SEABED ESTIMATION USING TRIPLE NMF METHOD.

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ABSTRACT

Spectral unmixing of hyperspectral remote sensing reflectance data is a challenging task, being the subject of many recent researches, and aims to retrieve both endmembers spectra and abundances. It turns out to be hardly feasible when the data are attenuated by additional mediums such as water column in the case of seabed estimation. In this case, a possible solution is to first correct the attenuation due to the water column and then proceed to the unmixing process. This paper presents a new approach, jointly estimating the attenuation, the endmembers spectra and the abundances with a triple non-negative matrix factorization (tri-NMF) method. The method has been tested on synthetic and real data and allow one to obtain accurate abundance maps of the seabed.

1. INTRODUCTION

Spectral unmixing (SU) is an important step for hyperspectral image analysis. It aims at estimating the spectral signatures of the pure materials (or *endmembers*) present in any hyperspectral image pixel and its corresponding fractions (or *abundances*) usually assuming that the mixture is linear. Since these two parameters are of physical nature, they are both constrained to be positive. Many works in the litterature focused on this resulting linear mixing model (LMM) and give interesting results. For a complete review on these works over the last decade, the interested reader is invited to consult [1].

In the context of coastal environments hyperspectral mapping, previously mentioned methods for SU are useless since the presence of water strongly attenuates the subsurface reflectance spectra. As underlined in [2], it is necessary to incorporate a bathymetric model in the unmixing process. The Maritorena's model [3] has shown very attracting properties when retrieving the subsurface reflectance is needed. This model have been employed in [4] for underwater target detection. The authors employ a maximum likelihood approach to recover the water column parameters allowing them to estimate the subsurface reflectance. However, this approach is very sensitive to noise and needs prior information on the water column. The approach proposed in [2] is also based on these two models and consists of estimating jointly the water column parameters and the abundance coefficients by a partial linear least squares method. Yet, it does not take into account the abundance constraints and assume the spectra are known.

In this contribution, we propose to solve the unmixing problem without directly estimating the subsurface reflectance, combining the Maritorena's bathymetric model and the LMM. The resulting problem can be solved using non-negative matrix factorization (NMF) [5]. Such techniques have been successfully applied to linear unmixing in [6] or in [7], where the abundances sum-to-one constraint has been dealt with by introducing a proper regularization term. As shown in the sequel of the paper, a so-called "triple NMF" (or tri-NMF) method [8] must be employed to jointly recover the spectra and abundance matrices but also the attenuation matrix stemming from the water column. It is worth noting that such method has been applied for clustering data in system management in [9] and never been applied to any related SU problem.

In section 2 the chosen bathymetric model for the water column attenuation and the linear mixing model are introduced before presenting the proposed triple NMF. Section 4.1 presents and discusses results for simulated data. Results on real image are given in Section 5. Finally, conclusions are reported in Section 6.

2. MODELISATION

This paper focuses on Maritorena's bathymetric model that approximates in a simple way the water column attenuation. Let $\boldsymbol{R}_{\text{t}}$ the observation matrix of size $L \times I$ with L the number of spectral bands and I the number of pixels.Since we are planning to use a matrix based method, the subsurface bathymetric model (the transition at the sea surface can be corrected separately) is written in matrix notations. In other terms

$$\boldsymbol{R}_{\text{t}} = \boldsymbol{K}\left(\boldsymbol{R}_{\text{f}} - \boldsymbol{r}_{\text{inf}}\mathbf{1}_{1I}\right) + \boldsymbol{r}_{\text{inf}}\mathbf{1}_{1I}, \tag{1}$$

with $\boldsymbol{K}$ the attenuation diagonal matrix of size $L \times L$ depending on the unknown depth H and water characteristics, $\boldsymbol{R}_{\text{f}}$ the reflectance matrix of the sea bottom, $\boldsymbol{r}_{\text{inf}}$ the L-dimension vector representing the subsurface reflectance over an optically deep water column, abusively renamed "infinite reflectance" in this paper, and $\mathbf{1}_{1I}$ the matrix of "ones" of size $1 \times I$.

