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Supervised Nonlinear Spectral Unmixing Using a Postnonlinear Mixing Model for Hyperspectral Imagery

Yoann Altmann, *Student Member, IEEE*, Abderrahim Halimi, *Student Member, IEEE*,
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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 nonlinear functions of pure spectral components contaminated by an additive white Gaussian noise. These nonlinear functions are approximated using polynomial functions leading to a polynomial postnonlinear mixing model. A Bayesian algorithm and optimization methods are proposed to estimate the parameters involved in the model. The performance of the unmixing strategies is evaluated by simulations conducted on synthetic and real data.

Index Terms—Hyperspectral imagery, postnonlinear model, spectral unmixing (SU).

I. INTRODUCTION

SPECTRAL UNMIXING (SU) is one of the major issues when analyzing hyperspectral images. SU consists of identifying the macroscopic materials present in an hyperspectral image and quantifying the proportions of these materials in the image pixels. Most SU strategies assume that pixel reflectances are linear combinations of pure component spectra [1]–[5]. The resulting linear mixing model (LMM) has been widely used in the literature and has provided interesting results. However, as explained in [6], the LMM can be inappropriate for some hyperspectral images, such as those containing sand, trees, or vegetation areas. Nonlinear mixing models provide an interesting alternative for overcoming the inherent limitations of the LMM. They have been proposed in the hyperspectral image literature for specific kinds of nonlinearities. More precisely, the bidirectional reflectance-based model proposed in [7] has been introduced for hyperspectral images including intimate mixtures. Conversely, the bilinear models recently studied in [8]–[11] address the problem of scattering effects, mainly observed in vegetation areas. Other more flexible unmixing techniques have been also proposed to handle a wider class of nonlinearity, including radial basis function networks [12], [13]

and kernel-based models [14], [15]. This paper considers a class of nonlinear mixing models referred to as *postnonlinear mixing models* (PNMMs). PNMMs are flexible generalizations of the standard LMMs that have been introduced in [16] and [17] for source separation problems. The main advantage of PNMMs is that they can accurately model many different nonlinearities (as will be shown in this paper). This paper addresses the problem of supervised SU of hyperspectral images using PNMMs. Note that “supervised” means that the endmembers contained in the image have been estimated by an endmember extraction algorithm (EEA). As a consequence, the only parameters to be estimated are the abundances and the nonlinearity coefficients for all pixels of the image. In the last decades, many EEAs have been developed to identify the pure spectral components contained in a hyperspectral image (the reader is invited to consult [18] for a recent review of these methods). Most EEAs implicitly rely on the LMM and might be inappropriate for nonlinear models such as PNMMs. However, as noticed in [6], geometric EEAs are still adapted to identify endmembers and can be reasonably employed when the mixing model involves nonlinearities. Therefore, this paper proposes to extract the endmembers contained in the hyperspectral image using a geometric EEA, known as *vertex component analysis* (VCA) [19]. The recent nonlinear EEA introduced in [20] is also considered. Once the endmembers have been extracted from the image, we propose to estimate the abundances and the nonlinearity parameters involved in the PNMM using estimation algorithms based on Bayesian and least-square (LS) methods.

In the Bayesian framework, appropriate prior distributions are chosen for the unknown PNMM parameters. The joint posterior distribution of these parameters is then derived. However, the classical Bayesian estimators cannot be easily computed from this joint posterior. To alleviate this problem, a Markov-chain Monte Carlo (MCMC) method is used to generate samples according to the posterior of interest. As in any Bayesian algorithm, the joint posterior distribution can be also used to compute confidence intervals for the parameter estimates. However, the resulting computational complexity can be too heavy for practical applications. In order to reduce this computational complexity, we propose to study LS methods that have already received considerable attention in the hyperspectral imagery [2], [10], [14]. A first method based on Taylor series expansions is proposed to iteratively solve the LS criterion associated with the PNMM observation model. The Taylor approximations allow quadratic optimization problems to be solved at each iteration.

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A second approach is based on a classical gradient method dedicated to constrained problems.

This paper is organized as follows: Section II introduces the PNM for hyperspectral image analysis. Section III presents a Bayesian unmixing algorithm associated with the proposed PNM. Section IV studies the two alternative unmixing algorithms based on LS methods. Some simulation results conducted on synthetic and real data are shown and discussed in Section V. Conclusions are finally reported in Section VI.

II. POLYNOMIAL PNM

This section defines the nonlinear mixing model used for hyperspectral image SU. More precisely, the L -spectrum $\mathbf{y} = [y_1, \dots, y_L]^T$ of a mixed pixel is defined as a nonlinear transformation \mathbf{g} of a linear mixture of R spectra \mathbf{m}_r contaminated by additive noise, i.e.,

$$\mathbf{y} = \mathbf{g} \left(\sum_{r=1}^R a_r \mathbf{m}_r \right) + \mathbf{n} = \mathbf{g}(\mathbf{M}\mathbf{a}) + \mathbf{n} \quad (1)$$

where $\mathbf{m}_r = [m_{r,1}, \dots, m_{r,L}]^T$ is the spectrum of the r th material present in the scene, a_r is its corresponding proportion, R is the number of endmembers contained in the image, and \mathbf{g} is an appropriate nonlinear function. Moreover, L is the number of spectral bands, and \mathbf{n} is an additive independent and identically distributed zero-mean Gaussian noise sequence with variance σ^2 , denoted as $\mathbf{n} \sim \mathcal{N}(\mathbf{0}_L, \sigma^2 \mathbf{I}_L)$, where \mathbf{I}_L is the $L \times L$ identity matrix. Note that the usual matrix and vector notations $\mathbf{M} = [\mathbf{m}_1, \dots, \mathbf{m}_R]$ and $\mathbf{a} = [a_1, \dots, a_R]^T$ have been used in the right-hand side of (1).

