

Politecnico of Milan

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MASTER THESIS

The DRPM Strikes Back: Improvements on a Bayesian Spatio-Temporal Clustering Model

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*to my cats Otto
and La Micia*

Abstract

Sommario

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Chapter 1

Introduction

Chapter 2

Description of the model

“Come on, gentlemen, why shouldn’t we get rid of all this calm reasonableness with one good kick, just so as to send all these logarithms to the devil and be able to live our own lives at our own sweet will?”
— Fëdor Dostoevskij, *Notes from the Underground*

The original model design (henceforth referred to as CDRPM).

$$\begin{aligned}
Y_{it}|Y_{it-1}, \boldsymbol{\mu}_t^*, \boldsymbol{\sigma}_t^{2*}, \boldsymbol{\eta}, \mathbf{c}_t &\stackrel{\text{ind}}{\sim} \mathcal{N}(\mu_{c_{it}}^* + \eta_{1i}Y_{it-1}, \sigma_{c_{it}}^{2*}(1 - \eta_{1i}^2)) \\
Y_{i1} &\stackrel{\text{ind}}{\sim} \mathcal{N}(\mu_{c_{i1}}^*, \sigma_{c_{i1}}^{2*}) \\
\xi_i = \text{Logit}(\tfrac{1}{2}(\eta_{1i} + 1)) &\stackrel{\text{ind}}{\sim} \text{Laplace}(a, b) \\
(\mu_{jt}^*, \sigma_{jt}^{2*}) &\stackrel{\text{ind}}{\sim} \mathcal{N}(\vartheta_t, \tau_t^2) \times \mathcal{U}(0, A_\sigma) \\
\vartheta_t|\vartheta_{t-1} &\stackrel{\text{ind}}{\sim} \mathcal{N}((1 - \varphi_1)\varphi_0 + \varphi_1\vartheta_{t-1}, \lambda^2(1 - \varphi_1^2)) \\
(\vartheta_1, \tau_t) &\stackrel{\text{iid}}{\sim} \mathcal{N}(\varphi_0, \lambda^2) \times \mathcal{U}(0, A_\tau) \\
(\varphi_0, \varphi_1, \lambda) &\sim \mathcal{N}(m_0, s_0^2) \times \mathcal{U}(-1, 1) \times \mathcal{U}(0, A_\lambda) \\
\{\mathbf{c}_t, \dots, \mathbf{c}_T\} &\sim \text{tRPM}(\boldsymbol{\alpha}, M) \text{ with } \alpha_t \stackrel{\text{iid}}{\sim} \text{Beta}(a_\alpha, b_\alpha) \quad (2.1)
\end{aligned}$$

The updated model design (henceforth referred to as JDRPM), with highlighted in dark red the changes and insertions that we made.

$$\begin{aligned}
Y_{it}|Y_{it-1}, \boldsymbol{\mu}_t^*, \boldsymbol{\sigma}_t^{2*}, \boldsymbol{\eta}, \mathbf{c}_t &\stackrel{\text{ind}}{\sim} \mathcal{N}(\mu_{c_{it}}^* + \eta_{1i}Y_{it-1} + \mathbf{x}_{it}^T \boldsymbol{\beta}_t, \sigma_{c_{it}}^{2*}(1 - \eta_{1i}^2)) \\
Y_{i1} &\stackrel{\text{ind}}{\sim} \mathcal{N}(\mu_{c_{i1}}^* + \mathbf{x}_{i1}^T \boldsymbol{\beta}_1, \sigma_{c_{i1}}^{2*}) \\
\boldsymbol{\beta}_t &\stackrel{\text{ind}}{\sim} \mathcal{N}_p(\mathbf{b}, s^2 I) \\
\xi_i = \text{Logit}(\tfrac{1}{2}(\eta_{1i} + 1)) &\stackrel{\text{ind}}{\sim} \text{Laplace}(a, b) \\
(\mu_{jt}^*, \sigma_{jt}^{2*}) &\stackrel{\text{ind}}{\sim} \mathcal{N}(\vartheta_t, \tau_t^2) \times \text{invGamma}(a_\sigma, b_\sigma) \\
\vartheta_t|\vartheta_{t-1} &\stackrel{\text{ind}}{\sim} \mathcal{N}((1 - \varphi_1)\varphi_0 + \varphi_1\vartheta_{t-1}, \lambda^2(1 - \varphi_1^2))
\end{aligned}$$

$$\begin{aligned}
(\vartheta_1, \tau_t^2) &\stackrel{\text{iid}}{\sim} \mathcal{N}(\varphi_0, \lambda^2) \times \text{invGamma}(a_\tau, b_\tau) \\
(\varphi_0, \varphi_1, \lambda^2) &\sim \mathcal{N}(m_0, s_0^2) \times \mathcal{U}(-1, 1) \times \text{invGamma}(a_\lambda, b_\lambda) \\
\{\mathbf{c}_t, \dots, \mathbf{c}_T\} &\sim \text{tRPM}(\boldsymbol{\alpha}, M) \text{ with } \alpha_t \stackrel{\text{iid}}{\sim} \text{Beta}(a_\alpha, b_\alpha)
\end{aligned} \tag{2.2}$$

