A REVERSIBLE-JUMP MCMC ALGORITHM FOR ESTIMATING THE NUMBER OF ENDMEMBERS IN THE NORMAL COMPOSITIONAL MODEL. APPLICATION TO THE UNMIXING OF HYPERSPECTRAL IMAGES.

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ABSTRACT

In this paper, we address the problem of unmixing hyperspectral images in a semi-supervised framework using the normal compositional model recently introduced by Eismann and Stein. Each pixel of the image is modeled as a linear combination of random *endmembers*. More precisely, endmembers are modeled as Gaussian vectors whose means belong to a known spectral library. This paper proposes to estimate the number of endmembers involved in the mixture, as well as the mixture coefficients (referred to as *abundances*) using a trans-dimensional algorithm. Appropriate prior distributions are assigned to the abundance vector (to satisfy constraints inherent to hyperspectral imagery), the noise variance and the number of components involved in the mixture model. The computational complexity of the resulting posterior distribution is alleviated by constructing an hybrid Gibbs algorithm which generates samples distributed according to this posterior distribution. As the number of endmembers is unknown, the sampler has to jump between spaces of different dimensions. This is achieved by a reversible jump Markov chain Monte Carlo method that allows one to handle the model order selection problem. The performance of the proposed methodology is evaluated thanks to simulations conducted on synthetic data.

Index Terms— Bayesian inference, Monte Carlo methods, reversible jump, spectral unmixing, hyperspectral images, normal compositional model.

1. INTRODUCTION

Spectral unmixing is a mandatory step in the analysis of hyperspectral images that has received much attention in the signal and image processing community (see [1] and references therein). It consists of decomposing a pixel spectrum of the image into a mixture of pure material spectra whose fractions (i.e., proportions) are referred to as abundances. The linear mixing model (LMM) is the most frequent observation model used in the community for spectral unmixing [1]. It assumes that the L-spectrum $\boldsymbol{y} = [y_1, \ldots, y_L]^T$ of a mixed pixel is modeled as

$$\boldsymbol{y} = \sum_{r=1}^{R} \boldsymbol{m}_r \alpha_r + \boldsymbol{n} \tag{1}$$

where $\boldsymbol{m}_r = [m_{r,1}, \ldots, m_{r,L}]^T$ denotes the spectrum of the r^{th} material (referred to as endmember), α_r is the fraction of the r^{th} material in the pixel (referred to as abundance), R is the number of pure materials present in the observed scene and L is the number of available spectral bands for the image. Due to obvious physical considerations, the abundances satisfy the following positivity and sum-to-one constraints

$$\begin{cases} \alpha_r \geq 0, \ \forall r = 1, \ldots, R \\ \sum_{r=1}^{R} \alpha_r = 1. \end{cases} \tag{2}$$

However, the LMM has shown some limitations for real images [1]. Indeed, the endmember extraction algorithms (EEA) (such as the N-FINDR [2], the vertex component analysis (VCA) [3] and the pixel purity index (PPI) [4]) based on the LMM can be inefficient when the image does not contain enough pure pixels [3].

An alternative model referred to as normal compositional model (NCM), recently proposed in [5], allows one to alleviate the problem mentioned above. In this model, the pixels of the hyperspectral image are linear combinations of random endmembers with known means (e.g., resulting from an EEA) providing more flexibility regarding the observed pixels and the endmembers. The NCM has been defined by the following mixture

$$\boldsymbol{y} = \sum_{r=1}^{R} \boldsymbol{\varepsilon}_r \alpha_r \tag{3}$$

where the $\boldsymbol{\varepsilon}_r$ are independent Gaussian vectors with known means extracted from a spectral library or estimated by an EEA. The covariance matrix of each endmember is assumed to be $\sigma^2 \boldsymbol{I}_L$, where $\boldsymbol{I}_L$ is the $L \times L$ identity matrix and σ^2 is the endmember variance in any spectral band[1].

