HYPERSPECTRAL UNMIXING VIA L1/4 SPARSITY-CONSTRAINED MULTILAYER NMF

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ABSTRACT

Hyperspectral unmixing, by extracting the fractional abundances of endmembers from the hyperspectral image (HSI), has raised wide attention in recent years. In last decade, non-negative matrix factorization (NMF) have been intensively studied for solving spectral unmixing problem. In this paper, we extend the multilayer NMF method by incorporating the $L_{1/4}$ sparsity constraint, named $L_{1/4}$-MLNMF. The $L_{1/4}$ regularizer induces sparsity effectively. We propose an iterative estimation algorithm for $L_{1/4}$-MLNMF, which provides sparser and more accurate results than MLNMF. Experiments on a synthetic dataset and a real dataset show that the proposed method outperforms the similar competitors.

Index Terms—Hyperspectral unmixing, hyperspectral image, nonnegative matrix factorization.

1. INTRODUCTION

Hyperspectral unmixing (HSU) is an important technique for remote sensing hyperspectral data exploitation. The task of HSU is to synchronously estimate the pure spectral signatures, called endmembers, and their corresponding fractions, called abundance, for each pixel of the hyperspectral image. Thus, the spectral of pixels is resolved into a weighted combination of the endmembers. HSU is widely applied for other hyperspectral intervals. According to the fundamental mixing models, the solutions of hyperspectral image unmixing can be separated into two types: non-linear model (NLMM) and linear model (LMM). Since the computational complexity of NLMM methods is usually high [1], the LMM methods are more practical in real applications [2], [3].

According to the employed searching strategy, LMM methods can be further categorized into geometrical, statistical and sparse regression based approaches. Among these methods, nonnegative matrix factorization (NMF) is intensively studied and widely used to unmix hyperspectral images [4]. As a natural solution to the nonnegativity constraint on LMM, NMF decomposes the mixed data into two nonnegative matrices. However, some NMF-based unmixing methods usually leads to an NP-hard optimization problem that cannot be solved in practice [5].

In this paper, a novel method called $L_{1/4}$ sparsity-constrained multilayer NMF ($L_{1/4}$-MLNMF) is proposed to improved the performance of NMF methods for spectral unmixing. Compared to the above mentioned three kinds of methods, $L_{1/4}$-MLNMF is much more different. The main contributions of this method are claimed as follow.

1) An inspiring and efficient unmixing structure is applied to extend the NMF method. With multilayer structure of ML-NMF [6], this method considers spectral signatures matrix as the product of a set of sparse matrices. It not only uses a creative model in practice, but also provides an effective extension for NMF-based unmixing methods.

2) An effective objective function is proposed in a novel point of view. In each layer of this method, the sparsity constraints on endmembers matrix is added to the cost function. Since the $L_{1/4}$ regularizer induces sparsity effectively [7], the proposed method provides sparser and more accurate results than MLNMF.

The remainder of this paper is organized as follows. Section II elaborates the proposed algorithm. Section III and IV summarizes the experiments and results on synthetic dataset and real dataset. Finally, we discuss and conclude this paper in Section V.

2. METHODOLOGY

This section details the proposed $L_{1/4}$-MLNMF method. First, the cost function of NMF method is introduced. Then, the multilayer NMF method is given. In the end, the objective function and iterative estimation algorithm for proposed $L_{1/4}$-MLNMF method are described.

2.1. Nonnegative Matrix Factorization for Linear Model

The linear mixture model (LMM) assumes that each pixel spectrum in any given spectral band can be linearly combined by the endmember spectrums, which means for each pixel the LMM can be mathematically expressed as

$$x_j = \sum_{i=1}^{q} a_{ij}s_i + n_j,$$

(1)

where $x_j$ is the measured value of the reflectivity for a mixed pixel on the spectral band $j$; $a_{ij}$ is the reflectivity of the end-
member \(i\) on the band \(j\); \(s_{ij}\) is the abundance values of endmember \(i\) in this mixed pixel; \(n_j\) is the process nose, and \(q\) is the number of endmembers.

