SPATIAL-SPECTRAL UNMIXING OF HYPERSPECTRAL DATA FOR DETECTION AND ANALYSIS OF ASTROPHYSICAL SOURCES WITH THE MUSE INSTRUMENT

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ABSTRACT

Detection and analysis of astrophysical sources from the forthcoming MUSE instrument is of greatest challenge mainly due to the high noise level and the three-dimensional translation variant blur effect of MUSE data. In this work, we use some realistic hypotheses of MUSE to reformulate the data convolution model into a set of linear mixing models corresponding to different, disjoint spectral frames. Based on the linear mixing models, we propose a spatial-spectral unmixing (SSU) algorithm to detect and characterize the galaxy spectra. In each spectral frame, the SSU algorithm identifies the pure galaxy regions with a theoretical guarantee, and estimate spectra based on a sparse approximation assumption. The full galaxy spectra can finally be recovered by concatenating the spectra estimates associated with all the spectral frames. The simulations were performed to demonstrate the efficacy of the proposed SSU algorithm.

Index Terms— MUSE instrument, astrophysical hyperspectral data, galaxy spectra, spatial-spectral unmixing, sparse representation

1. INTRODUCTION

MUSE (Multi-Unit Spectroscopic Explorer) is a very powerful integral field spectrograph, planned to be commissioned at Very Large Telescope (VLT) in Chile in the near future. MUSE will provide massive hyperspectral astrophysical data cube with images of 300×300 pixels and up to 4000 spectral bands, ranging from the visible to near-infrared (465nm to 930nm) wavelength. The data provided by MUSE will be in a very noisy condition with highly spectrally-varied power distribution, caused by the strong parasite emission of the atmosphere at specific wavelengths and by the instrumental limitations. In addition, when observed through MUSE, each source will be spread in spatial and spectral domains in the cube with the three-dimensional point spread function (PSF) due to the instrument and atmospheric effects [3].

Present efforts for analyzing the MUSE hyperspectral data can be mainly categorized by two groups: one for very distant galaxies [1, 2] while the other for stellar spectra [3]. In [1], under the hypothesis that spectra should be in sparse form, spectra restoration from line spread function (LSF) contaminated MUSE data can be accomplished by solving an ℓ_1-norm minimization problem, where a dictionary of elementary spectral features must be advisably given in advance. In [2], Bourguignon et al. consider the restoration problem with the PSF taken into account, employ sparse approximations to solve joint spatial-spectral restoration for full data cube, instead of objects only, and use prior knowledge of the field spread function (FSF) to retrieve the abundance maps. In the other group that considers stellar spectra, [3] presents a instantaneous, spectrally invariant linear mixing model and uses existing method, non-negative matrix factorization (NMF), to extract stellar spectra, but it cannot distinguish star types.

In this paper, we propose a spatial-spectral unmixing (SSU) algorithm to detect spectra and abundance maps associated with all the objects in order to characterize very distant emitting astrophysical sources from the PSF-corrupted MUSE data. We first reformulate the convolution model (for whole spectral range) into several linear mixing models associated with distinct, disjoint spectral frames. In each spectral frame, based on the pure pixel assumption, the proposed SSU algorithm identifies the pure galaxy regions. By considering the fact that each galaxy spectrum can be well approximated by suitable sparse representation [1], the estimation of galaxy spectra is formulated as a convex ℓ_1-norm minimization problem. The estimation of abundance maps can be formulated as a non-negative least-squares problem. Both problems can be solved by any available convex optimization solvers. Finally, the complete estimated spectra are obtained from those estimates of all the spectral frames through an advisable permutation. Some simulation results are presented to demonstrate the efficacy of the proposed SSU algorithm.

Notations: $\mathbb{R}$ ($\mathbb{R}_+$), $\mathbb{R}^N$ ($\mathbb{R}_+^N$) and $\mathbb{R}^{M\times N}$ ($\mathbb{R}_+^{M\times N}$) denote set of real (non-negative real) numbers, $N \times 1$ vectors and $M \times N$ matrices, respectively; $\delta[\mathbf{x}]$ is the discrete-time impulse function of $\mathbf{x}$; $\mathbf{1}$ is an all-one column vector with proper dimension; "$\|\cdot\|_p$", "$\|\cdot\|_F$" and "$\lceil\cdot\rceil$" stand for p-norm, Frobenius norm, and ceiling function, respectively; $\mathbf{P}_{\mathbf{C}}^{\perp}$ is the orthogonal complement projector of matrix $\mathbf{C}$.