This paper considers the scenario where the number of endmembers R participating in the mixture model is unknown. A model selection algorithm was recently studied to estimate the number of endmembers in the LMM model [7]. Due to the LMM limitations mentioned above, we propose here to adapt this algorithm to the NCM, assuming the endmember means in (3) belong to a given spectral library. Note that the nature and the number of endmember participating in the NCM are unknown. The algorithm is referred to as "semi-supervised" to reflect the partial knowledge about the endmembers present in the NCM mixture (the only assumption is that the endmembers belong to a known library). The proposed strategy relies on a hierarchical Bayesian model. Appropriate prior distributions are chosen for the NCM parameters, including the number of endmembers R. A vague prior distribution is also assigned to the hyperparameter involved in the NCM to define a hierarchical Bayesian model. The unknwon parameters and hyperparameter of the resulting model are then jointly estimated using their full posterior distribution. This distribution is too complex to derive closed-form expressions of the Bayesian estimators. Furthermore, the dimension of the abundance vector and endmember means depends on the unknown number R of endmembers involved in the mixture. Therefore, a reversible jump Markov Chain Monte Carlo (RJ-MCMC) algorithm [8] is proposed to generate samples distributed according to the posterior of interest. This dimension matching strategy allows moves between parameter spaces with different dimensions which is clearly relevant for the proposed unmixing problem.

[1]This assumption might be relaxed to handle colored noise, as in [6].

This paper is organized as follows. Section 2 derives the posterior distribution of the unknown parameter vector resulting from the NCM. Section 3 studies the RJ-MCMC sampling strategy that is used to generate samples distributed according to this posterior and to solve the model selection problem. Simulation results conducted on synthetic data are presented in Section 4. Conclusions are reported in Section 5.

2. HIERARCHICAL BAYESIAN MODEL

This section introduces the likelihood and the priors inherent to the proposed NCM for the spectral unmixing of hyperspectral images. A particular attention is devoted to the unknown number R of endmembers, and to the positivity and sum-to-one constraints for the abundances.

2.1. Likelihood

The NCM assumes that the endmembers $\boldsymbol{\varepsilon}_r$, $r = 1, ..., R$, are independent Gaussian vectors whose means belong to a known spectral library $\mathcal{S} = \{\boldsymbol{s}_1, \ldots, \boldsymbol{s}_{R_{\max}}\}$ ($\boldsymbol{s}_r$ representing the L-spectrum $[s_{r,1}, \ldots, s_{r,L}]^T$ of the rth material). Moreover, this paper assumes that the endmember spectrum components are independent from one band to another, i.e. $\boldsymbol{\varepsilon}_r|\boldsymbol{m}_r, \sigma^2 \sim \mathcal{N}(\boldsymbol{m}_r, \sigma^2\boldsymbol{I}_L)$ where $\boldsymbol{m}_r = [m_{r,1}, \ldots, m_{r,L}]^T$ is the mean vector of $\boldsymbol{\varepsilon}_r$, $\sigma^2\boldsymbol{I}_L$ is its covariance matrix and $\mathcal{N}(\boldsymbol{m}, \boldsymbol{\Sigma})$ denotes the Gaussian distribution with mean vector $\boldsymbol{m}$ and covariance matrix $\boldsymbol{\Sigma}$. Note that the number of components R, as well as the spectra involved in the mixture are unknown. Following the NCM (3) and the independence between the endmembers, the likelihood of the observed pixel $\boldsymbol{y}$ is

$$f\left(\boldsymbol{y}\,|\boldsymbol{\alpha}^+, \sigma^2, R, \boldsymbol{M}\right) = \frac{1}{\left[2\pi\sigma^2 c\left(\boldsymbol{\alpha}^+\right)\right]^{\frac{L}{2}}} \exp\left(-\frac{\|\boldsymbol{y} - \mu\left(\boldsymbol{\alpha}^+\right)\|^2}{2\sigma^2 c\left(\boldsymbol{\alpha}^+\right)}\right) \quad (4)$$

where $\|\boldsymbol{x}\| = \sqrt{\boldsymbol{x}^T\boldsymbol{x}}$ is the standard ℓ^2 norm, $\boldsymbol{\alpha}^+ = [\alpha_1, \ldots, \alpha_R]^T$, $\boldsymbol{M} = [\boldsymbol{m}_1, \ldots, \boldsymbol{m}_R]$ contains the endmember defining the mixture (3), $\mu\left(\boldsymbol{\alpha}^+\right) = \sum_{r=1}^R \boldsymbol{m}_r\alpha_r$ and $c\left(\boldsymbol{\alpha}^+\right) = \sum_{r=1}^R \alpha_r^2$. Note that the variance of this Gaussian distribution depends on the abundance vector $\boldsymbol{\alpha}^+$ contrary to the classical LMM. Note also that the dimensions of $\boldsymbol{\alpha}^+$ and $\boldsymbol{M}$ (via the quantities $\mu\left(\boldsymbol{\alpha}^+\right)$ and $c\left(\boldsymbol{\alpha}^+\right)$) depend on the unknown number of endmembers R.

