Blind hyperspectral unmixing by non-parametric non-Gaussianity measure

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Abstract: For linear mixing model (LMM) of hyperspectral unmixing in hyperspectral images processing problem, the endmember fractional abundances satisfy the sum-to-one constraint, which makes the well-known independent component analysis (ICA) based blind source separation (BSS) algorithms not well suited to blind hyperspectral unmixing (bHU). In this paper, an efficient non-parametric bHU algorithm consulting dependent component analysis (DCA) is presented. Based on the cumulative density function (CDF) and order statistics instead of traditional probability distribution function (PDF), the novel objective function is derived by maximising the non-parametric non-Gaussianity between the estimated endmember abundance of the endmember signatures and their corresponding original abundances. With the stochastic gradient rule of constrained optimisation method, an efficient dependent sources separation algorithm for bHU is obtained to fulfil the endmember signatures extraction and abundances estimation tasks. Simulations based on the synthetic data are performed to evaluate the validity of the proposed non-parametric non-Gaussianity HU (non-pNG-bHU) algorithm.

Keywords: independent component analysis; ICA; blind source separation; BSS; blind hyperspectral unmixing; bHU; dependent component analysis; DCA.


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1 Introduction

Over the last few years, with the rapid development of imaging spectroscopy and space technology, remotely sensed hyperspectral images have many potential applications such as space exploration, environmental detection and protection, national defence and security, et al. (Halimi et al., 2016; Li et al., 2016). Generally, due to the limited spatial resolution of state-of-the-art imaging sensors, each individual pixel in the hyperspectral image usually contains more than one pure spectral signature, weighted by their fractional abundances. Consequently, as an important problem in many hyperspectral image analysis, hyperspectral unmixing (HU) attempts to identify the endmember signatures and estimate the corresponding abundances from the spectral of each pixel (Halimi et al., 2016; Li et al., 2016).

Although several models have been built to describe the mixing process of mixing endmembers to hyperspectral images, as a compromise between model accuracy and tractability, linear mixing model (LMM) has been widely used to solve the HU problem for its implementing efficiency and flexibility in many applications (Halimi et al., 2016; Li et al., 2016; Heylen et al., 2011). Despite the fact that the LMM is not usually true and accurate, it is always considered as an acceptable model for most real-world scenarios except that special scenarios exhibit strong nonlinearity.

Many HU algorithms have been developed by exploiting the LMM model, which are mainly divided into two categories, semi-blind HU approaches and blind HU (bHU) approaches. Most semi-blind HU approaches require some or full knowledge of the existing materials (endmembers) and their spectral characteristics, which forms the endmember spectral signature matrix. If the endmember signature matrix is known, then the estimation of the abundance vector can be considered as a constrained linear least squares problems, which can be solved by classic convex optimisation methods and some advanced efficient modification implementations (Heylen et al., 2011).

Nevertheless, for real-world applications, obtaining full knowledge of endmember signature matrix is not an easy task, which is impossible to know exactly all the materials in the scene in most cases. To overcome this difficulty, some efforts were made to develop bHU approaches in recent years, which can identify the endmember signature matrix and the abundances vector simultaneously without any apriority. If the endmember signature matrix is seen as the mixing matrix and the abundances vector as sources vector respectively, the bHU problem falls into the scope of the popular blind source separation (BSS) technology, which has been comprehensively studied during the last two decades, especially for the case where the source signals are mutually statistically independent, which is called independent component analysis (ICA) (Comon et al., 2010).

However, in the framework of bHU, the endmember abundances are not statistically independent for their sum-to-one constraint (Nascimento et al., 2005). As a result, the classic ICA based BSS algorithms are usually not well suited for general bHU scheme.