2. PROBLEM STATEMENT

As reported in [1–3], MUSE data can be modeled by

$$y[\mathbf{r},\lambda] = x[\mathbf{r},\lambda] + w[\mathbf{r},\lambda] \in \mathbb{R},\ \forall \mathbf{r},\lambda, \tag{1}$$

where $y[\mathbf{r},\lambda]$ is the value of the MUSE data at voxel $[\mathbf{r},\lambda]$, $x[\mathbf{r},\lambda]$ is the noise-free counterpart, and $w[\mathbf{r},\lambda]$ is the noise. Also, $\mathbf{r} \in \mathbb{R}^2$ denotes the 2-D spatial coordinate and $\lambda \in \mathbb{R}_+$ denotes the wavelength. The noise-free MUSE data can be written as:

$$x[\mathbf{r},\lambda] = \sum_{i=1}^{N} x_i[\mathbf{r},\lambda],\ \forall \mathbf{r},\lambda, \tag{2}$$

where $x_i[\mathbf{r},\lambda]$ is the contribution of the ith galaxy to the voxel $[\mathbf{r},\lambda]$ after taking into account the PSF effect and N is the number of galaxies. Moreover, suppose that there are P_i pixels corresponding to the ith galaxy and each galaxy has a set of pixel indices $\mathcal{I}_i = \{\mathbf{r}_i^1, \mathbf{r}_i^2, \ldots, \mathbf{r}_i^{P_i}\}$ for $i = 1, \ldots, N$. Hence, the ith galaxy

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contribution $x_i[\mathbf{r},\lambda]$ in (2) can be further expressed as the following convolution model:

$$x_i[\mathbf{r},\lambda]=\sum_{\mathbf{z}}\sum_{\mu}\left(\sum_{j=1}^{P_i}c_i[j]a_i[\mu]\delta[\mathbf{z}-\mathbf{r}_i^j]\right)H_{\mathbf{z},\mu}[\mathbf{r},\lambda],\ \forall i,\quad (3)$$

where $\sum_{j=1}^{P_i}c_i[j]a_i[\mu]\delta[\mathbf{z}-\mathbf{r}_i^j]$ is the contribution of the ith galaxy spectrum $a_i[\mu]$, up to an unknown proportional factor $c_i[j]$ at jth pixel in $\mathcal{I}_i$, to the voxel $[\mathbf{z},\mu]$, and $H_{\mathbf{z},\mu}[\mathbf{r},\lambda]$ is the contribution of the PSF of voxel $[\mathbf{z},\mu]$ to voxel $[\mathbf{r},\lambda]$. Since the PSF is translation variant, it can not be written in the form $H(\mathbf{r}-\mathbf{z},\lambda-\mu)$.

The problem of spatial-spectral unmixing is to estimate the galaxy spectra $a_1[\lambda],\ldots,a_N[\lambda],\ \forall\lambda$ from the given MUSE data cube $y[\mathbf{r},\lambda],\ \forall\mathbf{r},\lambda$, under the following general assumptions:

- $(\mathbf{C1})$ The sum of factors associated with all the pixels in each galaxy is equal to unity, i.e., $\sum_{j=1}^{P_i}c_i[j]=1,\ i=1,\ldots,N.$
- $(\mathbf{C2})$ The PSFs are spatially invariant for each galaxy $\mathcal{I}_i$, i.e.,

$$H_{\mathbf{z},\mu}[\mathbf{r},\lambda]=H_\mu^i[\mathbf{r}-\mathbf{z},\lambda],\ \mathbf{z}\in\mathcal{I}_i,\ i=1,\ldots,N.$$

- $(\mathbf{C3})$ The PSF is separable in terms of FSF $F_{\mathbf{z},\mu}[\mathbf{r}]\in\mathbb{R}_+$ and LSF $L_{\mathbf{z},\mu}[\lambda]\in\mathbb{R}_+$, i.e., $H_{\mathbf{z},\mu}[\mathbf{r},\lambda]=F_{\mathbf{z},\mu}[\mathbf{r}]L_{\mathbf{z},\mu}[\lambda]\in\mathbb{R}_+$.
- $(\mathbf{C4})$ The FSF changes slowly spectrally, i.e.,

$$F_{\mathbf{z},\mu}[\mathbf{r}]=F_{\mathbf{z},\lambda_m}[\mathbf{r}],\ \mu\in\Lambda_m,$$

  where $\Lambda_m=\{\lambda_m+i\Delta\lambda\}_{i=-K_{\rm F}}^{K_{\rm F}}$ for some $K_{\rm F}$ and $m=1,\ldots,Q$, in which $\Delta\lambda$ is the spectral resolution and $Q\triangleq\lceil M/(2K_{\rm F}+1)\rceil$ is the total number of spectral frames, where M is the total number of spectral bands. The sum of the FSF coefficients is equal to unity, i.e., $\sum_{\mathbf{r}}F_{\mathbf{z},\mu}[\mathbf{r}]=1,\ \forall\mathbf{z},\mu$.
- $(\mathbf{C5})$ The LSF only spreads over few spectral samples, i.e.,

