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Cross-Validation of Blindly Separated Interstellar Dust Spectra

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Abstract: *In this paper, we investigate the validation of Blind Source Separation (BSS) methods applied to interstellar dust hyperspectral data cubes. Since the original source signals are unknown, we cannot measure the separation accuracy by means of classical objective criteria. As a consequence, we here propose a cross-validation of the extracted spectra by applying to the measured data various BSS techniques based on different criteria. We show that, with all these methods, we obtain quite the same (physically relevant) estimated interstellar dust spectra. Moreover, we then derive a spatial structure of the emission of the chemical species, which is not used in the separation step and which is physically relevant.*

I. INTRODUCTION

Blind Source Separation (BSS) is an inverse problem which consists in estimating a set of N unknown sources s_j from a set of P observations x_i resulting from mixtures of these sources through unknown propagation channels. These methods are thus called "blind" since both sources and mixing parameters are unknown. In order to achieve the separation, they generally make assumptions on the source signals, such as mutual independence [1], sparsity [2] and/or non-negativity [3]. BSS is a "generic" problem which finds a lot of applications [4], e.g. in the Astrophysics field that we here consider.

The InterStellar Medium (ISM) lies between stars in our galaxy and contains dust particles which play a major role in the chemical and physical evolutions of galaxies. These particles absorb the star ultra-violet light and re-emit this energy in the infra-red domain. To explain the shape of the infrared spectrum of our galaxy, astronomers invoke the presence of several populations of dust grains of different sizes and compositions [5] in Photo-Dissociation Regions (PDR).

The InfraRed Spectrograph (IRS) on board the Spitzer telescope can provide hyperspectral data cubes: two dimensions (resp. the third one) of a cube correspond to spatial (resp. spectral) coordinates. When a PDR is observed by Spitzer, we assume that for each spatial position (n,m), the observed spectrum $x_{(n,m)}$ consists of a linear mixture of N spectra:

$$x_{(n,m)}(\lambda) = \sum_{j=1}^{N} a_{(n,m),j}\, s_j(\lambda), \tag{1}$$

where $a_{(n,m),j}$ are unknown mixing coefficients and s_j are the grain spectra. When all the cube is considered (i.e. the P spatial positions (n,m)), we thus have a classical BSS problem which can be written in matrix form:

$$\underline{x}(\lambda) = A\,\underline{s}(\lambda), \tag{2}$$

where $\underline{x}(\lambda) = \left[x_1(\lambda) \quad \cdots \quad x_P(\lambda)\right]^T$ is the vector[1] of observations, $\underline{s}(\lambda) = \left[s_1(\lambda) \quad \cdots \quad s_N(\lambda)\right]^T$ is the vector of the unknown sources and $A = \left[a_{ij}\right]$ is the $P \times N$ mixing matrix.

[1] We do not take into account the spatial structure of observations: the spectra which are observed for all pixels are arranged in an arbitrary order to form a vector processed by BSS methods. As a consequence, mixing parameters $a_{(n,m),j}$ are also arranged in the same arbitrary order to form a matrix.

Since these spectra are real mixtures of unknown sources, we cannot directly measure the separation accuracy provided by a BSS approach. As an alternative, we here propose to cross-validate separated Spitzer spectra, using several BSS techniques based on different assumptions about sources. In particular, we will show that all the tested BSS methods yield quite the same separated spectra, up to some small differences that we will discuss below. Moreover, we will derive a physically relevant spatial structure of the presence of the different grains in the PDR, while we do not need this spatial information in the separation step. This kind of analysis has already been done in [6]. However, contrary to [6], we here consider a greater number of BSS methods.

The remainder of this paper proceeds as follows. Section II describes the BSS methods we used in this paper. We then present in Section III the pre-processing step applied to the considered hyperspectral datacube, the estimated spectra that we obtained and, lastly, the derived spatial distribution maps of the grains.

II. SOURCE SEPARATION METHODS

As introduced above, BSS methods aim at separating unknown source signals from a set of mixtures of them, while the mixing parameters are unknown too. In order to achieve the separation, these approaches make some assumptions on the sources, so that BSS methods generally belong to one of the following families.