2.2. Parameter priors

2.2.1. Endmember priors

A discrete uniform distribution on $[1, \ldots, R_{\max}]$ is chosen as prior distribution for the number of mixture components R

$$P(R = k) = \frac{1}{R_{\max}}, \quad k = 1, \ldots, R_{\max} \quad (5)$$

where $R_{\max}$ is the maximum number of pure elements that can be present in a pixel. Note that this uniform prior distribution does not favor any model order among $[1, \ldots, R_{\max}]$.

All combinations of R spectra belonging to the library $\mathcal{S}$ are assumed to be equiprobable conditionally upon the number of endmembers R leading to

$$P(\boldsymbol{M} = [\boldsymbol{s}_{i_1}, \ldots, \boldsymbol{s}_{i_R}]\,|R) = \binom{R_{\max}}{R}^{-1} \quad (6)$$

where $i_1, \ldots, i_R$ is an unordered sequence of R distinct elements of $[1, \ldots, R_{\max}]$.

2.2.2. Abundance prior

Because of the sum-to-one constraint inherent to the mixing model, the abundance vector is split into two part as $\boldsymbol{\alpha}^+ = \left[\boldsymbol{\alpha}^T, \alpha_R\right]^T$ with $\alpha_R = 1 - \sum_{r=1}^{R-1}\alpha_r$. To satisfy the positivity constraint, the abundance vector $\boldsymbol{\alpha}$ belongs to a simplex defined by

$$\mathbb{S} = \left\{\boldsymbol{\alpha} \;\middle|\; \alpha_r \geq 0, \forall r = 1, \ldots, R-1, \sum_{r=1}^{R-1}\alpha_r \leq 1\right\}. \quad (7)$$

A uniform distribution on this simplex is chosen as prior distribution for the partial abundance vector $\boldsymbol{\alpha}$

$$f(\boldsymbol{\alpha}|R) \propto \mathbf{1}_{\mathbb{S}}(\boldsymbol{\alpha}) \quad (8)$$

where $\propto$ means "proportional to" and $\mathbf{1}_{\mathbb{S}}(.)$ is the indicator function defined on the set $\mathbb{S}$. This prior ensures the positivity and sum-to-one constraints of the abundance coefficients and reflects the absence of other prior knowledge about these parameters.

2.2.3. Endmember variance prior

The prior distribution for the variance σ^2 is chosen as a conjugate inverse Gamma distribution

$$\sigma^2|\delta \sim \mathcal{IG}(\nu, \delta) \quad (9)$$

where ν and δ are the shape and scale parameters [9]. This paper classically assumes $\nu = 1$ (as in [10]) and estimates δ within a hierarchical Bayesian framework. Such approach require to define a prior distribution for the hyperparameter δ. This paper assumes that the prior of δ is a non-informative Jeffreys' prior defined by

$$f(\delta) \propto \frac{1}{\delta}\mathbf{1}_{\mathbb{R}^+}(\delta). \quad (10)$$

This prior reflects the lack of knowledge regarding δ.

2.3. Posterior distribution

The joint posterior distribution of the unknown parameter vector $\boldsymbol{\theta} = \left\{\boldsymbol{\alpha}, \sigma^2, \boldsymbol{M}, R\right\}$ and hyperparameter δ can be easily computed using the Bayes' rule, leading to

$$f(\boldsymbol{\theta}, \delta|\boldsymbol{y}) \propto \frac{\Gamma(R+1)\Gamma(R_{\max} - R + 1)}{R_{\max}\Gamma(R_{\max}+1)} \times \frac{1}{c\left(\boldsymbol{\alpha}^+\right)^{\frac{L}{2}}} \frac{1}{\sigma^{L+2}} \exp\left(-\frac{\|\boldsymbol{y} - \boldsymbol{\mu}(\boldsymbol{\alpha})\|^2}{2\sigma^2 c(\boldsymbol{\alpha})} - \delta\right) \mathbf{1}_{\mathbb{S}}(\boldsymbol{\alpha})\mathbf{1}_{\mathbb{R}^+}(\delta). \quad (11)$$

The posterior distribution (11) is too complex to derive the minimum mean squared error (MMSE) or maximum *a posteriori* (MAP) estimators of the unknown parameter vector $\boldsymbol{\theta}$. In particular, the dimension of $\boldsymbol{\theta}$ is unknown and depends on the number of endmembers R. RJ-MCMC methods provide efficient algorithms to generate samples according to a posterior distribution with unknown dimension (see [9] and [8]). The next section presents an RJ-MCMC method that generates samples distributed according to the joint posterior (11). These samples will be used to compute the Bayesian estimators associated to the NCM allowing one in particular to estimate the number of endmembers participating in the mixture (3).