$$\begin{cases}L_{\mathbf{z},\mu}[\lambda]>0, & \text{if } \lambda\in\{\mu+k\Delta\lambda\}_{k=-K_{\rm L}}^{K_{\rm L}}\\ L_{\mathbf{z},\mu}[\lambda]=0, & \text{otherwise}\end{cases}$$

  for some small K_L, and the sum of the LSF coefficients is equal to unity, i.e., $\sum_\lambda L_{\mathbf{z},\mu}[\lambda]=1,\ \forall\mathbf{z},\mu$.

Assumptions $(\mathbf{C1})$, $(\mathbf{C4})$ and $(\mathbf{C5})$ are realistic for MUSE data [3]. Assumption $(\mathbf{C2})$ is due to the fact that all the pixel locations in $\mathcal{I}_i$ are basically close to each other. Assumption $(\mathbf{C3})$ is widely used in the MUSE studies [2,3]. From $(\mathbf{C2})-(\mathbf{C4})$, the FSFs and LSFs located at the voxels of the ith galaxy can be expressed as:

$$F_{\mathbf{z},\mu}[\mathbf{r}]=F_{\lambda_m}^i[\mathbf{r}-\mathbf{z}],\ \mathbf{z}\in\mathcal{I}_i,\ \mu\in\Lambda_m,\quad (4a)$$
$$L_{\mathbf{z},\mu}[\lambda]=L_\mu^i[\lambda],\ \mathbf{z}\in\mathcal{I}_i,\quad (4b)$$

which will be utilized to derive the linear mixing models of the MUSE data for different, disjoint spectral frames.

3. LINEAR MIXING MODEL FORMULATION

From (3) and under $(\mathbf{C2})$, we can have

$$\begin{aligned}x_i[\mathbf{r},\lambda]&=\sum_\mu a_i[\mu]\sum_{j=1}^{P_i}c_i[j]H_\mu^i[\mathbf{r}-\mathbf{r}_i^j,\lambda]\\&=\sum_{m=1}^{Q}\left(\sum_{j=1}^{P_i}c_i[j]F_{\lambda_m}^i[\mathbf{r}-\mathbf{r}_i^j]\right)\sum_{\mu\in\Lambda_m}a_i[\mu]L_\mu^i[\lambda],\end{aligned}\quad (5)$$

where the second equality holds due to (4). Substituting (5) into (2) yields

$$x[\mathbf{r},\lambda]=\sum_{m=1}^{Q}\sum_{i=1}^{N}\left(\sum_{j=1}^{P_i}c_i[j]F_{\lambda_m}^i[\mathbf{r}-\mathbf{r}_i^j]\right)\sum_{\mu\in\Lambda_m}a_i[\mu]L_\mu^i[\lambda].\quad (6)$$

Considering the mth, shorten, spectral frame $\Psi_m\triangleq\{\lambda_m+i\Delta\lambda\}_{i=-K_{\rm F}+K_{\rm L}}^{K_{\rm F}-K_{\rm L}}$, by $(\mathbf{C5})$, (6) can be written as

$$x[\mathbf{r},\lambda]=\sum_{i=1}^{N}\left(\sum_{j=1}^{P_i}c_i[j]F_{\lambda_m}^i[\mathbf{r}-\mathbf{r}_i^j]\right)\sum_{\mu\in\Lambda_m}a_i[\mu]L_\mu^i[\lambda],\ \lambda\in\Psi_m,\quad (7)$$

which only involves the information of the mth spectral frame for $m=1,\ldots,Q$.

In order to have a vector-matrix representation of (7), let us perform the following change of variables:

- The noise-free data associated with the mth frame at pixel n:

$$\mathbf{x}_m[n]\triangleq[\,x[\mathbf{r},\lambda]\,]_{\lambda\in\Psi_m}\in\mathbb{R}_+^{2K_{\rm F}-2K_{\rm L}+1},$$

  where $[\,x[\mathbf{r},\lambda]\,]_{\lambda\in\Psi_m}$ denotes a column vector comprising $x[\mathbf{r},\lambda]$ for all λ in the set Ψ_m, and $n=(r_1-1)Z+r_2$, in which r_i is the ith entry of $\mathbf{r}$ and Z is the width of MUSE image.
- The ith galaxy spectrum in the mth spectral frame:

$$\mathbf{a}_i^m\triangleq[\,a_i[\mu]\,]_{\mu\in\Lambda_m}\in\mathbb{R}_+^{2K_{\rm F}+1}.$$

