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► **To cite this version:**

Afef Cherni, Elena Piersanti, Caroline Chaux. NMF-based sparse unmixing of complex mixtures. 2019. hal-02147290v1

HAL Id: hal-02147290

<https://hal.science/hal-02147290v1>

Preprint submitted on 4 Jun 2019 (v1), last revised 15 Jun 2019 (v2)

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NMF-based sparse unmixing of complex mixtures

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Abstract—In this work, we are interested in unmixing complex mixtures based on Nuclear Magnetic Resonance spectroscopy spectra. More precisely, we propose to solve a 2D blind source separation problem where signals (spectra) are highly sparse. The separation is formulated as a nonnegative matrix factorization problem that is solved using a block coordinate proximal gradient algorithm involving various sparse regularizations. An application to 2D NMR HSQC experience is presented and shows the good performances of the proposed method.

I. PROBLEM STATEMENT

Blind source separation (BSS) consists in separating a set of source signals from a set of mixture measurements with a limited information on sources or on mixtures. In this work, we focus on BSS problem given as follow

$$\mathbf{X} = \mathbf{A}\mathbf{S} + \mathbf{N} \approx \mathbf{A}\mathbf{S} \quad (1)$$

where $\mathbf{X} \in \mathbb{R}^{M \times L}$ corresponds to the measurements defined as a linear mixture of N unknown sources $\mathbf{S} \in \mathbb{R}^{N \times L}$ through a mixing matrix $\mathbf{A} \in \mathbb{R}^{M \times N}$ in the presence of some acquisition noise $\mathbf{N} \in \mathbb{R}^{M \times L}$. The BSS problem (1) is an inverse ill-posed problem which suffers from scale and order indeterminacies. The aim of this work is to solve the BSS problem in the case of 2D nuclear magnetic resonance (NMR) spectroscopy data where sources \mathbf{S} are characterized with a high level of sparsity as shown in Figure 1(a) and Figure 3. The crowded sparse spectra presenting an important spectral overlap and poor resolution increase the difficulty of the analysis step.

A commonly used strategy consists in formulating the problem under a variational approach thus giving rise to an optimization problem to be solved w.r.t. \mathbf{A} and \mathbf{S} of the form

$$\underset{\mathbf{A}, \mathbf{S}}{\text{minimize}} \quad \frac{1}{2} \|\mathbf{X} - \mathbf{A}\mathbf{S}\|_F^2 + \lambda_A \Psi_A(\mathbf{A}, \mathbf{S}) + \lambda_S \Psi_S(\mathbf{A}, \mathbf{S}) \quad (2)$$

where Ψ_A (resp. Ψ_S) encodes the prior information on \mathbf{A} (resp. \mathbf{S}). Ψ_A is usually defined as the indicator function ι_+ of the nonnegative set while Ψ_S should not only ensure the nonnegativity but also promote the sparsity of the solution. λ_A and λ_S are the regularization parameters of \mathbf{A} and \mathbf{S} respectively. The choice of Ψ_S presents the main locks of our problem.

II. PROPOSED SPARSITY-BASED REGULARIZATIONS

The most popular regularization function used in the case of sparse signals recovery is the ℓ_1 norm given by

$$(\forall \mathbf{Z} = (z_i)_{1 \leq i \leq L} \in \mathbb{R}^L) \quad \ell_1(\mathbf{Z}) = \sum_i |z_i|. \quad (3)$$

For years, the ℓ_1 norm was used as an efficient convex function to measure the sparsity level. However, some recent works [1], [2], [3] proposed new regularization functions to enforce sparsity based on

This work was supported by the Excellence Initiative of Aix-Marseille University - A*Mixex, a French “Investissements d’Avenir” program.