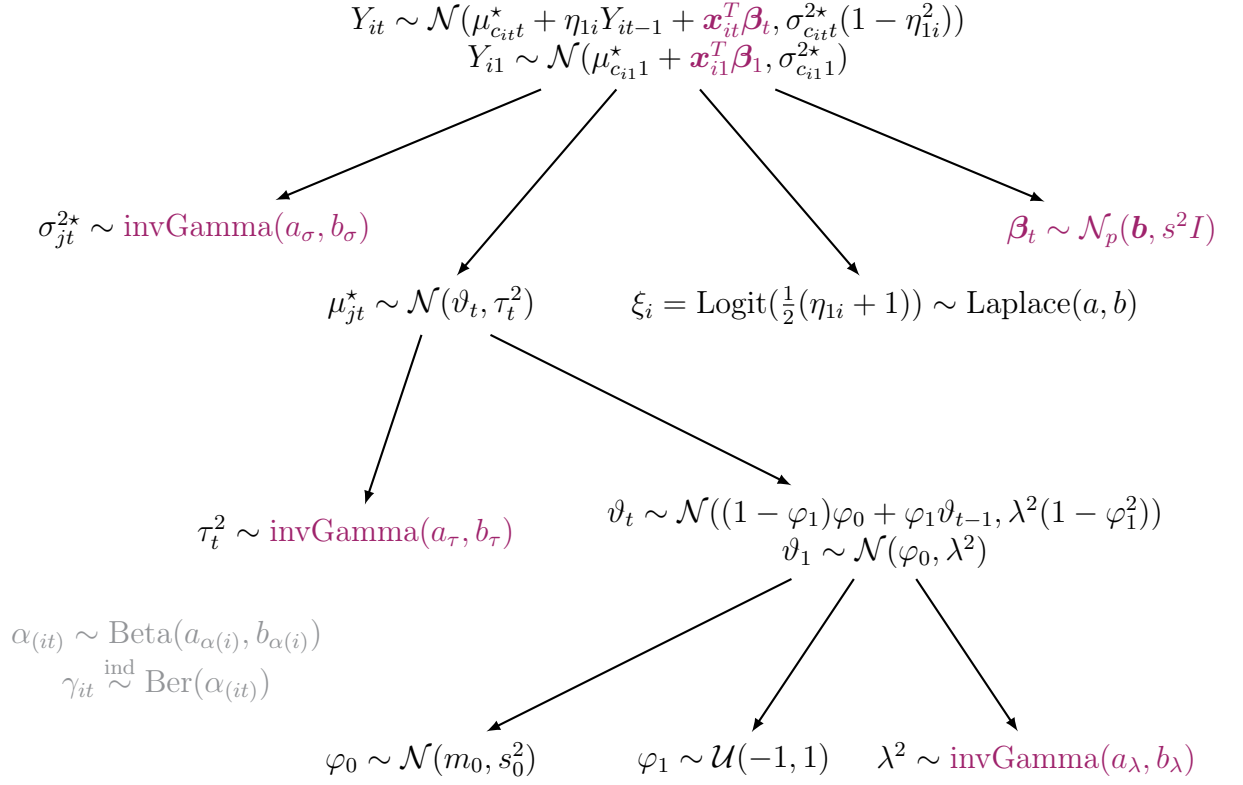


Figure 2.1: Graph visualization of the DRPM model, with highlighted in dark red the changes that we made to the original formulation and in gray the internal variables of the model.

2.1 Update rules derivation

We report here the full conditionals derivation for the parameters which had a conjugacy in the model (for the full computations see Appendix A). The other variables not included here, namely η_{1i} and φ_1 , involved instead the classical Metropolis update.

- update σ_{jt}^{2*}

for $t = 1$: $f(\sigma_{jt}^{2*} | -) \propto \text{kernel of a } \text{invGamma}(a_{\sigma(\text{post})}, b_{\sigma(\text{post})})$ with

$$a_{\tau(\text{post})} = a_\sigma + \frac{|S_{jt}|}{2} \quad b_{\tau(\text{post})} = b_\sigma + \frac{1}{2} \sum_{i \in S_{jt}} (Y_{it} - \mu_{jt}^* - \mathbf{x}_{it}^T \boldsymbol{\beta}_t)^2$$

for $t > 1$: $f(\sigma_{jt}^{2*} | -) \propto \text{kernel of a } \text{invGamma}(a_{\sigma(\text{post})}, b_{\sigma(\text{post})})$ with

$$a_{\tau(\text{post})} = a_{\sigma} + \frac{|S_{jt}|}{2} \quad b_{\tau(\text{post})} = b_{\sigma} + \frac{1}{2} \sum_{i \in S_{jt}} (Y_{it} - \mu_{jt}^* - \eta_{1i} Y_{it-1} - \mathbf{x}_{it}^T \boldsymbol{\beta}_t)^2 \quad (2.3)$$

- update μ_{jt}^*

for $t = 1$: $f(\mu_{jt}^* | -) \propto \text{kernel of a } \mathcal{N}(\mu_{\mu_{jt}^*}(\text{post}), \sigma_{\mu_{jt}^*}^2(\text{post}))$ with

$$\sigma_{\mu_{jt}^*}^2(\text{post}) = \frac{1}{\frac{1}{\tau_t^2} + \frac{|S_{jt}|}{\sigma_{jt}^{2*}}} \quad \mu_{\mu_{jt}^*}(\text{post}) = \sigma_{\mu_{jt}^*}^2(\text{post}) \left(\frac{\vartheta_t}{\tau_t^2} + \frac{\sum_{i \in S_{jt}} Y_{i1}}{\sigma_{jt}^{2*}} \right)$$

for $t > 1$: $f(\mu_{jt}^* | -) \propto \text{kernel of a } \mathcal{N}(\mu_{\mu_{jt}^*}(\text{post}), \sigma_{\mu_{jt}^*}^2(\text{post}))$ with

$$\sigma_{\mu_{jt}^*}^2(\text{post}) = \frac{1}{\frac{1}{\tau_t^2} + \frac{\sum_{i \in S_{jt}} \frac{1}{1 - \eta_{1i}^2}}{\sigma_{jt}^{2*}}} \quad \mu_{\mu_{jt}^*}(\text{post}) = \sigma_{\mu_{jt}^*}^2(\text{post}) \left(\frac{\vartheta_t}{\tau_t^2} + \frac{\sum_{i \in S_{jt}} \frac{Y_{it} - \eta_{1i} Y_{i,t-1}}{1 - \eta_{1i}^2}}{\sigma_{jt}^{2*}} \right) \quad (2.4)$$

- update $\boldsymbol{\beta}_t$

for $t = 1$: $f(\boldsymbol{\beta}_t | -) \propto \text{kernel of a } \mathcal{N}(\mathbf{b}_{(\text{post})}, A_{(\text{post})})$ with

$$A_{(\text{post})} = \left(\frac{1}{s^2} I + \sum_{i=1}^n \frac{\mathbf{x}_{it} \mathbf{x}_{it}^T}{\sigma_{c_{it}}^{2*}} \right)^{-1} \quad \mathbf{b}_{(\text{post})} = A_{(\text{post})} \left(\frac{\mathbf{b}}{s^2} + \sum_{i=1}^n \frac{(Y_{it} - \mu_{c_{it}}^*) \mathbf{x}_{it}}{\sigma_{c_{it}}^{2*}} \right)$$

i.e. $f(\boldsymbol{\beta}_t | -) \propto \text{kernel of a } \mathcal{N}\text{Canon}(\mathbf{h}_{(\text{post})}, J_{(\text{post})})$ with

$$\mathbf{h}_{(\text{post})} = \left(\frac{\mathbf{b}}{s^2} + \sum_{i=1}^n \frac{(Y_{it} - \mu_{c_{it}}^*) \mathbf{x}_{it}}{\sigma_{c_{it}}^{2*}} \right) \quad J_{(\text{post})} = \left(\frac{1}{s^2} I + \sum_{i=1}^n \frac{\mathbf{x}_{it} \mathbf{x}_{it}^T}{\sigma_{c_{it}}^{2*}} \right)$$

