Supervised mixture analysis and Source detection from multimodal measurements

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Abstract. The aim of this paper is to present a method for source detection within unknown chemical mixtures using several measurement modalities. Contrary to the well studied case of single source detection, this approach enables simultaneous detection of multiple chemical components by exploiting the mixing coefficients resulting from supervised linear unmixing and thresholded non-negative least squares. The first contribution of this work is to propose an automated procedure to compute an optimized binary classifier rule for each component independently using a database of known mixtures. The second contribution is to propose a global decision rule based on the fusion of the multimodal decisions using weighting schemes such as those used in multiple classifier systems (MCS). A real database of Ion Mobiliy Mass Spectrometry (IMMS) data is used to evaluate the detection performance. An increase of the detection accuracy is reached using the multiple thresholds within the independent classifiers approach as compared to single modality detection.

Keywords: Multimodal supervided spectral unmixing · Sensor fusion · Chemical mixture analysis.

1 Introduction

Source detection from spectral data is at the core of several applications of signal processing methods in physical sensing problems, such as chemical substance analysis [6], hyperspectral imaging [17]. The concept of a source signal is defined as the spectral signature associated to a chemical component.

Classical approaches for source detection and identification are based on the recognition of some discriminant patterns or features of the sought sources [24]. These features can be determined empirically [13,18] or learned from a large-scale database [10]. Often, the measured signal is interpreted as the linear combination of an unknown set of several sources. In such cases, multivariate analysis techniques [21] such as independent component analysis and non-negative matrix factorization can be used. But, even if these blind separation methods yield estimates of the source and their relative abundances (mixing coefficients), their identification as a physically meaningful components is not guaranteed in all situations.

Alternatively, one can consider a known set of sought sources and estimate the mixing coefficients by a linear regression under non-negativity constraint. These coefficients are then used to make a decision on the presence or the absence of each source in the mixture. In this supervised linear unmixing framework, various methods can be applied, such as thresholded non negative least squares [25], non-negative orthogonal greedy algorithms [20] or constrained sparse regression [1]. The main challenge in these approaches is to estimate the sparsity level corresponding to the appropriate number of mixture components. For non-negative least-squares (NNLS), hard thresholding based methods may require a tuning of the threshold level [25] or a setting of an appropriate stopping strategy of the iterative process [2]. For greedy algorithms, the sparsity level should be defined manually or estimated automatically by adopting an adequate stopping rule during the decomposition. In this paper, we explore more specifically the hard thresholding based approach for which we propose two enhancements. The first one is to adopt a source dependent threshold which allows more accurate detection. The second proposal is to use a training database of known mixtures to determine an optimized detection threshold for each sought source separately.

The abundance of each source in an observed mixture data depends on the sensitivity of the sensing modality to this source. Consequently, a lack of sensitivity to some sources in one modality leads to a poor detection of these sources using this modality and conversely an accurate detection will be achieved from another modality more sensitive to these sources. Exploiting multi-modality will therefore enhance detectability of all the sources present in a mixture [7, 11]. In the case of multiple measurements of the mixture recorded in the same modality, it has been shown that joint analysis of the data can enhance performance [5,27]. In the case where different measurement modalities are available, an appropriate fusion strategy should be defined. The second contribution of this paper is to adopt a decision fusion method based on a multiple classifier system (MCS) [9]. Finally, the proposed approaches of component-dependent thresholding and multimodal decision fusion are tested on a challenging example of chemical mixture analysis using Ion Mobility Mass Spectrometry (IMMS) data [12, 26], where spectral responses of the mixtures and the sources are recorded using four complementary measurement modalities (ionization modes).

