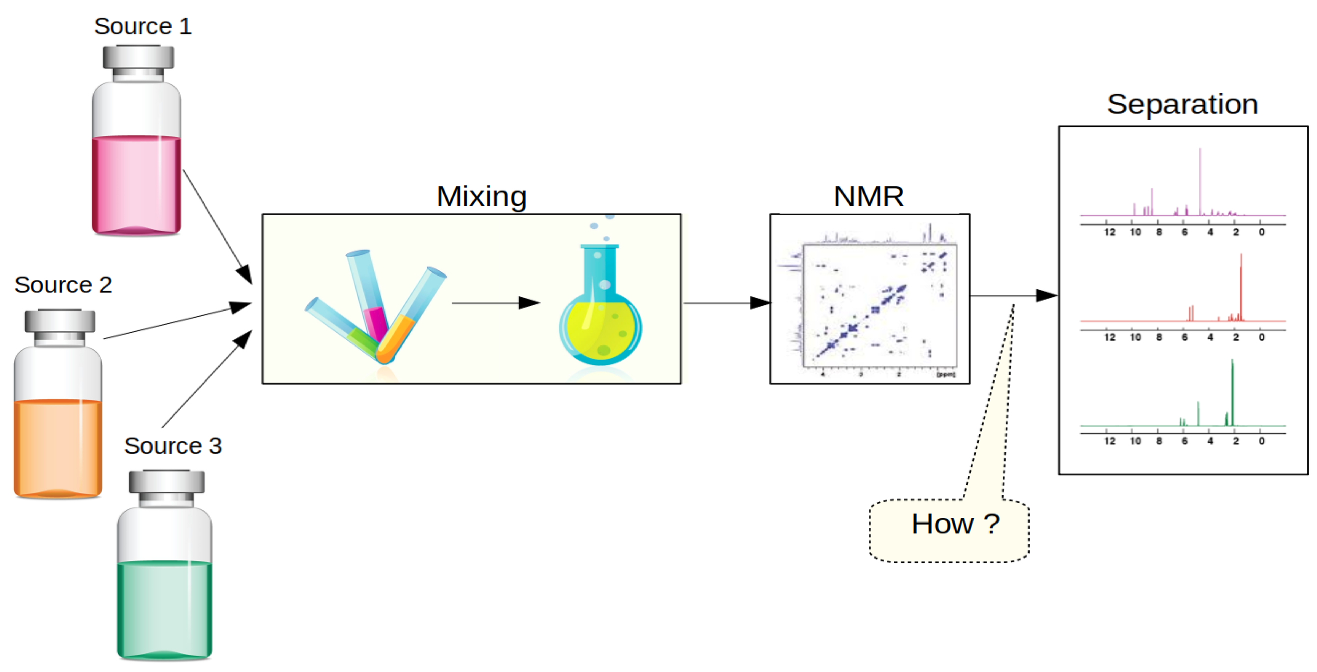
NMF-BASED SPARSE UNMIXING OF COMPLEX MIXTURES

Afef CHERNI*, Elena PIERSANTI*, Caroline CHAUX*

* Aix-Marseille Univ, CNRS, Centrale Marseille, I2M, Marseille, France
*Aix-Marseille Univ, CNRS, Centrale Marseille, iSm2, Marseille, France.

Overview



- **Aim:** Given the measurements $\mathbf{X} \in \mathbb{R}^{M\times L}$, find the unknown sources $\mathbf{S} \in \mathbb{R}^{N\times L}$ and the unknown mixing matrix $\mathbf{A} \in \mathbb{R}^{M\times N}$ related to $\mathbf{X}$ through