for $t > 1$: $f(\boldsymbol{\beta}_t | -) \propto \text{kernel of a } \mathcal{N}(\mathbf{b}_{(\text{post})}, A_{(\text{post})})$ with

$$A_{(\text{post})} = \left(\frac{1}{s^2} I + \sum_{i=1}^n \frac{\mathbf{x}_{it} \mathbf{x}_{it}^T}{\sigma_{c_{it}}^{2*}} \right)^{-1} \quad \mathbf{b}_{(\text{post})} = A_{(\text{post})} \left(\frac{\mathbf{b}}{s^2} + \sum_{i=1}^n \frac{(Y_{it} - \mu_{c_{it}}^* - \eta_{1i} Y_{it-1}) \mathbf{x}_{it}}{\sigma_{c_{it}}^{2*}} \right)$$

i.e. $f(\boldsymbol{\beta}_t | -) \propto \text{kernel of a } \mathcal{N}\text{Canon}(\mathbf{h}_{(\text{post})}, J_{(\text{post})})$ with

$$\mathbf{h}_{(\text{post})} = \left(\frac{\mathbf{b}}{s^2} + \sum_{i=1}^n \frac{(Y_{it} - \mu_{c_{it}}^* - \eta_{1i} Y_{it-1}) \mathbf{x}_{it}}{\sigma_{c_{it}}^{2*}} \right) \quad J_{(\text{post})} = \left(\frac{1}{s^2} I + \sum_{i=1}^n \frac{\mathbf{x}_{it} \mathbf{x}_{it}^T}{\sigma_{c_{it}}^{2*}} \right) \quad (2.5)$$

Here $\mathcal{N}\text{Canon}(\mathbf{h}, J)$ is the canonical formulation of the $\mathcal{N}(\boldsymbol{\mu}, \Sigma)$, with $\mathbf{h} = \Sigma^{-1} \boldsymbol{\mu}$ and $J = \Sigma^{-1}$. This other distribution facilitates the sampling, since these full conditional computations allow to derive directly the parameters of the canonical one, e.g. the inverse of the variance matrix, rather than the variance matrix itself; and therefore sampling through it does not require any inversion of matrices which would produce more computational load, numerical instabilities, and loss of accuracy. So in Julia we can write `rand(MvNormalCanon(h_star, J_star))`, rather than the riskier one `rand(MvNormal(inv(J_star)*h_star, inv(J_star)))`; which apart from the previously mentioned disadvantages would be a statistically equivalent form.

- update τ_t^2

$$f(\tau_t^2|-) \propto \text{kernel of a invGamma}(a_{\tau(\text{post})}, b_{\tau(\text{post})}) \text{ with}$$

$$a_{\tau(\text{post})} = \frac{k_t}{2} + a_{\tau} \quad b_{\tau(\text{post})} = \frac{\sum_{j=1}^{k_t} (\mu_{jt}^* - \vartheta_t)^2}{2} + b_{\tau} \quad (2.6)$$

- update ϑ_t

for $t = T$: $f(\vartheta_t|-) \propto \text{kernel of a } \mathcal{N}(\mu_{\vartheta_t(\text{post})}, \sigma_{\vartheta_t(\text{post})}^2)$ with

$$\sigma_{\vartheta_t(\text{post})}^2 = \frac{1}{\frac{1}{\lambda^2(1-\varphi_1^2)} + \frac{k_t}{\tau_t^2}}$$

$$\mu_{\vartheta_t(\text{post})} = \sigma_{\vartheta_t(\text{post})}^2 \left(\frac{\sum_{j=1}^{k_t} \mu_{jt}^*}{\tau_t^2} + \frac{(1-\varphi_1)\varphi_0 + \varphi_1\vartheta_{t-1}}{\lambda^2(1-\varphi_1^2)} \right)$$

for $1 < t < T$: $f(\vartheta_t|-) \propto \text{kernel of a } \mathcal{N}(\mu_{\vartheta_t(\text{post})}, \sigma_{\vartheta_t(\text{post})}^2)$ with

$$\sigma_{\vartheta_t(\text{post})}^2 = \frac{1}{\frac{1+\varphi_1^2}{\lambda^2(1-\varphi_1^2)} + \frac{k_t}{\tau_t^2}}$$

$$\mu_{\vartheta_t(\text{post})} = \sigma_{\vartheta_t(\text{post})}^2 \left(\frac{\sum_{j=1}^{k_t} \mu_{jt}^*}{\tau_t^2} + \frac{\varphi_1(\vartheta_{t-1} + \vartheta_{t+1}) + \varphi_0(1-\varphi_1)^2}{\lambda^2(1-\varphi_1^2)} \right)$$

for $t = 1$: $f(\vartheta_t|-) \propto \text{kernel of a } \mathcal{N}(\mu_{\vartheta_t(\text{post})}, \sigma_{\vartheta_t(\text{post})}^2)$ with

$$\sigma_{\vartheta_t(\text{post})}^2 = \frac{1}{\frac{1}{\lambda^2} + \frac{\varphi_1^2}{\lambda^2(1-\varphi_1^2)} + \frac{k_t}{\tau_t^2}}$$

$$\mu_{\vartheta_t(\text{post})} = \sigma_{\vartheta_t(\text{post})}^2 \left(\frac{\varphi_0}{\lambda^2} + \frac{\varphi_1(\vartheta_{t+1} - (1-\varphi_1)\varphi_0)}{\lambda^2(1-\varphi_1^2)} + \frac{\sum_{j=1}^{k_t} \mu_{jt}^*}{\tau_t^2} \right) \quad (2.7)$$

- update φ_0

$f(\varphi_0|-) \propto \text{kernel of a } \mathcal{N}(\mu_{\varphi_0(\text{post})}, \sigma_{\varphi_0(\text{post})}^2)$ with

$$\sigma_{\varphi_0(\text{post})}^2 = \frac{1}{\frac{1}{s_0^2} + \frac{1}{\lambda^2} + \frac{(T-1)(1-\varphi_1)^2}{\lambda^2(1-\varphi_1^2)}}$$

$$\mu_{\varphi_0(\text{post})} = \sigma_{\varphi_0(\text{post})}^2 \left(\frac{m_0}{s_0^2} + \frac{\vartheta_1}{\lambda^2} + \frac{1-\varphi_1}{\lambda^2(1-\varphi_1^2)} \sum_{t=2}^T (\vartheta_t - \varphi_1\vartheta_{t-1}) \right) \quad (2.8)$$

