Algorithm 1 Bayesian positive source separation algorithm (BPSS)

for $i = 1, \dots, N_{\mathrm{MC}}$ **do**
  % sampling the abundance hyperparameters
  for $p = 1, \dots, P$ **do**
    Draw λ_p from the pdf

$$f\left(\lambda_p \middle| \mathbf{a}_{p:}, \gamma_p\right) \propto \prod_{r=1}^{R} \left[\frac{\gamma_p^{\lambda_p}}{\Gamma\left(\lambda_p\right)} a_{p,r}^{\lambda_p}\right] e^{-\epsilon\lambda_p} \mathbf{1}_{\mathbb{R}^+}(\lambda_p).$$

  end for
  % sampling the abundance hyperparameters
  for $p = 1, \dots, P$ **do**
    Draw γ_p from the gamma distribution

$$\gamma_p \big| \lambda_p, \mathbf{a}_{p:} \sim \mathcal{G}\left(1 + R\lambda_p + \epsilon, \sum_{r=1}^{R} a_{p,r} + \epsilon\right).$$

  end for
  % sampling the abundance vectors
  for $p = 1, \dots, P$ and $r = 1, \dots, R$ **do**
    Draw $a_{p,r}$ from the pdf

$$f\left(a_{p,r} \middle| \lambda_p, \gamma_p, \mathbf{S}, \boldsymbol{\sigma}_{\mathrm{e}}^2, \mathbf{X}\right) \propto a_{p,r}^{\lambda_r - 1} \mathbf{1}_{\mathbb{R}^+}(a_{p,r}) \exp\left[-\frac{\left(a_{p,r} - \mu_{p,r}\right)^2}{2\delta_p^2} - \gamma_p a_{p,r}\right],$$

  end for
  % sampling the noise hyperparameter
  Draw ψ_{e} from the inverse-gamma distribution

$$\psi_{\mathrm{e}} \left| \boldsymbol{\sigma}_{\mathrm{e}}^2, \rho_{\mathrm{e}} \right. \sim \mathcal{IG}\left(\frac{P\rho_{\mathrm{e}}}{2}, \frac{1}{2}\sum_{p=1}^{P} \frac{1}{\sigma_{\mathrm{e},p}^2}\right).$$

  % sampling the noise variances
  for $p = 1, \dots, P$ **do**
    Draw $\sigma_{\mathrm{e},p}^2$ from the inverse-gamma distribution

$$\sigma_{\mathrm{e},p}^2 \left| \psi_{\mathrm{e}}, \mathbf{a}_{p:}, \mathbf{S}, \mathbf{x}_{p:} \right. \sim \mathcal{IG}\left(\frac{\rho_{\mathrm{e}} + L}{2}, \frac{\psi_{\mathrm{e}} + \|\mathbf{x}_{p:} - \mathbf{S}\mathbf{a}_{p:}\|^2}{2}\right).$$

  end for
  % sampling the source hyperparameters
  for $r = 1, \dots, R$ **do**
    Draw α_r from the pdf

$$f\left(\alpha_r \middle| \mathbf{s}_{r:}, \beta_r\right) \propto \prod_{l=1}^{L} \left[\frac{\beta_r^{\alpha_r}}{\Gamma\left(\alpha_r\right)} s_{r,l}^{\alpha_r}\right] e^{-\epsilon\alpha_r} \mathbf{1}_{\mathbb{R}^+}(\alpha_r).$$

  end for
  % sampling the source hyperparameters
  for $r = 1, \dots, R$ **do**
    Draw β_r from the gamma distribution

$$\beta_r \big| \alpha_r, \mathbf{s}_{r:} \sim \mathcal{G}\left(1 + L\alpha_r + \epsilon, \sum_{l=1}^{L} s_{r,l} + \epsilon\right).$$

  end for
  % sampling the source spectrum
  for $r = 1, \dots, R$ and $l = 1, \dots, L$ **do**
    Draw $s_{r,l}$ from the pdf

$$f\left(s_{r,l} \middle| \alpha_r, \beta_r, \mathbf{A}, \boldsymbol{\sigma}_{\mathrm{e}}^2, \mathbf{X}\right) \propto s_{r,l}^{\alpha_r - 1} \mathbf{1}_{\mathbb{R}^+}(s_{r,l}) \exp\left[-\frac{\left(s_{r,l} - \mu_{r,l}\right)^2}{2\delta_r^2} - \beta_r s_{r,l}\right],$$