According to the form of nonnegative matrix factorization (NMF) mentioned above, (1) can be generally presented as

\[
X \approx AS,
\]

subject to \(S \geq 0, 1_P^T S = 1_n^T\). \(\text{(2)}\)

where \(X \equiv [y_1, ..., y_n] \in \mathbb{R}^{d \times n}\) is the hyperspectral image matrix with \(n\) pixels and \(d\) spectral bands; \(A \equiv [m_1, ..., m_p] \in \mathbb{R}^{d \times p}\) is the mixing matrix with \(p\) endmembers; \(m_i\) is the \(i\)th endmember signature; \(S \equiv [s_1, ..., s_m] \in \mathbb{R}^{p \times n}\) is the abundance matrix; \(s_i\) denotes the endmember fractions, for pixels \(i = 1, ..., n\); \(S \geq 0\) is the nonnegative abundance constraint for the component-wise method. \(1_P^T S = 1_n^T\) is the abundance sum to one constraint for the physics characteristic of abundance vector. The cost function used for solving NMF problem is formulated as

\[
O_{NMF} = \frac{1}{2} \| X - AS \|^2_F, \text{ (3)}
\]

This cost function in Eq. (3) should also be minimized under the constraints in Eq. (2). Furthermore, sparsity constraints on the abundance fractions matrix can be added to improve the performance of NMF algorithm, such as \(L_{1/2}\) regularizer [8]. The cost function under this regularizer is given as

\[
O_{L_{1/2}-NMF} = \frac{1}{2} \| X - AS \|^2_F + \alpha \| S \|_{1/2}, \text{ (4)}
\]

where \(\alpha\) is a regularization parameter to control the effect of sparsity constraint [7].

### 2.2. MLNMF Method

To improve the performance of NMF-based methods for spectral unmixing, this paper introduced MLNMF method. MLNMF has been firstly proposed in in signal processing to solve blind source separation problem [9]. Then, it has been initially applied and improved in for spectral unmixing problem [6], where multilayer structure is used to decompose the observation matrix shown in Fig.1. In the first layer, basic decomposition results in \(A_1\) and \(S_1\). Then in the second layer, the obtained \(S_1\) is decomposed into \(A_2\) and \(S_2\). Above process will be repeated until the maximum number of layers \(L\). The mathematical expression of the multilayer structure is formulated as

\[
X = A_1S_1, S_1 = A_2S_2, ..., S_{L-1} = A_L S_L, \text{ (5)}
\]

\[
A = A_1A_2...A_L = \prod_{l=1}^{L} A_l, S = S_L, \text{ (6)}
\]

where the \(S_L\) resulted in the last layer is the estimated abundance fraction matrix for spectral unmixing and the product of \(A\) from all layers is the final mixing matrix.

#### 2.3. Proposed \(L_{1/4}-\text{MLNMF}\) Method

In this paper, in order to improve the performance of MLNMF method for spectral unmixing, \(L_{1/4}-\text{MLNMF}\) is proposed. The sparsity constraints for both spectral signatures and abundance fractions are used in the proposed method. The sparsity constraint on abundance fractions has been already discussed thoroughly in [7]. Then the MLNMF method in [6] has also attempted to add sparsity constraint on spectral signatures matrix, the result of which are not very satisfactory. Note that sometimes \(L_{1/4}\) regularizer works better than \(L_{1/2}\) regularizer. Considering the mentioned constraints, \(L_{1/4}-\text{MLNMF}\) cost function for the \(l\)th layer is defined as

\[
O_{L_{1/4}-\text{MLNMF}} = \frac{1}{2} \| X - A_lS_l \|^2_F + \alpha_A \| A_l \|_{1/4} + \alpha_S \| S_l \|_{1/2}. \text{ (7)}
\]

To increase the effect of sparsity constraints on spectral signatures and abundance fractions, we set \(\alpha_A\) and \(\alpha_S\) by

\[
\alpha_A = \alpha_0 e^{-\tau t}, \alpha_S = 2\alpha_A, \text{ (8)}
\]

where \(t\) is the iteration number; \(\alpha_0\) and \(\tau\) are constants to control the impact of constraints [10].

