EUSIPCO 2013 1569744375

BAYESIAN UNSUPERVISED UNMIXING OF HYPERSPECTRAL IMAGES USING A POST-NONLINEAR MODEL

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ABSTRACT

This paper presents a nonlinear mixing model for hyperspectral image unmixing. The proposed model assumes that the pixel reflectances are post-nonlinear functions of unknown pure spectral components (referred to as endmembers) contaminated by an additive white Gaussian noise. The nonlinear effects affecting endmembers are approximated by polynomial functions leading to a polynomial post-nonlinear mixing model. A Bayesian strategy is used to estimate the parameters of this model yielding an unsupervised nonlinear unmixing algorithm. Due to the large number of parameters to be estimated, an efficient constrained Hamiltonian Markov chain Monte Carlo method is developed to sample according to the posterior of the Bayesian model. The performance of the resulting unmixing strategy is evaluated on synthetic data.

Index Terms— Hyperspectral imagery, spectral unmixing, Hamiltonian Monte Carlo, post-nonlinear model.

1. INTRODUCTION

Identifying macroscopic materials and quantifying the proportions of these materials are major issues when analyzing hyperspectral images. This spectral unmixing (SU) problem has been widely studied for applications where the pixel reflectances are linear combinations of pure component spectra. However, as explained in [1], the linear mixing model (LMM) can be inappropriate for some hyperspectral images. Nonlinear mixing models provide an interesting alternative for overcoming the inherent limitations of the LMM. Several models have been studied in the literature to handle specific kinds of nonlinearities. In particular, the bilinear models recently studied in [2–5] address the problem of scattering effects, mainly observed in vegetation or urban areas. Other more flexible unmixing techniques have been also proposed to handle wider class of nonlinearities, including radial basis function networks and kernel-based models.

Part of this work has been supported by Direction Generale de l'armement, French Ministry of defence, and by the Hypanema ANR Project ANR Project n°ANR- 12-BS03-003.

This paper considers a polynomial post-nonlinear mixing model (PPNMM) that has recently shown interesting properties for the SU of hyperspectral images [6]. Precisely, we propose a fully unsupervised Bayesian unmixing algorithm based on the PPNMM (estimating jointly the endmembers and the other model parameters). However, the classical Bayesian estimators cannot be easily computed from the PPNMM posterior distribution. To alleviate this problem, a Markov chain Monte Carlo (MCMC) method is used to generate samples according to this posterior. Due to the large number of parameters to be estimated we propose to use Hamiltonian Monte Carlo (HMC) moves within a Gibbs sampler. HMCs are simulation strategies based on Hamiltonian dynamics which can improve the convergence and mixing properties of classical MCMC methods [7]. We investigate recent HMC methods handling constrained variables [7, Chap. 5] that can be applied to our Bayesian model for spectral unmixing.

The paper is organized as follows. Section 2 introduces the PPNMM for hyperspectral image analysis. Section 3 presents the hierarchical Bayesian model associated with the proposed PPNMM and its posterior distribution. A Gibbs sampling strategy coupling standard simulations (according to the full conditional of the posterior) and constrained HMC (CHMC) moves is presented in Section 4. Simulation results conducted on synthetic data are shown and discussed in Section 5. Conclusions are finally reported in Section 6.

2. PROBLEM FORMULATION

2.1. Polynomial Post-Nonlinear Mixing Model

This section recalls the nonlinear mixing model used in [6] for hyperspectral image SU. We consider a set of N observed spectra $\mathbf{y}_n = [y_{n,1}, \ldots, y_{n,L}]^T, n \in \{1, \ldots, N\}$ where L is the number of spectral bands. Each spectrum is defined as a nonlinear transformation $\boldsymbol{g}_n$ of a linear mixture of R endmembers $\mathbf{m}_r$ contaminated by additive noise

$$\mathbf{y}_n = \boldsymbol{g}_n \left(\sum_{r=1}^{R} a_{r,n} \mathbf{m}_r \right) + \mathbf{e}_n = \boldsymbol{g}_n \left(\mathbf{M} \boldsymbol{a}_n \right) + \mathbf{e}_n \qquad (1)$$

