Bayesian Blind Source Separation of Positive Non Stationary Sources

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Abstract. In this contribution, we address the problem of blind non negative source separation. This problem finds its application in many fields of data analysis. We propose herein a novel approach based on Gamma mixture probability priors: Gamma densities to constraint the unobserved sources to lie on the positive half plane; a mixture density with a first order Markov model on the associated hidden variables to account for eventual non stationarity on the sources. Posterior mean estimates are obtained via appropriate Monte Carlo Markov Chain sampling.

INTRODUCTION

Blind source separation has been largely considered in the scientific community these last two decades, many solutions has been presented [1, 9]. However in many data analysis applications (spectral analysis, image analysis ...) an additional constraint has to be enforced: positivity constraint on the sources and/or the mixing matrix elements. This is referred, in ICA community, as *non negative Independent Component Analysis*. In [4, 5], the authors considered a rectification nonlinearity in non linear Principal Components to propose algorithms for this particular problem.

The authors in [2, 8, 3] considered the non negative blind source separation under a Bayesian formulation: [2] considered a mixture of rectified Gaussian prior to enforce such a constraint on both the sources and mixing elements. The author in [8] considered a same rectified Gaussian prior to enforce such a constraint on the mixing elements. The authors in [3] considered a Gamma prior both for the sources and the mixing elements for a non negative source separation problem in mass spectrometry.

In this paper, we consider the problem of non negative source separation under a Bayesian framework, where we impose the positivity only on the sources (positivity constraint on the mixing elements can be accounted and the interested reader can refer to [3] for a possible extension). For that purpose, we model the sources by Gamma densities priors. We consider more particularly a non stationary prior distribution consisting of mixture of the Gamma densities, where the associated hidden variables are modeled by a first order Markov chain.

Such prior models (Gamma densities) are highly non linear, leading to posterior joint densities highly intractable and making explicit analysis not possible. For the optimization purpose, we make use of Monte Carlo integration to estimate posterior means where we propose appropriate proposal distributions in Markov Chain Monte Carlo methods combining Gibbs and Hastings Metropolis sampling.

PROBLEM STATEMENT AND BAYESIAN FORMULATION

The problem of instantaneous linear mixture blind source separation is described by:

$$\mathbf{x}(t) = \mathbf{A}\mathbf{s}(t) + \boldsymbol{\varepsilon}(t), \quad t \in \mathbb{Z} \quad (1)$$

where $\mathbf{x}(t)$ and $\boldsymbol{\varepsilon}(t)$ are m column vectors of the observed mixtures and observation noise respectively, $\mathbf{A}$ is the $(m \times n)$ unknown mixing matrix (containing the unknown mixing proportions of the sources) and $\mathbf{s}(t)$ is a n column vector of the unobservable sources. Each component of the unobservable sources $\mathbf{s}(t)$ is *constrained to lie on the positive half plane of $\mathbb{R}$* . This is the case in many fields of data analysis as mass spectrometry for example. In the sequel, noise $\boldsymbol{\varepsilon}(t)$ is assumed to be Gaussian spatially¹ independent and temporarily white:

$$\boldsymbol{\varepsilon}(t) \sim \mathcal{N}(\mathbf{0}, \mathbf{R}_{\boldsymbol{\varepsilon}}), \quad t \in \mathbb{Z} \quad (2)$$

We identify, in this problem, several unknown quantities to be estimated: the unobserved sources $\mathbf{s}(t)$, the mixing matrix $\mathbf{A}$, noise covariance $\mathbf{R}_{\boldsymbol{\varepsilon}}$ and additional parameters that may describe the prior models (detailed hereafter). The joint posterior distribution, according to Bayes rule, is given by:

$$p(\mathbf{s}, \mathbf{A}, \boldsymbol{\theta} | \mathbf{x}) \propto p(\mathbf{x} | \mathbf{s}, \mathbf{A}, \boldsymbol{\theta}) \pi(\mathbf{s}, \mathbf{A}, \boldsymbol{\theta}) \quad (3)$$