As a reminder, the LMM is written as $\boldsymbol{R}_{\mathrm{f}} = \boldsymbol{S}\boldsymbol{A} + \boldsymbol{N}$, with $\boldsymbol{S}$ representing the endmember matrix of size $L \times J$ (J being the number of endmembers), $\boldsymbol{A}$ the abundances matrix and $\boldsymbol{N}$ the L-dimension vector distributed according to a normal distribution with zero mean and same variance for each band $\mathcal{N}(\boldsymbol{0}_L, \sigma_n^2 \boldsymbol{I}_L)$. The LMM is subject to physical constraints, thus forcing the matrices $\boldsymbol{S}$ and $\boldsymbol{A}$ to be positive. Moreover, the sum of the column elements of $\boldsymbol{A}$ must equal 1, i.e. $\boldsymbol{1}_{1J}\boldsymbol{A} = \boldsymbol{1}_{1J}$. The following relation can then be established $\boldsymbol{r}_{\inf}\boldsymbol{1}_{1I} = \boldsymbol{r}_{\inf}\boldsymbol{1}_{1J}\boldsymbol{A}$. Letting $\boldsymbol{\rho} = \boldsymbol{R}_{\mathrm{t}} - \boldsymbol{r}_{\inf}\boldsymbol{1}_{1I}$ and $\boldsymbol{\rho_0} = \boldsymbol{S} - \boldsymbol{r}_{\inf}\boldsymbol{1}_{1J}$, we replace $\boldsymbol{r}_{\inf}\boldsymbol{1}_{1I}$ in (1) thus obtaining the resulting model

$$\boldsymbol{\rho} = \boldsymbol{K}\boldsymbol{\rho_0}\boldsymbol{A} + \boldsymbol{K}\boldsymbol{N}. \tag{2}$$

3. TRIPLE NMF ALGORITHM

We first remind the principle of NMF consisting of approximating a nonnegative matrix $\boldsymbol{R}_{\mathrm{f}}$ by a two matrices product [5, 8] $\boldsymbol{R}_{\mathrm{f}} \simeq \hat{\boldsymbol{S}}\hat{\boldsymbol{A}}$. These matrices can be found by solving the resulting optimisation problem

$$\min_{\boldsymbol{S},\boldsymbol{A}} D(\boldsymbol{R}_{\mathrm{f}}|\boldsymbol{S}\boldsymbol{A}) \text{ s. t. } \boldsymbol{S} \geq 0, \boldsymbol{A} \geq 0$$

where $D(\cdot|\cdot)$ is a divergence measure. The positivity hard constraint is fundamental to restrict the admissible solutions set, thus reinforcing the possibility to obtain unique solutions. This work will consider the reconstruction quadratic error as a divergence measure by default, i.e. $D(\boldsymbol{X}|\boldsymbol{A}\boldsymbol{S}) = \|\boldsymbol{X} - \boldsymbol{A}\boldsymbol{S}\|_F^2$.

An extension of the classic NMF problem to a three matrices product is proposed. Indeed, the so-called method "tri-NMF" [8, 9] can be applied to the resulting model (2) that allows one to jointly estimate the spectra $\boldsymbol{S}$, the abundances $\boldsymbol{A}$ and the attenuation matrix $\boldsymbol{K}$. The goal of this tri-NMF problem is to estimate three matrices $\boldsymbol{K}$, $\boldsymbol{S}$ and $\boldsymbol{A}$. In order to satisfy the sum-to-one constraint for hyperspectral data, a regularization term is added to the objective function

$$STU(\boldsymbol{A}) = \delta(\boldsymbol{1}_{1J}\boldsymbol{A} - \boldsymbol{1}_{1J})(\boldsymbol{1}_{1J}\boldsymbol{A} - \boldsymbol{1}_{1J})^T,$$

where δ is the positive real parameters of the sum-to-one regularization term, fixed to 1 in the sequel. Similarly, a regularization term $\boldsymbol{D_K}$ for $\boldsymbol{K}$ is included in the objective function, enforcing smoothed solutions. This regularization term is equal to the square of the numerical derivative of diagonal terms of $\boldsymbol{K}$ with respect to spectral bands. Finally, a dispersion regularization term presented in [7] $\lambda_S \boldsymbol{D_S}$ forces the spectra to remain flat and strictly depends on $\boldsymbol{S}$, λ_S being the positive regularization parameter. From this and (2), the following optimisation problem is established[1]

$$\begin{aligned} &\min_{\boldsymbol{K},\boldsymbol{A},\boldsymbol{S}} \|\boldsymbol{\rho} - \boldsymbol{K}\boldsymbol{\rho_0}\boldsymbol{A}\|_F^2 + STU(\boldsymbol{A}) + \boldsymbol{D_K} + \boldsymbol{D_S} \\ &\text{s. t. } \boldsymbol{K} \geq 0, \boldsymbol{A} \geq 0, \boldsymbol{S} \geq 0. \end{aligned} \tag{3}$$

[1] Note that it is not necessary to impose non-negativity on the three matrices for tri-NMF problem [8].