1. The most studied class of methods is called *Independent Component Analysis* (ICA) [1]. It supposes the sources to be statistically independent and recombines observations in order to obtain, as outputs of the separating system, independent signals (and so separated ones).
2. A more recent family of approaches assumes that the sources are "sparse" in an analysis domain (e.g. Fourier, time-frequency, time-scale, time-time domains), hence its name *Sparse Component Analysis* (SCA) [2]. A signal is said to be *sparse* if it contains a "few non-negligible values". Since this assumption is satisfied, these methods estimate columns of the mixing matrix in regions where only one source is active.
3. Another recent class of methods supposes that the sources and the mixing matrix are positive and is therefore called *Non-negative Matrix Factorization* (NMF) [3]. These methods use the positivity in order to factorize the matrix of observations in a product of two non-negative matrices: the mixing matrix and the matrix of unknown source signals.

The above source signal assumptions, i.e. independence, sparsity and positivity, can be used together, providing new methods for solving the BSS problem (e.g. ICA or NMF with sparse priors or non-negative ICA). We now introduce the methods we used in order to cross-validate the separated spectra of interstellar chemical species.

A. FastICA and Markovian ICA methods

ICA is the first means that has been proposed in the literature for solving the BSS problem. We tested FastICA [7] which is one of the most famous ICA methods. It assumes the sources to be stationary, centered, non-Gaussian (except for at most one source), and mutually statistically independent random signals. In order to achieve the separation, FastICA maximizes the non-Gaussianity of output signals. This criterion can be measured e.g. by the absolute value of the kurtosis defined as

$$\mathrm{kurt}(y) = \mathrm{E}\left\{y^4\right\} - 3\,\mathrm{E}\left\{y^2\right\}^2 \tag{3}$$

where $\mathrm{E}\{.\}$ stands for expectation and y is a zero-mean random variable. FastICA has been proposed in both deflation (where only one source is estimated at each iteration) and parallel versions (where all the sources are estimated at once). In our tests, we decided to use the deflation method, since it does not need to fix in advance the number of source signals present in the observations.

We also tested a maximum likelihood ICA method [8] which assumes the sources to be first-order markovian processes and possibly non-stationary. Contrary to FastICA, this method exploits not only non-Gaussianity but also correlation of adjacent spectral samples and non-stationarity of the source signals (which is considered by means of a blocking approach).

B. LI-TIFROM and LI-TIFCORR methods

SCA is a powerful tool for achieving separation. Indeed, it can process stationary, non-stationary and/or dependent sources. Most of SCA methods suppose that, in each atom of the considered sparsifying analysis domain, at most one source is active. This means that the supports of the sources are disjoint, which is a strong assumption. On the contrary, some methods such as the symmetrical version of LI-TIFROM[2] [9] and both versions of LI-TIFCORR [10], assume that there exists, for each source, an *analysis zone* (i.e. a set of adjacent atoms of the analysis domain) where only this source is active. Everywhere else, more than one source can be active, which is a very low sparsity assumption.

These methods have the same structure: they first find such *single-source* analysis zones and then estimate in these zones the column of the mixing matrix associated to the active source. However, they use different criteria: LI-TIFROM-S is based on ratios of time-frequency (TF) transforms[3] of observations while LI-TIFCORR-C and LI-TIFCORR-NC are based on cross-correlation coefficients of (resp. Centered and Non-Centered versions of) TF observations.

C. Lee & Seung's NMF Method

NMF is a class of BSS methods that has been proposed in the middle of the 90's and which has been popularized by Lee and Seung [11]. Their algorithm consists in factorizing a non-negative matrix X as a product of two non-negative matrices $X = AS$ by minimizing the divergence between X and the product of estimated matrices $\hat{A}$ and $\hat{S}$

$$\mathrm{div}\left(X \mid \hat{A}\hat{S}\right) = \sum_{i,j}\left\{X_{ij}\log\left(\frac{X_{ij}}{\left(\hat{A}\hat{S}\right)_{ij}}\right) - X_{ij} + \left(\hat{A}\hat{S}\right)_{ij}\right\}. \quad (4)$$

Contrary to ICA or SCA methods, the priors which are made on the sources and the mixing parameters are satisfied by the physics of the problem considered in this paper. Indeed, observed and source spectra are positive data (except for some rare wavelengths, due to data processing, as discussed in Subsection III.A). However, the uniqueness of the convergence point of Lee and Seung's algorithm is not guaranteed but, as explained in [6], convergence to local minima has not been encountered in our experiments.