where $\mathbf{m}_r = [m_{r,1}, \ldots, m_{r,L}]^T$ is the spectrum of the rth material present in the scene, $a_{r,n}$ is its corresponding proportion in the nth pixel, R is the number of endmembers contained in the image and $\boldsymbol{g}_n$ is a nonlinear function associated with the nth pixel. Moreover, $\mathbf{e}_n$ is an additive independent and identically distributed (i.i.d) zero-mean Gaussian noise sequence with variance σ^2, denoted as $\mathbf{e}_n \sim \mathcal{N}\left(\mathbf{0}_L, \sigma^2 \mathbf{I}_L\right)$. Note that the usual matrix and vector notations $\mathbf{M} = [\mathbf{m}_1, \ldots, \mathbf{m}_R]$ and $\boldsymbol{a}_n = [a_{1,n}, \ldots, a_{R,n}]^T$ have been used in the right hand side of (1). As in [6], the N nonlinear functions $\boldsymbol{g}_n$ are defined as second order polynomial nonlinearities defined by $\boldsymbol{g}_n(\mathbf{s}) = \mathbf{s} + b_n(\mathbf{s} \odot \mathbf{s})$, where $\mathbf{s} \in \mathbb{R}^L$, b_n is a real parameter, and $\odot$ denotes the Hadamard (termwise) product. An interesting property of the resulting PPNMM is that it reduces to the classical LMM for $b_n = 0$. Motivations for considering polynomial nonlinearities have been discussed in [6]. Straightforward computations allow the PPNMM observation matrix to be expressed as follows

$$\mathbf{Y} = \mathbf{MA} + [(\mathbf{MA}) \odot (\mathbf{MA})] \operatorname{diag}(\boldsymbol{b}) + \mathbf{E} \tag{2}$$

where $\mathbf{A} = [\boldsymbol{a}_1, \ldots, \boldsymbol{a}_N]$ is an $R \times N$ matrix, $\mathbf{Y} = [\mathbf{y}_1, \ldots, \mathbf{y}_N]$ and $\mathbf{E} = [\mathbf{e}_1, \ldots, \mathbf{e}_N]$ are $L \times N$ matrices, and $\boldsymbol{b} = [b_1, \ldots, b_N]^T$ is an $N \times 1$ vector containing the nonlinearity parameters. Moreover, $\operatorname{diag}(\boldsymbol{b})$ is an $N \times N$ diagonal matrix containing the elements of the vector $\boldsymbol{b}$.

2.2. Abundance reparametrization

Due to physical considerations, the abundance vectors $\boldsymbol{a}_n$ satisfy the following positivity and sum-to-one constraints

$$\sum_{r=1}^{R} a_{r,n} = 1, \;\; a_{r,n} > 0, \forall r \in \{1, \ldots, R\}. \tag{3}$$

To handle these constraints, we propose to reparameterize the abundance vectors belonging to the set

$$\mathcal{S} = \left\{ \boldsymbol{a} = [a_1, \ldots, a_R]^T \,\middle|\, a_r > 0, \sum_{r=1}^{R} a_r = 1 \right\}$$

using the following transformation

$$a_{r,n} = \left(\prod_{k=1}^{r-1} z_{k,n} \right) \times \begin{cases} 1 - z_{r,n} & \text{if } r < R \\ 1 & \text{if } r = R \end{cases}. \tag{4}$$

This transformation has been recently suggested in [8]. The main motivation for using the latent variables $z_{r,n}$ instead of $a_{r,n}$ is the fact that the constraints (3) (for the nth abundance vector $\boldsymbol{a}_n$) express as

$$0 < z_{r,n} < 1, \quad \forall r \in \{1, \ldots, R-1\} \tag{5}$$

for the nth coefficient vector $\boldsymbol{z}_n = [z_{1,n}, \ldots, z_{R-1,n}]^T$. As a consequence, the constraints (5) are much easier to handle for the sampling procedure than (3). The next section presents the Bayesian model associated with the PPNMM for SU.

3. BAYESIAN MODEL

This section generalizes the hierarchical Bayesian model introduced in [6] to estimate the unknown parameter vector associated with the PPNMM containing the reparameterized abundances $\mathbf{Z} = [\boldsymbol{z}_1, \ldots, \boldsymbol{z}_N]$, the endmember matrix $\mathbf{M}$, the nonlinearity parameter vector $\boldsymbol{b}$ and the additive noise variance σ^2. This section summarizes the likelihood and the parameters priors that are used for this estimation.