Prior laws assignment

We will make, first, assume that the sources $\mathbf{s}(t)$ and the mixing matrix $\mathbf{A}$ are statistically a priori independent, i.e:

$$\pi(\mathbf{s}, \mathbf{A}, \boldsymbol{\theta}) = \pi(\mathbf{s} | \boldsymbol{\theta}) \pi(\mathbf{A} | \boldsymbol{\theta}) \quad (4)$$

Mixing matrix prior distribution. The elements of the mixing matrix are considered a priori Gaussian and identically distributed:

$$a_{i,j} \sim \mathcal{N}(\mu_{i,j}^a, \tau_a), \quad (i, j) \in \{1, \dots, m\} \otimes \{1, \dots, n\} \quad (5)$$

This can be extended to the case where the elements of the mixing matrix are constrained to lie on the positive half plane, however this is out of the scope of this paper and the reader can refer to [3] for further details.

Sources prior distribution. The sources constrained to lie on the positive half plane are modeled by Gamma prior distributions of the form:

$$s_i(t) \sim \mathcal{G}(\alpha_i, \beta_i) \propto s_i(t)^{\alpha_i-1} e^{-s_i(t)/\beta_i} \mathbb{I}_{\mathbb{R}_+}, \quad t \in \mathbb{Z} \quad (6)$$

¹ we refer to the vector components s_i as the spatial dimension and to the time index t as the temporal dimension

with $\{\alpha_i, \beta_i\} \in \{\mathbb{R}_+^*, \mathbb{R}_+\}$. However, in order to account for any non stationarity of the sources, a mixture of these Gamma distributions is considered with a hidden variables modelisation of the form:

$$\begin{aligned} s_i(t) &\sim \sum_{k=1}^K p_{i,k} \mathcal{G}(s_i(t) | \alpha_{i,k}, \beta_{i,k}), \quad t \in \mathbb{Z} \\ &\sim \sum_{k=1}^K \text{Prob}[z_i(t) = k] \mathcal{G}(s_i(t) | \alpha_{i,k}, \beta_{i,k}) \end{aligned} \quad (7)$$

with $\sum_{k=1}^K p_{i,k} = 1$, where the sources, conditionally on the hidden variables, are Gamma densities of the form:

$$(s_i(t) | z_i(t) = k) \sim \mathcal{G}(s_i(t) | \alpha_{i,k}, \beta_{i,k}) \quad (8)$$

Hidden variables prior model: temporal non stationarity. In order to account for any non stationarity on the sources, the hidden variables are a priori modeled by a first order Markov chain of the form:

$$\pi[z_i(t) = k] = \sum_{k'=1}^K \pi[z_i(t-1) = k'] \pi[z_i(t) = k | z_i(t-1) = k'] \quad (9)$$

for $t = 2, \dots, T$ and $\pi[z_i(1) = k] = \pi_1(k)$.

Scale parameters prior distribution. The scale parameters are a priori modeled by inverse Gamma distributions of the form:

$$\pi(\theta) \sim \mathcal{G}^{-1}(\theta | r_0, v_0) \propto \frac{1}{\theta^{r_0+1}} e^{-\frac{1}{v_0\theta}} \quad (10)$$

where θ stands for the noise variances $\mathbf{R}_\epsilon = [\sigma_1^2, \dots, \sigma_m^2]'$ and for the sources prior scale parameter $\beta_{i,k}$ as well.