2 Problem Statement

Let us consider the case of a single measurement modality. The measurement vector of the mixture is noted $\boldsymbol{y} \in \mathbb{R}^M$, where M represents the number of samples provided by the sensor. Measurement vectors associated to N sources are gathered in a matrix $\boldsymbol{S} = [\boldsymbol{s}_1, ...\boldsymbol{s}_N] \in \mathbb{R}^{M \times N}$. The measurement model is assumed to be a linear mixing:

$$\boldsymbol{y} = \sum_{i=1}^{N} a_i \boldsymbol{s}_i + \boldsymbol{e}, \tag{1}$$

where the additive noise term $\boldsymbol{e}$ corresponds to measurement errors. Computing the vector of mixing coefficients $\boldsymbol{a} = [a_1, ..., a_N]^{\mathrm{t}} \in \mathbb{R}^N$ can be efficiently done by solving the following problem:

$$\hat{\boldsymbol{a}} = \arg\min_{\boldsymbol{a} \in \boldsymbol{C}} \|\boldsymbol{y} - \boldsymbol{S}\boldsymbol{a}\|_2^2, \tag{2}$$

where $\boldsymbol{C}$ denotes the constraint set of the coefficients. For the considered application, measured data correspond to mass spectrometry and ion mobility spectra and are assumed to follow a linear mixing model. The leas- squares problem above (2) is therefore solved under the constraint of non-negativity using a non-negative least squares algorithm (NNLS) [16] or an interior-point least squares (IPLS) [4]. The estimated mixing coefficients in each measurement modality are then used to retrieve the detection vector $\boldsymbol{d} = [d_1, ..., d_N]^{\mathrm{t}} \in \{0, 1\}^N$ from $\boldsymbol{a}$ where for $i \in 1, ..., N, d_i = 1$ when component i is present in the mixture and $d_i = 0$ otherwise.

In the case where L independent measurement modalities are available, for each modality $l \in 1, ..., L$, the measurement vector of the mixture is noted $\boldsymbol{y}^{(l)} \in \mathbb{R}^{M_l}$ and the spectra of the N sources are gathered in a matrix $\boldsymbol{S}^{(l)} = [\boldsymbol{s}_1^{(l)}, ...\boldsymbol{s}_N^{(l)}] \in \mathbb{R}^{M_l \times N}$ where M_l is the length of the data vector in the l-th modality. The observation model is then expressed as:

$$\boldsymbol{y}^{(l)} = \sum_{i=1}^{N} \boldsymbol{a}_i^{(l)} \boldsymbol{s}_i^{(l)} \tag{3}$$

with linearly independent abundance vectors $\boldsymbol{a}_i^{(l)}$. The detection of the components which are present in the mixture should therefore be realized by accounting for the values of the mixing coefficients in all modalities using a decision fusion strategy.

Figure 1 shows the proposed detection pipeline. It consists in firstly solving a non-negative linear regression problem in each modality and then deducing the binary detection vectors $(\boldsymbol{d}^{(1)}, ..., \boldsymbol{d}^{(L)})$. The proposed method to compute a fused

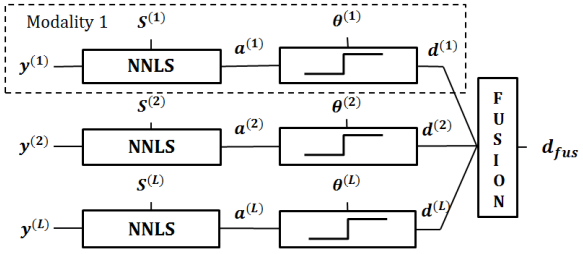


Fig. 1. Multimodal detection pipeline

detection vector $\boldsymbol{d}_{fus}$ from the L unimodal detection vectors $(\boldsymbol{d}^{(1)}, ..., \boldsymbol{d}^{(L)})$ is

presented in Section 4. Section 5 details an application of the proposed detection method in the case of chemical mixture analysis using IMMS spectrometry data.

3 Detection from single modality measurements

A first step of the proposed approach consists in estimating the mixing coefficients (a_i, for $i \in 1, ..., N$) by solving Problem (2). A NNLS algorithm [16] is used for this purpose. Dedicated optimisation algorithms [4] can be used in order to account for additional constraints (such as sum-to-one). The detection of each mixture components from these mixing coefficient values is addressed as a binary classification problem between two states: presence or absence of each source.

3.1 Detection approach

The decision rule related to the two states leads to a binary classifier $h_{\theta_i}(a_i) : \mathbb{R} \to \{0, 1\}$ according to:

$$h_i(a_i; \theta_i) = \begin{cases} 1 \text{ if } \ a_i \geq \theta_i \\ 0 \ \ \text{otherwise} \end{cases} \tag{4}$$

Our proposal consists in adopting thresholds θ_i which are specific to each source in the considered measurement modality. It allows to account for the different sensitivities of the measurement modalities on the sought sources. The detection vector is then given by $d_i = h_i(a_i; \theta_i)$ for $i \in 1, ..., N$. The values of the thresholds θ_i are defined by optimization of the detection performances on a training database of known mixtures. The best detection threshold values are chosen in such a way to reach a balance between sensitivity and specificity of the binary classifier.