3.1. Likelihood

Assuming prior independence between the observed pixels and using (2), the joint likelihood of the observation matrix $\mathbf{Y}$ can be expressed as

$$f(\mathbf{Y}|\mathbf{M}, \mathbf{Z}, \boldsymbol{b}, \sigma^2) \propto \sigma^{-NL} \operatorname{etr}\left[-\frac{(\mathbf{Y} - \boldsymbol{X})^T (\mathbf{Y} - \boldsymbol{X})}{2\sigma^2} \right] \tag{6}$$

where $\propto$ means "proportional to", $\operatorname{etr}(\cdot)$ denotes the exponential trace and $\boldsymbol{X} = \mathbf{MA} + [(\mathbf{MA}) \odot (\mathbf{MA})] \operatorname{diag}(\boldsymbol{b})$ is an $L \times N$ matrix.

3.2. Parameter priors

To reflect the lack of prior knowledge about the abundances, we propose to assign a prior distribution to the vector $\boldsymbol{z}_n$ ensuring that $\boldsymbol{a}_n$ is uniformly distributed in its definition domain. More precisely, we assign beta priors $z_{n,r} \sim \mathcal{B}e(R - r, 1), r \in \{1, \ldots, R-1\}$ and assume prior independence between the elements of $\boldsymbol{z}_n$. As explained in [8], this choice yields an abundance vector $\boldsymbol{a}_n$ uniformly distributed in the set $\mathcal{S}$. Assuming prior independence between the coefficient vectors $\{\boldsymbol{z}_n\}_{n=1,\ldots,N}$ leads to

$$f(\mathbf{Z}) = \prod_{r=1}^{R-1} \left\{ \frac{1}{B(R-r,1)^N} \prod_{n=1}^{N} z_{n,r}^{R-r-1} \right\} \tag{7}$$

where $B(\cdot, \cdot)$ is the Beta function.

Each endmember $\mathbf{m}_r = [m_{r,1}, \ldots, m_{r,L}]^T$ is a reflectance vector satisfying the following constraints

$$0 \leq m_{r,\ell} \leq 1, \forall r \in \{1, \ldots, R\}, \forall \ell \in \{1, \ldots, L\}. \tag{8}$$

For each endmember $\mathbf{m}_r$, we propose to use a Gaussian prior truncated on $[0,1]^L$ to satisfy the constraints (8), i.e.,

$$\mathbf{m}_r \sim \mathcal{N}_{[0,1]^L}(\bar{\mathbf{m}}_r, s^2 \mathbf{I}_L). \tag{9}$$

This prior requires to define the mean vectors $\bar{\mathbf{m}}_r$ and the noise variance s^2. We propose to select the mean vectors $\bar{\mathbf{m}}_r$ as the pure components previously identified by the nonlinear EEA studied in [9] and referred to as "Heylen". The variance s^2 reflects the degree of confidence given to this prior information ($s^2 = 50$ in our simulations).

The PPNMM reduces to the LMM for $b_n = 0$. Since the LMM is probably relevant for most observed pixels it makes sense to assign prior distributions to the nonlinearity parameters that enforce sparsity for the vector $\boldsymbol{b}$. Consequently, the following conjugate Bernoulli-Gaussian prior is assigned to each parameter b_n

$$f(b_n|w,\sigma_b^2) = (1-w)\delta(b_n) + w\frac{1}{\sqrt{2\pi\sigma_b^2}}\exp\left(-\frac{b_n^2}{2\sigma_b^2}\right) \quad (10)$$

where $\delta(\cdot)$ denotes the Dirac delta function. Note that the prior distributions for $\{b_n\}_{n=1,\ldots,N}$ share the same hyperparameters $w \in [0,1]$ and $\sigma_b^2 \in]0,+\infty[$. Moreover, the weight w is the prior probability of having a nonlinearly mixed pixel in the image. Assuming prior independence between the nonlinearity parameters $\{b_n\}_{n=1,\ldots,N}$, the joint prior distribution of the nonlinearity parameter vector $\boldsymbol{b}$ is given by

$$f(\boldsymbol{b}|w,\sigma_b^2) = \prod_{n=1}^{N} f(b_n|w,\sigma_b^2). \quad (11)$$

A Jeffreys' prior is assigned to the noise variance σ^2

$$f(\sigma^2) \propto \frac{1}{\sigma^2}\mathbf{I}_{+}(\sigma^2) \quad (12)$$

which reflects the absence of knowledge for this parameter.

