})^2}{2\delta_y^2}} \)

\[ r = C_{(:,k)} - \tilde{C}_{(:,k)} \]

\[ \text{Ssq}(r) \rightarrow \text{the solution is unique} \]
THE EFFECT OF IPCs ON THE EXTENT OF ROTATIONAL AMBIGUITY IN MCR-ALS OF HSI

M. Gaffari et al. ACA, 2019

2D-Gaussian components (diffusion, emulsions)

Uniform and spatially-structured components (remote sensing)

Spiky and randomly distributed components (pharmaceutic. tablets)

Heavily mixed spectra but clear spatial information
THE EFFECT OF IPCs ON THE EXTENT OF ROTATIONAL AMBIGUITY IN MCR-ALS OF HSI

M. Gaffari et al. ACA, 2019

2D Gaussian Segmentation Sparseness
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 closer to the true one
References

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

Effect of image processing constraints on the effect of rotational ambiguity of HSI images
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

Edge-Preserving Image Smoothing Constraint in Multivariate Curve Resolution–Alternating Least Squares (MCR-ALS) of Hyperspectral Data
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

On the implementation of spatial constraints in multivariate curve resolution alternating least squares for hyperspectral image analysis
CAC 2020 AT THE TOP

XVIII CHEMOMETRICS IN ANALYTICAL CHEMISTRY

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

\[ \min \|I - I_{TV}\|^2 + \lambda \sum_{x,y} \sqrt{(i_{x+1,y} - i_{x,y})^2 + (i_{x,y+1} - i_{x,y})^2} \]

\[ \min \|I - I_{TV}\|^2 + \lambda \# \{p \mid \|\delta_x i\|_0 + \|\delta_y i\|_0 \neq 0\} \]

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 also can be discussed further in our email group.
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)
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

\[ \tilde{C}_{(,k)} = A \exp \left( - \frac{(x-x_{center})^2}{2\delta_x^2} + \frac{(y-y_{center})^2}{2\delta_y^2} \right) \]

MCR-ALS with NN + Gaussian shape constraint

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

\[
\min_{x,y} \| I - I_{TV} \|^2 + \lambda \sum_{x,y} \sqrt{(i_{x+1,y} - i_{x,y})^2 + (i_{x,y+1} - i_{x,y})^2}
\]

\[
\min_{x,y} \| I - I_{TV} \|^2 + \lambda \# \{ p \mid \| \delta_x i \|_0 + \| \delta_y i \|_0 \neq 0 \}
\]

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

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
To reduce the distortion (noise and blur) due to the measurement process by post-processing the image → To recover the true latent image

Scene, Object
(True latent Image)

Camera, Microscope
(Blurring operator)

Image
(Blurred and noisy)
To reduce the distortion (noise and blur) due to the measurement process by post-processing the image.

Scene, Object (True latent Image)

Camera, Microscope (Blurring operator)

Image (Blurred and noisy)

Image processing
To reduce the distortion (noise and blur) due to the measurement process by post-processing the image, the true latent image Scene, Object (True latent Image) can be recovered.
The why wheel (C. Fitness)
(Hyper)spectral imaging data
Unfolding
Multivariate image analysis

$p_i$
Image processing constraints

\[ \hat{c} = (I' I + \lambda W)^{-1} I' c \]
Hyperspectral imaging data
Hyperspectral imaging data
Unfolding
Hyperspectral imaging data

Unfolding

Multivariate Image Analysis

Classification (Class membership $p$)
Curve resolution ($C$ and $S$)
...

Pixels

Wavelength
Hyperspectral imaging data
Image processing

Smoothing

Edge enhancement

Deconvolution
Imaging processing
Multivariate curve resolution

MCR-ALS with \textbf{NN} and \textbf{image processing (TV)} constraint on C (LOF: 5.46 %)
Hyperspectral imaging data
MCR-ALS OF PROCESS SPECTROSCOPY DATA

TIME

Spectral information

Kinetic model
\((A \rightarrow B \rightarrow C)\)

*Constraints set conditions on \(C\) and \(S\) within ALS*
Constraints for HSI data?

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

\[ D = C S^T \]
\[ D = (CR)(R^{-1}S^T) \]
\[ C = D(S^T)^+ \]
\[ S^T = C^+D \]

Constraints on C and S

(Tauler, 1995, de Juan et al.; 2004)
Spectral information
Spatial-spectral information

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

- Smoothness
- Sparseness
Segmentation
- Edge preserving smoothing
(\text{TV, RTV})