- The contribution of ith galaxy (through the FSF) to the mth spectral frame at pixel n, or called the abundance fraction:

$$s_i^m[n]\triangleq\sum_{j=1}^{P_i}c_i[j]F_{\lambda_m}^i[\mathbf{r}-\mathbf{r}_i^j]\in\mathbb{R}_+.$$

- The matrix form of the LSF of ith galaxy associated with the mth spectral frame $\mathbf{H}_i^m\in\mathbb{R}_+^{(2K_{\rm F}-2K_{\rm L}+1)\times(2K_{\rm F}+1)}$, whose (p,q)th element $H_i^m(p,q)$ is

$$L_{\lambda_m-(K_{\rm F}-K_{\rm L})\Delta\lambda+(q-1)\Delta\lambda}^i[\lambda_m-(K_{\rm F}-K_{\rm L})\Delta\lambda+(p-1)\Delta\lambda],$$

  which is nonzero over the following set (by $(\mathbf{C5})$)

$$\{(p,q)\mid 1\leq p\leq 2K_{\rm F}-2K_{\rm L}+1,\ p\leq q\leq p+2K_{\rm L}\}.$$

With $\mathbf{x}_m[n]$, $\mathbf{a}_i^m$, $s_i^m[n]$, $\mathbf{H}_i^m$ defined above, and by (1) and (7), the noisy MUSE pixel vector associated with the mth spectral frame $\mathbf{y}_m[n]\triangleq[\,y[\mathbf{r},\lambda]\,]_{\lambda\in\Psi_m}$ for $m\in\{1,2,...,Q\}$ can be expressed as

$$\mathbf{y}_m[n]=\sum_{i=1}^{N}s_i^m[n]\mathbf{H}_i^m\mathbf{a}_i^m+\mathbf{w}_m[n],\ n=1,...,L,\quad (8)$$

where $\mathbf{w}_m[n]\triangleq[\,w[\mathbf{r},\lambda]\,]_{\lambda\in\Psi_m}\in\mathbb{R}^{2K_{\rm F}-2K_{mL}+1}$ is a zero-mean Gaussian noise vector with covariance matrix $\mathbf{\Sigma}_m[n]=\sigma[n]\mathbf{C}_m$, in which $\mathbf{C}_m$ is a known diagonal matrix, $\sigma[n]$ is a known constant [1], and L is the total number of observed pixel vectors.

Now, the problem to be solved for each spectral frame becomes a blind source separation problem for the estimation of galaxy spectra $\mathbf{a}_1^m,\ldots,\mathbf{a}_N^m$, with the given noisy pixel vectors $\mathbf{y}_m[1],\ldots,\mathbf{y}_m[L]$ given by (8) , LSF matrices $\{\mathbf{H}_i^m\}_{i=1}^N$, and the number of galaxies N. The full spectra $\mathbf{a}_1,\ldots,\mathbf{a}_N$ can finally be obtained from the spectra estimates of all the Q frames. Based on $(\mathbf{C1})-(\mathbf{C4})$, we have the following two facts:

- $(\mathbf{F1})$ Abundance fractions are non-negative, i.e., $s_i^m[n]\geq 0,\ \forall\,i,n,m.$
- $(\mathbf{F2})$ Sum of all the abundance fractions of ith galaxy is equal to unity for each spectral band, i.e., $\sum_{n=1}^{L}s_i^m[n]=1,\ \forall\,i,m.$

Besides, we make two assumptions to the linear mixing model (8):

($\mathbf{A1}$) $\min\{L, 2K_{\mathrm{F}} - 2K_{\mathrm{L}} + 1\} \geq N$ and the LSF corrupted galaxy spectra $\{\mathbf{H}_1^m \mathbf{a}_1^m, \ldots, \mathbf{H}_N^m \mathbf{a}_N^m\}$ are linearly independent.

($\mathbf{A2}$) (Pure pixel assumption) The pure pixel region associated with the ith galaxy is identical for all the spectral bands, and there exists a set of indices $\{\ell_1^m, ..., \ell_N^m\}$ such that $\mathbf{x}_m[\ell_i^m] = s_i^m[\ell_i^m]\mathbf{H}_i^m \mathbf{a}_i^m, \ \forall\, i$.

Assumption ($\mathbf{A1}$) describes the fact that the number of galaxies of interest are less than the number of pixels and the number of spectral bands in each spectral frame. Assumption ($\mathbf{A2}$) is realistic because the object field is not very dense, as illustrated in Figure 1.