- update λ^2

$f(\lambda^2|-) \propto \text{kernel of a invGamma}(a_{\lambda(\text{post})}, b_{\lambda(\text{post})})$ with

$$a_{\lambda(\text{post})} = \frac{T}{2} + a_{\lambda}$$

$$b_{\lambda(\text{post})} = \frac{(\vartheta_1 - \varphi_0)^2}{2} + \sum_{t=2}^T \frac{(\vartheta_t - (1-\varphi_1)\varphi_0 - \varphi_1\vartheta_{t-1})^2}{2} + b_{\lambda} \quad (2.9)$$

- update α

if global α : $f(\alpha|-) \propto \text{kernel of a Beta}(a_{\alpha(\text{post})}, b_{\alpha(\text{post})})$ with

$$a_{\alpha(\text{post})} = a_{\alpha} + \sum_{i=1}^n \sum_{t=1}^T \gamma_{it} \quad b_{\alpha(\text{post})} = b_{\alpha} + nT - \sum_{i=1}^n \sum_{t=1}^T \gamma_{it}$$

if time specific α : $f(\alpha_t|-) \propto \text{kernel of a Beta}(a_{\alpha(\text{post})}, b_{\alpha(\text{post})})$ with

$$a_{\alpha(\text{post})} = a_{\alpha} + \sum_{i=1}^n \gamma_{it} \quad b_{\alpha(\text{post})} = b_{\alpha} + n - \sum_{i=1}^n \gamma_{it}$$

if unit specific α : $f(\alpha_i|-) \propto \text{kernel of a Beta}(a_{\alpha(\text{post})}, b_{\alpha(\text{post})})$ with

$$a_{\alpha(\text{post})} = a_{\alpha i} + \sum_{t=1}^T \gamma_{it} \quad b_{\alpha(\text{post})} = b_{\alpha i} + T - \sum_{t=1}^T \gamma_{it}$$

if time and unit specific α : $f(\alpha_{it}|-) \propto \text{kernel of a Beta}(a_{\alpha(\text{post})}, b_{\alpha(\text{post})})$ with

$$a_{\alpha(\text{post})} = a_{\alpha i} + \gamma_{it} \quad b_{\alpha(\text{post})} = b_{\alpha i} + 1 - \gamma_{it} \quad (2.10)$$

- update a missing observation Y_{it}

for $t = 1$: $f(Y_{it}|-) \propto \text{kernel of a } \mathcal{N}(\mu_{Y_{it}(\text{post})}, \sigma_{Y_{it}(\text{post})}^2)$ with

$$\sigma_{Y_{it}(\text{post})}^2 = \frac{1}{\frac{1}{\sigma_{c_{it}t}^{2*}} + \frac{\eta_{1i}^2}{2\sigma_{c_{it+1}t+1}^{2*}(1-\eta_{1i}^2)}}$$

$$\mu_{Y_{it}(\text{post})} = \sigma_{Y_{it}(\text{post})}^2 \left(\frac{\mu_{c_{it}t}^* + \mathbf{x}_{it}^T \boldsymbol{\beta}_t}{\sigma_{c_{it}t}^{2*}} + \frac{\eta_{1i}(Y_{it+1} - \mu_{c_{it+1}t+1}^* - \mathbf{x}_{it+1}^T \boldsymbol{\beta}_{t+1})}{\sigma_{c_{it+1}t+1}^{2*}(1-\eta_{1i}^2)} \right)$$

for $1 < t < T$: $f(Y_{it}|-) \propto \text{kernel of a } \mathcal{N}(\mu_{Y_{it}(\text{post})}, \sigma_{Y_{it}(\text{post})}^2)$ with

$$\sigma_{Y_{it}(\text{post})}^2 = \frac{1 - \eta_{1i}^2}{\frac{1}{\sigma_{c_{it}t}^{2*}} + \frac{\eta_{1i}^2}{\sigma_{c_{it+1}t+1}^{2*}}}$$

$$\mu_{Y_{it}(\text{post})} = \sigma_{Y_{it}(\text{post})}^2 \left(\frac{\mu_{c_{it}t}^* + \eta_{1i}Y_{it-1} + \mathbf{x}_{it}^T \boldsymbol{\beta}_t}{\sigma_{c_{it}t}^{2*}(1-\eta_{1i}^2)} + \frac{\eta_{1i}(Y_{it+1} - \mu_{c_{it+1}t+1}^* - \mathbf{x}_{it+1}^T \boldsymbol{\beta}_{t+1})}{\sigma_{c_{it+1}t+1}^{2*}(1-\eta_{1i}^2)} \right)$$

for $t = T$: $f(Y_{it}|-) \propto \text{kernel of a } \mathcal{N}(\mu_{Y_{it}(\text{post})}, \sigma_{Y_{it}(\text{post})}^2)$ with

$$(2.11)$$

2.2 Spatial cohesions analysis

To include spatial information, the idea is to extend the PPM from being a function of just $C(S_{jt})$ to the more informed one $C(S_{jt}, \mathbf{s}_{jt}^*)$, where S_{jt} is the j -th cluster at time instant t , and \mathbf{s}_{jt}^* is the subset of spatial coordinates of the units inside S_{jt} . For the sake of clarity, in this section where we are just interested in analysing the cohesions we employ the S_h notation, to indicate a general h -th cluster, rather than the more precise S_{jt} .

Regarding the computation of spatial cohesion, several choices are available [PQ15]. The main common idea of the following formulas is to favour few spatially

connected clusters rather than a lot of singleton ones; therefore most of them employ also the term $M \cdot \Gamma(|S_h|)$ which resembles the DP partitioning method that helps in reaching such goal.

We will now describe briefly all the cohesions which are implemented in the JDRPM model (and were implemented as well in CDRPM) and conduct test on each of them, to see how the tuning of their parameters affects the computed values. All the tests of Figures 2.3 and 2.4 refer to the partition of Figure 2.2, taken as test case here from a general fit on the same spatio-temporal dataset of Chapter 4.

