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A DECISION FUSION FOR SOURCE DETECTION BASED ON MULTIMODAL SUPERVISED SPECTRAL UNMIXING

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ABSTRACT

This paper addresses the problem of source detection in unknown chemical mixtures in the context of multimodal measurements of spectral data. The proposed approaches are based on supervised linear spectral unmixing under non-negativity and sparsity constraints with adapted variants of the orthogonal matching pursuit algorithm. Two detection strategies are introduced: fusion of independent unimodal detection results and fusion by a joint multimodal decomposition and detection. Results are evaluated using a real database of ion mobility mass spectrometry (IMMS) data. A significant increase of the detection accuracy is obtained using the joint decomposition based decision as compared to the single modality detection results.

Index Terms— multimodal supervised spectral unmixing, joint sparse recovery, signal separation, chemical mixture analysis

1. INTRODUCTION

Source detection from spectral data is a signal processing problem encountered in several applications of physical sensing. Typical examples include chemical substance analysis [1] and hyperspectral imaging [2]. Single source identification has been extensively studied and successfully applied in various fields [3]. In the context of signal detection from spectral measurements, existing approaches are mainly based on a spectral matching between the observed data and the available library of known sources [4, 5]. Other approaches explore a large amount of mixture data to identify the discriminant features that could be used by a binary classifier [6]. However, in several chemical sensing applications, the measured data are assumed to be a linear mixture of several sources and the most challenging problem lies in the identification of the entire set of sources which are present in the considered mixture [7, 8].

Multivariate analysis methods [9] and blind source separation algorithms has been already applied for this purpose [10]. These techniques perform a joint estimation of the source signals and their relative abundances in the mixture data. However, defining the actual number of sources and

linking the estimated sources to meaningful physical components may not be successful in all situations. The present work proposes to narrow down the identification problem by recording directly the set of target source spectra in order to focus on the detection. The proposed processing pipeline is therefore based on supervised regression techniques under the constraint of non-negativity. The estimated mixing coefficients are then used by a binary classifier to deduce the subset of the more likely present sources.

In the case where several mixture data, composed by the same sources, are available it has proven useful to jointly process these data using the multiple measurement formulation of sparse recovery problem [11] or the simultaneous orthogonal matching algorithm (S-OMP) [12]. These studies focus on the case where all the measurements are acquired using the same modality and can be gathered in a single matrix with a joint row sparsity hypothesis. This paper however is concerned with the application cases where both the mixture and the sources are observed with multiple measurement modalities thus yielding multiple heterogeneous data. It is obviously assumed that taking advantage of several modalities will improve detection as it is the case with multiple measurement from a single modality. However, existing methods have yet to be adapted to take in account multimodality. The challenge is to find an adequate fusion strategy to obtain accurate detection of the entire set of sources.

In that respect, the main concern of this paper is to propose two fusion strategies. The first strategy consists in independent processing of each modality data and fusion of the detection using a voting scheme. The second adopted strategy is to perform a joint sparse unmixing using a multimodal greedy algorithm.

2. PROBLEM STATEMENT

Let us consider the case where L independent measurement modalities are available. The measurement vector of the mixture in the l -th modality is noted $\mathbf{y}^{(l)} \in \mathbb{R}^{M_l}$, where M_l is the length of the data vector in the l -th modality. The K spectral sources are gathered in matrix $\mathbf{S}^{(l)} = [\mathbf{s}_1^{(l)}, \dots, \mathbf{s}_K^{(l)}] \in \mathbb{R}^{M_l \times K}$. The measurement model is assumed to be a linear

mixing:

$$\mathbf{y}^{(l)} = \sum_{i=1}^K a_k^{(l)} \mathbf{s}_k^{(l)} = \mathbf{S}^{(l)} \mathbf{a}^{(l)}, \quad (1)$$

where each mixing coefficient $a_k^{(l)}$ depends on the abundance of the k -th source in the mixture and on the sensitivity of the l -th measurement modality to this source. Moreover, the mixing coefficient vectors $\mathbf{a}^{(l)} = [a_1^{(l)}, \dots, a_K^{(l)}]^T$, for $l = 1, \dots, L$ are linearly independent.

By assuming a dictionary of $N > K$ known sources, the identification of the sources which are present in the mixture is achieved using a two step approach. In a first step, a spectral unmixing is performed under the constraint of non-negativity and sparsity [13, 14]. The estimated mixing coefficients are then used in a second step to detect the sources which are present in the mixture. The estimation of the mixing coefficients $\mathbf{a}^{(l)}$ in each measurement modality, under the Gaussian noise hypothesis, is performed according to:

$$\hat{\mathbf{a}}^{(l)} = \arg \min_{\mathbf{a}^{(l)} \in \mathcal{C}} \|\mathbf{y}^{(l)} - \mathbf{S}^{(l)} \mathbf{a}^{(l)}\|_2^2, \text{ for } l = 1, \dots, L, \quad (2)$$

where \mathcal{C} denotes the constraint set on the coefficients and $\mathbf{S}^{(l)} \in \mathbb{R}^{M_l \times N}$. In order to perform a joint estimation of the mixing coefficients and the detection vectors, a greedy algorithm, the non-negative orthogonal matching pursuit (NNOMP), is used hereafter [15] and we propose its extension to the case of multimodal data, either by adding a fusion stage after the decomposition in each modality or during the source selection step in the joint multimodal decomposition.