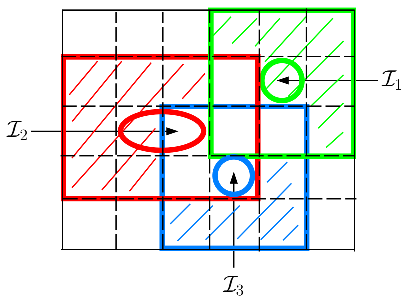

Fig. 1. Illustration of ($\mathbf{A2}$). Three galaxies located at $\mathcal{I}_1, \mathcal{I}_2, \mathcal{I}_3$ and their associated abundance supports (through the FSF) are marked by respective color regions. The so-called pure pixel regions are denoted by the oblique line regions.

4. THE PROPOSED SSU ALGORITHM FOR MUSE DATA

In this section, we elaborate the procedure of the proposed SSU algorithm for analyzing MUSE data.

4.1. Noise Pre-Whitening and Noise Reduction

As the covariance matrix of noise at each pixel (i.e., $\mathbf{\Sigma}_m[n], \ \forall n$) are known in advance [2], we perform noise-prewhitening as follows

$$\begin{aligned}\boldsymbol{y}_m[n] &\triangleq \mathbf{\Sigma}_m[n]^{-\frac{1}{2}} \mathbf{y}_m[n] \\ &= \sum_{i=1}^{N} s_i^m[n] \mathbf{\Sigma}_m[n]^{-\frac{1}{2}} \mathbf{H}_i^m \mathbf{a}_i^m + \mathbf{\Sigma}_m[n]^{-\frac{1}{2}} \mathbf{w}_m[n], \ \forall n,\end{aligned} \tag{9}$$

where the noise term $\mathbf{\Sigma}_m[n]^{-1/2}\mathbf{w}_m[n]$ becomes white Gaussian [1, 2]. Then, by letting $\mathbf{V}_m \in \mathbb{R}^{(2K_{\mathrm{F}} - 2K_{\mathrm{L}} + 1) \times N}$ be the matrix containing the first N left singular vectors of $[\ \boldsymbol{y}_m[1], \ldots, \boldsymbol{y}_m[L]\ ]$ and since $\mathbf{\Sigma}_m[n] = \sigma[n]\mathbf{C}_m$, we can obtain the noise reduced data

$$\tilde{\mathbf{y}}_m[n] \triangleq \mathbf{V}_m \mathbf{V}_m^T \boldsymbol{y}_m[n] = \sum_{i=1}^{N} e_i^m[n] \mathbf{b}_i^m + \mathbf{v}_m[n], \ \forall n, \tag{10}$$

where $e_i^m[n] = \sigma[n]^{-1/2} s_i^m[n]$, $\mathbf{b}_i^m = \mathbf{V}_m \mathbf{V}_m^T \mathbf{C}_m^{-1/2} \mathbf{H}_i^m \mathbf{a}_i^m$, and $\mathbf{v}_m[n] = \mathbf{V}_m \mathbf{V}_m^T \mathbf{\Sigma}_m[n]^{-1/2} \mathbf{w}_m[n]$.

4.2. Pure Pixel Indices Search

The noise reduced data (10) will then be used to estimate pure pixel indices. We first normalize the noise reduced data (10) as

$$\bar{\mathbf{y}}_m[n] \triangleq \tilde{\mathbf{y}}_m[n] / \mathbf{1}^T \tilde{\mathbf{y}}_m[n] = \sum_{i=1}^{N} \bar{e}_i^m[n] \bar{\mathbf{b}}_i^m + \bar{\mathbf{v}}_m[n], \ \forall n, \tag{11}$$

where $\bar{e}_i^m[n] = e_i^m[n] \mathbf{1}^T \mathbf{b}_i^m / \mathbf{1}^T \tilde{\mathbf{y}}_m[n]$ denotes the normalized abundance fraction, $\bar{\mathbf{b}}_i^m = \mathbf{b}_i^m / \mathbf{1}^T \mathbf{b}_i^m$ denotes the ith normalized LSF corrupted galaxy spectrum, and $\bar{\mathbf{v}}_m[n] = \mathbf{v}_m[n] / \mathbf{1}^T \tilde{\mathbf{y}}_m[n]$ denotes the normalized noise. Since $\mathbf{v}_m[n]$ is zero-mean, one can easily show that

$$\sum_{i=1}^{N} \bar{e}_i^m[n] \cong 1, \ \forall n. \tag{12}$$

It has been shown in [4, Lemma 4] that under ($\mathbf{F1}$), ($\mathbf{A1}$), ($\mathbf{A2}$) and the absence of noise (i.e., $\sum_{i=1}^{N} \bar{e}_i^m[n] = 1, \ \forall n$), the pure pixel indices can be identified by