Power parameter prior distribution. In order to define an a priori distribution for the power parameter $\{\alpha_{i,k}\}$, we first look at the likelihood of the parameter:

$$\begin{aligned} p(s_{i,1 \dots T} | z_{i,1 \dots T} = k, \alpha_{i,k}, \beta_{i,k}) &\propto \prod_{t_k=1}^{T_{i,k}} p(s_i(t_k) | z_i(t_k), \alpha_{i,k}, \beta_{i,k}) \\ &\propto \left(\frac{(\tilde{s}_{i,k} / \beta_{i,k})^{\alpha_{i,k}}}{\Gamma(\alpha_{i,k})} \right)^{T_{i,k}} \mathbb{I}_{\mathbb{R}_+} \end{aligned} \quad (11)$$

where $\tilde{s}_{i,k} = \sqrt[T_{i,k}]{s_i(1) \times \dots \times s_i(T_{i,k})}$. The geometrical mean $\tilde{s}_{i,k}$ presents a major drawback: it is null whenever one of the $s_i(t_k)$'s is null, making thus the Gamma probability density function undefined at zero. In order to overcome this problem, the Gamma mixture prior of equation 7 needs to be redefined giving:

$$s_i(t) \sim p_{i,1} \mathcal{E}xp(s_i(t) | \lambda_i) + \sum_{k=2}^K p_{i,k} \mathcal{G}(s_i(t) | \alpha_{i,k}, \beta_{i,k}), \quad t \in \mathbb{Z} \quad (12)$$

with $\alpha_{i,k} \in]1, +\infty[$ and $\{\lambda_i, \beta_{i,k}\} \in \mathbb{R}_+$ and a new constraint on the $\alpha_{i,k}$'s.

MONTE CARLO SAMPLING

As an estimate of the different parameters of interest, we choose the posterior mean, and to achieve this we will approach it by means of Monte Carlo Markov Chain sampling. The posterior distribution 3 is quite intractable, thus Gibbs and Hastings-Metropolis procedures are alternated as described in the sequel:

Mixing matrix sampling. The posterior distribution of the mixing matrix conditioned on $(\mathbf{s}, \theta)$ is given by:

$$\begin{aligned} p(\mathbf{A}|\mathbf{s}, \theta, \mathbf{x}, \phi) &\propto p(\mathbf{x}|\mathbf{s}, \mathbf{A}, \mathbf{R}_\varepsilon) \pi(\mathbf{A}|\mu_A, \mathbf{R}_A) \propto \mathcal{N}(\mathbf{x}|\mathbf{A}\mathbf{s}, \mathbf{R}_\varepsilon) \mathcal{N}(\mathbf{A}|\mu_A, \mathbf{R}_A) \\ &\propto \mathcal{N}(\mathbf{A}|\hat{\mu}_A, \hat{\mathbf{R}}_A) \end{aligned} \quad (13)$$

where

$$\begin{aligned} \hat{\mathbf{R}}_A &= (\mathbf{R}_\varepsilon^{-1} \otimes \mathbf{R}_{ss} + \mathbf{R}_A^{-1})^{-1}, \\ \hat{\mu}_A &= \hat{\mathbf{R}}_A [(\mathbf{R}_\varepsilon^{-1} \otimes \mathbb{I}_n) \text{Vect}(\mathbf{R}_{xs}) + \mathbf{R}_A^{-1} \mu_A] \end{aligned}$$

and $\mathbf{R}_A = \tau_a \mathbb{I}_{mn}$, $\mu_A = [\mu_{1,1}^a, \mu_{1,2}^a, \dots, \mu_{m,n}^a]'$, $\mathbf{R}_{ss} = \sum_t \mathbf{s} \mathbf{s}'$ and $\mathbf{R}_{xs} = \sum_t \mathbf{x} \mathbf{s}'$. $\text{Vect}(\cdot)$ is a row-wise column vectorization defined by:

$$\text{Vect} \left(\begin{bmatrix} a_{1,1} & \dots & a_{1,n} \\ \vdots & \ddots & \vdots \\ a_{m,1} & \dots & a_{m,n} \end{bmatrix} \right) = [a_{1,1}, a_{1,2}, \dots, a_{m,n}]'$$