3. REVERSIBLE JUMP MCMC ALGORITHM

A stochastic simulation algorithm is proposed to sample according to $f(\boldsymbol{\alpha}, \sigma^2, \boldsymbol{M}, R, \delta|\boldsymbol{y})$. The vectors to be sampled belong to a space whose dimension depends on R, requiring to use a dimension matching strategy as in [11]. More precisely, the proposed algorithm, consists of four different moves

1. updating the means of endmembers in the matrix $\boldsymbol{M}$,
2. updating the abundance vector $\boldsymbol{\alpha}$,
3. updating the variance σ^2,
4. updating the hyperparameter δ.

These steps are scanned systematically as in [11] and are briefly presented below.

3.1. Updating the endmember matrix M

In a first step, we propose three moves to update the endmember means involved in the mixture. The two first moves (referred to as "birth", "death") consist of increasing or decreasing the number of pure components R by 1, using the RJ-MCMC method introduced by Green [8]. The third move (referred to as "switch" move) replaces a selected spectrum by another member from the library, requiring the use of a standard Metropolis-Hastings (MH) acceptance procedure. Assume that at iteration t, the current model is defined by $(\boldsymbol{\alpha}^{(t)}, \boldsymbol{M}^{(t)}, R^{(t)})$. The "birth", "death" and "switch" moves are randomly chosen with probabilities $b_{R^{(t)}}$,$d_{R^{(t)}}$ and $u_{R^{(t)}}$ that follow three conditions[2]

- $b_{R^{(t)}} + d_{R^{(t)}} + u_{R^{(t)}} = 1$,
- $d_1 = 0$ (a *death* move is not allowed for $R = 1$),
- $b_{R_{\max}} = 0$ (a *birth* move is impossible for $R = R_{\max}$),

As a result, $b_{R^{(t)}} = d_{R^{(t)}} = u_{R^{(t)}} = \frac{1}{3}$ for $R \in \{2, R_{\max} - 1\}$ and $b_1 = d_{R_{\max}} = u_1 = u_{R_{\max}} = \frac{1}{2}$.
The acceptance probabilities of the *birth* and *death* move are $\rho = \min\{1, A_b\}$ and $\rho = \min\{1, A_d\}$ with

$$A_{\mathrm{b}} = \left[\frac{c(\boldsymbol{\alpha}^{(t)})}{c(\boldsymbol{\alpha}^*)}\right]^{\frac{L}{2}} \frac{d_{R^{(t)}+1}}{b_{R^{(t)}}} \frac{R^{(t)}}{g_{1,R^{(t)}}(w^*)} (1 - w^*)^{R^{(t)}-1} \times \exp\left[\frac{\|\boldsymbol{y} - \boldsymbol{\mu}(\boldsymbol{\alpha}^{(t)})\|^2}{2c(\boldsymbol{\alpha}^{(t)})} - \frac{\|\boldsymbol{y} - \boldsymbol{\mu}(\boldsymbol{\alpha}^*)\|^2}{2c(\boldsymbol{\alpha}^*)}\right] \quad (12)$$

where $g_{a,b}$ denotes the probability density function (pdf) of the Beta distribution $\mathcal{B}e(a, b)$, $w^* \sim \mathcal{B}e(1, R^{(t)})$ that is added to the full abundance vector, and, with $R^{(t)} \neq 2$

$$A_{\mathrm{d}} = \exp\left[\frac{\|\boldsymbol{y} - \boldsymbol{\mu}(\boldsymbol{\alpha}^{(t)})\|^2}{2c(\boldsymbol{\alpha}^{(t)})} - \frac{\|\boldsymbol{y} - \boldsymbol{\mu}(\boldsymbol{\alpha}^*)\|^2}{2c(\boldsymbol{\alpha}^*)}\right] \times \left[\frac{c(\boldsymbol{\alpha}^{(t)})}{c(\boldsymbol{\alpha}^*)}\right]^{\frac{L}{2}} \frac{b_{R^{(t)}-1}}{d_R} \frac{g_{1,R^{(t)}-1}(\alpha^*_{R^{(t)}})}{R^{(t)} - 1} (1 - \alpha^*_{R^{(t)}})^{R^{(t)}-2}. \quad (13)$$

