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Unsupervised Source Separation with Learned Regularization

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***Abstract*—Blind source separation (BSS) algorithms are unsupervised methods that allow for physically meaningful decompositions of multispectral data. Being ill-posed inverse problems, BSS algorithms must rely on efficient regularization schemes to better distinguish between the sources and yield interpretable solutions. For that purpose, we propose a semi-blind source separation approach coined sGMCA [1] in which we combine a projected alternate least-squares algorithm with a learning-based regularization scheme.**

I. Introduction

Multispectral data are found in various fields, ranging from astrophysics to biology or remote sensing for instance. Under the linear mixture model, a multispectral measurement $\mathbf{X}_j \in \mathbb{R}^P$ at a channel $j \in [1 \,..\, J]$ can be expressed as the weighted sum of elementary sources $\{\mathbf{S}_i\}_{i\in[1\,..\,I]}$: $\mathbf{X}_j = \sum_{i=1}^{I} \mathbf{A}_j^i \mathbf{S}_i + \mathbf{N}_j$, where $\mathbf{A}_j^i$ is the contribution of source i at channel j and $\mathbf{N}_j$ is some additive noise. The former equation can be recast with matrices, yielding $\mathbf{X} = \mathbf{AS} + \mathbf{N}$ where $\mathbf{X} \in \mathbb{R}^{J\times P}$, $\mathbf{A} \in \mathbb{R}^{J\times I}$ and $\mathbf{S} \in \mathbb{R}^{I\times P}$. The columns of the so-called mixing matrix $\mathbf{A}$ include the electromagnetic spectra of the sources.

In the scope of BSS, the objective is to jointly estimate $\mathbf{A}$ and $\mathbf{S}$ from the sole knowledge of $\mathbf{X}$. When applied to real data, the challenges of BSS are twofold: *(i)* to build efficient priors to better discriminate between the sources so as to limit leakages and *(ii)* to provide physically interpretable results. Altogether, these challenges mandate the design of regularizations that allow injecting physics-driven information by accounting for the fact that real signals naturally live on a low-dimensional manifold.

To capture the underlying manifold structure of signals, we introduced the interpolatory autoencoder (IAE) framework [2]. The gist of IAE is to learn how to travel on a manifold by non-linear interpolation between so-called "anchor points", which are samples that belong to the manifold. The IAE allows to build an efficient physics-driven regularization scheme in a variational inference approach by constraining signals to belong to modeled manifolds. In contrast to the usual data-driven methods [3], we show that the IAE scheme can perform well even when training samples are scarce.

In this contribution, we adapt and apply the IAE framework in the context of BSS to constrain the spectra. The resulting procedure, which associates a standard variational approach with a learned prior, is built upon the sparse BSS algorithm GMCA [4], [5] and dubbed semi-blind GMCA (sGMCA).

II. Methodology

Let $\mathbb{M} \subset [1 \,..\, I]$ be the indices of the components whose spectra are modeled by an IAE. The following cost function is considered:

$$\min_{\mathbf{A},\mathbf{S}} \frac{1}{2}\|\mathbf{X}-\mathbf{AS}\|_2^2 + \left\|\mathbf{\Lambda}\odot\left(\mathbf{SW}^\top\right)\right\|_1 + \sum_{i\in\mathbb{M}} \iota_{\mathcal{M}_{m_i}}\left(\mathbf{A}^i\right) + \sum_{i\notin\mathbb{M}} \iota_{\mathcal{O}}\left(\mathbf{A}^i\right). \quad (1)$$

If a spectrum is modeled, it is enforced to belong to the manifold $\mathcal{M}_{m_i}$ associated to the corresponding IAE model m_i. If not, it is constrained to belong to the intersection of the unit Euclidean sphere with the nonnegative orthant $\mathcal{O}$; the unit-norm constraint prevents scale degeneracies of the product $\mathbf{AS}$. In addition, the sources are assumed to be sparse in a given domain $\mathbf{W}$, such as a wavelet representation, hence the ℓ_1 penalization of sparsity parameters $\mathbf{\Lambda}$.

Equation (1) is non-convex. It is convex with respect to $\mathbf{S}$ when $\mathbf{A}$ is fixed. This is however not the case for the update with respect to $\mathbf{A}$ since the projections onto the manifolds are likely not convex. Fortunately, if the inputs are decent and not drowned by leakages from other components, the projections tend to converge to stationary points. Though it is not convex, it generally leads to stable projections that allow using traditional proximal minimization schemes.

The proposed algorithm sGMCA [1] builds upon a projected alternate least-squares minimization scheme, which allows for simple and fast updates. Each variable is updated alternatively with the other being fixed; firstly, a least-squares minimization is performed to minimize the data-fidelity term, secondly the constraints are enforced by applying the corresponding proximal operators. The main update of the algorithm lies in the update of $\mathbf{A}$; if a spectrum is known and modeled by an IAE, it is projected onto the associated learned manifold, using the AdaGrad iterative algorithm.

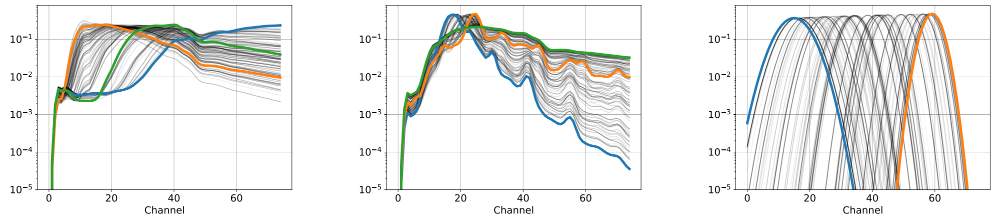
III. Numerical experiments

The proposed method is evaluated on a realistic astrophysical toy model (see Fig. 1 and 2) and compared to common BSS algorithms.