Referring to the update rules mentioned in [7], we can calculate Eq.(7) by replacing the terms related to \(L_{1/2}\) constraints. The obtained multiplicative update rules for \(L_{1/4}-\text{MLNMF}\) problem are defined as

\[
A_l \leftarrow A_l \cdot \frac{(X l^T S_l)}{(A_l S_l S_l^T + \frac{1}{2} \alpha_A A_l^{-3/4})}, \text{ (9)}
\]

\[
S_l \leftarrow S_l \cdot \frac{(A_l^T X_l)}{(A_l^T A_l S_l + \frac{1}{2} \alpha_S S_l^{-1/2})}, \text{ (10)}
\]

where \((\cdot)^T\) is the transpose of a matrix and the constraints in Eq.(2) are still considered in above equations. Then we set the stopping criteria as

\[
\| O_{L_{1/4}-\text{MLNMF}}_{new} - O_{L_{1/4}-\text{MLNMF}}_{old} \| < \epsilon, \text{ (11)}
\]

where \(\epsilon\) is the error which is set to \(10^{-4}\) in our experiments. And another important setting is using VCA as initialization, which usually gives robust results [11]. In summary, the \(L_{1/4}-\text{MLNMF}\) algorithm is shown in Algorithm 1.
Algorithm 1 $L_{1/4}$-MLNMF Algorithm

**Input:** Hyperspectral image matrix $X$; Parameters: $\alpha_0$, $\tau$, $\epsilon$, $L$, $T_{\text{max}}$.

1. $X_1 = X$
2. for $l = 1$ to $L$ do
   3. Initialize $A_l$ and $S_l$ using VCA in the first layer and random initialization for other layers
   4. for $t = 1$ to $T_{\text{max}}$ do
      5. update $A_l$ using Eq.(9)
      6. update $S_l$ using Eq.(10)
      7. if $\epsilon$ in Eq.(11) then break
   8. end for
3. $X_{l+1} = S_l$
4. end for
5. $A = \prod_{l=1}^{L} A_l$ and $S = S_L$ in Eq.(6)

**Output:** Estimated spectral signatures $A$ and abundance fractions $S$

3. EXPERIMENTS AND RESULTS

In this section, the proposed $L_{1/4}$-MLNMF method is tested by synthetic dataset and real dataset. First, the evaluation of the proposed method and quantitative results are shown for synthetic dataset. Then, the visual results are given for real dataset.

3.1. Synthetic Dataset

In synthetic dataset experiment, spectral signatures from USGS library is used to generate simulated data. Six signatures of this library are chosen randomly and shown in Fig.2. Then the product in has been used to creat a $58 \times 58$-sized synthetic images without pure pixels. Finally, white noise is added into the data to simulate the sensor noise.

![Fig. 2. Six signatures chosen from library.](image-url)

For evaluation purpose, two different measures is used: root mean square of spectral angle distance (rmsSAD) and abundance angle distance (rmsAAD). The rmsSAD measures the similarity between original spectral signatures ($m_i$) and the estimated ones ($\hat{m}_i$). The rmsAAD measures the similarity between original abundance fractions ($a_i$) and the estimated ones ($\hat{a}_i$). They are given by

\[
\text{rmsSAD} = \left( \frac{1}{P} \sum_{i=1}^{P} \cos^{-1} \left( \frac{m_i \mathbf{T} \hat{m}_i}{\| m_i \| \| \hat{m}_i \|} \right) \right)^{1/2},
\]

\[
\text{rmsAAD} = \left( \frac{1}{N} \sum_{i=1}^{N} \cos^{-1} \left( \frac{a_i^T \hat{a}_i}{\| a_i \| \| \hat{a}_i \|} \right) \right)^{1/2}.
\]

In this experiment, parameters are selected as: $\alpha_0 = 0.1$, $\tau = 25$, $L = 10$ and $T_{\text{max}} = 400$, which are selected to get the best result. Estimated spectral signatures and the original ones are obtained in Fig.3 when SNR is 30dB.