$$\mathbf{X} = \mathbf{AS} + \mathbf{N} \approx \mathbf{AS} \qquad (1)$$

- **Application:** Nuclear Magnetic Resonance (NMR) spectroscopy

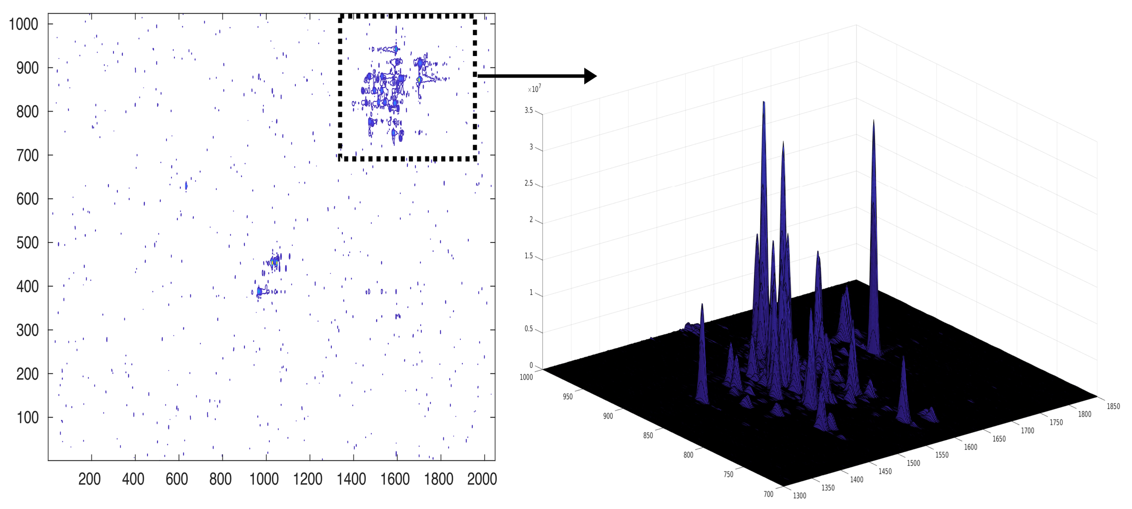
$\mathbf{A}$ represents the concentrations in the mixtures:

☞ positive constraint.

$\mathbf{S}$ represents source coefficients:

☞ positive and sparse constraints.

- **Existing solutions:** BSS techniques (NMF, JADE, ICA, etc.).
- **Difficulties:**
  - 2D NMR spectra present a hight level of sparsity with a spectral overlap and poor resolution.
  - Scale and order indeterminacies [3].



Practical implementation

- **Algorithm: Block-Coordinate Variable Metric Forward-Backward**

Inputs: $\mathbf{X}, \geq 0, \epsilon > 0$

Initialization: $\mathbf{A}_0$, $\mathbf{S}_0$

For $k = 0, 1, \ldots$

$$\mathbf{A}_{k+1} = \underset{\mathbf{A}}{\operatorname{argmin}} \ \tfrac{1}{2}\|\mathbf{X} - \mathbf{A}\mathbf{S}_k\|_F^2 + \Psi_{\mathbf{A}}(\mathbf{A})$$

$$\mathbf{S}_{k+1} = \underset{\mathbf{S}}{\operatorname{argmin}} \ \tfrac{1}{2}\|\mathbf{X} - \mathbf{A}_{k+1}\mathbf{S}\|_F^2 + \Psi_{\mathbf{S}}(\mathbf{S})$$

If $\|\mathbf{A}_{k+1}\mathbf{S}_{k+1} - \mathbf{X}\|^2 \leq \epsilon$:

$\hat{\mathbf{A}} = \mathbf{A}_{k+1}$ and $\hat{\mathbf{S}} = \mathbf{S}_{k+1}$

Outputs: $\hat{\mathbf{A}}$, $\hat{\mathbf{S}}$

- **Proximity operator**

For every $\Psi : \mathbb{R} \to]-\infty, +\infty]$, lower semi continuous (lsc) and proper function, the proximity operator of Ψ relative to the metric induced by a symmetric positive and definite matrix $\mathbf{P} \in \mathbb{R}^{L\times L}$ is defined as

$$\operatorname{prox}_{\mathbf{P},\Psi} : \mathbf{Z} \to \underset{\mathbf{Y}\in\mathbb{R}^L}{\operatorname{argmin}} \left(\Psi(\mathbf{Y}) + \frac{1}{2}\|\mathbf{Y} - \mathbf{Z}\|_{\mathbf{P}}^2 \right)$$

