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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  $\Psi_A$  (resp.  $\Psi_S$ ) encodes the prior information on  $\mathbf{A}$  (resp.  $\mathbf{S}$ ).  $\Psi_A$  is usually defined as the indicator function  $\iota_+$  of the nonnegative set while  $\Psi_S$  should not only ensure the nonnegativity but also promote the sparsity of the solution.  $\lambda_A$  and  $\lambda_S$  are the regularization parameters of  $\mathbf{A}$  and  $\mathbf{S}$  respectively. The choice of  $\Psi_S$  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  $\ell_1$  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  $\ell_1$  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

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entropies. On the one hand, in [1] and [2], a new combination between the  $\ell_1$  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  $\ell_1$  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) [5] of  $\Psi_A$  and  $\Psi_S$  (Table I).

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

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

For  $k = 0, 1, \dots$

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

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

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## 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  $\Psi_S$  ( $\ell_1$ ,  $\Psi_1$  and  $\Psi_2$ ). 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(b), (c) and (d) show that the three regularizations ensure a good estimation of the 2D HSQC sources. Moreover, according to Table II, the  $\ell_1$  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  $\lambda_S$  are used for each regularization function. Future works will address the adaptation of  $\lambda_S$  for each source according to its sparsity level. In addition, we will investigate on the combination between generalized entropy and  $\ell_1$  norm with multiresolution transforms and new sparse NMF algorithms [9].

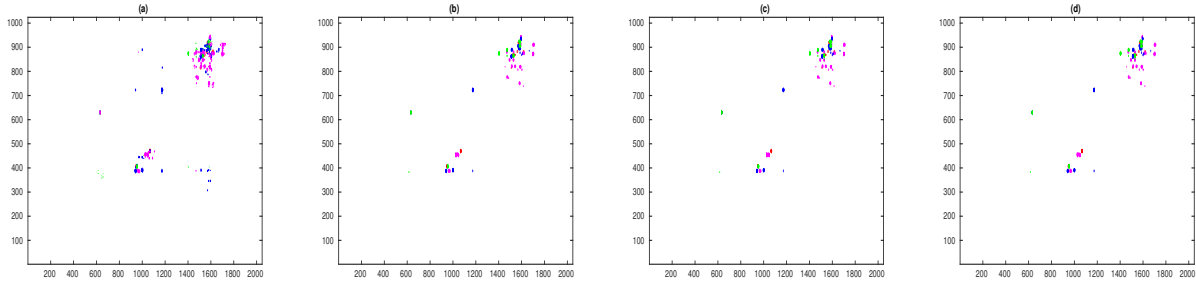


Figure 1. 2D HSQC data (4 sources: Limonene (red), Nerol (blue),  $\alpha$ -Terpinolene (green) and  $\beta$ -Caryophyllene (magenta)): (a) original sources with size ( $4 \times 1024 \times 2048$ ), (b) estimated sources using  $\ell_1$  norm, (c) estimated sources using  $\Psi_1$ , (d) estimated sources using  $\Psi_2$ .

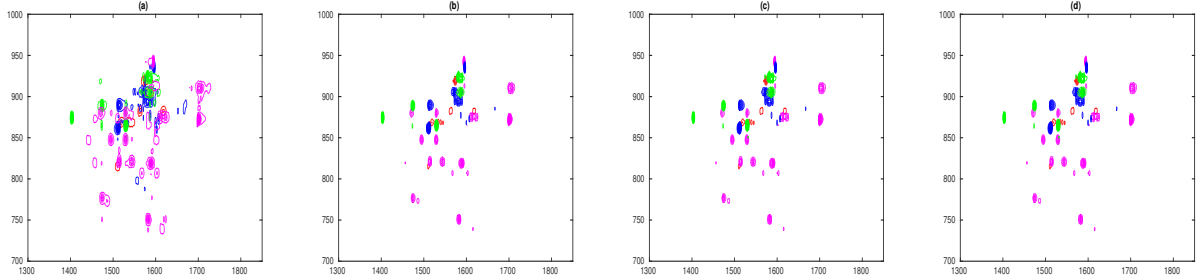


Figure 2. Zoom on the most important terpene zone [1300 : 1850, 700 : 1000]: (a) original sources, (b) estimated sources using  $\ell_1$  norm, (c) estimated sources using  $\Psi_1$ , (d) estimated sources using  $\Psi_2$ .

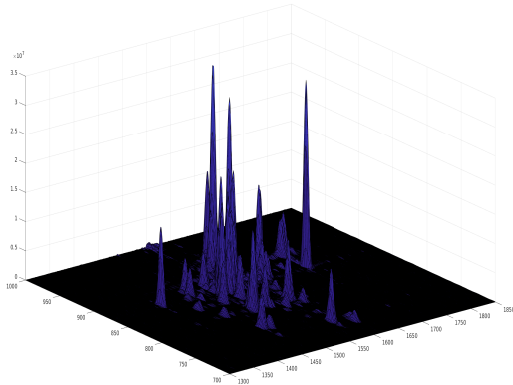


Figure 3. 3D representation of Figure 2 (a)

$\Psi_S$	Proximal operator of $\Psi_S$
$\ell_1$ (Eq. (3))	Computed [8]
$\Psi_1$ (Eq. (4))	Computed [1]
$\Psi_2$ (Eq. (5))	Approximated algorithm [3]

Table I

PROXIMITY OPERATORS OF DIFFERENT REGULARIZATION FUNCTIONS.

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	$\ell_1$ (Eq. (3))	$\Psi_1$ (Eq. (4))	$\Psi_2$ (Eq. (5))
SIR	<b>40.10</b>	34.11	34.04
	42.98	44.58	<b>50.23</b>
	30.72	31.58	<b>33.18</b>
	<b>35.87</b>	29.03	28.13
SDR	<b>25.93</b>	24.56	24.70
	18.41	18.10	<b>18.78</b>
	<b>15.14</b>	14.46	15.08
	<b>11.06</b>	9.63	10.09
SAR	<b>26.10</b>	25.07	25.25
	18.42	18.11	<b>18.79</b>
	<b>15.26</b>	14.55	15.15
	<b>11.08</b>	9.68	10.17
Amari index	<b>0.01</b>	0.05	0.05

Table II

QUALITY PERFORMANCES USING DIFFERENT REGULARIZATION FUNCTIONS.

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