3.3. Hyperparameter priors

The performance of the proposed Bayesian model for spectral unmixing depends on the values of the hyperparameters σ_b^2 and w. When the hyperparameters are difficult to adjust, it is classical to include them in the unknown parameter vector, resulting in a hierarchical Bayesian model [6, 10]. A conjugate inverse-gamma prior is assigned to σ_b^2, i.e., $\sigma_b^2 \sim \mathcal{IG}(\gamma,\nu)$ where (γ,ν) are real parameters fixed to obtain a flat prior for the variance σ_b^2 ((γ,ν) will be set to $(10^{-1},10^{-1})$ in the simulation section). A uniform prior distribution is assigned to the hyperparameter w, i.e., $w \sim \mathcal{U}_{[0,1]}(w)$ since there is no *a priori* information regarding the proportions of linearly and nonlinearly mixed pixels in the image.

3.4. Joint posterior distribution

The joint posterior distribution of the unknown parameters $\boldsymbol{\theta} = \{\mathbf{Z},\mathbf{M},\boldsymbol{b},\sigma^2,\sigma_b^2,w\}$ can be computed using

$$f(\boldsymbol{\theta}|\mathbf{Y}) \propto f(\mathbf{Y}|\boldsymbol{\theta})f(\boldsymbol{\theta}) \quad (13)$$

where $f(\mathbf{Y}|\boldsymbol{\theta})$ has been defined in (6). By assuming *a priori* independence between the parameters $\mathbf{Z}$, $\mathbf{M}$, $\boldsymbol{b}$ and σ^2 and between the hyperparameters σ_b and w, the joint prior distribution of the $\boldsymbol{\theta}$ can be expressed as

$$f(\boldsymbol{\theta}) = f(\mathbf{Z})f(\mathbf{M})f(\sigma^2)f(\boldsymbol{b}|\sigma_b^2,w)f(\sigma_b^2)f(w). \quad (14)$$

Unfortunately, it is difficult to obtain closed form expressions for the standard Bayesian estimators associated with (13). Thus we propose to generate samples asymptotically distributed according to (13). Due to the large number of parameters to be sampled, we use HMC moves which allow the number of sampling steps to be reduced and the mixing properties of the sampler to be improved. The basic principles of the HMC methods that are used to sample asymptotically from (13) can be found in [11]. The generated samples are then used to compute the MMSE estimator of $\boldsymbol{\theta}$. The next section defines the Gibbs sampler (including constrained HMC moves) used to sample from (13).

4. GIBBS SAMPLER

The principle of the Gibbs sampler is to sample according to the conditional distributions of the posterior of interest [12, Chap. 10]. Due to the large number of parameters to be estimated, it makes sense to use a block Gibbs sampler to improve the convergence of the sampling procedure. More precisely, we propose to sample sequentially $\mathbf{M}, \mathbf{Z}, \boldsymbol{b}, \sigma^2, \sigma_b^2$ and w using six moves that are detailed in the next sections.

4.1. Sampling the coefficient matrix Z

Sampling from $f(\mathbf{Z}|\mathbf{Y},\mathbf{M},\boldsymbol{b},\sigma^2,\sigma_b^2,w)$ is difficult due to the complexity of this distribution. In this case, it is classical to use an accept/reject procedure to update the coefficient matrix $\mathbf{Z}$ (leading to a hybrid Metropolis-within-Gibbs sampler). It can be shown that

$$f(\mathbf{Z}|\mathbf{Y},\mathbf{M},\boldsymbol{b},\sigma^2,\sigma_b,w) = \prod_{n=1}^{N} f(\boldsymbol{z}_n|\mathbf{y}_n,\mathbf{M},b_n,\sigma^2), \quad (15)$$

i.e., the N coefficients vectors $\{\boldsymbol{z}_n\}_{n=1,\ldots,N}$ are *a posteriori* independent and can be sampled independently (in a parallel manner). Straightforward computations lead to