$$\ell_j^m \in \begin{cases} \arg\max_{n=1,\ldots,L} \|\bar{\mathbf{y}}_m[n]\|_2, & j = 1 \\ \arg\max_{n=1,\ldots,L} \|\mathbf{P}^{\perp}_{\mathbf{\Gamma}_{1:(j-1)}} \bar{\mathbf{y}}_m[n]\|_2, & j > 1 \end{cases} \tag{13}$$

where $\mathbf{\Gamma}_{1:k} = [\bar{\mathbf{y}}_m[\ell_1^m], \ldots, \bar{\mathbf{y}}_m[\ell_k^m]]$. We denote the extracted pure pixel indices in the noisy scenario by $\{\hat{\ell}_1^m, \ldots, \hat{\ell}_N^m\}$.

4.3. Galaxy Spectra Unmixing

Given the pure pixel indices $\{\hat{\ell}_1^m, \ldots, \hat{\ell}_N^m\}$ estimated above, by (9) and ($\mathbf{A2}$), we have

$$\boldsymbol{y}_m[\hat{\ell}_i^m] = s_i^m[\hat{\ell}_i^m] \mathbf{\Sigma}_m[\hat{\ell}_i^m]^{-\frac{1}{2}} \mathbf{H}_i^m \mathbf{a}_i^m + \mathbf{\Sigma}_m[\hat{\ell}_i^m]^{-\frac{1}{2}} \mathbf{w}_m[\hat{\ell}_i^m], \forall i. \tag{14}$$

Also, we suppose that each galaxy spectrum $\mathbf{a}_i^m$ can be sparsely represented by a dictionary [1]:

$$\mathbf{a}_i^m = \mathbf{D}_m \mathbf{u}_i^m, \ i = 1, \ldots, N, \tag{15}$$

where $\mathbf{u}_i^m$ is a sparse vector, and $\mathbf{D}_m \in \mathbb{R}^{(2K_{\mathrm{F}}+1) \times 22604}$ is the dictionary matrix composed of line spectra, step-like spectra and continuous spectra. Substituting (15) into (14) yields

$$\boldsymbol{y}_m[\hat{\ell}_i^m] = \mathbf{\Sigma}_m[\hat{\ell}_i^m]^{-\frac{1}{2}} \mathbf{H}_i^m \mathbf{D}_m \boldsymbol{\mu}_i^m + \mathbf{\Sigma}_m[\hat{\ell}_i^m]^{-\frac{1}{2}} \mathbf{w}_m[\hat{\ell}_i^m], \forall i, \tag{16}$$

where $\mathbf{\Sigma}_m[\hat{\ell}_i^m]$, $\mathbf{H}_i^m$, $\mathbf{D}_m$ are known *a priori*, and $\boldsymbol{\mu}_i^m \triangleq s_i^m[\hat{\ell}_i^m]\mathbf{u}_i^m$ should be sparse since $\mathbf{u}_i^m$ is sparse. Hence, we can estimate $\hat{\boldsymbol{\mu}}_i^m, \ \forall i$ by solving the following ℓ_1-norm minimization problem subject to the maximum fitting error in (16) upper-bounded by $\varepsilon \triangleq \sqrt{2K_{\mathrm{F}} - 2K_{\mathrm{L}} + 1}$ (standard deviation of $\mathbf{\Sigma}_m[\hat{\ell}_i^m]^{-1/2}\mathbf{w}_m[\hat{\ell}_i^m]$):

$$\hat{\boldsymbol{\mu}}_i^m = \arg \min_{\|\boldsymbol{y}_m[\hat{\ell}_i^m] - \mathbf{\Sigma}_m[\hat{\ell}_i^m]^{-\frac{1}{2}} \mathbf{H}_i^m \mathbf{D}_m \boldsymbol{\mu}_i^m\|_2 \leq \varepsilon} \|\boldsymbol{\mu}_i^m\|_1, \forall i. \tag{17}$$

The scaled galaxy spectra can be estimated by

$$s_i^m[\hat{\ell}_i^m]\mathbf{a}_i^m = s_i^m[\hat{\ell}_i^m]\mathbf{D}_m \mathbf{u}_i^m = \mathbf{D}_m \hat{\boldsymbol{\mu}}_i^m, \ \forall i. \tag{18}$$

By (9) and (18), we can estimate the scaled abundance fractions

$$\kappa_i^m[n] \triangleq s_i^m[n] / s_i^m[\hat{\ell}_i^m], \ \forall i, n, \tag{19}$$

by solving the non-negative least-squares problem

$$\min_{\substack{\kappa_i^m[n] \geq 0, \\ i=1,\ldots,N}} \|\boldsymbol{y}_m[n] - \sum_{i=1}^{N} \kappa_i^m[n] \mathbf{\Sigma}_m[n]^{-\frac{1}{2}} \mathbf{H}_i^m \mathbf{D}_m \hat{\boldsymbol{\mu}}_i^m\|_2. \tag{20}$$