The choice of an appropriate nonlinearity \mathbf{g} deserves a specific attention. Polynomials, sigmoids, and combinations of polynomial and sigmoidal nonlinearities have shown interesting properties for source separation [17]. This paper focuses on second-order polynomial nonlinearities \mathbf{g}_b defined by

$$\mathbf{g}_b : [0, 1]^L \rightarrow \mathbb{R}^L \\ \mathbf{s} \mapsto [s_1 + bs_1^2, \dots, s_L + bs_L^2]^T \quad (2)$$

with $\mathbf{s} = [s_1, \dots, s_L]^T$. An interesting property of the resulting nonlinear model referred to as polynomial PNM (PPNM) is that it reduces to the classical LMM for $b = 0$. Thus, we can expect unmixing results at least as good as those presented in [21] and [2] where Bayesian and LS methods were investigated. Another motivation for using the PPM is the Weierstrass approximation theorem, which states that any continuous function defined on a bounded interval can be uniformly approximated by a polynomial with any desired precision [22, p. 15]. As explained in [9], it is reasonable to consider polynomials with first- and second-order terms (since higher order terms can generally be neglected), which leads to (2). Higher order terms could be considered in the presence of more than two reflections. However, the resulting interaction spectra are, in practice, of low amplitude and are hardly distinguishable from the noise. Straightforward computations allow the PPM observation vector (for a given pixel of the image) to be expressed as follows:

$$\mathbf{y} = \mathbf{g}_b(\mathbf{M}\mathbf{a}) + \mathbf{n} = \mathbf{M}\mathbf{a} + b(\mathbf{M}\mathbf{a}) \odot (\mathbf{M}\mathbf{a}) + \mathbf{n} \quad (3)$$

where \odot denotes the Hadamard (term-by-term) product. Note that the resulting PPM includes bilinear terms such as those considered in [8]–[11]. However, the nonlinear terms are characterized by a single amplitude parameter b , leading to a less complex model when compared with the models introduced in [8], [9], and [11]. Note that endmember \mathbf{m}_r (contained in \mathbf{M}) can be obtained in the noise free case ($\mathbf{n} = \mathbf{0}_L$) by setting $b = 0$ and $\mathbf{a} = [\mathbf{0}_{r-1}, 1, \mathbf{0}_{R-r}]^T$ in (3).

Due to physical considerations, the abundance vector \mathbf{a} satisfy the following positivity and sum-to-one constraints:

$$\sum_{r=1}^R a_r = 1, a_r \geq 0, \forall r \in \{1, \dots, R\}. \quad (4)$$

It is straightforward to show that the function $\mathbf{s} \mapsto \mathbf{g}_b(\mathbf{s})$ is noninjective for a fixed b . However, the unmixing problem is identifiable since the application

$$\mathbf{g} : \mathbb{R}^R \times \mathbb{R} \rightarrow \mathbb{R}^L \\ (\mathbf{a}, b) \mapsto \mathbf{M}\mathbf{a} + b(\mathbf{M}\mathbf{a}) \odot (\mathbf{M}\mathbf{a})$$

is injective under specific conditions related to the pure component spectra (see [23] for details).

III. BAYESIAN ESTIMATION

This section generalizes the hierarchical Bayesian model introduced in [21] to the PPM. The unknown parameter vector associated with the PPM contains the pixel abundances \mathbf{a} [satisfying constraints (4)], the nonlinearity parameter b , and the additive noise variance σ^2 . This section summarizes the likelihood and the parameter priors associated with the proposed hierarchical Bayesian PPM.

A. Likelihood

Equation (3) shows that $\mathbf{y}|\mathbf{a}, b, \sigma^2$ are distributed according to a Gaussian distribution with mean $\mathbf{g}_b(\mathbf{M}\mathbf{a})$ and covariance matrix $\sigma^2 \mathbf{I}_L$ (denoted as $\mathbf{y}|\mathbf{a}, b, \sigma^2 \sim \mathcal{N}(\mathbf{g}_b(\mathbf{M}\mathbf{a}), \sigma^2 \mathbf{I}_L)$). As a consequence, the likelihood function of the observation vector \mathbf{y} can be expressed as

$$f(\mathbf{y}|\mathbf{a}, b, \sigma^2) = \left(\frac{1}{2\pi\sigma^2} \right)^{\frac{L}{2}} \exp \left(-\frac{\|\mathbf{y} - \mathbf{g}_b(\mathbf{M}\mathbf{a})\|^2}{2\sigma^2} \right) \quad (5)$$

where $\|\mathbf{x}\| = \sqrt{\mathbf{x}^T \mathbf{x}}$ is the standard ℓ^2 norm.

B. Parameter Priors

In order to satisfy the sum-to-one constraint, the abundance vector can be rewritten¹ $\mathbf{a} = [\mathbf{a}_{\setminus R}, a_R]^T$ with $a_R = 1 - \sum_{r=1}^{R-1} a_r$ and where notation $\mathbf{a}_{\setminus R}$ indicates that the R th component of \mathbf{a} has been removed, i.e., $\mathbf{a}_{\setminus R} = [a_1, \dots, a_{R-1}]^T$. The positivity constraints in (4) impose that $\mathbf{a}_{\setminus R}$ belongs to the following simplex \mathcal{S}

$$\mathcal{S} = \left\{ \mathbf{a}_{\setminus R} \mid a_r \geq 0, \forall r \neq R, \sum_{r=1}^{R-1} a_r \leq 1 \right\}. \quad (6)$$

¹Note that the proposed parameterization is chosen for notation simplicity. However, the component to be discarded can be randomly chosen.

A uniform prior distribution on \mathcal{S} is chosen for $\mathbf{a}_{\setminus R}$ to reflect the absence of prior knowledge about the abundance vector. A Jeffreys prior is chosen for σ^2

$$f(\sigma^2) \propto \frac{1}{\sigma^2} \mathbf{1}_{\mathbf{R}^+}(\sigma^2) \quad (7)$$

which also reflects the absence of knowledge for this parameter (see [24] for details). A conjugate Gaussian prior is finally chosen for the nonlinearity parameter b , i.e.,

$$b|\sigma_b^2 \sim \mathcal{N}(0, \sigma_b^2). \quad (8)$$

The Gaussian prior is zero mean since the value of b can be equally likely positive or negative. Moreover, it favors small values of b and is a conjugate prior for parameter b , which will simplify the computations.