3.2 Specification of the detection thresholds

Let $\boldsymbol{Y} = [\boldsymbol{y}_1, ..., \boldsymbol{y}_K] \in \mathbb{R}^{M \times K}$ denote a matrix of K mixtures with a subset of known sources among a set of N sources. The detection performances for each binary classifier corresponding to the i-th source are evaluated in terms of true positive rate and false positive rate

$$\mathrm{TPR}_i\ (\theta_i) = \frac{\mathrm{TP}_i}{\mathrm{TP}_i + \mathrm{FN}_i} \quad \text{and} \quad \mathrm{FPR}_i(\theta_i) = \frac{\mathrm{FP}_i}{\mathrm{FP}_i + \mathrm{TN}_i}, \quad \text{for } i = 1, \ldots, N,$$

where TP (True Positive) and FP (False Positive), correspond to the number of times that sources are detected as present by the binary classifier and they are actually present (resp. absent) in the mixture. TN (False Negative) and FN (False Negative) correspond to the cases where components are detected as absent by the binary classifier and they are actually absent (resp. present) in

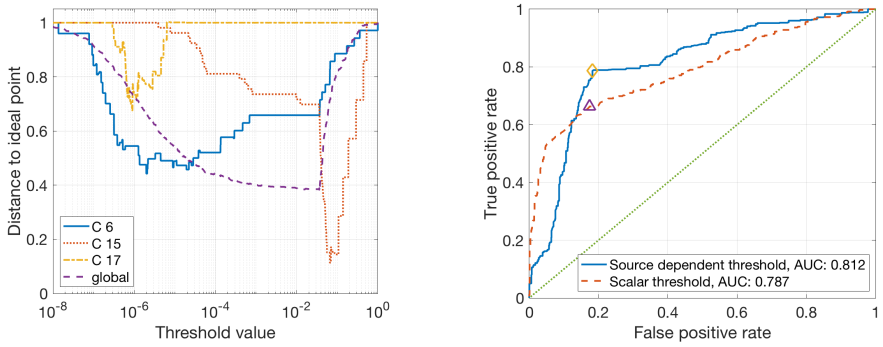
the mixture. The best compromise between sensitivity (TPR) and specificity (1-FPR) is achieved by defining the threshold values according to

$$\hat{\theta}_i = \arg\min_{\theta_i \in \mathbb{R}} \|(\mathrm{TPR}_i(\theta_i), \mathrm{FPR}_i(\theta_i)) - (1,0)\|_2^2. \quad (5)$$

Note that the ideal point $(1,0)$ corresponds to the detection of the source (sensitivity) when it is present in the mixtures and without any false positive detection (specificity).

3.3 Illustration on a real mixture data set

A real database of IMMS data from 85 lubricant mixtures is considered. Each mixture contains between 5 and 7 components among 20 possible ones. More details on this data set are given in Section 5. Figure 2-(a) gives the distance between the receiver operating characteristic (ROC) curve for the detection of different sources. It can be noted that the optimal detection thresholds for the considered sources (C6, C15 and C17) are different, which suggests to use a source dependent threshold. Moreover, the global threshold seems to be appropriate for C15 but it is not optimal for the two other sources (C6 and C17).



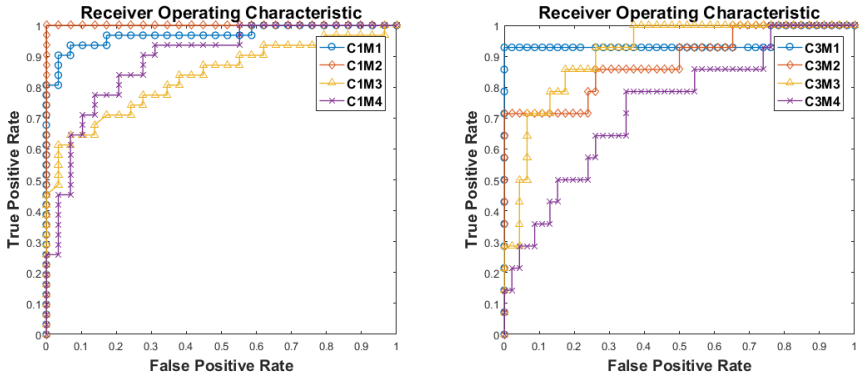
(a) Distance to ideal point (0,1) (b) ROC curves