Noise variance sampling. The noise conditional posterior distribution is given by:

$$\begin{aligned} p(\tau_i|\mathbf{x}, \mathbf{A}\mathbf{s}) &\propto p(\mathbf{x}_i|[\mathbf{A}\mathbf{s}]_i, \tau_i) \pi(\tau_i) \propto \mathcal{N}(\mathbf{x}_i|[\mathbf{A}\mathbf{s}]_i, \tau_i) \mathcal{G}^{-1}(\tau_i|r_0, v_0) \\ &\propto \mathcal{G}^{-1}(\tau_i|r, v) \end{aligned} \quad (14)$$

for $i = 1, \dots, m$ where $r = T/2 + r_0$ and

$$\frac{1}{v} = \frac{1}{2} \sum_t (x_i(t) - [\mathbf{A}\mathbf{s}(t)]_i)^2 + \frac{1}{v_0}$$

Gamma priors scale parameter sampling. The conditional posterior distribution of the scale parameter of the mixture prior (equation 7) is given by:

$$\begin{aligned} p(\beta_{i,k}|\mathbf{s}_{i,1\dots T_k}) &\propto p(\mathbf{s}_{i,1\dots T_k}|\beta_{i,k}) \pi(\beta_{i,k}) \propto \mathcal{G}(\mathbf{s}_{i,1\dots T_k}|\alpha_{i,k}, \beta_{i,k}) \mathcal{G}^{-1}(\beta_{i,k}|r_0, v_0) \\ &\propto \mathcal{G}^{-1}(\beta_{i,k}|r, v) \end{aligned} \quad (15)$$

for $i = 1, \dots, n$; $k = 1, \dots, K$ where $r = \alpha_{i,k} T_{i,k}/2 + r_0$ and²

$$\frac{1}{v} = \sum_{t_k=1}^{T_{i,k}} s_i(t_k) + \frac{1}{v_0}$$

Power parameter sampling. The conditional posterior probability density function of the power parameter of the Gamma mixture prior (equation 7) is given by:

$$\begin{aligned} p(\alpha_{i,k} | s_{i,1 \dots T_k}, \beta_k) &\propto p(s_{i,1 \dots T_k} | \beta_{i,k}, \alpha_{i,k}) \pi(\alpha_{i,k}) \propto \left(\frac{(\tilde{s}_{i,k}/\beta_{i,k})^{\alpha_{i,k}}}{\Gamma(\alpha_{i,k})} \right)^{T_{i,k}} \mathbb{I}_{]1, +\infty[} \\ &\propto \left(\frac{w^{\alpha_{i,k}}}{\Gamma(\alpha_{i,k})} \right)^{T_{i,k}} \mathbb{I}_{]1, +\infty[} \end{aligned} \quad (16)$$

$w = \tilde{s}_{i,k}/\beta_{i,k}$. The distribution between brackets would be the Poisson distribution for $\alpha_{i,k}$ if the latter would have been discrete.

We make use of the Metropolis Hastings algorithm in order to generate conditional posterior samples from distribution 16 with a proposal distribution given by:

$$g(y) = \mathcal{G}(y | \vartheta, \gamma)$$

ϑ and γ are such that:

$$\begin{cases} \vartheta &= \hat{\alpha}^2 / \varphi \\ \gamma &= \varphi / \hat{\alpha} \end{cases}$$

where $\Psi(\alpha) = \frac{\partial \ln \Gamma}{\partial \alpha}(\alpha)$, $\hat{\alpha} = \Psi^{-1}(\ln(w))$ and $\varphi = \frac{1}{T_{i,k}} \left(\frac{\partial \Psi}{\partial \alpha}(\vartheta) \right)^{-1}$.