C. Hyperparameter Prior

The hyperparameter σ_b^2 is also included within the Bayesian model. A conjugate inverse-gamma prior is assigned to σ_b^2

$$\sigma_b^2 \sim \mathcal{IG}(\gamma, \nu) \quad (9)$$

where (γ, ν) are fixed to obtain a flat prior, reflecting the absence of knowledge about variance σ_b^2 [(γ, ν) will be set to $(1, 10^{-2})$ in the simulation section].

D. Posterior Distribution of $\boldsymbol{\theta}$

The joint posterior distribution of the unknown parameter vector $\boldsymbol{\theta} = \{\mathbf{a}_{\setminus R}, b, \sigma^2, \sigma_b^2\}$ can be computed using the following hierarchical structure:

$$f(\boldsymbol{\theta}|\mathbf{y}) \propto f(\mathbf{y}|\boldsymbol{\theta})f(\mathbf{a}_{\setminus R}, b, \sigma^2|\sigma_b^2)f(\sigma_b^2) \quad (10)$$

where \propto means ‘‘proportional to’’ and $f(\mathbf{y}|\boldsymbol{\theta})$ is defined in (5). By assuming that parameters σ^2 , b , and $\mathbf{a}_{\setminus R}$ are *a priori* independent, the joint prior distribution of the unknown parameter vector can be expressed as

$$f(\boldsymbol{\theta}) = f(\mathbf{a}_{\setminus R})f(\sigma^2)f(b|\sigma_b^2)f(\sigma_b^2). \quad (11)$$

The joint posterior distribution $f(\boldsymbol{\theta}, \sigma_b^2|\mathbf{y})$ can then be computed up to a multiplicative constant, i.e.,

$$f(\boldsymbol{\theta}|\mathbf{y}) \propto \frac{1}{\sigma^2} \left(\frac{1}{\sigma_b^2}\right)^{\frac{3}{2}+\gamma} f(\mathbf{y}|\mathbf{a}_{\setminus R}, \sigma^2, b) \times \exp\left(-\frac{b^2+2\nu}{2\sigma_b^2}\right) \mathbf{1}_{\mathcal{S}}(\mathbf{a}_{\setminus R}). \quad (12)$$

Unfortunately, it is difficult to obtain closed form expressions of the standard Bayesian estimators [including the maximum *a posteriori* (MAP) and the minimum mean square error (MMSE) estimators] associated with (12). The last part of this section studies an MCMC method that can be used to generate samples asymptotically distributed according to (12). These generated samples are then used to compute the MAP or MMSE estimators of the unknown parameter vector $\boldsymbol{\theta}$.

E. Metropolis-Within-Gibbs Sampler

The principle of the Gibbs sampler is to sample according to the conditional distributions of the posterior of interest [25, Chap. 10]. The probability density functions (pdf) associated with (12) are studied below.

1) *Conditional pdf* $f(a_r|\mathbf{y}, \boldsymbol{\theta}_{\setminus a_r})$: Straightforward computations lead to

$$f(a_r|\mathbf{y}, \boldsymbol{\theta}_{\setminus a_r}) \propto \exp\left(-\frac{\|\mathbf{y} - \mathbf{g}_b(\mathbf{M}\mathbf{a})\|^2}{2\sigma^2}\right) \mathbf{1}_{\mathcal{S}}(\mathbf{a}_{\setminus R}) \quad (13)$$

where $r = 1, \dots, R-1$. Since it is not easy to sample according to (13) [mainly because of the indicator function $\mathbf{1}_{\mathcal{S}}(\mathbf{a}_{\setminus R})$], we propose to update the abundance a_r using a Metropolis–Hasting move. More precisely, a new abundance coefficient is proposed following a Gaussian random walk procedure (the variance of the proposal distribution has been adjusted to obtain an acceptance rate close to 0.5, as recommended in [26, p. 8]). The generated abundance is accepted or rejected with an appropriate probability provided in Algorithm 1.

2) *Conditional pdf* $f(b|\mathbf{y}, \boldsymbol{\theta}_{\setminus b})$: Using (5), it can be easily shown that b is distributed according to the following Gaussian distribution:

$$b|\mathbf{y}, \boldsymbol{\theta}_{\setminus b} \sim \mathcal{N}(m_b, s_b^2) \quad (14)$$

where

$$m_b = \frac{\sigma_b^2(\mathbf{y} - \mathbf{M}\mathbf{a})^T \mathbf{h}(\mathbf{a})}{\sigma_b^2 \mathbf{h}(\mathbf{a})^T \mathbf{h}(\mathbf{a}) + \sigma^2} \quad s_b^2 = \frac{\sigma_b^2 \sigma^2}{\sigma_b^2 \mathbf{h}(\mathbf{a})^T \mathbf{h}(\mathbf{a}) + \sigma^2}$$

and $\mathbf{h}(\mathbf{a}) = (\mathbf{M}\mathbf{a}) \odot (\mathbf{M}\mathbf{a})$. As a consequence, sampling according to (14) is straightforward.

3) *Conditional pdf* $f(\sigma^2|\mathbf{y}, \boldsymbol{\theta}_{\setminus \sigma^2})$: Looking carefully at (12), it can be shown that $\sigma^2|\mathbf{y}, \boldsymbol{\theta}_{\setminus \sigma^2}$ is distributed according to the following inverse-gamma distribution:

$$\sigma^2|\mathbf{y}, \boldsymbol{\theta}_{\setminus \sigma^2} \sim \mathcal{IG}\left(\frac{L}{2}, \frac{\|\mathbf{y} - \mathbf{g}_b(\mathbf{M}\mathbf{a})\|^2}{2}\right) \quad (15)$$

from which it is easy to sample.