Consequently, the above mentioned bHU problem is actually a problem of blind separation of dependent source signals from their linearly instantaneous mixtures, which is usually called dependent component analysis (DCA) in the BSS society and has received much attention in recent years. In this paper, inspired by the existing DCA method (Caiafa et al., 2008), we propose a bHU algorithm called non-parametric non-Gaussianity (NG) bHU (non-pNG-bHU) algorithm, which exploits the fact that maximisation the NG of the abundances can separate the latent endmember abundances and the endmember signatures, even if there have some dependencies existed between abundances. The algorithm proposed in Caiafa et al. (2008) is a parametric method by utilising NG measure, which is realised by assuming the parametric model of the probability distribution function (PDF) of latent sources. On the contrary, the approach proposed in this paper is derived based on the order statistics (OS), which is a non-parametric scheme and as a result, it has more application cases. The feasibility of applying ICA to HU is analysed from theory to simulations in Nascimento et al. (2005), nevertheless, efficient algorithm for HU is not proposed for bHU problem.

Inspiring by this principle, the novel cost function to be optimised is derived based on the cumulative density function (CDF) and OS instead of traditional PDF based approaches. By executing the stochastic gradient rule of constrained optimisation method, the final non-parametric maximum NG measure algorithm for bHU is obtained and then based on the proposed algorithm, the endmember signature matrix (mixing matrix) can be estimated efficiently. Eventually, the original endmember abundances (source signals) vector can be estimated properly.

The rest of this paper is organised as follows, Section 2 introduces the bHU model and briefly reviews some BSS based algorithm for bHU problem. In Section 3, we present the proposed non-pNG-bHU algorithm. Experimental results are shown in Section 4. Finally, in Section 5, our main conclusions are outlined.

2 bHU model

For any fixed pixel \( l \) in the hyperspectral image, let \( x_m[l] \) denote the hyperspectral camera’s measurement at spectral band \( m \). Suppose we have \( M \) spectral channels, then \( x[l] = [x_1[l], \ldots, x_M[l]]^T \in \mathbb{R}^M \), the LMM can be written as follows,

\[
x[l] = \sum_{i=1}^{N} a_i s_i[l] + v[l] = A s[l] + v[l],
\]

(1)

for \( l = 1, \ldots, L \), \( L \) denotes the number of pixels. Each \( a_i \in \mathbb{R}^M, i = 1, \ldots, N \), is termed as an endmember signature vector, which contains the spectral components of a specific material in the scene indexed by \( i \). \( N \) is the number of
endmembers in the scene. $A = [a_1, \ldots, a_N] \in \mathbb{R}^{M \times N}$ is called the endmember matrix (mixing matrix in BSS). $s[l] = [s_1[l], \ldots, s_N[l]]^T \in \mathbb{R}^N$ is called the endmember abundances vector (sources in BSS) at pixel $l$, $v[l] = [v_1[l], \ldots, v_M[l]]^T \in \mathbb{R}^M$ denotes an additive noise at pixel $l$, which contains the modelling errors, system noise, etc. For a certain pixel $l$, the endmember abundance $s[l]$ represents the fractional area occupied by the $i$-th endmember. Therefore, in the LMM, all the source signals $s[l]$ in a special pixel is greater or equal to zero,

$$s[l] \geq 0, \; i = 1, \ldots, N, \; \forall l \in \{1, \ldots, L\}$$

(2)

Furthermore, $s[l]$ are the percentage contribution of each endmember in the pixel $l$, they should sum-to-one constraint, that is,

$$\sum_{i=1}^{N} s_i[l] = 1, \; \forall l \in \{1, \ldots, L\}$$

(3)

Obviously, the sum-to-one constraint (3) imposes dependence among the source signals $s[l]$. That is, every source signal $s[l]$ can be expressed as a linear combination of the other $N - 1$ ones and this leads to the dependences between different source signals.

If the endmember signature matrix $A$ is known, an estimation of the source signals can be obtained by

$$\hat{s}[l] = A^+ x[l]$$

(4)

where $A^+$ is the Moore-Penrose pseudo inverse of $A$, i.e., $A^+ = (A^T A)^{-1} A^T$.