![Fig. 3. Estimated spectral signatures in blue lines and the original ones in yellow lines using $L_{1/4}$-MLNMF.](image-url)

Table.1 shows the quantitative results of the proposed method compared to VCA [12], $L_{1/2}$-NMF [7], MLNMF [6] methods in terms of rmsSAD and rmsAAD for 20 runs. As we can see in this table, our proposed method outperforms the other methods.

<table>
<thead>
<tr>
<th>SNR(dB)</th>
<th>Index</th>
<th>VCA</th>
<th>$L_{1/2}$-NMF</th>
<th>MLNMF</th>
<th>$L_{1/4}$-MLNMF</th>
</tr>
</thead>
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<tr>
<td>20</td>
<td>rmsSAD</td>
<td>0.1765</td>
<td>0.1138</td>
<td>0.0630</td>
<td><strong>0.0490</strong></td>
</tr>
<tr>
<td></td>
<td>rmsAAD</td>
<td>0.6128</td>
<td>0.4610</td>
<td>0.3094</td>
<td><strong>0.2737</strong></td>
</tr>
<tr>
<td>30</td>
<td>rmsSAD</td>
<td>0.1826</td>
<td>0.1044</td>
<td>0.0509</td>
<td><strong>0.0486</strong></td>
</tr>
<tr>
<td></td>
<td>rmsAAD</td>
<td>0.4613</td>
<td>0.3934</td>
<td>0.2876</td>
<td><strong>0.2410</strong></td>
</tr>
<tr>
<td>40</td>
<td>rmsSAD</td>
<td>0.2108</td>
<td>0.0976</td>
<td>0.0454</td>
<td><strong>0.0472</strong></td>
</tr>
<tr>
<td></td>
<td>rmsAAD</td>
<td>0.5097</td>
<td>0.2981</td>
<td>0.1985</td>
<td><strong>0.2144</strong></td>
</tr>
</tbody>
</table>

3.2. Real Dataset

The Jasper Ridge dataset is a popular hyperspectral data used in NMF-based methods. In this paper, a $100 \times 100$-pixel sub-scene of this dataset is used as in Fig.4. After removing water
vapor and atmosphere absorption bands, we remain 198 channels to use in this experiment. And there are four endmembers latent in this dataset used as the true signatures.

![Image of reflectance values](image)

**Fig. 4.** OA curves on Salinas Scene for different band selection methods, in which $m$ is set from 3 to 30 each 3 intervals.

The parameters are set as $\alpha_0 = 0.1$, $\tau = 25$, $L = 10$ and $T_{max} = 400$ in this experiment. The abundance fractions maps and signatures extracted by proposed method are demonstrated in Fig. 5. And estimated signatures also have been compared with corresponding true signatures from USGS library in this figure. As it can be seen in these comparisons, the proposed method performances well for spectral unmixing.

![Image of abundance fractions maps](image)

**Fig. 5.** The abundance fractions maps and signatures extracted by $L_{1/4}$-MLNMF method.

4. CONCLUSION

In this paper, we present a $L_{1/4}$ sparsity-constrained multilayer nonnegative matrix factorization method for spectral unmixing. We apply multilayer structure of MLNMF to extend the NMF methods. Sparsity constraints for both abundance fractions and spectral signatures are added in our method to improve the results. The proposed method is tested by synthetic and real datasets. Results and comparisons show that the proposed algorithm excels the other methods.

5. ACKNOWLEDGEMENT

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