4) *Conditional pdf* $f(\sigma_b^2|\mathbf{y}, \boldsymbol{\theta}_{\setminus \sigma_b^2})$: Finally, by looking at the posterior distribution (12), it can be seen that $\sigma_b^2|\mathbf{y}, \boldsymbol{\theta}_{\setminus \sigma_b^2}$ is distributed according to the following inverse-gamma distribution:

$$\sigma_b^2|\mathbf{y}, \boldsymbol{\theta}_{\setminus \sigma_b^2} \sim \mathcal{IG}\left(\frac{1}{2} + \gamma, \frac{b^2}{2} + \nu\right). \quad (16)$$

The resulting Metropolis-within-Gibbs sampler used to sample according to (12) is summarized in Algorithm 1.

After generating samples using the procedures defined previously, the MMSE estimator of the unknown parameters can be approximated by computing the empirical averages of these samples, after an appropriate burn-in period.² Even if the sampling strategy has been observed to converge very fast, its computational complexity can be heavy for practical applications. The next section studies LS estimators, which allow this computational complexity to be significantly reduced.

²The length of the burn-in period has been determined using appropriate convergence diagnoses [26].

ALGORITHM 1

Gibbs Sampler

- 1: **Initialization** ($t = 0$)
 Sample $\mathbf{a}^{(0)}, b^{(0)}, \sigma^{2(0)}, \sigma_b^{2(0)}$ according to their prior distributions.
 - 2: **Iterations** ($t \geq 1$)
 - 3: Set $\mathbf{c} = [c_1, \dots, c_{R-1}]^T = \mathbf{a}_{\setminus R}^{(t-1)}$
 - 4: **for** $r = 1 : R - 1$ **do**
 - 5: Sample a candidate ζ_r using a Gaussian proposal distribution $\mathcal{N}(a_r^{(t-1)}, \sigma_r^2)$.
 Compute $\rho = \min \left\{ \frac{f(\zeta_r | \mathbf{y}, b, \mathbf{c}_{\setminus r}, \sigma^2, \sigma_b^2)}{f(c_r | \mathbf{y}, b, \mathbf{c}_{\setminus r}, \sigma^2, \sigma_b^2)}, 1 \right\}$
 Set $c_r = \begin{cases} \zeta_r & \text{with probability } \rho \\ c_r & \text{with probability } 1 - \rho \end{cases}$
 - 6: **end for**
 - 7: Set $\mathbf{a}_{\setminus R}^{(t)} = [c_1, \dots, c_{R-1}]^T$
 - 8: Set $a_R^{(t)} = 1 - \sum_{r=1}^{R-1} a_r^{(t)}$
 - 9: Sample $b^{(t)}$ from (14)
 - 10: Sample $\sigma^{2(t)}$ from (15)
 - 11: Sample $\sigma_b^{2(t)}$ from (16)
 - 12: Set $t = t + 1$.
-
-

IV. LS METHODS

LS methods have been successfully used for linear SU [2]. The LS method associated with the observation equation (3) consists of minimizing the following criterion:

$$J(\mathbf{a}, b) = \frac{1}{2} \|\mathbf{y} - \mathbf{g}_b(\mathbf{M}\mathbf{a})\|^2 = \frac{1}{2} \|\mathbf{y} - \mathbf{M}\mathbf{a} - b(\mathbf{M}\mathbf{a}) \odot (\mathbf{M}\mathbf{a})\|^2 \quad (17)$$

under the positivity and sum-to-one constraints (4). This optimization problem is not easy to handle mainly because of constraints (4). However, the cost function $J(\mathbf{a}, b)$ is quadratic with respect to parameter b . As a consequence, by differentiating $J(\mathbf{a}, b)$ with respect to b , the following closed-form expression for b can be obtained

$$b = \frac{(\mathbf{y} - \mathbf{M}\mathbf{a})^T \mathbf{h}(\mathbf{a})}{\mathbf{h}(\mathbf{a})^T \mathbf{h}(\mathbf{a})} = \beta(\mathbf{a}). \quad (18)$$

After replacing (18) in $J(\mathbf{a}, b)$, we obtain

$$J(\mathbf{a}) = J[\mathbf{a}, \beta(\mathbf{a})] = \frac{1}{2} \|\mathbf{y} - \phi(\mathbf{a})\|^2 \quad (19)$$

where

$$\phi(\mathbf{a}) = \mathbf{M}\mathbf{a} + \beta(\mathbf{a})(\mathbf{M}\mathbf{a}) \odot (\mathbf{M}\mathbf{a}). \quad (20)$$

We introduce below two strategies to compute the optimal abundance vector

$$\hat{\mathbf{a}} = \arg \min_{\mathbf{a}} J(\mathbf{a})$$

under constraints (4). Note that, once $\hat{\mathbf{a}}$ has been computed, the nonlinearity parameter b can be estimated as follows:

$$\hat{b} = \beta(\hat{\mathbf{a}}). \quad (21)$$

A. Taylor Approximation

Motivated by the method introduced in [10], we propose to approximate function $\phi(\cdot)$ defined in (20) using the first-order terms of a Taylor series expansion. Let $\mathbf{a}^{(t)}$ denotes the estimated abundance vector estimate at the t th iteration, and its corresponding estimated spectrum $\phi(\mathbf{a}^{(t)})$ following (20). The Taylor approximation of $\phi(\cdot)$ at $\mathbf{a}^{(t)}$ can be written

$$\phi(\mathbf{a}) \approx \phi(\mathbf{a}^{(t)}) + \nabla \phi(\mathbf{a}^{(t)}) (\mathbf{a} - \mathbf{a}^{(t)}) \quad (22)$$

where $\nabla \phi(\mathbf{a}^{(t)})$ is the gradient matrix of $\phi(\mathbf{a}^{(t)})$ of size $L \times R$ and \mathbf{a} is the unknown parameter vector to be estimated. The r th column of $\nabla \phi(\mathbf{a}^{(t)})$ can be derived from (3) as