Note that (17) and (20) are convex and can be solved by any standard convex optimization solvers, such as CVX [5]. The issue that remains is how to fix the scaling ambiguity $s_i^m[\hat{\ell}_i^m]$ in (18) and (19). Under ($\mathbf{F2}$) and (19), we can further estimate the scale factors by

$$\begin{aligned}&\sum_{n=1}^{L} \kappa_i^m[n] = \sum_{n=1}^{L} s_i^m[n] / s_i^m[\hat{\ell}_i^m] = 1 / s_i^m[\hat{\ell}_i^m] \\ &\Longrightarrow \hat{s}_i^m[\hat{\ell}_i^m] = 1 / \sum_{n=1}^{L} \hat{\kappa}_i^m[n], \ i = 1, \ldots, N.\end{aligned} \tag{21}$$

Table 1. The pseudo-codes of the proposed SSUm and SSU algorithms.

SSUm Algorithm		**SSU Algorithm**	
Given	$\{\mathbf{y}_m[n]\}_{n=1}^{L}$, N, $\{\mathbf{\Sigma}_m[n]\}_{n=1}^{L}$, $\{\mathbf{H}_i^m\}_{i=1}^{N}$ and $\mathbf{D}_m$.	**Given**	$\{\mathbf{y}_m[1],\ldots,\mathbf{y}_m[L]\}_{m=1}^{Q}$, N, and initial $m=1$.
Step 1.	obtain $\boldsymbol{y}_m[n],\ \forall n$ by (9), $\tilde{\mathbf{y}}_m[n],\ \forall n$ by (10) and $\bar{\mathbf{y}}_m[n],\ \forall n$ by (11). Then, obtain $\{\hat{\ell}_1^m,\ldots,\hat{\ell}_N^m\}$ by (13).	**Step 1.**	obtain $\{(\hat{\mathbf{a}}_1^m,\hat{\mathbf{s}}_1^m),\ldots,(\hat{\mathbf{a}}_N^m,\hat{\mathbf{s}}_N^m)\}$ by the proposed SSUm algorithm.
Step 2.	obtain $\hat{\boldsymbol{\mu}}_i^m,\ \forall i$ by (17) and then obtain $\{\hat{\kappa}_i^m[n]\}_{i=1}^{N},\ \forall n$ by (20).	**Step 2.**	obtain $\hat{\mathbf{P}}_m$ by (25).
Step 3.	obtain $\hat{\mathbf{a}}_i^m,\ \forall i$ by (22).	**Step 3.**	obtain $\hat{\mathbf{B}}_m$ by (26).
Step 4.	obtain $\{\hat{s}_i^m[n]\}_{i=1}^{N},\ \forall n$ by (23) and then obtain $\hat{\mathbf{s}}_i^m,\ \forall i$ by (24).	**Step 4.**	if $m<Q$, then set $m:=m+1$, and go to **Step 1**, else output the the ith column of $\hat{\mathbf{A}}=[\hat{\mathbf{B}}_1^T,\hat{\mathbf{B}}_2^T,\ldots,\hat{\mathbf{B}}_Q^T]^T$ as the estimated spectrum of the ith galaxy for all i.
Step 5.	output $\{\hat{\mathbf{a}}_1^m,\ldots,\hat{\mathbf{a}}_N^m\}$ as the estimated galaxy spectra and $\{\hat{\mathbf{s}}_1^m,\ldots,\hat{\mathbf{s}}_N^m\}$ as the estimated abundance maps.		

Substituting (21) into (18) and (19), the estimated galaxy spectra and abundance fractions in the mth spectral frame can be recovered by

$$\hat{\mathbf{a}}_i^m = \mathbf{D}_m \hat{\boldsymbol{\mu}}_i^m \sum_{n=1}^{L} \hat{\kappa}_i^m[n],\ \forall i. \tag{22}$$

$$\hat{s}_i^m[n] = \hat{\kappa}_i^m[n] / \sum_{n=1}^{L} \hat{\kappa}_i^m[n],\ \forall i, n. \tag{23}$$

The estimates by (23) are collected as column vectors

$$\hat{\mathbf{s}}_i^m = [\hat{s}_i^m[1], \ldots, \hat{s}_i^m[L]]^T,\ \forall i. \tag{24}$$

The above procedure presented in subsections 4.1, 4.2, 4.3 for estimating the galaxy spectra $\{\hat{\mathbf{a}}_1^m,\ldots,\hat{\mathbf{a}}_N^m\}$ and abundance maps $\{\hat{\mathbf{s}}_1^m,\ldots,\hat{\mathbf{s}}_N^m\}$ associated with the mth spectral frame is termed as SSUm and summarized in Table 1 (left part).