$$f(\boldsymbol{z}_n|\mathbf{y}_n,\mathbf{M},b_n,\sigma^2) \propto \exp\left(-\frac{\|\mathbf{y}_n-\boldsymbol{x}_n\|^2}{2\sigma^2}\right) \times \mathbf{1}_{(0,1)^{R-1}}(\boldsymbol{z}_n)\prod_{r}^{R-1} z_{n,r}^{R-r-1} \quad (16)$$

where $\boldsymbol{x}_n = \boldsymbol{g}_n(\mathbf{M}\boldsymbol{a}_n)$, $\mathbf{1}_{(0,1)^{R-1}}(\cdot)$ denotes the indicator function over $(0,1)^{R-1}$. The distribution (16) can be related to a potential energy that is then used within a CHMC method to update the vector $\boldsymbol{z}_n$. For space limitations, we do not detail this CHMC method. The reader is invited to consult a separate technical report for more details [11].

4.2. Sampling the endmember matrix M

From (13) and (14), it can be seen that

$$f(\mathbf{M}|\mathbf{Y},\mathbf{Z},\boldsymbol{b},\sigma^2,s^2,\widetilde{\mathbf{M}}) = \prod_{\ell=1}^{L} f(\mathbf{m}_{\ell,:}|\mathbf{y}_{\ell,:},\mathbf{Z},\boldsymbol{b},\sigma^2,s^2,\bar{\mathbf{m}}_{\ell,:})$$

where $\mathbf{m}_{\ell,:}$ (resp. $\bar{\mathbf{m}}_{\ell,:}$ and $\mathbf{y}_{\ell,:}$) is the ℓth row of $\mathbf{M}$ (resp. of $\widetilde{\mathbf{M}}$ and $\mathbf{Y}$) and

$$f(\mathbf{m}_{\ell,:}|\mathbf{y}_{\ell,:},\mathbf{Z},\boldsymbol{b},\sigma^2,s^2,\bar{\mathbf{m}}_{\ell,:}) \propto \exp\left(-\frac{\|\mathbf{y}_{\ell,:}-\boldsymbol{t}_\ell\|^2}{2\sigma^2}\right) \times \exp\left(-\frac{\|\mathbf{m}_{\ell,:}-\bar{\mathbf{m}}_{\ell,:}\|^2}{2s^2}\right)\mathbf{1}_{(0,1)^R}(\mathbf{m}_{\ell,:}) \quad (17)$$

with $\boldsymbol{t}_\ell = \mathbf{A}^T\mathbf{m}_{\ell,:} + \text{diag}(\boldsymbol{b})\left[\left(\mathbf{A}^T\mathbf{m}_{\ell,:}\right)\odot\left(\mathbf{A}^T\mathbf{m}_{\ell,:}\right)\right]$. Thus, the rows of the endmember matrix $\mathbf{M}$ can be sampled independently similarly to the CHMC procedure described in the previous section by introducing the L potential energies associated with each $\mathbf{m}_{\ell,:}$ (see [11] for details).

4.3. Sampling the nonlinearity parameter vector $\boldsymbol{b}$

Using (13) and (14), it can be easily shown that the conditional distribution of $b_n|\mathbf{y}_n,\mathbf{M},\boldsymbol{z}_n,\sigma^2,w,\sigma_b^2$ is the following Bernoulli-Gaussian distribution

$$b_n|\mathbf{y}_n,\mathbf{M},\boldsymbol{z}_n,\sigma^2,w,\sigma_b^2 \sim (1-w_n^*)\delta(b_n) + w_n^*\mathcal{N}\left(\mu_n,s_n^2\right) \quad (18)$$

where

$$\mu_n = \frac{\sigma_b^2\left(\mathbf{y}_n-\mathbf{M}\boldsymbol{a}_n\right)^T\boldsymbol{h}_n}{\sigma_b^2\boldsymbol{h}_n^T\boldsymbol{h}_n+\sigma^2}, \quad s_n^2 = \frac{\sigma_b^2\sigma^2}{\sigma_b^2\boldsymbol{h}_n^T\boldsymbol{h}_n+\sigma^2}$$

and $\boldsymbol{h}_n = (\mathbf{M}\boldsymbol{a}_n)\odot(\mathbf{M}\boldsymbol{a}_n)$. Moreover,

$$w_n^* = \frac{w}{\beta_n+w(1-\beta_n)}, \quad \beta_n = \frac{\sigma_b}{s_n}\exp\left(-\frac{\mu_n^2}{2s_n^2}\right). \quad (19)$$

For each b_n, the conditional distribution (18) does not depend on $\{b_k\}_{k\neq n}$. Consequently, the nonlinearity parameters $\{b_n\}_{n=1,\ldots,N}$ can be sampled independently.