III. OBTAINED RESULTS

In this section, we analyze the separation provided by the above methods on Spitzer spectra in PDRs. In particular, we consider the reflection nebula Ced 201 which lies in the Cepheus constellation and is considered as a good case for the study of the photochemical evolution of interstellar very small particles [6]. The datacube dimension is $39\times29\times331$ (i.e. 1131 spectra of 331 samples corresponding to wavelengths ranging from 5 to $35\mu m$). As in [6], we only keep $P = 370$ spectra of interest (i.e. spectra with magnitudes above user-defined thresholds at 9.3 and $20.6\mu m$).

A. Observations: Pre-processing Stage

Depending on the considered BSS method, a pre-processing stage is applied before the separation stage. Indeed, the Spitzer IRS acquisitions contain a strong and wavelength-dependent noise [6] which has not been taken into account in the mixing model (1) and which can be reduced thanks to a pre-processing stage. As a consequence,

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[2] Matlab code of this method is available at: http://www.ast.obs-mip.fr/bss-softwares

[3] SCA methods are generally applied to audio signals which are expressed in the time domain. In this paper, what we call "time-frequency transforms of observations" corresponds to Short-Time Fourier Transforms applied to observations $x_i(\lambda)$. Such transformed observations are thus expressed with respect to the wavelength λ and its dual λ^{-1}.

- for ICA and SCA methods, we first center and normalize the observed signals and then, since astrophysicists supposed the number N of sources to be drastically lower than the number P of observations, we apply a Principal Component Analysis to observations in order to (i) reduce the data complexity and (ii) reduce the noise contained in observations.
- For Lee and Seung's algorithm, as the above pre-processing makes observations negative, we directly apply NMF to the 370 observations. However, these spectra contain some rare negative values for the lowest wavelengths. This is possibly due to the Spitzer pipeline which revises observed data. As a consequence, we propose two possible scenarii introducing two different pre-processing stages:
    1. the first ones consists in considering negative magnitudes of the spectra as outliers that we do not have to take into account. We thus keep the wavelengths associated to positive magnitudes, i.e. we only keep 304 samples (among 331) for which NMF is applied. Once this method has converged, we can e.g. estimate the sources for all the wavelengths by left-multiplying observations by the pseudo-inverse of the estimated mixing matrix $\widehat{A}$.
    2. On the contrary, we can suppose that the Spitzer pipeline introduces an error translating the actual magnitudes of observed spectra. We thus propose to add a small positive constant α_i to each observation $x_i(\lambda)$ containing negative values so that

$$x_i(\lambda) + \alpha_i \geq 0, \quad \forall \lambda. \tag{5}$$

B. Comparison of Estimated Source Spectra

We now analyze the performance obtained by the above BSS methods. Figure 1 provides mean values (dark line) and envelope (gray area enclosing all estimated spectra) of the separated signals. All of them have been made positive and scaled so that their maximum value is equal to 1. The first estimated spectra corresponds to Very Small Grains (VSG) spectrum, which is dominated by a continuum in the highest wavelengths. The second ones are associated to Polycyclic Aromatic Hydrocarbons (PAH) and exhibit hydrogen emission bands. Even if all these BSS methods provide quite the same estimated signals, they yield small differences that we now discuss.