$\Psi_{\mathbf{S}}$	Proximity operator
ℓ_1 (Eq. 4)	Computed [4]
Ψ_1 (Eq. 5)	Computed [2]
Ψ_2 (Eq. 6)	Approximated algorithm [5]

Optimization tools

$$\underset{\mathbf{A},\mathbf{S}}{\text{minimize}} \ \frac{1}{2}\|\mathbf{X} - \mathbf{AS}\|_F^2 + \lambda_{\mathbf{A}}\Psi_{\mathbf{A}}(\mathbf{A},\mathbf{S}) + \lambda_{\mathbf{S}}\Psi_{\mathbf{S}}(\mathbf{A},\mathbf{S}) \qquad (2)$$

- $\Psi_{\mathbf{A}}$: encodes the nonnegativity of $\mathbf{A}$.

$$(\forall \mathbf{Z} \in \mathbb{R}^L) \quad \iota_+ : z_i \to \begin{cases} 0 & \text{if } z_i \geq 0\,, \\ +\infty & \text{elsewhere.} \end{cases} \qquad (3)$$

- $\Psi_{\mathbf{S}}$: encodes the nonnegativity and the sparsity of $\mathbf{S}$.
  - classical choice: ℓ_1 norm

$$\ell_1(\mathbf{Z}) = \sum_i |z_i|. \qquad (4)$$

  - new proposition: entropy functions

Shannon entropy + ℓ_1 norm [1, 2]:

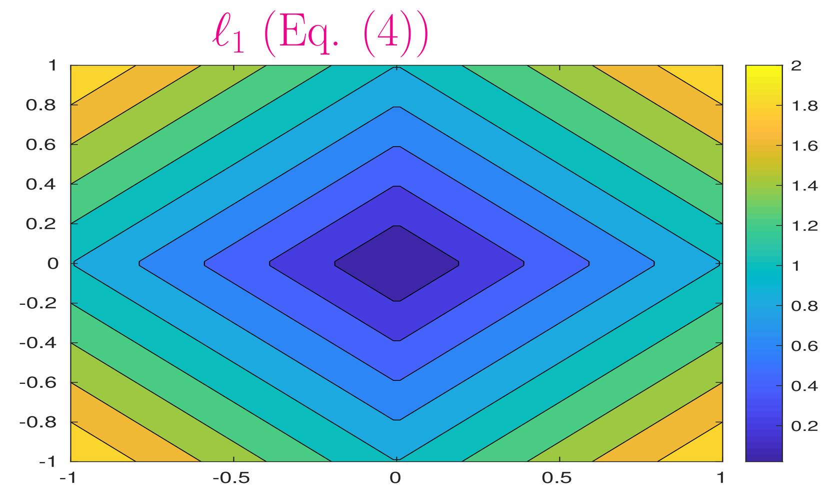
$$\Psi_1(\mathbf{Z}) = \sum_i (z_i \log(z_i) + z_i + \iota_+(z_i))\,. \qquad (5)$$

Generalized entropy function [5]:

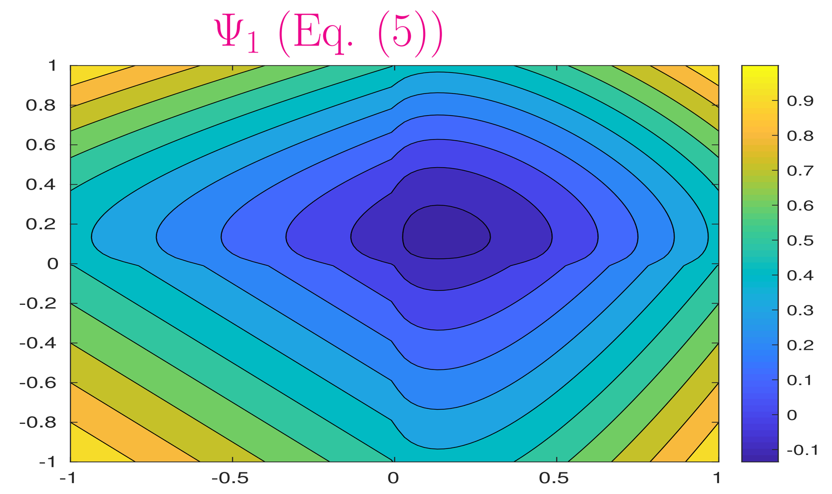
$$\Psi_2(\mathbf{Z}) = -\sum_i \frac{|z_i|^p}{\|\mathbf{Z}\|_p^p} \log\left(\frac{|z_i|^p}{\|\mathbf{Z}\|_p^p}\right). \qquad (6)$$

- $\lambda_{\mathbf{A}}$, $\lambda_{\mathbf{S}}$: regularization parameters.

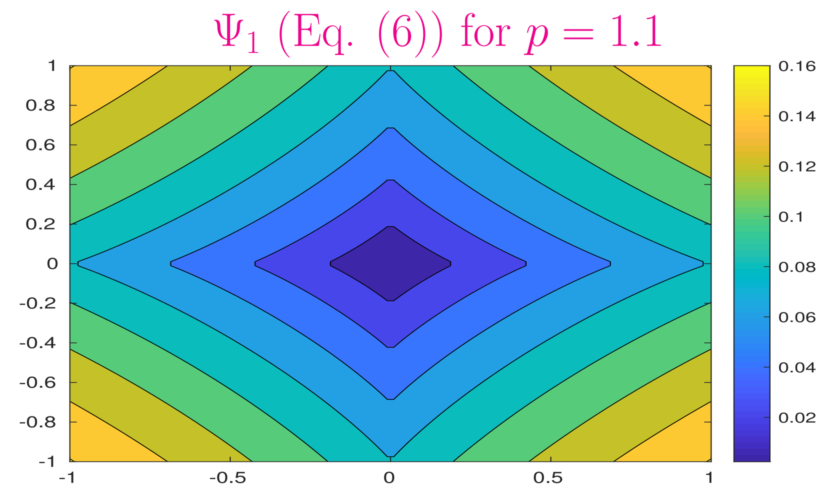
ℓ_1 (Eq. (4))



Ψ_1 (Eq. (5))