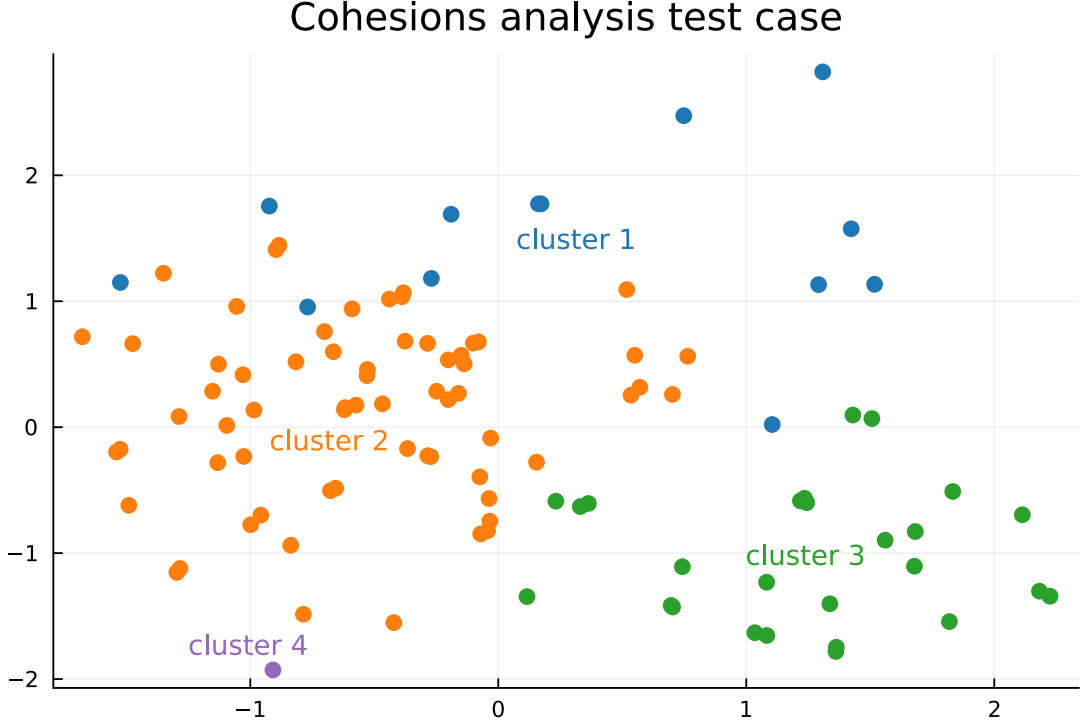


Figure 2.2: Partition considered to analyse the spatial cohesions.

The first cohesion uses a tessellation idea from [DH01] that considers $\mathcal{D}_h = \sum_{i \in S_h} \|s_i - \bar{s}_h\|$ as the total distance from the units to the cluster centroid \bar{s}_h . The computation is then an adjustment of a decreasing function in terms of \mathcal{D}_h , to give an higher weight on clusters which are denser, i.e. clusters that have lower \mathcal{D}_h , with an additional parameter α to provide more control on the penalization.

$$C_1(S_h, \mathbf{s}_h^*) = \begin{cases} \frac{M \cdot \Gamma(|S_h|)}{\Gamma(\alpha \mathcal{D}_h) \mathbb{1}_{[\mathcal{D}_h \geq 1]} + \mathcal{D}_h \mathbb{1}_{[\mathcal{D}_h < 1]}} & \text{if } |S_h| > 1 \\ M & \text{if } |S_h| = 1 \end{cases} \quad (2.12)$$

The second function provides, instead, a hard cluster boundary, where the weight is set to 1 only if all units inside the cluster are “close enough” to each other. The strictness of that requirement can be tuned trough the parameter a .

$$C_2(S_h, \mathbf{s}_h^*) = M \cdot \Gamma(|S_h|) \cdot \prod_{i,j \in S_h} \mathbb{1}_{[\|s_i - s_j\| \leq a]} \quad (2.13)$$

According to this cohesion, from Figure 2.3 we can see how the purple cluster is considered the one with the highest weight, being a singleton. The runner-up is the green cluster because it's the first among all the non-singletons which activates cohesion 2 when increasing the parameter a . In fact, cohesion 2 returns a value of 1 only if the cluster is quite compact, i.e. if the distances between all possible pairs of points are below the threshold parameter. The orange and blue clusters, instead, appear as less dense since they require an higher value of a to “pass” that distance check.

Anyway, cohesions C_1 and C_2 do not preserve the exchangeability property, meaning that if we would marginalize the random partition model over the last of m units, we would not get to the same model as if we only had $m - 1$ units. This coherence property, known as sample size consistency or addition rule [De +15], is instead often desirable, for theoretical or computational purposes, and the following two cohesions are able to provide it [MQR11].

Cohesion 3, called marginal likelihood or prior predictive distribution, treats the spatial coordinates \mathbf{s}^* as if they were random, applying on them a model such as the Normal/Normal-Inverse-Wishart, where $\boldsymbol{\xi} = (\mathbf{m}, V)$, $\mathbf{s}|\boldsymbol{\xi} \sim \mathcal{N}(\mathbf{m}, V)$ and $\boldsymbol{\xi} \sim \mathcal{NIW}(\boldsymbol{\mu}_0, \kappa_0, \nu_0, \Lambda_0)$. The idea is to assign a larger weight on clusters which produce large marginal likelihood values.

$$C_3(S_h, \mathbf{s}_h^*) = M \cdot \Gamma(|S_h|) \cdot \int \prod_{i \in S_h} q(\mathbf{s}_i | \boldsymbol{\xi}_h) q(\boldsymbol{\xi}_h) d\boldsymbol{\xi}_h \quad (2.14)$$

On the same line there is cohesion 4, the double dipper cohesion [QMP15], which it now employs a posterior predictive distribution, rather than the prior predictive distribution of cohesion 3.

$$C_4(S_h, \mathbf{s}_h^*) = M \cdot \Gamma(|S_h|) \cdot \int \prod_{i \in S_h} q(\mathbf{s}_i | \boldsymbol{\xi}_h) q(\boldsymbol{\xi}_h | \mathbf{s}_h^*) d\boldsymbol{\xi}_h \quad (2.15)$$

Another idea comes from [PQ18], which will also come back also for the covariates similarities case. In fact, cohesions 5 and 6 employ two variations of the cluster variance/entropy similarity function, with the parameter φ to provide control on the penalization.

$$C_5(S_h, \mathbf{s}_h^*) = \exp \left\{ -\varphi \sum_{i \in S_h} \|\mathbf{s}_i - \bar{\mathbf{s}}\| \right\} \quad (2.16)$$

$$C_6(S_h, \mathbf{s}_h^*) = \exp \left\{ -\varphi \log \left(\sum_{i \in S_h} \|\mathbf{s}_i - \bar{\mathbf{s}}\| \right) \right\} \quad (2.17)$$

2.3 Covariates similarities analysis

A wide spectrum of choice is also available for covariates similarities [PQ18]. To account for them, the idea consists in extending the PPM to make it function of S_{jt} ,