Figure 3 shows the estimated spectra along with the estimation errors. The three BSS methods are particularly prone to interferences, which is problematic for astrophysical interpretations. On the contrary, sGMCA manages to remove most interferences and recovers satisfactory spectra. Figure 4 shows the estimates of the synchrotron source and the associated estimation errors. Remnants of other sources and/or reconstruction artifacts are clearly visible in the estimation errors of the three blind methods. The sGMCA algorithm provides a more accurate source, whose error equally originates from interference, noise contamination and artifacts.

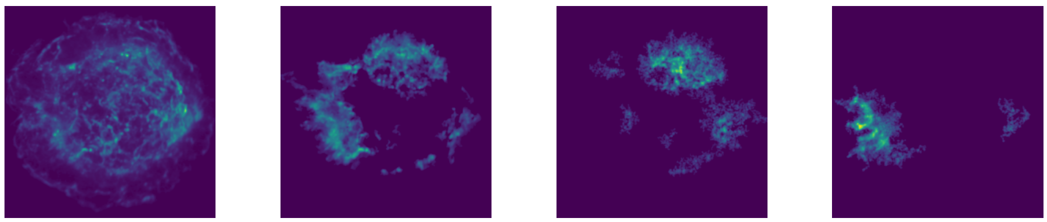
IV. Conclusion

We introduce a novel unsupervised source separation approach to tackle physical multispectral data. It makes use of a learned, physic-driven, prior on the spectra of the sought-after sources in a standard variational framework. We show that the introduced regularization on the spectra efficiently rejects inter-source leakages, thus improving significantly the estimations of both the sources and the spectra, including in challenging settings (involving strong noise, highly correlated spectra and unbalanced sources). The numerical experiments will be presented during the conference.



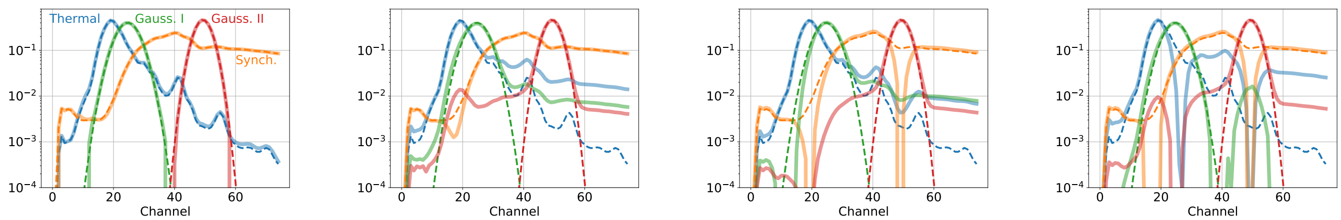
(a) Synchrotron (b) Thermal (c) Gaussian line emission

Fig. 1. Examples of spectra. The colored thick spectra are the chosen anchor points for the IAE model.



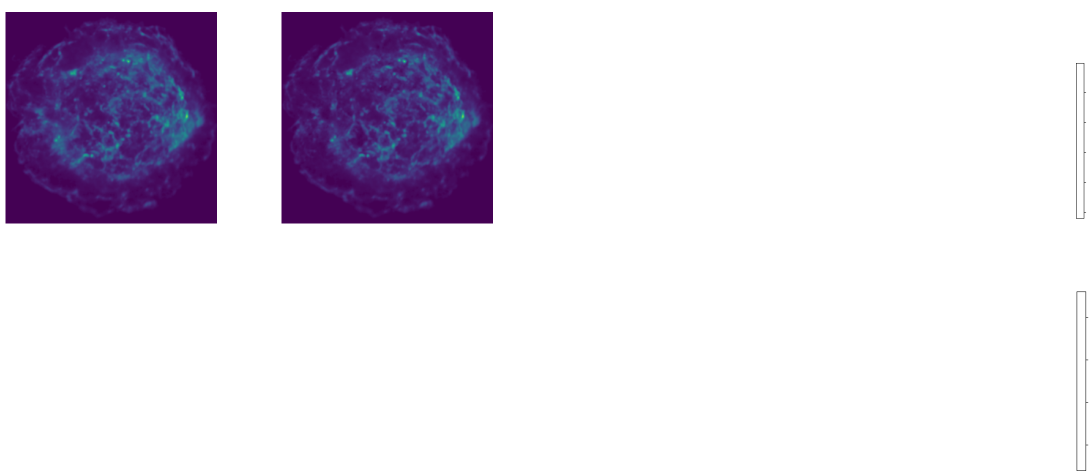
(a) Synchrotron (b) Thermal (c) Gaussian I (d) Gaussian II

Fig. 2. Spatial templates obtained from Chandra X-ray observations of the Cassiopeia A supernova remnant (logarithmic scale).



(a) sGMCA (b) GMCA (c) HALS [6] (d) SNMF [7]

Fig. 3. Example of estimated spectra, with SNR = 40 dB. Solid lines: estimation. Dashed lines: ground truth. The plots share the same ordinate range.



(a) sGMCA (b) GMCA (c) HALS [6] (d) SNMF [7]

Fig. 4. Example of the estimated synchrotron source, with SNR = 40 dB (logarithmic scale). Top: estimations, bottom: absolute error. The figures on a same row share the same color scale.

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