Sampling the hidden variables. Two alternatives are possible to sample the hidden variables with a Markov chain prior model (equation 9): an exact method based on the Baum & Walsh procedure [6] and an approximate one based on Gibbs sampling procedure [7]. In this work, we adopt the second one being simpler and faster to implement, it is detail hereafter:

$$\begin{aligned} (z_i(t) = k | s_i(t), z_{i,-t}, \theta_k) &\sim \mathcal{G}(s_i(t) | \alpha_{i,k}, \beta_{i,k}) \\ &\times \pi[z_i(t+1) | z_i(t) = k] \pi[z_i(t) = k | z_i(t-1)] \end{aligned} \quad (17)$$

for $t = 2, \dots, T-1$, where $z_{i,-t} = [\dots, z_i(t-1), z_i(t+1), \dots]$ and

$$\begin{aligned} (z_i(1) = k | s_i(1), z_{i,-1}, \theta_k) &\sim \mathcal{G}(s_i(1) | \alpha_{i,k}, \beta_{i,k}) \pi[z_i(2) | z_i(1) = k] \\ (z_i(T) = k | s_i(T), z_{i,-T}, \theta_k) &\sim \mathcal{G}(s_i(T) | \alpha_{i,k}, \beta_{i,k}) \pi[z_i(T) | z_i(T-1) = k] \end{aligned}$$

² recall that $\beta_{i,1} = \lambda_i$ and $\alpha_{i,1} = 1$

Sampling the sources. The conditional posterior distribution of the sources is given by:

$$\begin{aligned} p(\mathbf{s}|\mathbf{x}, \mathbf{z}, \mathbf{A}, \Theta) &\propto p(\mathbf{x}|\mathbf{s}, \mathbf{A}, \mathbf{R}_\varepsilon) \pi(\mathbf{s}|\mathbf{z}, \theta) \\ &\propto \left(\prod_{i=1}^n s_i^{\alpha_{i,k}-1} \right) \exp\left(-\frac{1}{2} \mathbf{Q}(\mathbf{s}|\mathbf{x}, \mathbf{A}, \Theta)\right) \end{aligned} \quad (18)$$

where $\mathbf{Q}(\cdot)$ is a quadratic function on $\mathbf{s}$ given by:

$$\mathbf{Q}(\mathbf{s}|\mathbf{x}, \mathbf{A}, \Theta) = (\mathbf{s} - \boldsymbol{\mu}_s)' \boldsymbol{\Sigma} (\mathbf{s} - \boldsymbol{\mu}_s)$$

where $\boldsymbol{\Sigma} = \mathbf{A}' \mathbf{R}_\varepsilon^{-1} \mathbf{A}$ and $\boldsymbol{\mu}_s = \boldsymbol{\Sigma}^{-1} (\mathbf{A}' \mathbf{R}_\varepsilon^{-1} \mathbf{x} - \boldsymbol{\beta}^{-1})^3$. A hybrid Gibbs Hastings-Metropolis scheme is used to generate samples from the distribution 18:

The conditional posterior distribution of source s_i is given by:

$$p(s_i) \propto s_i^{\alpha_{i,k}-1} e^{-\frac{\zeta_i}{2}(s_i - \mu_i)^2} \mathbb{I}_{\mathbb{R}_+} \quad (19)$$

where $\zeta_i = \boldsymbol{\Sigma}[i, i]$ and $\mu_i = ([\boldsymbol{\Sigma} \boldsymbol{\mu}_s]_i - \sum_{j \neq i} \boldsymbol{\Sigma}[i, j] s_j) / \boldsymbol{\Sigma}[i, i]$. We distinguish mainly three cases:

$\mu_i = 0$: the distribution 19 rewrites

$$p(s_i) \propto s_i^{\alpha_{i,k}-1} e^{-\frac{\zeta_i}{2} s_i^2} \mathbb{I}_{\mathbb{R}_+}$$

In this case $s_i = \sqrt{y/\zeta_i}$ where $y \sim \chi^2(\alpha_{i,k}) \propto y^{\alpha_{i,k}/2-1} e^{-y/2} \mathbb{I}_{\mathbb{R}_+}$.

$\mu_i < 0$: we can rewrite the distribution 19 as:

$$p(s_i) \propto s_i^{\alpha_{i,k}-1} e^{-\zeta_i |\mu_i| s_i} e^{-\frac{\zeta_i}{2} s_i^2} \mathbb{I}_{\mathbb{R}_+}$$

then $y \sim \mathcal{G}(y|\alpha_{i,k}, \frac{1}{\zeta_i |\mu_i|})$, where the rejection probability is given by:

$$\rho = \min\left(1, e^{-\frac{\zeta_i}{2}(y^2 - s_i^{(l),2})}\right)$$

the quantity l stands for the iteration index.