$$\frac{\partial \phi(\mathbf{a})}{\partial a_r} = \mathbf{m}_r + \frac{\partial \beta(\mathbf{a})}{\partial a_r} \mathbf{h}(\mathbf{a}) + \beta(\mathbf{a}) \frac{\partial \mathbf{h}(\mathbf{a})}{\partial a_r} \quad (23)$$

where $r = 1, \dots, R$ and the partial derivatives of $\beta(\cdot)$ and $\mathbf{h}(\cdot)$ are available in [23]. Approximating $\phi(\cdot)$ in (19) using (22), vector $\mathbf{a}^{(t+1)}$ can be estimated by solving the following constrained LS problem:

$$\mathbf{a}^{(t+1)} = \arg \min_{\mathbf{a}} \left\| \mathbf{z}^{(t)} - \tilde{\mathbf{M}}^{(t)} \mathbf{a} \right\|^2 \quad (24)$$

under constraints (4), where

$$\mathbf{z}^{(t)} = \mathbf{y} - \phi(\mathbf{a}^{(t)}) + \nabla \phi(\mathbf{a}^{(t)}) \mathbf{a}^{(t)} \quad (25)$$

and $\tilde{\mathbf{M}}^{(t)} = \nabla \phi(\mathbf{a}^{(t)})$ is the $L \times R$ gradient matrix. Problem (24) can be finally solved by the FCLS algorithm [2]. More precisely, the sum-to-one constraint of the abundances is considered by penalizing (24), leading to

$$\mathbf{a}^{(t+1)} = \arg \min_{\mathbf{a}} \left[\left\| \mathbf{z}^{(t)} - \tilde{\mathbf{M}}^{(t)} \mathbf{a} \right\|^2 + \delta (1 - \mathbf{1}_R^T \mathbf{a})^2 \right] \quad (26)$$

subject to the nonnegativity constraints for the parameter vector \mathbf{a} , where $\delta \in \mathbb{R}^+$ controls the impact of the sum-to-one constraint. Procedure (26) is repeated until convergence. The convergence of this iterative procedure to the global minimum of the objective function (21) is difficult to prove because of constraints (4) in (24). The next section introduces an alternative subgradient-based algorithm whose convergence (to a local minimum of the associated objective function) is ensured.

B. Subgradient-Based Optimization

A gradient approach could be used to solve the cost function defined in (19) in the absence of constraints. However, the problem is more complicated when constraints (4) have to be considered. The estimation method studied in this section is based on a subgradient optimization (SO) algorithm [27, p. 339] that is appropriate for constrained problems. More precisely, subgradient-based optimization allows each abundance a_1, \dots, a_r to be independently updated. Due to the sum-to-one constraint of the abundance vector, the cost function (19) can be expressed as a function of $\mathbf{a}_{\setminus R}$ by setting $a_R = 1 - \sum_{r=1}^{R-1} a_r$. In that case, the cost function (19) can be rewritten as

$$\bar{J}(\mathbf{a}_{\setminus R}) = \frac{1}{2} \left\| \mathbf{y} - \bar{\phi}(\mathbf{a}_{\setminus R}) \right\|^2 \quad (27)$$

where

$$\bar{J}(\mathbf{a}_{\setminus R}) = J \left(a_1, \dots, a_{R-1}, 1 - \sum_{r=1}^{R-1} a_r \right) \quad (28)$$

$$\bar{\phi}(\mathbf{a}_{\setminus R}) = \phi \left(a_1, \dots, a_{R-1}, 1 - \sum_{r=1}^{R-1} a_r \right). \quad (29)$$

At a given point $\mathbf{a}_{\setminus R}$, the SO algorithm performs sequential line searches along directions d_r defined by the partial derivatives with respect to a_r (for $r = 1, \dots, R-1$), i.e.,

$$d_r = -\frac{\partial \bar{J}(\mathbf{a}_{\setminus R})}{\partial a_r} = \left[\mathbf{y} - \bar{\phi}(\mathbf{a}_{\setminus R}) \right]^T \frac{\partial \bar{\phi}(\mathbf{a}_{\setminus R})}{\partial a_r}$$

where the partial derivatives of $\bar{\phi}(\mathbf{a}_{\setminus R})$ are provided in [23]. Finally, the line search procedure solves the following problem:

$$\hat{\lambda}_r = \arg \min_{\lambda_r} \bar{J}(\mathbf{a}_{\setminus R} - \lambda_r \mathbf{u}_r) \quad (30)$$

where $\mathbf{u}_r = [0, \dots, \text{sign}(d_r), 0, \dots, 0]^T$ is a direction vector of size $(R-1) \times 1$, $0 \leq \lambda_r \leq \lambda_{r,M}$ and $\lambda_{r,M} \in \mathbb{R}^+$ (for $r = 1, \dots, R-1$) are upper bounds for the line search parameters. More precisely, upper bounding λ_r according to the rule

$$\lambda_{r,M} = \begin{cases} 0, & \text{if } d_r = 0 \\ a_r, & \text{if } d_r > 0 \\ a_r - \sum_{i=1, i \neq r}^{R-1} a_i, & \text{if } d_r < 0 \end{cases}$$

ensures that constraints (4) are satisfied. Problem (30) can be solved using the golden section method [27, p. 270]. The abundances are then updated component by component (see [23] for more details about the algorithm). Here again, the procedure is repeated until convergence. The next section presents the performance of the proposed algorithms on synthetic and real hyperspectral images.