4.4. Sampling the noise variance σ^2

By considering the posterior distribution (13), it can be shown that $\sigma^2|\mathbf{Y},\mathbf{M},\mathbf{Z},\boldsymbol{b}$ is distributed according to the following inverse-gamma distribution

$$\sigma^2|\mathbf{Y},\mathbf{M},\mathbf{Z},\boldsymbol{b} \sim \mathcal{IG}\left(\frac{NL}{2},\frac{\text{tr}\left((\mathbf{Y}-\boldsymbol{X})^T(\mathbf{Y}-\boldsymbol{X})\right)}{2}\right) \quad (20)$$

with $\text{tr}(\cdot)$ the matrix trace, from which it is easy to sample.

4.5. Sampling the hyperparameters σ_b^2 and w

Looking carefully at the posterior distribution (13), it can be seen that $\sigma_b^2|\boldsymbol{b},\gamma,\nu$ is distributed according to the following inverse-gamma distribution

$$\sigma_b^2|\boldsymbol{b},\gamma,\nu \sim \mathcal{IG}\left(\frac{n_1}{2}+\gamma,\sum_{n\in I_1}\frac{b_n^2}{2}+\nu\right) \quad (21)$$

with $I_1 = \{n|b_n\neq 0\}$, $n_0 = \|\boldsymbol{b}\|_0$ (where $\|\cdot\|_0$ is the ℓ_0 norm, i.e., the number of elements of $\boldsymbol{b}$ that differ from zero) and $n_1 = N-n_0$. Similarly, we obtain

$$w|\boldsymbol{b} \sim \mathcal{B}e(n_1+1,n_0+1). \quad (22)$$

Of course, sampling according to (21) and (22) is straightforward.

The small number of sampling steps is due to the high parallelization properties of the procedure used to generate the N coefficient vectors $\{\boldsymbol{z}_n\}_{n=1,\ldots,N}$, the N nonlinearity parameters $\{b_n\}_{n=1,\ldots,N}$ and the L reflectance vectors $\{\mathbf{m}_{\ell,:}\}_{\ell=1,\ldots,L}$. After generating N_{MC} samples using the moves detailed above, the MMSE estimator of the unknown parameters can be approximated by computing the empirical averages of these samples, after an appropriate burn-in period[1]. The next section studies the performance of the proposed algorithm for synthetic hyperspectral images.

5. SIMULATIONS

The performance of the proposed SU algorithm is first evaluated by unmixing three synthetic images I_1, I_2, I_3 with $N = 2500$ pixels. The $R = 3$ endmembers observed at $L = 207$ different spectral bands and contained in these images have been extracted from the spectral libraries provided with the ENVI software. The first image I_1 has been generated using the LMM. The image I_2 has been generated according to the PPNMM and I_3 has been generated according to the generalized bilinear mixing model (GBM) presented in [5]. For each image, the abundance vectors have been randomly generated according to a uniform distribution in the admissible set defined by $\mathcal{S}_{\text{t}} = \left\{\boldsymbol{a}\left|0<a_r<0.9,\sum_{r=1}^R a_r=1\right.\right\}$ to ensure that there is no pure pixel in the images. All images have been corrupted by an i.i.d Gaussian noise sequence of variance $\sigma^2 = 10^{-4}$, corresponding to an average signal-to-noise ratio $\text{SNR}\simeq 21$dB for the three images. The nonlinearity coefficients are uniformly drawn in the set $[0,1]$ for the GBM. The parameters b_n have been generated uniformly in the set $[-0.3,0.3]$ for the PPNMM.