Strictly speaking, this is not a NMF optimization problem since the positivity constraint is on the spectra $\boldsymbol{S}$ which is actually indirectly present in the divergence to minimize. Nevertheless, the constraints are sufficiently strong that this problem can still be considered as a generalization of NMF problem.

To solve this NMF problem, two optimization algorithms can be chosen : an alternated Projected Gradient (PG) algorithm [10] or a Hierarchical Alternating Least Squares (HALS) algorithm, which has been shown to be more performant [8, 11]. However, for technical reason, essentially due to the shape of matrix $\boldsymbol{K}$, the PG algorithm will be employed for our proposed tri-NMF method. This algorithm iteratively updates $\boldsymbol{K}$, $\boldsymbol{S}$ and $\boldsymbol{A}$ and forces the attenuation matrix $\boldsymbol{K}$ to be positive and diagonal. The spectra and abundances matrices are only forced to be positive. For each iteration, the update rules are

$$\begin{aligned} &\boldsymbol{K} \longleftarrow P\left[\boldsymbol{K} - \alpha_K \left(\boldsymbol{K}\boldsymbol{\rho_0}\boldsymbol{A} - \boldsymbol{\rho}\right)\boldsymbol{A}^T\boldsymbol{\rho_0}^T + \boldsymbol{\nabla_K}\boldsymbol{D_K}\right], \\ &\boldsymbol{S} \longleftarrow P\left[\boldsymbol{\rho_0} - \alpha_S \boldsymbol{K}^T\left(\boldsymbol{K}\boldsymbol{\rho_0}\boldsymbol{A} - \boldsymbol{\rho}\right)\boldsymbol{A}^T + \boldsymbol{\nabla_S}\boldsymbol{D_S}\right] + \boldsymbol{r}_{\inf}\boldsymbol{1}_{1J}, \\ &\boldsymbol{A} \longleftarrow P\left[\boldsymbol{A} - \alpha_A \tilde{\boldsymbol{K}}^T\tilde{\boldsymbol{\rho_0}}^T\left(\tilde{\boldsymbol{K}}\tilde{\boldsymbol{\rho_0}}\boldsymbol{A}^T - \tilde{\boldsymbol{\rho}}\right)\right], \end{aligned} \tag{4}$$

where α_K, α_S and α_A are the step sizes that guarantee convegence of the PG algorithm. They are estimated at each iteration using a modified Armijo rule described in [12]. The projection P ensures strong constraints. The regularization term $STU(\boldsymbol{A})$ can be included in $\boldsymbol{K}$, $\boldsymbol{\rho_0}$ and $\boldsymbol{\rho}$ with $\tilde{\boldsymbol{K}}$ is the matrix $\boldsymbol{K}$ augmented with a 1 as a new diagonal term and $\tilde{\boldsymbol{\rho_0}} = \left[\boldsymbol{\rho_0}^T\boldsymbol{1}_{J1}\right]^T$, $\tilde{\boldsymbol{\rho}} = \left[\boldsymbol{\rho}^T\boldsymbol{1}_{I1}\right]^T$.

4. SIMULATION ON SYNTHETIC DATA

The proposed approach is compared with the former one, the NMF-HALS approach developed in [11], where the bottom reflectance is preliminary found using the bathymetric model by using a maximum likelihood procedure derived in [4].

4.1. Simulation results

The proposed method has been tested and compared on a 50×50 pixels synthetic image that contains two distinct pairs of targets and two disctincts varieties of backgrounds. In this work, the number of spectral bands for this synthetic image is $L = 61$ from 400 nm to 700 nm, since subsurface data can be observed only in the visible. Therefore, the $J = 4$ endmembers spectra that are present in the image have been cut off to these bands. They are given Fig. 1 (left) and correspond to Plagioclase minerals, a steady mixture of sand and Phlogopite, grey tarpaulin and black tarpaulin spectra. The abundances are generated using a normal distribution truncated to the simplex with different means, whether the pixel belongs to the bottom or to the targets. The original abundance maps are

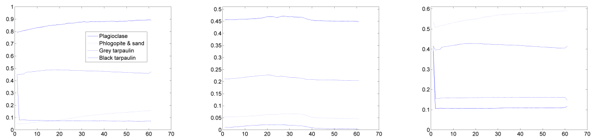

Fig. 1. Spectra used for the mixture (left), estimated spectra using the proposed method (center) and the MV+HALS method (right).