Note that when $R^{(t)} = 2$, the death move yields $R^* = 1$, i.e., one single pure element is present in the proposed model, which leads obviously to $\boldsymbol{\alpha}^* = 1$. Thus, $\boldsymbol{\alpha}^*$ is deterministic and

$$A_{\mathrm{d}} = \left[\frac{c(\boldsymbol{\alpha}^{(t)})}{c(\boldsymbol{\alpha}^*)}\right]^{L/2} \frac{b_{R^{(t)}-1}}{d_R^{(t)}} \times \exp\left[\frac{\|\boldsymbol{y} - \boldsymbol{\mu}(\boldsymbol{\alpha}^{(t)})\|^2}{2c(\boldsymbol{\alpha}^{(t)})} - \frac{\|\boldsymbol{y} - \boldsymbol{\mu}(\boldsymbol{\alpha}^*)\|^2}{2c(\boldsymbol{\alpha}^*)}\right]. \quad (14)$$

The acceptance probability of the *switch* move is given by the standard MM ratio $\rho = \min\{1, A_{\mathrm{s}}\}$ with

$$A_{\mathrm{s}} = \left[\frac{c(\boldsymbol{\alpha}^{(t)})}{c(\boldsymbol{\alpha}^*)}\right]^{L/2} \exp\left[\frac{\|\boldsymbol{y} - \boldsymbol{\mu}(\boldsymbol{\alpha}^{(t)})\|^2}{2c(\boldsymbol{\alpha}^{(t)})} - \frac{\|\boldsymbol{y} - \boldsymbol{\mu}(\boldsymbol{\alpha}^*)\|^2}{2c(\boldsymbol{\alpha}^*)}\right]. \quad (15)$$

Once the endmember matrix $\boldsymbol{M}$ has been obtained, the abundances, the endmember variances and the hyperparameter δ are generated following the distributions presented below using a Metropolis-within-Gibbs procedure [9].

3.2. Generating samples according to $f(\boldsymbol{\alpha}|\boldsymbol{y}, R, \sigma^2, \boldsymbol{M}, \delta)$

The Bayes' theorem $f(\boldsymbol{\alpha}|\boldsymbol{y}, R, \sigma^2, \boldsymbol{M}, \delta) \propto f(\boldsymbol{y}|\boldsymbol{\theta}) f(\boldsymbol{\alpha}|R)$ (where $\propto$ means "proportional to") easily leads to

$$f(\boldsymbol{\alpha}|\boldsymbol{y}, R, \sigma^2, \boldsymbol{M}, \delta) = f(\boldsymbol{\alpha}|\boldsymbol{y}, R, \sigma^2, \boldsymbol{M}) \propto \frac{1}{[\sigma^2 c(\boldsymbol{\alpha})]^{L/2}} \times \exp\left(-\frac{\|\boldsymbol{y} - \boldsymbol{\mu}(\boldsymbol{\alpha})\|^2}{2\sigma^2 c(\boldsymbol{\alpha})}\right) \mathbf{1}_{\mathbb{S}}(\boldsymbol{\alpha}). \quad (16)$$

Note that the conditional distribution of $\boldsymbol{\alpha}$ is defined on the simplex $\mathbb{S}$ ensuring the abundance vector $\boldsymbol{\alpha}^+$ satisfies the positivity and sum-to-one constraints (2) inherent to the NCM. The generation of $\boldsymbol{\alpha}$ according to (16) can be achieved using a Metropolis-within-Gibbs move with a uniform prior distribution (8) as proposal distribution.

3.3. Generating samples according to $f(\sigma^2|\boldsymbol{y}, R, \boldsymbol{\alpha}, \boldsymbol{M}, \delta)$

The conditional distribution of the noise variance is the following inverse Gamma distribution

$$\sigma^2|\boldsymbol{y}, R, \boldsymbol{\alpha}, \boldsymbol{M}, \delta \sim \mathcal{IG}\left(\frac{L}{2} + 1, \frac{\|\boldsymbol{y} - \boldsymbol{\mu}(\boldsymbol{\alpha})\|^2}{2c(\boldsymbol{\alpha})} + \delta\right). \quad (17)$$

3.4. Generating samples according to $f(\delta|\boldsymbol{y}, R, \boldsymbol{\alpha}, \sigma^2, \boldsymbol{M})$

The conditional distribution of δ is the Gamma distribution

$$\delta|\boldsymbol{y}, R, \boldsymbol{\alpha}, \sigma^2, \boldsymbol{M} \sim \mathcal{G}\left(1, \frac{1}{\sigma^2}\right) \quad (18)$$

where $\mathcal{G}(a, b)$ denotes the Gamma distribution with shape parameter a and scale parameter b [9, p. 581].