$\mu_i > 0$: in this particular case, a proposal distribution is given by:

$$g(y) \propto y^{\alpha_{i,k}-1} e^{-\zeta_i |y - \mu_i|} \mathbb{I}_{\mathbb{R}_+}$$

with a rejection probability given by

$$\rho' = \begin{cases} e^{-\frac{\zeta_i}{2}(y - s_i^{l-1})(y + s_i^{l-1} - 2\mu_i - 2)} & \text{when } (y - \mu_i, s_i^{l-1} - \mu_i) \geq 0, \\ e^{-\frac{\zeta_i}{2}(y - s_i^{l-1} + 2)(y + s_i^{l-1} - 2\mu_i)} & \text{when } (\mu_i - y, s_i^{l-1} - \mu_i) \geq 0, \\ e^{-\frac{\zeta_i}{2}(y - s_i^{l-1} - 2)(y + s_i^{l-1} - 2\mu_i)} & \text{when } (y - \mu_i, \mu_i - s_i^{l-1}) \geq 0, \\ e^{-\frac{\zeta_i}{2}(y - s_i^{l-1})(y + s_i^{l-1} - 2\mu_i + 2)} & \text{when } (\mu_i - y, \mu_i - s_i^{l-1}) \geq 0 \end{cases}$$

³ $\boldsymbol{\beta}^{-T}$ defines the point wise inverse of the vector $\boldsymbol{\beta}$

and $\rho = \min(1, \rho')$.

SIMULATIONS

The proposed approach has been tested on the data set presented on figure 1: the two sources (middle) are realizations of Gamma mixture densities with the associated discrete variables (top). The observations (bottom) have been obtained with a mixing matrix $\mathbf{A} = \begin{bmatrix} 1, .5 \\ .5, 1 \end{bmatrix}$ and a low level centered white Gaussian noise (the observation signal to noise ratio (SNR) is of about 25dB), with:

$$\text{SNR}_{\text{dB}}(i) = 10 \log \left(\frac{\|[\mathbf{A} * \mathbf{s}(t)]_i\|_2^2}{\|\boldsymbol{\varepsilon}_i(t)\|_2^2} \right), \quad i = 1, \dots, m \quad (20)$$

FIGURE 1. Hidden variables representing the different states of the original sources at different time instants (top); original unobserved sources (middle), observations (bottom)

On figure 2, we present the obtained estimates with the outlined MCMC algorithm: the estimated hidden states (top) and the estimated sources (bottom). We give, for comparison, the proportions of the miss-estimated hidden states for each source. For this let us first define:

$$\eta_i(k) = \frac{\text{Card}\{t | \hat{z}_i(t) = k\} - \text{Card}\{t | z_i(t) = k\}}{\text{Card}\{t | z_i(t) = k\}}$$

then

$$\begin{aligned} \eta_1 &= [.028646, .285156, .101562] \\ \eta_2 &= [.036364, .246951, .370546] \end{aligned}$$

FIGURE 2. Estimated data: a. Hidden variables representing the different states of the sources at different time instants, b. Estimated unobserved sources

CONCLUSION

We presented in this paper a novel approach for separating non negative sources in a blind source separation problem based on a Bayesian formulation of the problem. The proposed approach is based on Markov Chain Monte Carlo methods. The prior model for the sources is a Gamma mixture model: the Gamma density function constrains the sources to lie on the right half plane while the mixture model enables to model any sources non stationarity. Simulation results allowed us to show the performances of the proposed approach.

A direct extension of this work would be to incorporate an estimation step for the number of the hidden states, and a natural way to do this in a Bayesian approach with MCMC methods is through Reversible Jump sampling.

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