Fig. 2. Influence of the threshold values on the detection performance

Figure 2-(b) shows a comparison between the average ROC curve obtained when applying a source dependent threshold and the ROC curve obtained by using the same threshold for all the sources. Both the Area Under Curve (AUC) and the average performance at the optimal point are higher in the case of source dependent thresholds.

4 Detection strategy in the multimodal case

This section addresses the detection in the case where $L > 1$ independent measurement modalities are available. To illustrate the relevance of this strategy let us compare the ROC curves, shown in Figure 3, obtained with two different sources C1 and C3 in the four modalities offered by the IMMS spectrometer. The ROC curves of modality M2 (to the left) yields the best performance and M3 the worst performance for source C1. In contrast, for component C3, the best detection is obtained by modality M1 and the worst detection is obtained with modality M4. This example illustrates the complementarity of the different modalities and the need for a decision fusion strategy for an accurate detection of the entire set of sources.



(a) Source C1 (b) Source C3

Fig. 3. ROC curves for source detection in four modalities

4.1 Weighting schemes

The fusion of the independent binary classifiers $(h_i^{(1)}, \ldots, h_i^{(L)})$ in the L modalities is performed using a linear combination rule according to

$$g_i\left(a_i^{(1)}, \ldots a_i^{(L)}\right) = \sum_{l=1}^{L} \omega_i^{(l)}\ h_i^{(l)}\left(a_i^{(l)}; \theta_i^{(l)}\right), \tag{6}$$

where $\theta_i^{(l)}$ and $\omega_i^{(l)}$ correspond to the detection threshold and the decision weight associated to the detection of i-th component in the l-th measurement modality. A resulting fused decision corresponds to a Multiple Classifier System [9] defined subsequently as:

$$d_i^{\text{fus}} = \begin{cases} 1 & \text{if } \ g_i\left(a_i^{(1)}, \ldots a_i^{(L)}\right) \geq 0.5 \\ 0 & \text{otherwise} \end{cases} \tag{7}$$

Depending on the values assigned to the decision weights, one can distinguish mainly three different fused classifiers.

a) Majority Vote (MV). It consists of retaining the decision taken by the absolute majority of classifiers [3]. It is defined as below:

$$\omega_i^{(l)} = \frac{1}{L}. \tag{8}$$

However, the MV classifier doesn't account for the performance of the binary classifiers in the different measurement modalities.

b) Weighted Majority Vote (WMV). Weighted Majority Vote [15], [19] is a decision fusion rule in the case of independent classifiers and the weights are defined as:

$$\omega_i^{(l)} = \log \frac{\mu_i^{(l)}}{1 - \mu_i^{(l)}} \tag{9}$$

where $\mu_i^{(l)}$ is the considered measure of the i-th classifier performance (distance to ideal point, global accuracy, balanced accuracy, etc.) in the l-th modality.

c) Dynamic Classifier Selection (DCS). DCS [8] is a simple and powerful multiple classifier fusion strategy consisting in selecting the most efficient classifier for each source and discarding the others. The chosen decision weights in (6) depend on the performance index of the binary classifiers in each modality. The values of $\omega_i^{(l)}$ are set according to:

$$\omega_i^{(l)} = \begin{cases} 1 & \text{if } \mu_i^{(l)} = \max_{k \in [\![1,L]\!]} \{\mu_i^{(k)}\}. \\ 0 & \text{otherwise.} \end{cases} \tag{10}$$

4.2 Performance index

The weighting schemes for decision fusion are based on classifier performance. The most commonly used performance measure is the detection accuracy (ACC), defined as:

$$\mu_i^{\text{acc}} = \frac{\text{TP}_i + \text{TN}_i}{\text{TP}_i + \text{TN}_i + \text{FP}_i + \text{FN}_i}. \tag{11}$$

This index is commonly used for evaluation of classifiers with balanced occurrences of presence/absence of the sources.