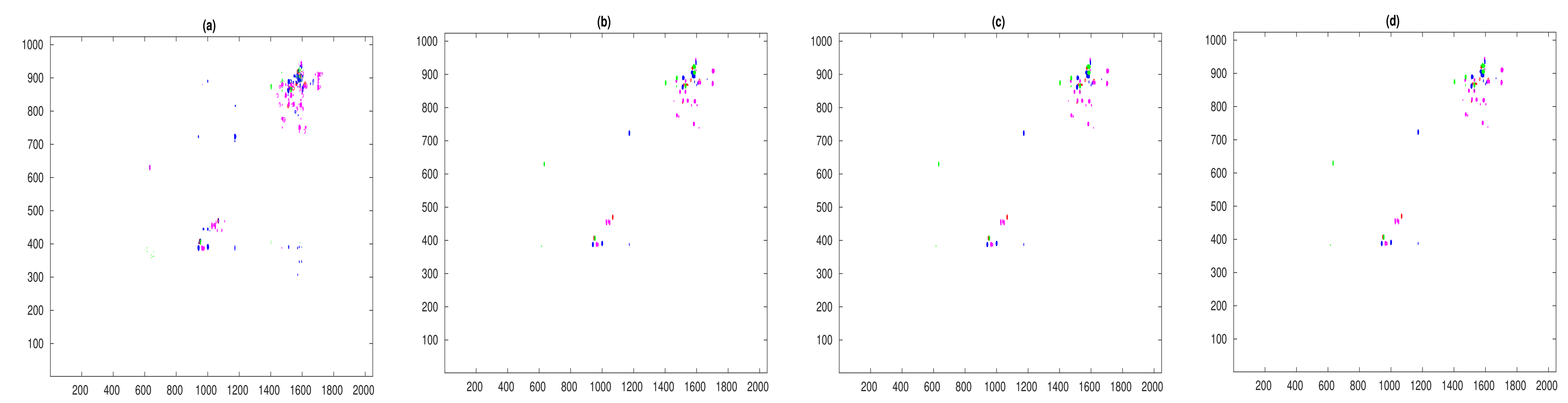


Ψ_1 (Eq. (6)) for $p = 1.1$



Results

- **2D HSQC data:** Limonene (red), Nerol (blue), α-Terpinolene (green), β-Caryophyllene (magenta)
- **Dimensions:** $N = 4$, $M = 5$, $L = (1024 \times 2048)$



Simulated data | Estimated sources using ℓ_1 | Estimated sources using Ψ_1 | Estimated sources using Ψ_2 ($p = 1.1$)

2D HSQC data: original (a) and estimated sources ((b)-(c)-(d))

		ℓ_1(Eq. (4))	Ψ_1 (Eq. (5))	Ψ_2 (Eq. (6))
SIR	S1	**40.10**	34.11	34.04
	S2	42.98	44.58	**50.23**
	S3	30.72	31.58	**33.18**
	S4	**35.87**	29.03	28.13
SDR	S1	**25.93**	24.56	24.70
	S2	18.41	18.10	**18.78**
	S3	**15.14**	14.46	15.08
	S4	**11.06**	9.63	10.09
SAR	S1	**26.10**	25.07	25.25
	S2	18.42	18.11	**18.79**
	S3	**15.26**	14.55	15.15
	S4	**11.08**	9.68	10.17
Amari index		**0.01**	0.05	0.05

Quality performances using different regularization functions

- **Interpretations**

✓ The ℓ_1, Ψ_1 and Ψ_2 ensure a good estimation of the 2D HSQC sources.

✓ ℓ_1 and Ψ_2 are the most efficient functions.

✓ Generalized entropy Ψ_2 seems to be an efficient function to estimate sparse signals.

- **Perspectives**

✓ Adapt the p value of the generalized entropy to better estimate 2D HSQC sources.

✓ Investigate on the combination of generalized entropy function Ψ_2 and ℓ_1 norm.

✓ Explore multiresolution transforms with new sparse NMF algorithms.

References

[1] A. Cherni, E. Chouzenoux, and M.-A. Delsuc. Proximity operators for a class of hybrid sparsity+ entropy priors application to dosy NMR signal reconstruction. In *Int. Symp. on Image Video Communications*, pages 120–125, 2016.

[2] A. Cherni, E. Chouzenoux, and M.-A. Delsuc. Palma, an improved algorithm for dosy signal processing. *Analyst*, 142(5):772–779, 2017.

[3] A. Cherni, E. Piersanti, S. Anthoine, C. Chaux, L. Shintu, M. Yemloul, and B. Torrésani. Challenges in the decomposition of 2D NMR spectra of mixtures of small molecules. *Faraday Discussions*, 2019.

[4] P.-L. Combettes and J.-C. Pesquet. Proximal splitting methods in signal processing. In *Fixed-point algorithms for inverse problems in science and engineering*, pages 185–212. Springer, 2011.

[5] S. Huang and T.-D. Tran. Sparse signal recovery via generalized entropy functions minimization. *IEEE Trans. Signal Process.*, 67(5):1322–1337, March 2019.

SPARS 2019, Toulouse 1-4 July.