entropies. On the one hand, in [1] and [2], a new combination between the ℓ_1 norm and Shannon entropy defined as

$$(\forall \mathbf{Z} \in \mathbb{R}^L, z_i > 0) \quad \Psi_1(\mathbf{Z}) = \sum_i z_i \log(z_i) + z_i \quad (4)$$

was shown to be a good choice to estimate signals in mass spectroscopy application. On the other hand, a generalized entropy function proposed in [3] and defined as

$$(\forall \mathbf{Z} \in \mathbb{R}^L, p > 0) \quad \Psi_2(\mathbf{Z}) = - \sum_i \frac{|z_i|^p}{\|\mathbf{Z}\|_p^p} \log \left(\frac{|z_i|^p}{\|\mathbf{Z}\|_p^p} \right) \quad (5)$$

was used for sparse signal recovery and was shown to be more effective than the ℓ_1 norm. Note that the effectiveness of these functions was shown considering inverse ill-posed problems involving a known mixing matrix. In the present work, we propose to use such sparsity promoting regularizations in the BSS context, by integrating them into a proximal framework.

Problem (2) is solved using the Block Coordinate Variable Metric Forward-Backward (BC-VMFB) algorithm [4]. It requires to compute the partials gradients of $\frac{1}{2} \|\mathbf{X} - \mathbf{A}\mathbf{S}\|_F^2$ w.r.t. \mathbf{A} and \mathbf{S} and the proximity operators (associated with a Symmetric Positive Definite matrix) of Ψ_A and Ψ_S [5].

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

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

For $k = 0, 1, \dots$

$$\left[\begin{array}{l} \mathbf{A}_{k+1} = \underset{\mathbf{A}}{\text{argmin}} \quad \frac{1}{2} \|\mathbf{X} - \mathbf{A}\mathbf{S}_k\|_F^2 + \Psi_A(\mathbf{A}) \quad (I) \end{array} \right.$$

$$\left[\begin{array}{l} \mathbf{S}_{k+1} = \underset{\mathbf{S}}{\text{argmin}} \quad \frac{1}{2} \|\mathbf{X} - \mathbf{A}_{k+1}\mathbf{S}\|_F^2 + \Psi_S(\mathbf{S}) \quad (II) \end{array} \right.$$

$$\left[\begin{array}{l} \text{If } \|\mathbf{A}_{k+1}\mathbf{S}_{k+1} - \mathbf{X}\|^2 \leq \epsilon : \hat{\mathbf{A}} = \mathbf{A}_{k+1} \text{ and } \hat{\mathbf{S}} = \mathbf{S}_{k+1} \end{array} \right.$$

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

III. APPLICATION TO 2D NMR HSQC EXPERIENCE

We process here 2D Heteronuclear single quantum coherence (HSQC) data where mixtures \mathbf{X} of size $5 \times 1024 \times 2048$ are generated from HSQC sources \mathbf{S} with size $(4 \times 1024 \times 2048)$. We apply the proposed algorithm to estimate the 4 sources from the 5 mixtures and we test different regularization functions Ψ_S (ℓ_1 , Ψ_1 and Ψ_2). To evaluate the quality of estimated sources \mathbf{S} , we use the SIR, SDR and SAR metrics [6] expressed in dB. Moreover, we use the Moreau-Amari index [7] to evaluate the estimation of the mixing matrix \mathbf{A} . Figures 1(a), (b) and (c) show that the three regularizations ensure a good estimation of the 2D HSQC sources. Moreover, according to Table II, the ℓ_1 norm (Eq. (3)) and the generalized entropy (Eq. (5)) seem to be the most efficient functions with slightly increased performances. Note that fixed regularization parameters λ_S are used for each regularization function. Future works will address the adaptation of λ_S for each source according to its sparsity level. In addition, we will investigate on the combination of generalized entropy, ℓ_1 norm together with multiresolution transforms.