In the case of our application, the source component are more often absent than present in the mixtures which leads trivial classifiers with high rejection rate to yield good global accuracy scores. This phenomenon called "curse of accuracy" [14] is avoided by choosing a more adapted performance index such as the Mathews Correlation Coefficient (MCC) [23], which is defined as

$$\mu_i^{\text{mcc}} = \frac{\text{TP}_i \times \text{TN}_i - \text{FP}_i \times \text{FN}_i}{\sqrt{(\text{TP}_i + \text{FP}_i)(\text{TP}_i + \text{FN}_i)(\text{TN}_i + \text{FP}_i)(\text{TN}_i + \text{FN}_i)}}. \tag{12}$$

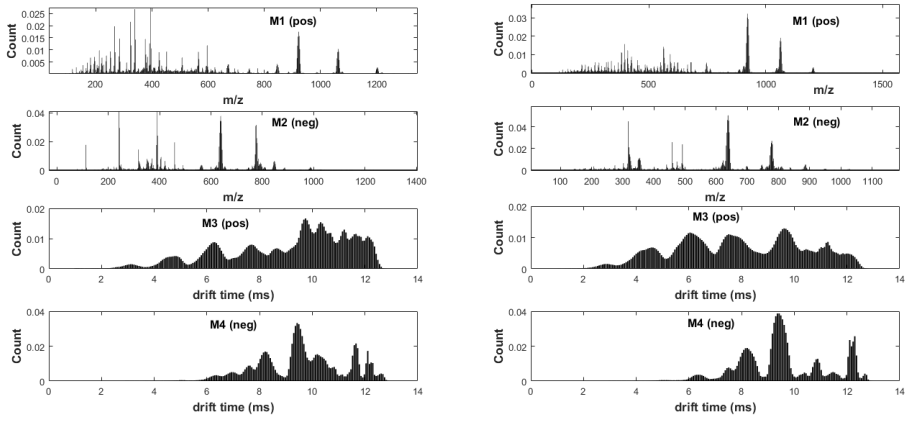
This index is considered as one of the best binary classifier performance metrics since it is not affected by class imbalances in the training set. An ideal classifier leads to $\mu_i^{\text{mcc}} = 1$, a random classifier gives $\mu_i^{\text{mcc}} = 0$ whether or not the training set is balanced, meanwhile a classifier systematically predicting the exact opposite of the ground truth will hace an MCC value $\mu_i^{\text{mcc}} = -1$.

5 Application to mixture analysis by IMMS spectrometry

In this section, detection performances of the presented MCS are compared to the performance obtained separately on each modality on a supervised chemical mixture analysis by an IMMS spectrometer.

5.1 Mixture synthesis

A database of 85 mixture made from 20 different chemical components has been designed. Each mixture contains 5, 6 or 7 components randomly chosen from a set of 20 classical components involved in lubricant formulation [22]. Samples from each mixture and each source components have been analysed twice with an IMMS spectrometer [12]. This spectrometer ionizes the analyte sample to create a swarn of ions. In a second step, bidimensional maps corresponding to distribution of drift times and time of flight of the ions through two separation chambers are recorded. The distribution of drift time through the first chamber is called the ion mobility spectrum and the distribution of time of flight in the second chamber leads to the mass spectrum. Mass spectra and ion mobility spectra are considered as the spectral signatures of the analyte sample.



(a) Mixture 10 (b) Source C16

Fig. 4. Spectral responses of a mixture and one source in four measurement modalities

Two distinct ionization modes have been used, therefore 4 one-dimensional spectra are recorded for each sample. Those modalities are called M1, M2, M3 and M4, corresponding to positive ionisation mass spectra, negative ionisation mass spectra, positive ion mobility spectra and negative ion mobility spectra. The spectral signatures of one of the mixture are presented in Figure 4-(a). Figure 4-(b) shows the spectral signatures of one component of this mixture.