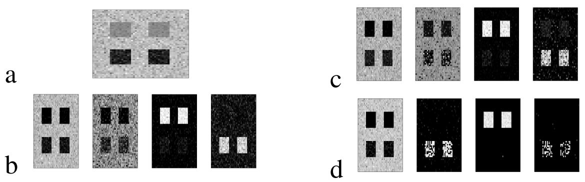

Fig. 2. a) observed image averaged in L bands, b) abundance maps of the corresponding generated seabed, c) abundance maps estimated using the proposed method, d) abundance maps estimated using HALS method (from left to right: plagioclase, phlogopite and sand, grey tarpaulin, black tarpaulin)

given in Fig. 2b. After building the subsurface image, the water column is added according to the bathymetric model with a height of $H = 10$ meters and the following concentrations of phytoplankton $C_{\phi} = 0.7$, suspended matter $C_{SM} = 2.8$ and colored dissolved organic matter $C_{CDOM} = 0.08$. The averaged observed image is given Fig.2a). The attenuation matrix $\boldsymbol{K}$ has been built according to Maritorena's model. Finally, the $\boldsymbol{r}_{\text{inf}}$ vector is supposed to be known.

At first, the proposed algorithm has been tested without noise ($\text{SNR} = Inf$), with $H = 10$ and compared with ML + NMF-HALS [11] method, where spectra are initialized using VCA algorithm [13] while the abundances are initialized using the resulting Moore-Penrose pseudoinverse. In the proposed method, the diagonal matrix $\boldsymbol{K}$ is initialized as the mean of all the observation $\boldsymbol{R}_t$. Then the product $\boldsymbol{K}\boldsymbol{\rho_0}$ is computed using VCA, allowing thus the spectra $\boldsymbol{S}$ and the abundances $\boldsymbol{A}$ to be initialized using pseudoinverse. The spectra regularization parameter λ_S has been empirically fixed to 1.

Figure 1 shows the spectra respectively estimated by the proposed method (center) and the MV+HALS method (right). While the proposed method gives flat spectra, the shape of the ones found by MV+HALS are much more closer to the original ones than those estimated by "Triple NMF". Nevertheless, the two methods presents the same scaling issues. The abundance maps obtained by the two algorithms are represented in Fig. 2c and d. The maps estimated by the proposed algorithm are closer to the original maps than the ones found by the MV+HALS method. Indeed, the bottom and the targets appears distinctly contrary to the results obtained with ML + HALS.

4.2. Influence of the noise

The following simulations have been achieved on the same data for different values of the SNR varying from 40dB to an infinite value, with $H = 10$. The proposed method is still compared with the NMF-HALS method, preceded by the maximum likelihood for the attenuation matrix estimation. The mean squared errors have been computed for the spectra and the abundances (respectively known as SME and AME) as comparison criterion.

Table 1. Performance comparison of the method "Triple NMF" with the method "ML+HALS" as a function of SNR and $H = 10$.

	SNR = 40dB	SNR = 60dB	SNR = 80dB	SNR = ∞
$\text{SME}_{\text{ML+HALS}}$	0.25	0.24	0.4	$\mathbf{4.6 \times 10^{-2}}$
$\text{AME}_{\text{ML+HALS}}$	1.8×10^5	7.6×10^5	71.2	7.8×10^{-2}
$\text{SME}_{\text{Tri-NMF}}$	**0.13**	**0.19**	**0.17**	0.12
$\text{AME}_{\text{Tri-NMF}}$	$\mathbf{7.2 \times 10^{-2}}$	$\mathbf{5 \times 10^{-2}}$	$\mathbf{3.5 \times 10^{-2}}$	$\mathbf{2.9 \times 10^{-2}}$

The results, obtained after averaging 10 experiments, are given in Table 1. Contrary to the NMF-HALS method that depends on the maximum likelihood step, the noise has very little influence on the proposed method. In presence of noise, the Triple NMF method is more performing than ML+HALS. This tendency is reversing when there is no noise, except for abundance estimation results.

4.3. Influence of the water column height

We also tested the influence of the water column height H with three different values. The results, averaged after 10 experiments, are reported in Table 2.