When we consider VSG spectra, Figure 1 shows that there are some non-negligible differences between estimated signals in the lowest wavelengths (between 5 and 12 μm). Indeed, one spectrum exhibits absorption bands (visible on the envelope) which do not have any physical meaning. These absorptions are obtained with the NMF method using the pre-processing step associated to the first above scenario. On the contrary, the second scenario yields estimated VSG spectra really close to those estimated by the Markovian ICA method and LI-TIFROM-S, LI-TIFCORR-C and LI-TIFCORR-NC methods[4]. The envelope also shows an emission band in the same wavelengths. In fact, this emission is only obtained with FastICA. This is possibly due to the fact that FastICA is only intented for stationary signals unlike all other tested methods, and that the data in this paper are non-stationary. When FastICA is applied to non-stationary signals such as speech, we have already shown in [8,10] that it is really less accurate than Markovian and SCA methods.

Let us now analyze estimated PAH spectra. All emission bands present the same location and the same magnitude (envelope is really close to the mean spectra in this part of the spectra). However, when we consider the longest wavelengths (above 20 μm), we can see in Figure 1 that the envelope is quite far from the mean value. In fact, all the estimated spectra are slightly above the mean value except one, estimated with FastICA which corresponds to the lowest part of the envelope. However, this spectrum slightly decreases and thus shows a low absorption which have no physical sense. This last result confirms that FastICA provides the less accurate separation. Note that the same decreasing PAH spectrum is obtained with the Markovian ICA or the SCA approaches when their parameters (resp. the considered number of blocks and the TF parameters) are not "well" selected.

[4] The VSG spectrum we here obtain with NMF slightly differs from the one in [6]. This is due to the fact that the observed data were not processed through the same pipeline in both studies.

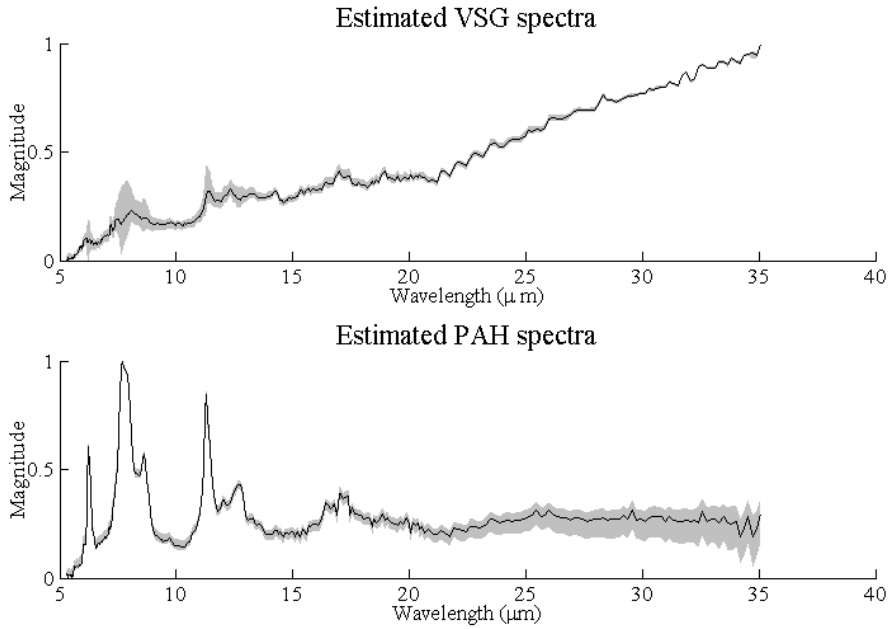

Fig. 1: Spectra estimated by BSS methods from Ced 201 data. The lines (resp. the gray areas) represent mean values (resp. the envelope) of the separated signals.

C. Spatial distributions of the extracted spectra

Once output signals of the BSS system, which are theoretically equal to sources up to a permutation $k = \sigma(j)$ and a scale factor η_j

$$y_k(\lambda) = \eta_j \, s_j(\lambda), \tag{6}$$

have been estimated, their magnitude in each pixel (n,m) can be estimated thanks to covariance. Indeed, since the source signals are assumed to be uncorrelated, by resp. denoting hereafter $y_k(\lambda)$ and $x_{(n,m)}(\lambda)$ the centered versions of the output signals and the observations, the cross-covariance between $y_k(\lambda)$ and $x_{(n,m)}(\lambda)$ reads

$$c(n,m,k) = E\left\{x_{(n,m)}(\lambda) y_k(\lambda)\right\} = a_{(n,m),j} \, \eta_j \, E\left\{s_j(\lambda)^2\right\}. \tag{7}$$

As η_j and $E\left\{s_j(\lambda)^2\right\}$ do not depend on the considered pixel (n,m), the covariance $c(n,m,k)$ is proportional to the mixing parameter $a_{(n,m),j}$ and can be estimated on each pixel of the cube.