  end for
end for

Algorithm 2 Fully constrained Bayesian positive source separation algorithm (BPSS2)

for $i = 1, \dots, N_{\mathrm{MC}}$ **do**
  % sampling the abundance vectors
  for $p = 1, \dots, P$ **do**
    Draw $\mathbf{a}_{p:}$ from the pdf

$$f\left(\mathbf{a}_{p:} \middle| \mathbf{A}, \boldsymbol{\sigma}_{\mathrm{e}}^2, \mathbf{X}\right) \propto \exp\left[-\frac{1}{2}\left(\mathbf{a}_{p:} - \boldsymbol{\mu}_p\right)^{\top} \boldsymbol{\Lambda}_p^{-1} \left(\mathbf{a}_{p:} - \boldsymbol{\mu}_p\right)\right] \mathbf{1}_{\mathbb{S}}(\mathbf{a}_{p:}).$$

    with

$$\mathbb{S} = \left\{\mathbf{a}_{p:}; a_{p,r} \geq 0, \ \forall r = 1, \dots, R, \ \sum_{r=1}^{R} a_{p,r} = 1\right\}.$$

  end for
  % sampling the noise hyperparameter
  Draw ψ_{e} from the inverse-gamma distribution

$$\psi_{\mathrm{e}} \left| \boldsymbol{\sigma}_{\mathrm{e}}^2, \rho_{\mathrm{e}} \right. \sim \mathcal{IG}\left(\frac{P\rho_{\mathrm{e}}}{2}, \frac{1}{2}\sum_{p=1}^{P} \frac{1}{\sigma_{\mathrm{e},p}^2}\right).$$

  % sampling the noise variances
  for $p = 1, \dots, P$ **do**
    Draw $\sigma_{\mathrm{e},p}^2$ from the inverse-gamma distribution

$$\sigma_{\mathrm{e},p}^2 \left| \psi_{\mathrm{e}}, \mathbf{a}_{p:}, \mathbf{S}, \mathbf{x}_{p:} \right. \sim \mathcal{IG}\left(\frac{\rho_{\mathrm{e}} + L}{2}, \frac{\psi_{\mathrm{e}} + \|\mathbf{x}_{p:} - \mathbf{S}\mathbf{a}_{p:}\|^2}{2}\right).$$

  end for
  % sampling the source hyperparameters
  for $r = 1, \dots, R$ **do**
    Draw α_r from the pdf

$$f\left(\alpha_r \middle| \mathbf{s}_{r:}, \beta_r\right) \propto \prod_{l=1}^{L} \left[\frac{\beta_r^{\alpha_r}}{\Gamma\left(\alpha_r\right)} s_{r,l}^{\alpha_r}\right] e^{-\epsilon\alpha_r} \mathbf{1}_{\mathbb{R}^+}(\alpha_r).$$

  end for
  % sampling the source hyperparameters
  for $r = 1, \dots, R$ **do**
    Draw β_r from the gamma distribution

$$\beta_r \big| \alpha_r, \mathbf{s}_{r:} \sim \mathcal{G}\left(1 + L\alpha_r + \epsilon, \sum_{l=1}^{L} s_{r,l} + \epsilon\right).$$

  end for
  % sampling the source spectrum
  for $r = 1, \dots, R$ and $l = 1, \dots, L$ **do**
    Draw $s_{r,l}$ from the pdf

$$f\left(s_{r,l} \middle| \alpha_r, \beta_r, \mathbf{A}, \boldsymbol{\sigma}_{\mathrm{e}}^2, \mathbf{X}\right) \propto s_{r,l}^{\alpha_r - 1} \mathbf{1}_{\mathbb{R}^+}(s_{r,l}) \exp\left[-\frac{\left(s_{r,l} - \mu_{r,l}\right)^2}{2\delta_r^2} - \beta_r s_{r,l}\right],$$

  end for
end for

time on an x86 processor architecture, while the changes to the code have been minimal. Furthermore, most dataset come as single precision.

3) OS Architecture: It is interesting to note that MATLAB© is limited in terms of memory usage (regardless of the size of physical memory). This depends on the Operating System (OS) and on the MATLAB version (see Table II-A3).

Therefore, a 32-bits LINUX architecture has been chosen.

4) Parallelization: MATLAB© contains libraries dedicated to automatically parallelize parts of the algorithms on a single computer. BPSS has been run on a 4-core machine. The underlying matrix libraries already provide a certain level of parallelism depending on the number of available cores. However, in the future, parts of the code could be parallelized