Different estimation procedures have been considered for the three mixing models. Two unmixing algorithms have been considered for the LMM. The first strategy extracts the endmembers using the N-FINDR algorithm [14] and estimates the abundances using the FCLS algorithm [15] (it is referred to as "SLMM" for supervised LMM). The second strategy is a Bayesian algorithm which jointly estimates the endmembers and the abundance matrix [10] (it is referred to as "ULMM" for unsupervised LMM). Two approaches have also been considered for the PPNMM. The first strategy uses the nonlinear endmember extraction algorithm (EEA) studied in [9] and the gradient-based approach based on the PPNMM studied in [6]

[1]The length of the burn-in period has been determined using appropriate convergence diagnoses [13].

for estimating the abundances and the nonlinearity parameters. This strategy is referred to as "SPPNMM" (supervised PPNMM). The second strategy is the proposed unmixing procedure referred to as "UPPNMM" (unsupervised PPNMM). The unmixing strategy used for the GBM is the EEA studied in [9] and the Bayesian algorithm presented in [5] for abundance estimation.

The quality of the unmixing procedures can be evaluated by the root normalized mean square error (RNMSE) defined by $\text{RNMSE} = \sqrt{\sum_{n=1}^{N} \|\hat{\boldsymbol{a}}_n - \boldsymbol{a}_n\|^2/(NR)}$, where $\boldsymbol{a}_n$ and $\hat{\boldsymbol{a}}_n$ are the actual and estimated abundance vectors for the nth pixel of the image. Table 1 shows the RNMSEs associated with the images I_1 to I_3 for the different estimation methods. These results show that the UPPNMM performs better (in term of RNMSE) than the other considered unmixing methods for the three images. Moreover, the proposed method provides similar results when compared with the ULMM for the linearly mixed image I_1.

The quality of endmember estimation is evaluated by the spectral angle mapper (SAM) defined by

$$\text{SAM} = \arccos\left(\frac{\langle \hat{\mathbf{m}}_r, \mathbf{m}_r \rangle}{\|\hat{\mathbf{m}}_r\| \, \|\mathbf{m}_r\|}\right)$$

where $\mathbf{m}_r$ is the rth actual endmember and $\hat{\mathbf{m}}_r$ its estimate. Table 2 compares the performance of the different endmember estimation algorithms using the SAM (averaged over the $R = 3$ endmembers (ASAM)). This table shows that the proposed UPPNMM yields accurate endmember estimations. Moreover, these results illustrate the robustness of the PPNMM regarding model mis-specification. Note that the ULMM and the UPPNMM provide similar results (in term of ASAM) for the image I_1 generated according to the LMM. Additional simulation results including reconstruction performance and simulations with different numbers of endmembers can be found in [11].

Table 1. Abundance RNMSEs ($\times 10^{-2}$): synthetic images.

		I_1 (LMM)	I_2 (PPNMM)	I_3 (GBM)
LMM	SLMM	3.78	13.21	6.83
	ULMM	0.66	10.87	4.21
PPNMM	SPPNMM	4.18	6.04	4.13
	UPPNMM	**0.37**	**0.81**	**1.38**
GBM		4.18	11.15	5.02

Table 2. SAMs ($\times 10^{-2}$): synthetic images.

	N-Findr	ULMM	Heylen	UPPNMM
I_1	4.95	0.52	6.38	**0.42**
I_2	7.44	8.23	7.92	**0.39**
I_3	7.46	4.66	7.19	**1.63**

6. CONCLUSIONS AND FUTURE WORK

We proposed a new hierarchical Bayesian algorithm for unsupervised nonlinear spectral unmixing of hyperspectral images. This algorithm assumed that each pixel of the image is a post-nonlinear mixture of the endmembers contaminated by additive Gaussian noise. Due to the complexity of the posterior distribution associated with the proposed Bayesian model, constrained Hamiltonian Monte Carlo moves were included into a Gibbs sampler to sample according to this posterior. The MMSE estimator of the unknown model parameters was then computed from the generated samples. Simulations conducted on synthetic data illustrated the interest of the proposed model for linear and nonlinear spectral unmixing and provided promising results. An important advantage of this model is its flexibility regarding the absence of pure pixels in the image. Future work includes the estimation of the number of endmembers contained in the image and mixed using the proposed post-nonlinear mixing model.

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