4. SIMULATION RESULTS

This section studies the accuracy of the semi-supervised algorithm presented in Sections 2 and 3 for unmixing a synthetic pixel, resulting from the combination of $R = 3$ random endmembers with variance $\sigma^2 = 0.002$ and abundance vector $\boldsymbol{\alpha}^+ = [0.5,\ 0.15,\ 0.35]^T$. The endmember means are the spectra of construction concrete, green grass and micaceous loam, observed in $L = 276$ spectral bands. The spectrum library $\mathcal{S}$ used in this simulation contains six elements defined as construction concrete, green grass, micaceous loam, olive green paint, bare red brick and galvanized steel metal depicted in

[2]The case $R = 1$ has been accepted for the semi-supervised algorithm as a pixel can be spectrally pure.

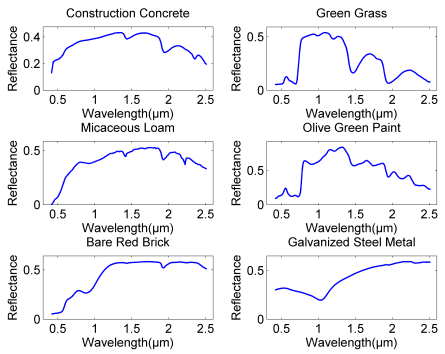

Fig. 1. Endmember spectra of the library.

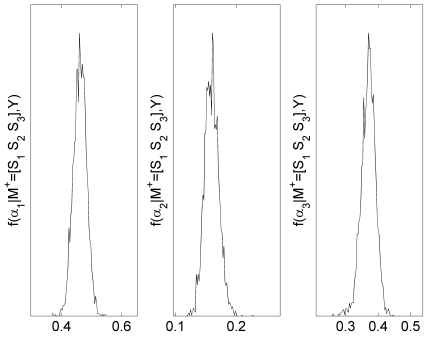

Fig. 3. Posterior distribution of the estimated abundances.

Fig. 1. These spectra have been extracted from the spectral libraries provided with the ENVI software [12]. The first step of the analysis estimates the number of components R. The posterior distribution of R depicted in Fig. 2 is clearly in good agreement with the actual value of R since its maximum is obtained for $R = 3$. The second step of the analysis estimates the *a posteriori* probabilities of all spectrum combinations, conditioned to $R = 3$. For this example, 100% of the sampled spectrum combinations are composed of the first three spectra of the library which are the actual spectra defining the mixture. The posterior distributions of the corresponding abundance coefficients are finally estimated and depicted in Fig. 3. The posteriors are in good agreement with the actual values of these parameters, i.e., $\boldsymbol{\alpha}^+ = [0.5,\ 0.15,\ 0.35]^T$.

It is interesting to note that the proposed model selection strategy allows one not only to estimate the number of endmembers participating in the NCM but also to recover the spectral signatures associated to these endmembers (extracted from a library). To our knowledge, there is no known method from the literature that could be used to handle this model selection problem for a single pixel of the image.

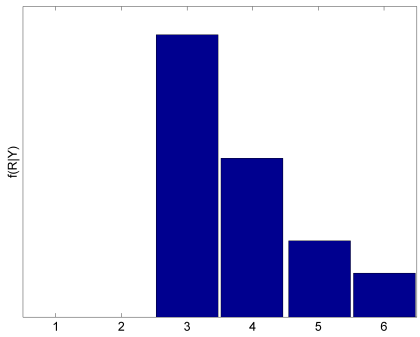

Fig. 2. Posterior distribution of the number of components R.

5. CONCLUSION

A new semi-supervised unmixing algorithm, based on the normal compositional model was derived for hyperspectral images. An RJ-MCMC algorithm was proposed to generate samples distributed according to the joint posterior distribution associated to this model. These samples were then used to estimate the parameters of interest, i.e., the number and the nature of the endmembers involved in the mixture, as well as their corresponding abundances. The proposed algorithm showed several advantages versus the standard model selection strategies. In particular, it allows one to estimate which components from a spectral library participate in the mixture. The simulation results on synthetic data showed very promising results. Future works include the generalization of the NCM algorithm to models involving spatial correlation between the pixels of the image.

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