V. SIMULATIONS

A. Synthetic Data

The performance of the proposed nonlinear SU algorithms is first evaluated by unmixing four synthetic images of size 50×50 pixels. The $R = 3$ endmembers contained in these images have been extracted from the spectral libraries provided with the ENVI software [28] (i.e., green grass, olive-green paint, and galvanized steel metal). The first synthetic image I_1 has been generated using the standard LMM. A second image I_2 has been generated according to the bilinear mixing model introduced in [10], referred to as ‘‘Fan model’’ (FM). A third image I_3 has been generated according to the generalized bilinear mixing model (GBM) presented in [11], whereas a fourth image I_4 has been generated according to the PNM. For each image, the abundance vectors \mathbf{a}_p , $p = 1, \dots, 2500$, have been randomly generated according to a uniform distribution over the admissible set defined by the positivity and sum-to-one constraints. All images have been corrupted by an additive white Gaussian noise of variance $\sigma^2 = 2.8 \times 10^{-3}$, corresponding to a signal-to-noise ratio $\text{SNR} = L^{-1} \sigma^{-2} \|\mathbf{g}_b(\mathbf{a})\|^2 \simeq 15$ dB. The nonlinearity coefficients are uniformly drawn in the set $(0, 1)$ for the GBM, and parameter b has been uniformly generated in the set $(-0.3, 0.3)$ for the PNM. Different estimation procedures have been considered for the four mixing models.

- 1) For the LMM, we have considered the standard FCLS algorithm [2] and the Bayesian algorithm of [21].
- 2) The FM has been unmixed using the LS method introduced in [10] and a Bayesian algorithm similar to the one derived in [11] but assuming all the nonlinearity coefficients are equal to 1.
- 3) The unmixing strategies used for the GBM are the three algorithms presented in [29], i.e., a Bayesian algorithm and two LS methods.

TABLE I
ABUNDANCE RMSEs ($\times 10^{-2}$): SYNTHETIC IMAGES

		I_1 (LMM)	I_2 (FM)	I_3 (GBM)	I_4 (PPNMM)
LMM	Bayesian [21]	<u>1.58</u>	27.54	15.16	18.88
	FCLS [2]	<u>1.58</u>	24.72	9.49	16.87
FM	Bayesian	22.67	1.51	13.63	16.84
	Taylor [10]	22.67	1.49	12.61	26.33
GBM	Bayesian [29]	3.24	17.49	9.09	16.18
	Taylor [29]	6.32	14.67	7.07	15.61
	Gradient [29]	4.28	4.26	3.01	15.05
PPNMM	Bayesian	2.75	3.43	3.22	2.93
	Taylor	2.70	3.83	3.26	3.33
	Gradient	2.93	3.43	3.43	2.93

4) The Bayesian and LS algorithms presented in Sections III and IV have been used for unmixing the proposed PPNMM. Note that all results presented in this paper have been obtained using the Bayesian MMSE estimator.

The quality of the unmixing procedures can be measured by comparing the estimated and actual abundance vector using the root mean square error (RMSE) defined by

$$\text{RMSE} = \sqrt{\frac{1}{P} \sum_{p=1}^P \|\hat{\mathbf{a}}_p - \mathbf{a}_p\|^2} \quad (31)$$

where \mathbf{a}_p and $\hat{\mathbf{a}}_p$ are the actual and estimated abundance vectors for the p th pixel of the image and P is the number of image pixels. Table I shows the RMSEs associated with images I_1, \dots, I_4 for the different estimation procedures. Note that the best results (in terms of RMSE) for each image have been represented in underlined bold, whereas the second best results have been depicted in bold. Table I shows that the abundances estimated by the Bayesian algorithm and the LS methods are similar for the PPNMM. Moreover, for these four images, the PPNMM seems to be more robust than the other mixing models to deviations from the actual model. Indeed, the PPNMM provides small abundance RMSEs for the four images I_1, \dots, I_4 .

The unmixing quality can be also evaluated by the reconstruction error (RE) defined as

$$\text{RE} = \sqrt{\frac{1}{PL} \sum_{p=1}^P \|\hat{\mathbf{y}}_p - \mathbf{y}_p\|^2} \quad (32)$$

where \mathbf{y}_p is the p th observation vector and $\hat{\mathbf{y}}_p$ is its estimate. Table II compares the REs obtained for the different synthetic images. These results show that the REs are close for the different unmixing algorithms. Again, the proposed PPNMM seems to be more robust than the other mixing models to deviations from the actual model in terms of RE.

Fig. 1 shows the estimated distributions of b for images I_1, \dots, I_4 using the three presented algorithms (i.e., Bayesian, linearization, and subgradient). This figure shows that the algorithms similarly perform for the estimation of the nonlinearity parameter b .

Table III shows the execution times of MATLAB implementations on a 1.66-GHz Dual Core of the proposed algorithms for unmixing the proposed images (2500 pixels for each image). The linearization-based algorithm has the lowest computational

TABLE II
RES ($\times 10^{-2}$): SYNTHETIC IMAGES

		I_1 (LMM)	I_2 (FM)	I_3 (GBM)	I_4 (PPNMM)
LMM	Bayesian [21]	<u>5.28</u>	6.54	5.65	5.89
	FCLS [2]	<u>5.28</u>	5.74	5.42	5.48
FM	Bayesian	5.61	5.29	5.38	5.76
	Taylor [10]	5.61	5.28	5.38	5.75
GBM	Bayesian [29]	5.29	5.49	5.33	5.44
	Taylor [29]	5.31	5.40	5.30	5.42
	Gradient [29]	5.29	5.30	5.28	5.41
PPNMM	Bayesian	<u>5.28</u>	5.29	5.28	5.28
	Taylor	5.29	5.29	5.28	5.28
	Gradient	5.29	5.29	5.28	5.28

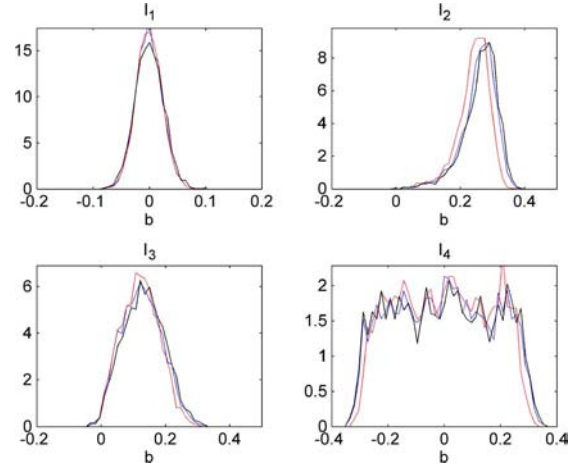


Fig. 1. Histograms of the estimated nonlinearity parameter \hat{b} for the four synthetic images estimated by the (black) Bayesian, (red) linearization-based and (blue) subgradient-based algorithms.