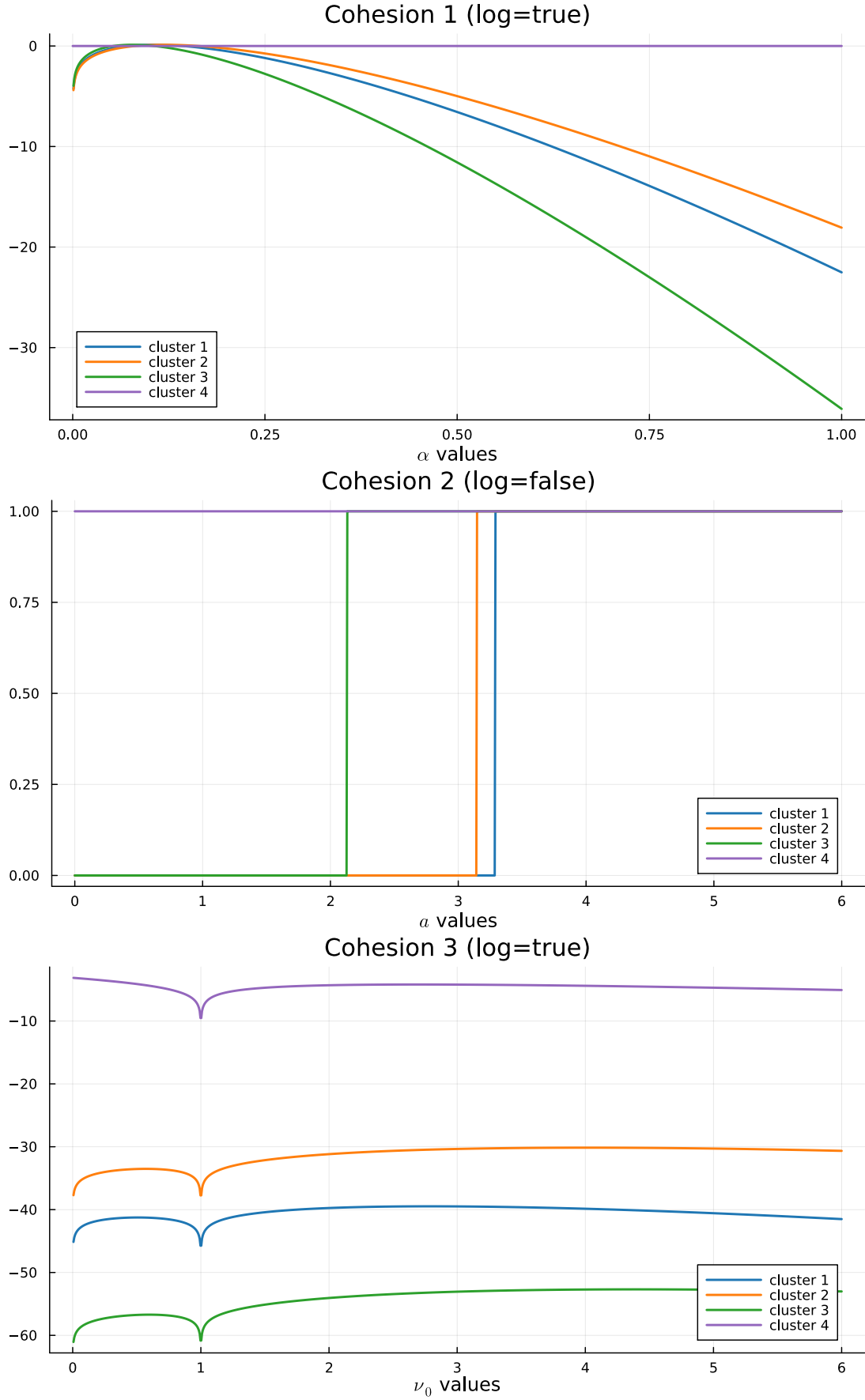


Figure 2.3: Cohesions 1, 2, and 3 computed on the test case partition, with respect to different values of their tuning parameter. Cohesion 2 is without the logarithm applied just for plotting purposes, since otherwise the values would have been $-\infty$ and 0.