In most cases, the endmember signature matrix can not be accessed easily and HU need to be executed in a blind manner, i.e., without knowing matrix $A$, which makes the HU problem more complicated and generally called bHU. The problem of bHU falls into the class of BSS problem in signal processing and the desired results of bHU are to estimate the endmember signature matrix and the corresponding abundances from the observed hyperspectral images, with no or little prior information of the mixing system. Being given little information to solve the problem, bHU is a challenging, but also fundamentally intriguing, problem with many possibilities (Nascimento et al., 2005; Lin et al., 2015).

Most of the methods of BSS perform a spatial decorrelation preprocessing over $x[l]$ to obtain the decorrelated observations $z[l] = [z_1[l], \ldots, z_M[l]]^T$. So, the global mixture is expressed as $z[l] = Vx[l]$, where $V$ is an unknown orthogonal matrix (Comon et al., 2010; Szabo et al., 2012). After separation algorithms are utilised to preprocessed data $z[l]$, one can find a linear unitary transformation $B$ and get the estimation of the source signals $y[l],

$$y[l] = Bz[l]$$

(5)

3 Proposed NG based bHU algorithm

3.1 non-pNG-bHU algorithm

The maximum NG method consists of searching for the linear combinations of mixtures that give source estimates with maximum NG distributions and restricts the searching space to the unit-variance signals space. More specifically, sources are estimated through relation $y[l] = Bz[l]$ over the space of invertible separating matrices $B$ providing signals $\{y_1[l], \ldots, y_M[l]\}$ with unit-variances (Caiafa et al., 2008). The NG measure is defined as,

$$d(y, g) = \left( \int |p_s(u) - p_g(u)|^2 du \right)^{1/2}$$

(6)

where the integral is defined in the Lebesgue sense and is taken on all the range of variable $u$ and $p_s(u)$ is the normalised Gaussian PDF. So, equation (6) is the square of the distance between functions $p_s(u)$ and $p_g(u)$ in $L^2$ space. Let us call $F_s$ and $F_g$ the CDF to be analysed and its Gaussian equivalent one, respectively. Then, the NG measure based on CDF is defined as,

$$d(F_s, F_g) = \left( \int \left( F_s(u) - F_g(u) \right)^2 du \right)^{1/2}$$

(7)

As done in Blanco et al. (2003), the previous definitions hold the following distance property,

$$d(F_s, F_g) = 0 \iff c = 2, \text{ and } d(F_s, F_g) > 0, \forall c \neq 2,$$

(8)

where $c$ is the Gaussianity parameter in the generalised Gaussian density (GGD) function (Wang et al., 2008). Consequently, the distance measure is NG measure since it offers a global minimum. For the property (8), the close relationship between CDF $F$ and its inverse $Q$ can be generalised as

$$D(Q_s, Q_g) = 0 \iff c = 2, \text{ and } D(Q_s, Q_g) > 0, \forall c \neq 2.$$  

(9)

As a result,

$$D(Q_s, Q_g) = \max_{u \in \mathbb{R}} |Q_s(u) - Q_g(u)|$$

(10)

is also an appropriate NG measure. The estimation of $Q_s$ can be performed very robustly in a simple practical way by using the set of OS $y_1(1) < y_2(2) < \ldots < y_M(\infty)$. Eventually, as shown in Blanco et al. (2003), the efficient estimation of NG measure (10) can be represented as

$$D(Q_s, Q_g) = \left| y_{ik} - y_{il} + 2Q_g\left(\frac{\zeta}{\alpha}\right) \right|$$

(11)

with \( \{k, l = 80\%n, 20\%n\}, \text{ or } \{k, l = n, 1\}. \)
As described in Blanco et al. (2003), we get that the proposed NG measure presents a local maximum at any output channel if $b_i$ is forced to be unitary. Therefore, a multistage procedure will be applied to obtain a different component at each output channel: the NG measure is maximised at each output channel successively under the constriction that the vector $b_i$ has to be orthonormal to the previously obtained vectors.