TABLE III
COMPUTATIONAL TIMES OF THE UNMIXING ALGORITHMS FOR 2500 PIXELS
(IN SECOND)

	I_1	I_2	I_3	I_4
Bayesian	5960	6200	6600	5970
Taylor	5	10	8	7
Subgradient	84	102	96	101

cost and also provides accurate estimations. Note that the computational cost of the Bayesian algorithm (which allows prior knowledge to be included in the unmixing procedure) can be prohibitive for larger images and a high number of endmembers. However, the computational cost of the two proposed optimization methods (linearization and gradient based) is very reasonable, which make them very useful for practical applications.

The next set of simulations analyzes the performance of the proposed nonlinear SU algorithms for different numbers of endmembers ($R \in \{3, 6, 9, 12\}$) by unmixing four synthetic images of 500 pixels. The endmembers contained in these images have been randomly selected from the 14 endmembers extracted by VCA from the full Cuprite scene described in [30]. For each image, the abundance vectors \mathbf{a}_p , ($p = 1, \dots, 500$), have been randomly generated according to a uniform distribution over the admissible set defined by the positivity and sum-to-one constraints. All images have been corrupted by an additive white

TABLE IV
AVERAGE RMSES ($\times 10^{-2}$): SYNTHETIC IMAGES

	Bayesian		Taylor	Gradient
	MMSE	MAP		
R=3	12.99	18.06	16.34	16.31
R=6	18.46	27.86	30.99	29.79
R=9	17.07	28.68	35.69	34.24
R=12	16.38	27.98	38.66	36.66

TABLE V
AVERAGE RES ($\times 10^{-2}$): SYNTHETIC IMAGES

	Bayesian		Taylor	Gradient
	MMSE	MAP		
R=3	4.18	4.22	4.17	4.17
R=6	4.22	4.24	4.20	4.20
R=9	4.27	4.29	4.24	4.24
R=12	4.18	4.19	4.13	4.13

Gaussian noise corresponding to a signal-to-noise ratio SNR = 20 dB. The nonlinearity coefficient b is uniformly drawn in the set $(-0.3, 0.3)$. Tables IV and V compare the performance of the three proposed methods in terms of abundance estimation and RE. These results show that the three methods similarly perform in terms of RE. The Bayesian estimators tend to provide more accurate abundance estimations (i.e., smaller RMSEs) for large values of R . Indeed, the Taylor and gradient algorithms may be trapped in local minima of the LS criterion (17) for large values of R .

B. Real Data

The first real image considered in this section is composed of $L = 189$ spectral bands and was acquired in 1997 by the airborne visible infrared imaging spectrometer (AVIRIS) over the Cuprite mining site in Nevada. A subimage of size 50×50 pixels has been chosen here to evaluate the proposed unmixing procedures. The scene is mainly composed of muscovite, alunite, and kaolinite, as explained in [31]. The endmembers extracted by VCA [19] and the nonlinear EEA proposed in [20] (referred to as ‘‘Heylen’’), with $R = 3$, are depicted in Fig. 2. The endmembers obtained by the two methods have similar shapes. This result confirms the fact that the geometric EEAs (such as VCA) can be used as a first approximation for endmember estimation [6]. The estimation algorithms presented in Sections III and IV have been applied to each pixel of the scene using the endmembers extracted by the two EEAs. Examples of abundance maps obtained for endmembers estimated using Heylen’s method are presented in Fig. 3 (see [23] for similar results obtained with endmembers estimated by VCA). The advantage of the PPNMM is that it allows the nonlinearities between the observations and the abundance vectors to be analyzed. For instance, Fig. 4 shows the estimated maps of b for the Cuprite image. These results show that the observations are nonlinearly related to the endmembers (since $b \neq 0$). However, the nonlinearity is weak since the estimated values of b are close to 0.

The second real image considered in this section is composed of $L = 189$ spectral bands and was acquired in 1997 by the satellite AVIRIS over the Moffett Field, CA. A subimage of size

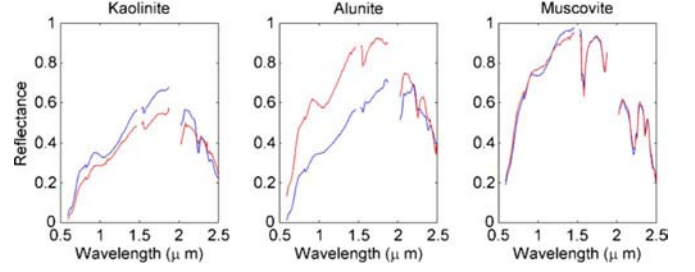


Fig. 2. $R = 3$ endmembers estimated by (blue lines) VCA and (red lines) Heylen for the Cuprite scene.

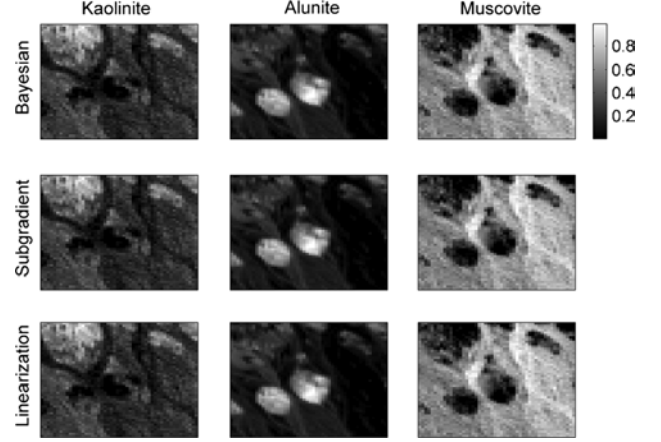


Fig. 3. Abundance maps estimated by the Bayesian, linearization, and subgradient methods for the Cuprite scene.