Figure 2 provides the maps of the above cross-covariance obtained with NMF (run with the second pre-processing scenario mentioned in Subsection II.A). PAH grains are mainly located in the central part of the nebula, which is especially close to the position of a star illuminating Ced 201. On the contrary, the VSG grains dominate the periphery of the nebula, i.e. far from the star. This result highlights a physical structure that BSS methods did not need in the separation step and which is an argument in favor of the relevance of their results from an astrophysicist point of view.

IV. CONCLUSION

In this paper, we investigated the cross-validation of separated interstellar dust spectra when they are estimated using various BSS methods based on different source assumptions. Indeed, when observed data are real mixtures of unknown sources, we cannot measure the separation accuracy provided by the separation system. We showed that (i) all the BSS methods yield almost the same results, except for some differences that we discussed in the paper, and (ii) the estimated separated spectra are physically relevant from an astrophysicist point of view. Lastly, we derived spatial chemical species distributions thanks to the covariance between estimated sources and original mixtures. These distributions show a

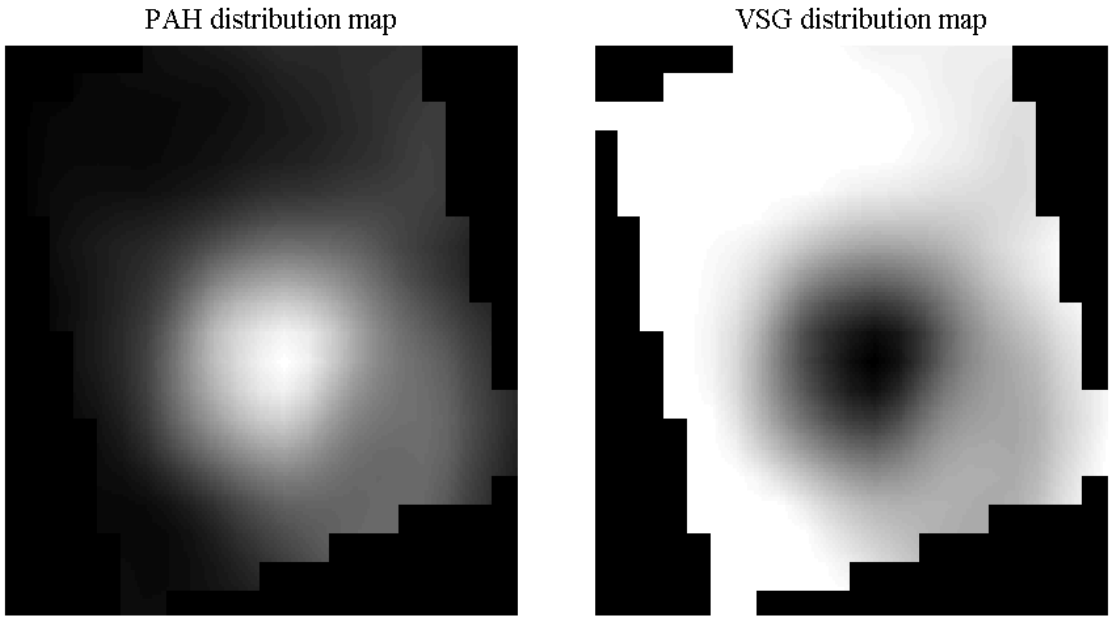

Fig. 2: Estimated grain distribution maps. Clear (resp. dark) zones correspond to high (resp. low) emissions of the considered source.

spatial structure which has a physical sense and provide another argument to verify the relevance of the elementary spectra extracted by the BSS methods.

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