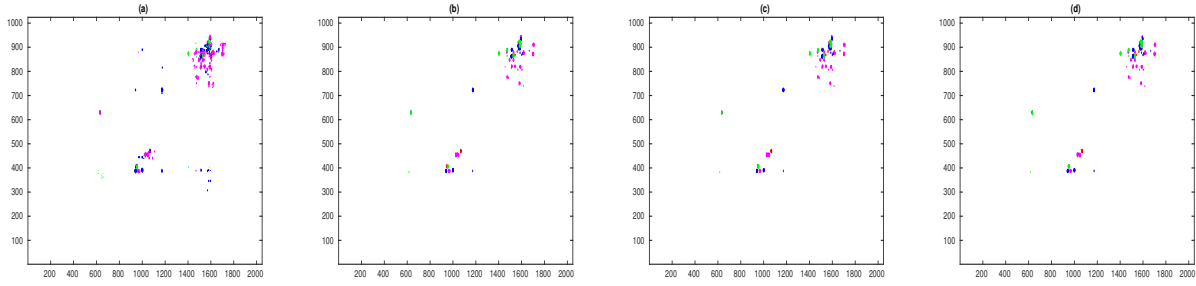


Figure 1. 2D HSQC data (4 sources: Limonene (red), Nerol (blue), α -Terpinolene (green) and β -Caryophyllene (magenta)): (a) original sources with size ($4 \times 1024 \times 2048$), (b) estimated sources using ℓ_1 norm, (c) estimated sources using Ψ_1 , (d) estimated sources using Ψ_2 .

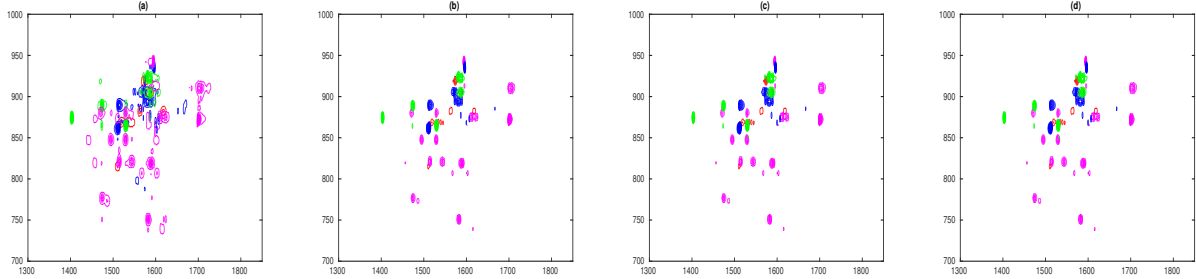


Figure 2. Zoom on the most important terpene zone [1300 : 1850, 700 : 1000]: (a) original sources, (b) estimated sources using ℓ_1 norm, (c) estimated sources using Ψ_1 , (d) estimated sources using Ψ_2 .

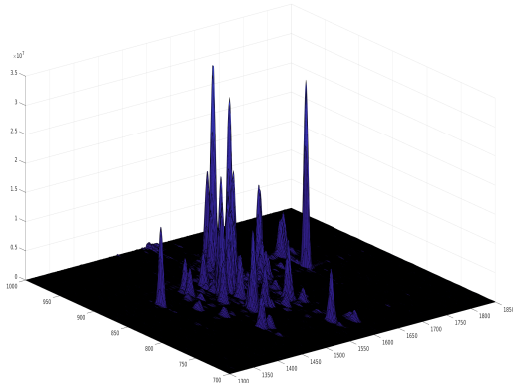


Figure 3. 3D representation of Figure 2 (a)

Ψ_S	Proximal operator of Ψ_S
ℓ_1 (Eq. (3))	Computed [8]
Ψ_1 (Eq. (4))	Computed [1]
Ψ_2 (Eq. (5))	Approximated algorithm [3]

Table I

PROXIMITY OPERATORS OF DIFFERENT REGULARIZATION FUNCTIONS.

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	ℓ_1 (Eq. (3))	Ψ_1 (Eq. (4))	Ψ_2 (Eq. (5))
SIR	40.10	34.11	34.04
	42.98	44.58	50.23
	30.72	31.58	33.18
	35.87	29.03	28.13
SDR	25.93	24.56	24.70
	18.41	18.10	18.78
	15.14	14.46	15.08
	11.06	9.63	10.09
SAR	26.10	25.07	25.25
	18.42	18.11	18.79
	15.26	14.55	15.15
	11.08	9.68	10.17
Amari index	0.01	0.05	0.05

Table II

QUALITY PERFORMANCES USING DIFFERENT REGULARIZATION FUNCTIONS.

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