The estimated set of non-zero mixing coefficients in the different modalities are then used to retrieve the detection vector $\mathbf{d} = [d_1, \dots, d_N]^T \in \{0, 1\}^N$ where for $i = 1, \dots, N$, $d_i = 1$ when the source i is estimated present in the mixture and $d_i = 0$ otherwise.

3. MULTIMODAL DECISION FUSION

The proposed detection pipeline consists in firstly performing a sparse spectral unmixing, in each modality independently, under the constraint of non-negativity by using a greedy approach. Then, the resulting detection vectors $\mathbf{d}^{(l)}$ corresponding to the detected sources in different modalities are fused using a decision fusion scheme based on a multiple voting strategy.

3.1. Step 1: single modality spectral unmixing

Sparse spectral unmixing is performed using a greedy approach based the non-negative matching pursuit algorithm [16, 15]. The inputs of this algorithm are the measurement vector $\mathbf{y}^{(l)} \in \mathbb{R}^{M_l}$, the source matrix $\mathbf{s}^{(l)} \in \mathbb{R}^{M_l \times N}$ and K , the expected number of sources (sparsity level). The outputs after K iterations are: the list of detected sources, $\Gamma_K^{(l)} \subset \{1, \dots, N\}$, their mixing coefficients $\mathbf{a}_K^{(l)} \in \mathbb{R}^K$ and

the decomposition residual $\mathbf{r}_K^{(l)} \in \mathbb{R}^{M_l}$.

The NNOMP procedure is initialized with the initial support $\Gamma_0^{(l)} = \{\emptyset\}$, $\mathbf{r}_0^{(l)} = \mathbf{y}^{(l)}$ and the set of candidate sources $\Lambda_0^{(l)} = \{1, \dots, N\}$. Each iteration $k = 1, \dots, K$ proceeds with four steps:

1. Detection of the index of the source the mostly correlated to the current residual according to:

$$p_k^{(l)} = \arg \max_{j \in \Lambda_k^{(l)}} \langle \mathbf{s}_j^{(l)}, \mathbf{r}_k^{(l)} \rangle, \quad (3)$$

where $\langle \cdot, \cdot \rangle$ denotes the scalar product.

2. Incorporation of the detected source index $p_k^{(l)}$ in $\Gamma_{k-1}^{(l)}$ and its removal from $\Lambda_k^{(l)}$.
3. Estimation of the mixing coefficients of the detected sources:

$$\hat{\mathbf{a}}_k^{(l)} = \min_{\mathbf{a} \geq 0} \|\mathbf{y}^{(l)} - \mathbf{F}_k^{(l)} \mathbf{a}\|_2^2 \quad (4)$$

where $\mathbf{F}_k^{(l)}$ is the matrix formed by the selected sources (columns of indexes $\Gamma_k^{(l)}$ in $\mathbf{S}^{(l)}$). This minimization is performed using the NNLS algorithm [17].

4. Update of the residual according to:

$$\mathbf{r}_{k+1}^{(l)} = \mathbf{y}^{(l)} - \mathbf{F}_k^{(l)} \hat{\mathbf{a}}_k^{(l)} \quad (5)$$

This iterative process is run until the identification of K sources. It can also be stopped when adding a new source does not yield a sufficient decrease of the relative residual norm:

$$\frac{\|\mathbf{r}_k\| - \|\mathbf{r}_{k+1}\|}{\|\mathbf{r}_k\|} < \epsilon, \quad (6)$$

where $\epsilon > 0$. This stopping rule allows an unsupervised assessment of the source number. Finally, the detection vector $\mathbf{d}^{(l)}$ in each modality is obtained from the list of selected atoms:

$$\forall i \in \{1, \dots, N\}, \quad d_i^{(l)} = \begin{cases} 1 & \text{if } i \in \Gamma_K^{(l)} \\ 0 & \text{otherwise} \end{cases} \quad (7)$$

3.2. Step 2: decision fusion by majority voting

Fusion at the decision level is subsequently obtained by using a Majority Voting (MV) scheme [18, 19]. Given the L detection vectors $\mathbf{d}^{(1)}, \dots, \mathbf{d}^{(L)}$ obtained using the method described above 3.1, a voting score \mathbf{v} is defined as:

$$\mathbf{v} = \frac{1}{L} \sum_{l=1}^L \mathbf{d}^{(l)}, \quad (8)$$

The fused detection vector is then obtained by:

$$\forall i \in \{1, \dots, N\}, \quad d_i^{\text{fus}} = \begin{cases} 1 & \text{if } v_i \geq \frac{1}{2} \\ 0 & \text{otherwise} \end{cases} \quad (9)$$

More sophisticated fusion approaches of decision fusion [20, 21] can also be envisaged to account for the detection reliability in each measurement modality.