5.2 Mixture analysis

The IPLS algorithm [4] is used for the mixing coefficient estimation under non-negativity constraint. Among the 85 observed mixtures, a set of randomly chosen 60 mixtures, with balanced occurrences of each component, are retained for training the algorithms in terms of optimal threshold values setting and decision weights calculation. The remaining set of 25 observed mixtures are retained for the performance evaluation. This procedure is repeated with 60 independent realizations to get statistically robust global performance indexes.

5.3 Unimodal detection and majoruty vote

Global performance of each optimized unimodal classifier and the majority vote of the 4 modalities on the database are presented in Table 1. It can be noted that modality M2 seems to present the best global performance in terms of true positive rate, false negative rate and overall accuracy. It can be noted that a naive global fusion scheme such as MV leads to an improvement of specificity (lower TPR) but at the expense of sensitivity (higher FPR). This results suggests adopting alternative fusion strategies

Table 1. Performances of unimodal detection

	Modalities				**Fusion**
Score	***M1***	***M2***	***M3***	***M4***	***MV***
TPR (%)	74.2	**77.7**	59.8	63.8	62.5
FPR (%)	21.5	18.4	26.3	29.2	**8.2**
MCC	0.50	**0.57**	0.31	0.32	**0.57**
ACC (%)	77.4	80.8	69.7	69.3	**83.9**

5.4 Decision fusion for multimodal detection

The results of the application of the two fusion strategies based on binary classifier performances are reported in Table 2. Two weighting strategies based either on ACC and MCC indices are considered. For all the presented metrics, one can notice that these weighted methods (WMV and DCS) outperform the best of unimodal classifiers. More specifically, a significant improvement in ACC and

MCC indices is achieved. An accuracy value of 87.9 % for the MCC based WMV. It notably reduced the rate of false positives (5.1%) while being less sensitive than the modality M2. However, the MCC based DCS classifier is the most sensitive one (82.3 %) and presents a moderate rate of false alarms (13.2 %).

Table 2. Performance of fusion strategies based on either ACC or MCC measures.

	ACC		**MCC**	
Score	**WMV**	**DCS**	***WMV***	***DCS***
TPR (%)	77.3	81.5	68.3	**82.3**
FPR (%)	11.8	12.5	**5.1**	13.2
MCC	0.65	**0.67**	0.62	**0.67**
ACC (%)	85.5	86.0	**87.9**	85.6

5.5 Discussion on component detection

Figure 5 shows the detection results of two groups of sources. In the first group, the sources are well detected by positive ionization mode while in the second group, the sources are better detected using negative ionization mode. For each group of components, unimodal detection results are compared to the multimodal detection. In both cases, the performance of the fused decision is equivalent to the best of all the unimodal classifiers. The proposed framework has therefore been able to fully exploit the complementarity of the modalities.

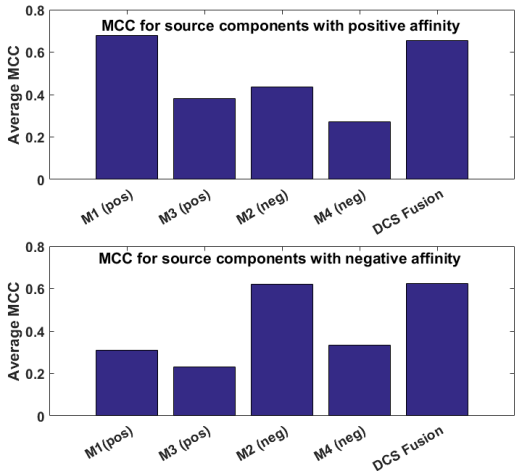


Fig. 5. Detection performance using measurements with two ionization modes

6 Conclusion

The concrete problem of identifying chemical components in an unknown mixture from multi-model spectrometric data, while being an instance of the well-known source separation problem, poses many challenges among which the source-dependent response sensitivity and need to derive robust decision fusion strategies to combine information provided by the different modalities. It has been shown on real data that a more accurate detection is achieved by proposing a component-specific threshold in each modality and adopting a decision fusion scheme exploiting the detection performances in each modality, measured in a training database. We also noted that DCS classifiers tend to be very sensitive while WMV are more specific. Future works will be directed at investigating methods based on greedy sparse recovery, proposing adequate rules for the joint decomposition of the observed data with multiple modalities. Another perspective proposal of decision rules based on machine learning approaches and that will not requite the linear mixing model hypothesis.

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