4.4. Whole Galaxy Spectra Combining

So far, there is still an ambiguity yet to be solved— order mismatch of the estimated spectra and abundance maps from frame to frame. It can be resolved by permuting $\{(\hat{\mathbf{a}}_i^m,\hat{\mathbf{s}}_i^m), i=1,\ldots,N\}$ so as to have the best match with that of the first frame. The permutation matrix can be obtained by solving the following problem [6]:

$$\hat{\mathbf{P}}_m = \arg\min_{\mathbf{P}_m\in\Phi} \left\| \hat{\mathbf{S}}_1 - \hat{\mathbf{S}}_m \mathbf{P}_m \right\|_F, \tag{25}$$

where $\hat{\mathbf{S}}_m = [\hat{\mathbf{s}}_1^m,\ldots,\hat{\mathbf{s}}_N^m]$ and Φ is the set of $N\times N$ permutation matrices. Then, we can obtain the column-permutation fixed $\hat{\mathbf{A}}_m$ as

$$\hat{\mathbf{B}}_m = \hat{\mathbf{A}}_m \hat{\mathbf{P}}_m \in \mathbb{R}^{(2K_{\mathrm{F}}+1)\times N}, \tag{26}$$

where $\hat{\mathbf{A}}_m = [\hat{\mathbf{a}}_1^m,\ldots,\hat{\mathbf{a}}_N^m]$.

Repeating the above procedure for all the spectral frames $m = 1, ..., Q$, and concatenating all the obtained Q galaxy spectra estimated by (26) provides

$$\hat{\mathbf{A}} = [\hat{\mathbf{B}}_1^T, \hat{\mathbf{B}}_2^T, \ldots, \hat{\mathbf{B}}_Q^T]^T \in \mathbb{R}^{M\times N}, \tag{27}$$

where the ith column of $\hat{\mathbf{A}}$ is the final spectrum estimate of the ith galaxy. We summarize the SSU algorithm in Table 1 (right part).

5. SIMULATION AND CONCLUSION

In this section, we use synthetic MUSE data to test the performance of the proposed SSU algorithm. The results for the estimated galaxy spectra and abundance maps are shown in Figures 2-4 in the supplementary document at `http://www.ee.nthu.edu.tw/cychi/SSD_SuppDoc.pdf`, due to the space limit. We simulate a 5×5 spatial dimension scene, composed of three galaxies $N=3$: One corresponds to extended source containing two pixels with factors $c_1[j]=0.5,\ j=1,2$, while the other two are close sources each of which containing 1 pixel with factors $c_i[1]=1,\ i=2,3$, as shown in Figure 2(a). The associated three galaxy spectra were generated by linear, random superposition of the synthesized dictionary [1]. The synthetic noise-free data were generated following (6) for $Q=2$, where FSFs all are 3×3 circular Gaussian with different variances, and LSFs are of $2K_{\mathrm{L}}+1=11$-point Gaussian with different variances, shown in Figure 2(b). Then we added zero mean Gaussian noise vectors with the same covariance as in [2, Fig. 1] for each pixel to obtain the observed noisy data shown in Figure 2(c). Two performance indices were used in the simulations. The root-mean-square (rms) spectral angle distance between simulated galaxy spectra and their estimates, denoted as ϕ (in degrees), was used as the error performance measure [4]. The computation time T (in secs) of the algorithm (implemented in Mathworks Matlab R2008a) running in a desktop computer equipped with Core i7-930 CPU 2.80 GHz, 12GB memory was used as the computational complexity measure.

The proposed SSU algorithm was applied to the noise-free and noisy data. The rms spectral angles and computation time of the SSU algorithm for the noise-free data are $\phi = 0.09$ (degrees) and $T = 153.16$ (secs), respectively, and those for noisy data are $\phi = 14.07$ (degrees) and $T = 173.28$ (secs), respectively. The corresponding results for noise-free and noisy data are demonstrated in Figure 3 and Figure 4, respectively. One can see that the proposed SSU algorithm performs well for both cases. Especially, for the noiseless case, almost perfect unmixing is achieved in spite of some small error (i.e., $\phi\approx0$) because the ℓ_1-norm minimization is an approximation for sparse representation of the galaxy spectra [7].

In conclusion, we have presented an SSU algorithm to process MUSE data for estimation of galaxy spectra. The simulation results have shown the superior efficacy of the proposed SSU algorithm.

6. REFERENCES

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