4. FUSION BY JOINT MULTIMODAL UNMIXING

The sparse multimodal unmixing aims at jointly recovering a set of mixing coefficients vectors $\{\mathbf{a}^{(l)} \in \mathbb{R}^N, l \in \{1, \dots, L\}\}$ solution to the set of problems:

$$\mathbf{a}^{(l)} = \arg \min_{\mathbf{a} \in \Gamma_K} \|\mathbf{y}^{(l)} - \mathbf{S}^{(l)} \mathbf{a}\|_2^2 \text{ for } l = 1, \dots, L.$$

where Γ_K corresponds to the set defined by the K detected sources. Consequently:

$$\Gamma_K \triangleq \left\{ i \in \{1, \dots, N\}; \exists l \in \{1, \dots, L\}, a_i^{(l)} \neq 0 \right\}. \quad (10)$$

It can be highlighted here that the main difference with the single modality spectral unmixing is that the list of selected sources is common to all measurement modalities. The estimation of this list can also be performed using a greedy approach similar to the case of the MMV formulation of the non-negative sparse recovery [12, 22]. However, since the decomposition is performed on measurement data acquired in different modalities, and hence different dictionaries, an adaptation of the source selection strategy is proposed.

The main steps of the joint unmixing algorithm:

1. In order to select the same source for all the modalities at each iteration, a global correlation criterion is computed according to:

$$J(\mathbf{S}_k^{(1)}, \dots, \mathbf{S}_k^{(L)}) \triangleq \sum_{l=1}^L \alpha_{kl} \max \{ \langle \mathbf{s}_j^{(l)}, \mathbf{r}_k^{(l)} \rangle, 0 \}, \quad (11)$$

where the weighting coefficients α_{kl} allow to control the balance between the correlation measures in different measurement modalities. A simple weighting strategy would be to choose these weights according to

$$\alpha_{kl} = \frac{1}{\|\mathbf{r}_k^{(l)}\|}.$$

Alternately, to the original S-NNOMP approach, these coefficients combine normalized correlation scores in different modalities which is not affected by the different scaling of the data in the measurement modalities. This method is referred to as Multimodal Non-negative OMP (MM-NNOMP). A possible extension of the approach would concern the search of the optimal set of weights allowing to optimize the detection accuracy.

2. Once the index of the mostly correlated source across all modalities is identified, the estimation of the mixing

coefficients of the selected sources $\{\mathbf{F}_k^{(1)}, \dots, \mathbf{F}_k^{(L)}\}$ such that $\forall l \in \{1, \dots, L\}, \mathbf{F}_k^{(l)} = \{\mathbf{S}_j^{(l)}; j \in \Gamma_k\}$, is performed using the NNLS algorithm.

3. The residual vector in each modality is updated as in Equation (5).
4. The average relative variation of the residual norm is used as a stopping criterion of the iterative process:

$$\frac{1}{L} \sum_{m=1}^L \frac{\left| \|\mathbf{r}_k^{(m)}\| - \|\mathbf{r}_{k+1}^{(m)}\| \right|}{\|\mathbf{r}_k^{(m)}\|} < \epsilon. \quad (12)$$

Finally, the detection vector \mathbf{d}_{fus} is obtained in the same way as in Equation (7).

5. EXPERIMENTAL RESULTS

A real database of 85 lubricant mixtures containing between 5 and 7 components randomly taken from a set of 20 chemical components has been designed. The abundance of each source is taken randomly. The spectral mixture data are acquired using an ion mobility mass spectrometer [23]. This device records spectral measurements of ion mobility spectra, mass spectra with two ionization mode modes: positive (POS) and negative (NEG). Therefore, four one-dimensional spectra have been recorded for each mixture and each source. Those modalities are called hereafter M1, M2, M3 and M4, corresponding to positive and negative mass spectra and positive and negative ion mobility spectra, respectively. Figure 1 illustrates the spectra of one source in the four modalities.