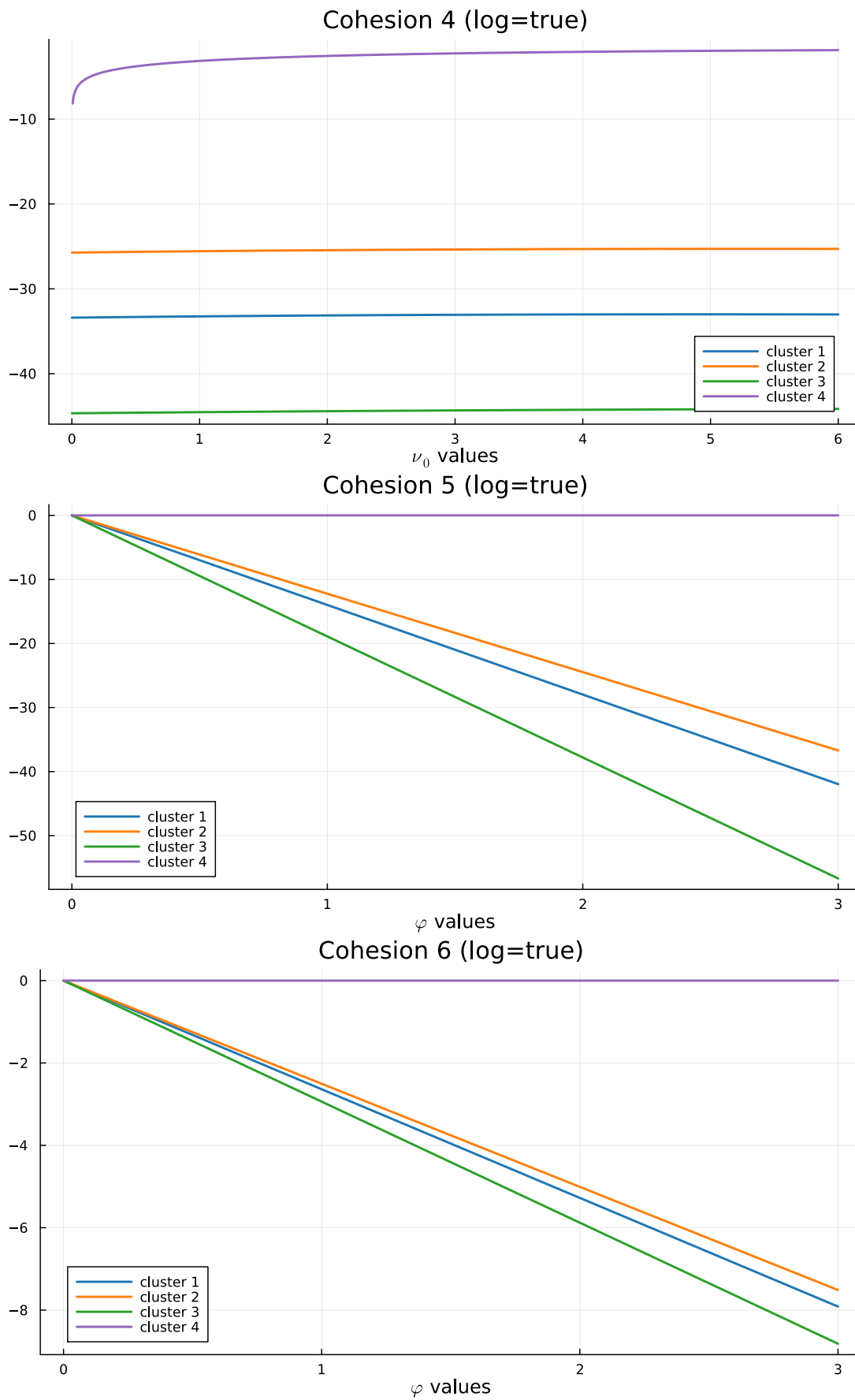


Figure 2.4: Cohesions 4, 5, and 6 computed on the test case partition, with respect to different values of their tuning parameter.

\mathbf{s}_{jt}^* , and now also of X_{jt}^* , being this the $p \times |S_{jt}|$ matrix storing the covariates of the units belonging to cluster j at time t , i.e. $X_{jt}^* = \{\mathbf{x}_{it}^* = (x_{it1}, \dots, x_{itp})^T : i \in S_{jt}\}$.

For the current implementation of JDRPM we decided to treat each covariate individually, therefore the PPM will actually be function of the set of unidimensional vectors which record the different p covariates of the units inside cluster jt , meaning $\mathbf{x}_{jt1}^*, \dots, \mathbf{x}_{jtp}^*$, of which all contributions will be considered independently one to each other. In this way, the final PPM form will be

$$P(\rho) \propto \prod_{h=1}^{k_t} C(S_{jt}, \mathbf{s}_{jt}^*) \left(\prod_{r=1}^p g(S_{jt}, \mathbf{x}_{jtr}^*) \right) \quad (2.18)$$

where \mathbf{x}_{jtr}^* represents the vector recording the r -th covariate values for all the units inside cluster S_{jt} , i.e. row r of matrix X_{jt}^* . A unified and multidimensional consideration of the covariates is nonetheless possible, as we will illustrate in the following description of the similarities, and would have lead to a PPM of the form

$$P(\rho) \propto \prod_{h=1}^{k_t} C(S_{jt}, \mathbf{s}_{jt}^*) g(S_{jt}, X_{jt}^*) \quad (2.19)$$

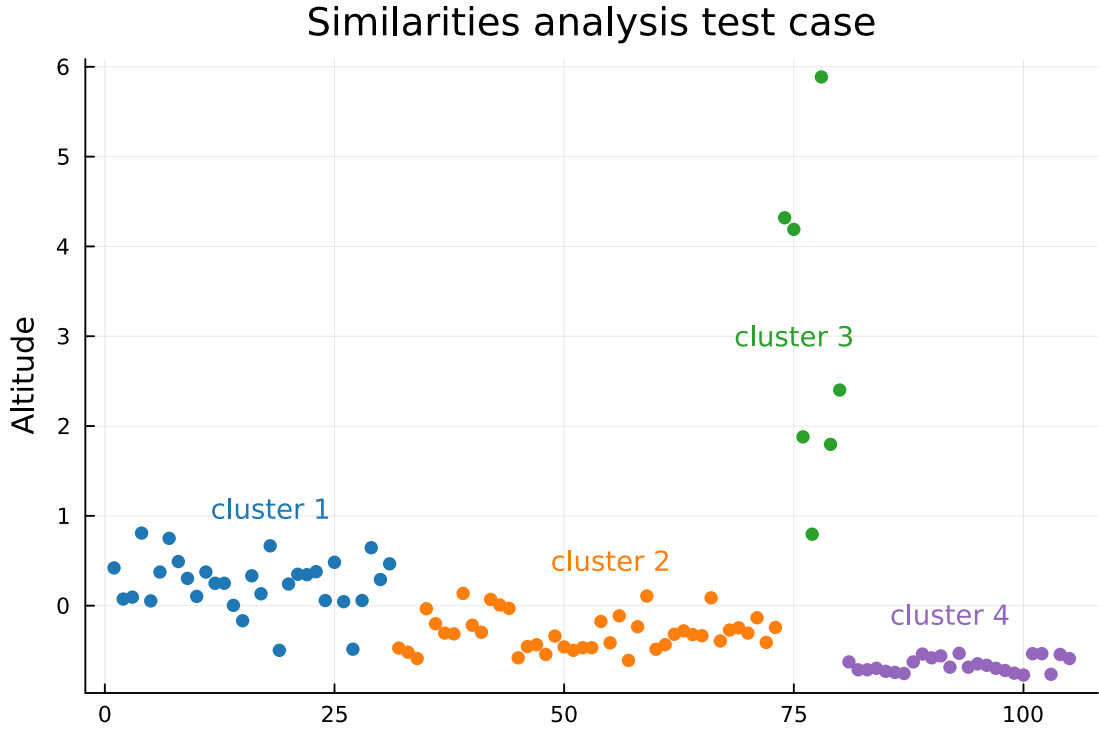


Figure 2.5: Partition considered to analyse the covariate similarities. The order of the units has been modified to plot together all units belonging to the same cluster.

As in the previous section, we will now discuss all the similarities implemented in the JDRPM model and perform test on each of the. All the tests will be referred to the test case partition displayed in Figure 2.5.

The first similarity is the cluster variance/entropy similarity function, which as the name suggest can work with both numerical and categorical variables. The general form is

$$g_1(S_h, \mathbf{x}_h^*) = \exp \{-\varphi H(S_h, \mathbf{x}_h^*)\} \quad (2.20)$$

with $H(S_h, \mathbf{x}_h^*) = \sum_{i \in S_h} (x_i - \bar{x})^2$ for numerical covariates, being \bar{x} the mean value of the \mathbf{x}_h^* vector, and $H(S_h, \mathbf{x}_h^*) = -\sum_{c=1}^C \hat{p}_c \log(\hat{p}_c)$ for categorical covariates, with \hat{p}_c indicating the computed relative frequency at which each factor appears. The parameter φ can control the amount of penalization to apply. This function can also be extended quite easily in the multidimensional case, at least for numerical covariates, where e.g. the H function could become $H(S_h, \mathbf{X}_h^*) = \sum_{r=1}^p \|\mathbf{x}_r - \bar{\mathbf{x}}\|$.