Table 2. Performance comparison of the method "Triple NMF" with the method "NMF-HALS" combined with maximum likelihood as a function of depth H and $\text{SNR} = Inf$.

	$H = 1$	$H = 10$	$H = 20$
$\text{SME}_{\text{ML+HALS}}$	0.18	$\mathbf{6.4 \times 10^{-2}}$	0.25
$\text{AME}_{\text{ML+HALS}}$	1.6×10^{11}	8.7×10^{-2}	1.3×10^7
$\text{SME}_{\text{Tri-NMF}}$	$\mathbf{3.1 \times 10^{-2}}$	0.15	**0.16**
$\text{AME}_{\text{Tri-NMF}}$	$\mathbf{2.1 \times 10^{-2}}$	$\mathbf{2.7 \times 10^{-2}}$	$\mathbf{2.4 \times 10^{-2}}$

The ML estimation step shows obvious sign of instability for small and large heights ($H = 1, 20$) of the water column and consequently do not allow efficient unmixing with HALS-NMF for shallow and deep waters. It is known that for such cases the depth of the water column is too small or too large to estimate the water parameters. In comparison, the proposed method has not these instability issues since it outperforms MV+HALS for the abundance estimates. However, the endmember spectra are better estimated using MV+HALS with $H = 10$. A possible explanation of these results would

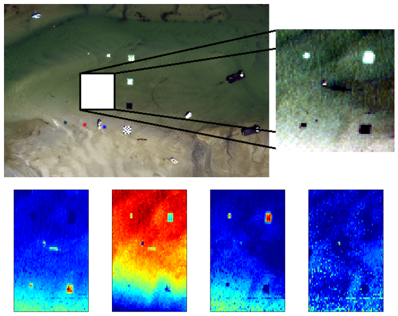

Fig. 3. Top: region of interest in true colors. Bottom: abundance maps obtained by the proposed algorithm.

be that forcing $\boldsymbol{K}$ to be diagonal introduces new constraints that limit the solution domain. By using the tri-NMF, we add $L^2 - L$ constraints enforcing $\boldsymbol{K}$ to be diagonal, while only L degrees of freedom come from the diagonal values. Moreover, this method is sensitive to the initialisation. Since $\boldsymbol{K}$, it is difficult to obtain good initialisations of the spectra $\boldsymbol{S}$.

5. SIMULATION RESULTS ON REAL IMAGE

The proposed algorithm is tested on real data that have been collected by ACTIMAR[2] as part of the HYPLITT project, supported by the Office for Advanced Research and Innovation (DGA/MRIS), France. These data have been acquired over Quiberon Peninsula, on the West coast of France. The hyperspectral sensor Hyspex VNIR-1600 has a spatial resolution of 0.4 m and a spectral resolution of about 4.5 nm. The region of interest of size 66×68 pixels, shown Fig. 3 (top), represents 4 targets (black and grey tarpaulin) that are placed on a sandy bottom at a depth of almost $H = 0.44$m, and the number of bands is $L = 81$. This small region of interest allows us to be very selective on the number of spectra. Indeed, HySime [14] has been employed to estimate this number and found $J = 4$. Using the same initialization than previously, the proposed method is then applied to the data. Estimated spectra have scaling issues and are not represented here for brevity. In spite of these problems, the black and grey tarpaulin targets can be easily recovered as can be seen on the resulting abundance maps in 3 (bottom). Note that the depth H has been fixed in the model while this depth is in fact varying : from the bottom of the scene to the top, the depth is growing. This can explain the lack of consistency on the second abundance map.

6. CONCLUSION

This paper presents a new algorithm for sea bottom analysis. By combining the linear mixing model and Maritorena's model, a NMF approach can be employed to recover the endmember, abundance and water attenuation matrix without the knowledge of water column parameters. Adding proper regularization terms and using a projected gradient algorithm, the proposed method is robust to noise and is able to estimate accurately the abundances, while the spectra still suffer from scaling issues. However, this algorithm would be suited for mapping of sea bottom especially for difficult cases such as high noise level or high depths. In future works, the bathymetric model will be more sophisticated, especially when modelling the attenuation matrix and the variation of the depth. Improving the initialization of $\boldsymbol{K}$ and its related regularization term is also under investigation.

[2]ACTIMAR is a firm specialised in a broad range of expertise areas within the marine environment sector, especially high resolution remote sensing applied to coastal zone management and deep ocean mapping.

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