Taking into account (5) in vector form, $y_i[l] = b_i^T z[l]$, where $b_i^T$ is the $i$-row of the separation matrix $B$, the goal is to update $b_i$ at each stage by optimising an objective function $J(b_i)$. We take $J(b_i) = D(Q_y, Q_x)$ and it will be optimised by the stochastic gradient rule of the constrained optimisation method at $r$-th iteration (Blanco et al., 2003),

$$b_i[+1] = b_i[r] + \mu V J(b_i[r]) b_i[r]$$

subject to:

$b_i$ is orthonormal to $[b_1, \cdots, b_{i-1}]$.

The gradient of $J(b_i)$ is,

$$\nabla J(b_i) = S \frac{d(y_{i(k)} - y_{i(l)})}{d b_i}$$

where $S = \text{sign} \left( y_{i(k)} - y_{i(l)} + 2Q_x \left( \frac{l}{n} \right) \right)$. By applying the chain rule, we have,

$$\frac{d(y_{i(k)} - y_{i(l)})}{d b_i} = Z \left( \frac{d y_{i(k)}}{d y_{i[l]}} \frac{d y_{i(l)}}{d y_{i[l]}} \right)$$

where

$$\frac{d y_{i[l]}}{d y_{i[l]}} = e_r = [0, \cdots, 0, 1, 0, \cdots, 0]^T$$

and

$$e_r(j) = \begin{cases} 1 & \text{if } y_{i(j)} = y_{i(l)}, j = 1, \cdots, N. \\ 0 & \text{else} \end{cases}$$

After each iteration procedure, $b_i$ must be normalised and projected over the orthonormal subspace $C_{l-1}$ to the vectors obtained at every previous stage, wherein $C_{l-1}$ is expressed as,

$$C_{l-1} = I - (B_{l-1} B_{l-1}^H)^{-1} B_{l-1}^H$$

where $B_{l-1} = [b_1, \cdots, b_{l-1}]$.

Once we get the estimation of the separation matrix $B$, based on the whiten matrix $V$, endmember signature matrix $A$ can be obtained easily. As a consequence, the original endmember abundances (source signals) can be solved by

$$\hat{s}[l] = A^s x[l].$$

4 Simulation results

In this section, simulation experiments using MATLAB are presented to confirm the validity and performance of the proposed non-pNG-bHU algorithm.

Six mineral signatures used in the simulations are extracted from the United States Geological Survey (USGS) (http://speclab.cr.usgs.gov/spectral-lib.html) spectral library, where the wavelength is 224 ($M = 224$), which forms the signature matrix (mixing matrix) $A \in \mathbb{R}^{224 \times 6}$. The abundance matrix (source signal) $S \in \mathbb{R}^{6 \times 1296}$ is generated randomly using the MATLAB function rand(). In order to test the anti-interference ability of the proposed non-pNG-bHU algorithm to additive noise, some Gaussian noises are added to the mixtures, where the signal-to-noise ratio (SNR) is defined as

$$\text{SNR} = 10 \log_{10} \frac{E(\hat{x}^H \hat{x})}{E(\hat{v}^H \hat{v})}$$

The following performance index is adopted to evaluate the performance of the proposed algorithm called Amari performance index (API) $(Li et al., 2004)$ and $0 \leq C \leq 1$, the perfect separation implies that $C = 0$. Another performance index is called the signal-to-interface ratio (SIR) between source signals $s_i[l]$ and their estimates $\hat{s}_i[l]$ which were calculated to measure the accuracy of the estimations of the source signals (Comon et al., 2010). In conventional BSS algorithms, it can be considered as getting meaningful results when SIR $\geq 10$ dB.

Firstly, we consider the noiseless case. The original true endmember signatures are shown in the left column of Figure 1, one of the separation results are presented at the middle column in Figure 1 and the estimation errors are depicted in the right column of Figure 1. From the first two columns in Figure 1, we can obtain that the waveforms of the original true endmember signatures and their estimators are very similar. In order to quantify the estimation error, we calculate the Euclid norm of the estimation errors, which are 0.0835, 0.3689, 0.0859, 0.2128, 0.4958 and 0.0196 respectively. From these results, we can conclude that the proposed non-pNG-bHU algorithm can estimate the endmember signatures accurately.
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Figure 1  Comparisons of the true endmember signatures with the separated endmember signatures based on the proposed non-pNG-bHU algorithm (see online version for colours)

Notes: left column: original true signatures; middle column: estimated signatures; right column: estimation error.