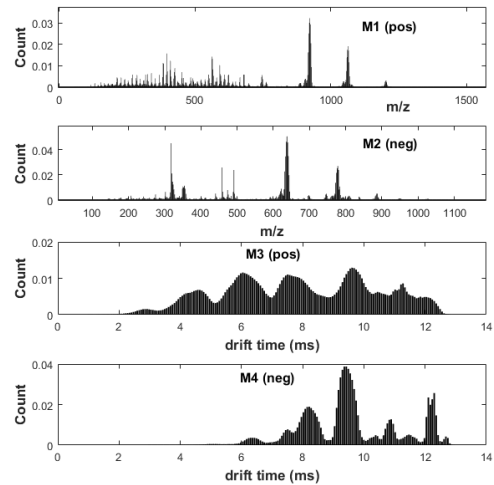


Fig. 1. Source C16 in the four measurement modalities.

5.1. Analysis of the detection accuracy

Figure 2 shows the Receiver Operating Characteristic (ROC) of the detection in the four modalities and for both fusion strategies. It has been obtained for different predefined values of $K \in \{1, \dots, N\}$.

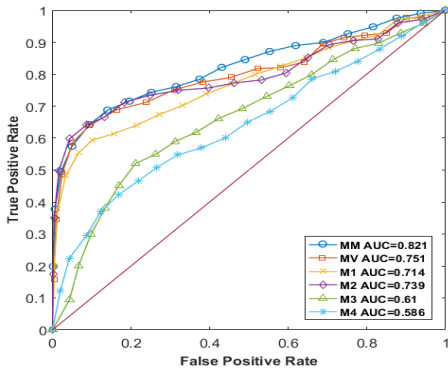


Fig. 2. Comparison of unidimensional OMP vs. fusion methods for predefined number of iterations

It can be noted that the MM-NNOMP outperforms all the single modalities as well as the voting scheme strategy. The best accuracy reached by the MM-NNOMP method has been obtained for $K = 6$ which is very close to the average value of the number of components in the mixtures ($\bar{K} = 5.72$ components). For each modality, the value of K giving the best detection accuracy are shown in Table 1. The detection accuracy of the joint unmixing is better than the fusion of the independent detection in the different modalities.

Table 1. Performance for optimal values of K

	M1	M2	M3	M4	MM	MV
K	6	7	8	8	6	6
acc (%)	77.6	79.5	66.1	67.0	81.4	80.5

5.2. Estimation of the number of sources

In real applications, the number of sources present in the mixture is generally unknown. The detection algorithms therefore need an automated value of the stopping threshold ϵ allowing the estimation of the number of components. Each method has been run for different values of ϵ in the range of $[0, 1]$ and the corresponding ROC curves are reported in Figure 3. Once again, one can notice that the joint unmixing leads to the best performance. Moreover, the area under curve (AUC) of the MM-NNOMP approach controlled by the relative residual norm is higher than when the algorithm is controlled by the number of components.

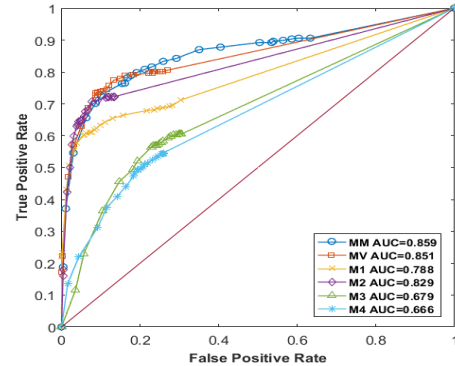


Fig. 3. Comparison of unidimensional OMP vs fusion methods with relative residual norm convergence criterion

For each method, the optimal value of ϵ corresponds to the ROC curve point which is the closest to the ideal point $(1,0)$. The corresponding accuracy and the average number of detected sources are shown in Table 2. Adopting the relative residual norm variation as a stopping criterion leads to a better estimation of the source number. This stopping strategy is adequate for automated estimation of the unknown number of sources.

Table 2. Performance for optimal values of ϵ

	M1	M2	M3	M4	MM
ϵ_{opt}	10^{-4}	10^{-5}	$9 \cdot 10^{-6}$	$2 \cdot 10^{-6}$	$8 \cdot 10^{-3}$
$K_{average}$	5.87	5.33	6.79	6.65	5.55
acc (%)	74.4	81.0	66.5	69.7	81.4

6. CONCLUSION

Two strategies for multimodal supervised mixture analysis have been proposed in this work. The joint spectral unmixing method (MM-NNOMP) was found to lead to better detection performance as compared to the decision fusion approach using majority voting scheme. It was shown that accounting for the multimodality outperformed the best of the unimodal detection schemes and therefore was able to take advantage from the complementarity of the multiple measurements. Subsequent tuning of the stopping criterion of the greedy algorithm allowed a successful automated detection of the number of components. Future work will be directed at setting optimized tuning multimodal source selection criterion involved in the MM-NNOMP, the proposal of adapted weighted majority voting schemes for the detection fusion and a complete comparison with respect to alternative approaches of source detection in spectral mixtures, including more recent approaches based on deep neural networks.

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