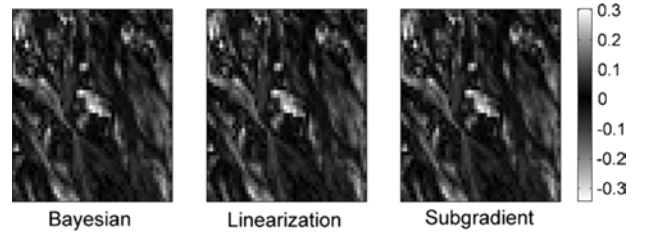


Fig. 4. Maps of the nonlinearity parameter b estimated by the Bayesian, linearization, and subgradient methods for the Cuprite scene.

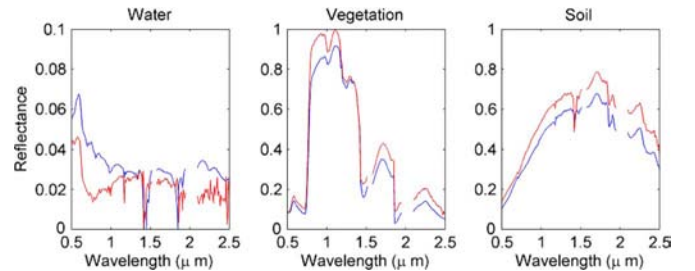


Fig. 5. $R = 3$ endmembers estimated by (blue lines) VCA and (red lines) Heylen for the Moffett scene.

50×50 pixels has been also chosen here to evaluate the proposed unmixing procedures. The scene is mainly composed of water, vegetation, and soil. The endmembers extracted by VCA and the Heylen’s method with $R = 3$ are depicted in Fig. 5. Again, the endmembers obtained by the two methods are similar. Examples of abundance maps estimated by the proposed

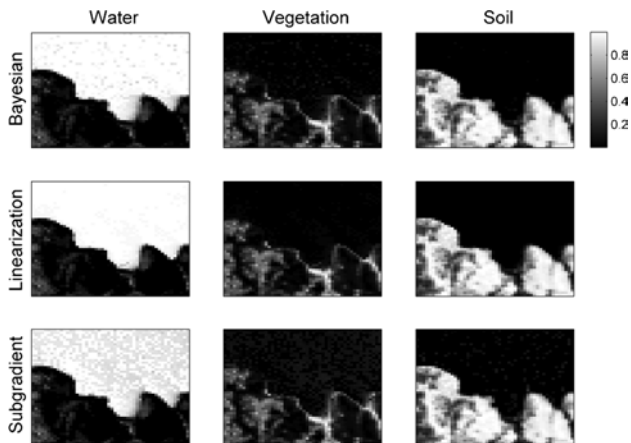


Fig. 6. Abundance maps estimated by the Bayesian, linearization, and subgradient methods for the Moffett scene.

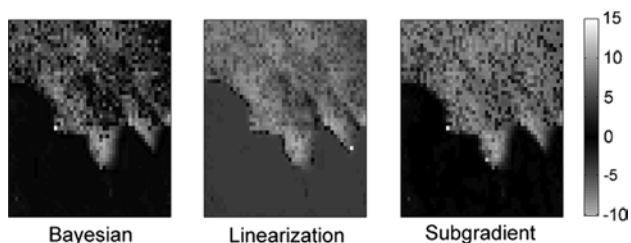


Fig. 7. Maps of the nonlinearity parameter b estimated by the Bayesian, linearization, and subgradient methods for the Moffett scene.

TABLE VI
RES ($\times 10^{-2}$): CUPRITE AND MOFFETT IMAGES

		VCA		Heylen	
		Cuprite	Moffett	Cuprite	Moffett
LMM	Bayesian [21]	2.14	2.70	2.35	2.02
	FCLS [2]	2.11	2.62	2.10	2.00
FM	Bayesian	7.36	2.31	2.30	1.92
	Taylor [10]	3.05	2.29	2.29	1.92
GBM	Bayesian [29]	2.24	2.57	2.11	1.99
	Taylor [29]	2.34	2.41	2.03	2.01
	Gradient [29]	2.02	2.30	2.04	1.93
PPNMM	Bayesian	1.19	1.59	1.91	1.85
	Taylor	1.19	1.54	1.90	1.84
	Gradient	1.19	1.55	1.90	1.87

algorithms are presented in Fig. 6 (endmembers have been estimated using Heylen's method). They are similar to the abundance maps obtained with estimation algorithms associated with the LMM (available in [21]). Fig. 7 shows the estimated maps of b for the Moffett image. In the water area, the observations are nonlinearly related to the endmembers (since $b \neq 0$). These nonlinearities can be due to the low amplitude of the water spectrum and possible nonlinear bathymetric effects.

The quality of unmixing is finally evaluated using the REs for both real images. These REs are compared in Table VI with those obtained by assuming other mixing models. The proposed PPNMM provides smaller REs when compared with other models, which is a very encouraging result. Additional results on the full Cuprite scene are available in [23].

VI. CONCLUSION AND FUTURE WORKS

A Bayesian and two least squares algorithms were presented for nonlinear spectral unmixing of hyperspectral images. These algorithms assumed that the hyperspectral image pixels are related to the endmembers by a polynomial post-nonlinear mixing model. In the Bayesian framework, the constraints related to the unknown parameters were ensured by using appropriate prior distributions. The posterior distribution of the unknown parameter vector was then derived. The corresponding minimum mean square error estimator was approximated from samples generated using Markov chain Monte Carlo methods. Least squares methods were also investigated for unmixing the PPNMM. These methods provided results similar to the Bayesian algorithm with a reduced computational cost, making them very attractive for hyperspectral image unmixing. Results obtained on synthetic and real images illustrated the accuracy of the PPNMM and the performance of the corresponding estimation algorithms. Future works include the study of nonlinear EEAs appropriate for the proposed parametric PPNMM. Deriving nonlinearity detectors based on the proposed parametric PPNMM is also under investigation.

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