Additionally, the true abundances and their estimations are depicted in Figure 2. The estimation errors are demonstrated in the right column in Figure 2. After 100 simulations, the mean API 0.042, the SIR means of six estimated abundances are: SIR1 = 32.27 dB, SIR2 = 31.39 dB, SIR3 = 37.17 dB, SIR4 = 36.21 dB, SIR5 = 33.65, SIR6 = 39.29 dB. It is obvious that the proposed non-pNG-bHU algorithm can separate original abundances properly. Then, we evaluate the performance of the proposed algorithm by relative estimation error $\varsigma$ which is executed by the Frobenius norm of the estimation errors and defined as

$$\varsigma = \frac{\|\mathbf{S}_i - \hat{\mathbf{S}}_i\|_F}{\|\mathbf{S}_i\|_F}$$

(18)

where $\|\cdot\|_F$ denotes the Frobenius norm of a matrix. The corresponding relative estimation errors of the six abundances are 0.0177, 0.0274, 0.0271, 0.0181, 0.0173 and 0.0105 respectively. This result also verifies the effectiveness of the proposed algorithm.

Then, we illustrate the performances comparisons of the proposed non-pNG-bHU algorithm with other two algorithms terms as fastICA algorithm (Nascimento et al., 2005) and MaxNG algorithm (Caiafa et al., 2008) under different noise conditions with a simulated scenario given by $N = 6$. Figure 3 shows the unmixing results obtained by the proposed algorithm, fastICA algorithm and MaxNG algorithm with different noise levels, which include 20, 30 and 40 dB. The averaged API and SIR with error bars are demonstrated in Figure 3 to evaluate the performance. As shown in Figure 3, when the noise level is moderately low (i.e., SNR greater than 30 dB), the proposed algorithm can obtain good unmixing results compared with other two algorithms. Otherwise, when the level of noise significantly increases (i.e., SNR less than 20 dB), the quality of the unmixing results of all algorithms decrease, particularly with regard to the fastICA algorithm. Although MaxNG algorithm can also achieve good unmixing, it is not as robust as the proposed non-pNG-bHU algorithm. Moreover, it should be noted that 20 dB is not a realistic noise level given the SNR of current imaging spectrometers. As a result, we can conclude that the results reported in Figure 3 indicate very high robustness to noise by the proposed non-pNG-bHU algorithm.
Figure 2  Comparisons of the true abundances with the estimated abundances based on the proposed non-pNG-bHU algorithm (see online version for colours)

Notes: left column: original true abundances; middle column: estimated abundances; right column: estimation errors.

Figure 3  Comparisons of the unmixing results obtained by the proposed non-pNG-bHU with fastica and maxng algorithms in a simulated scenario of $N = 6$ with different noise level over 100 Monte Carlo simulations, wherein SNR values are 20, 30 and 40 dB (see online version for colours)

Notes: Left three columns illustrate the sir performance with different SNRs; right three columns indicates the API performance with different SNRs.
5 Conclusions

As an important research topic of hyperspectral image processing, bHU aims at finding the endmember signature matrix and corresponding fractional abundances from the measured mixed hyperspectral images blindly. From signal processing perspective, bHU is a typical BSS problem. ICA, the most popular BSS method, has been proposed as a tool to solve bHU. Unfortunately, the assumption of mutually independent among source signals is always violated in applications, which makes ICA method not well suited to bHU. In this paper, a novel bHU algorithm is presented by exploiting the maximum non-parametric NG between the estimated source signals for LMM model to extract the endmember signatures and their corresponding abundances. According to simulation results, the performance of the proposed non-pNG-bHU algorithm is slightly more appropriate than fastICA and MaxNG algorithms for bHU problem. Our next research will focus on the extension of the proposed approach to non-LMM for HU problem, especially for the post-nonlinear situation.

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