Another popular choice is the Gower similarity function [Gow71]. This similarity was originally designed for a multivariate context, where vectors of covariates are compared to each other; as a consequence some work was required to adapt it to the univariate case. The simple idea of comparing all cluster-specific pair-wise similarities leads to the following average Gower similarity

$$g_2(S_h, \mathbf{x}_h^*) = \exp \left\{ -\alpha \sum_{i,j \in S_h, i \neq j} d(x_i, x_j) \right\} \quad (2.21)$$

This function, however, is strictly increasing with respect to the cluster size, meaning that it will naturally tend to propose a large number of small clusters. For that reason, a correction can be applied, accounting for the size of the cluster S_h , which leads to the average Gower similarity.

$$g_3(S_h, \mathbf{x}_h^*) = \exp \left\{ -\frac{2\alpha}{|S_h|(|S_h| - 1)} \sum_{i,j \in S_h, i \neq j} d(x_i, x_j) \right\} \quad (2.22)$$

In both functions, $d(x_i, x_j)$ is the Gower dissimilarity between x_i and x_j , with $d(x_i, x_j) = |x_i - x_j|/R$ in the case of numerical covariates, being $R = \max(\mathbf{x}_h^*) - \min(\mathbf{x}_h^*)$ the range of the covariate vector, while $d(x_i, x_j) = \mathbb{1}_{[x_i \neq x_j]}$ in the case of categorical covariates. This is a dissimilarity since values closer to 0 denote similar data, while values closer to 1 refer to dissimilar data; therefore the minus sign inside g_2 and g_3 exponents converts the function to a similarity. For the multidimensional design there are natural extensions to the function $d(\mathbf{x}_i, \mathbf{x}_j)$.

The last similarity recalls the structure of the spatial cohesion 3, where now the covariates are treated as if they were random variables. However, since we chose to deal with each covariate individually, in this unidimensional setting a Normal/Normal-Inverse-Gamma model is employed, with $\boldsymbol{\xi} = (\mu, \sigma^2)$, $x|\boldsymbol{\xi} \sim \mathcal{N}(\mu_0, \sigma^2)$, and $\mu \sim \mathcal{N}(\mu_0, \sigma^2/\lambda_0)$, $\sigma^2 \sim \text{invGamma}(a_0, b_0)$, i.e. $\boldsymbol{\xi} \sim \mathcal{N}\text{invGamma}(\mu_0, \lambda_0, a_0, b_0)$. Therefore a multivariate extension is possible trough the same modelling style of the spatial coordinates case.

$$g_4(S_h, \mathbf{x}_h^*) = \int \prod_{i \in S_h} q(x_i|\boldsymbol{\xi}_h) q(\boldsymbol{\xi}_h) d\boldsymbol{\xi}_h \quad (2.23)$$

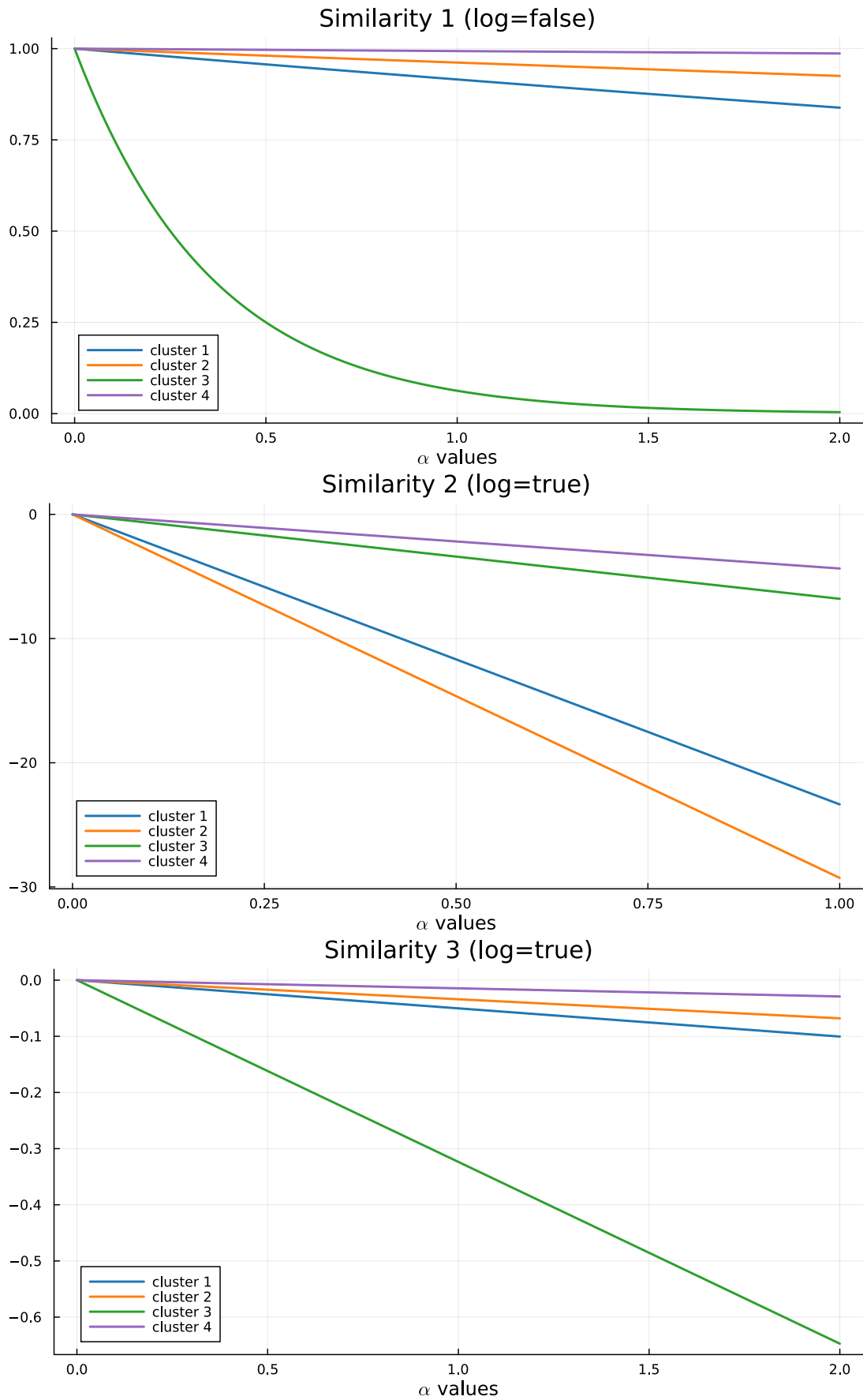


Figure 2.6: Similarities 1, 2 and 3 computed on the test case partition, with respect to different values of their tuning parameter. Similarity 1 is without the logarithm applied just for plotting purposes, to see more clearly the gap among the clusters.

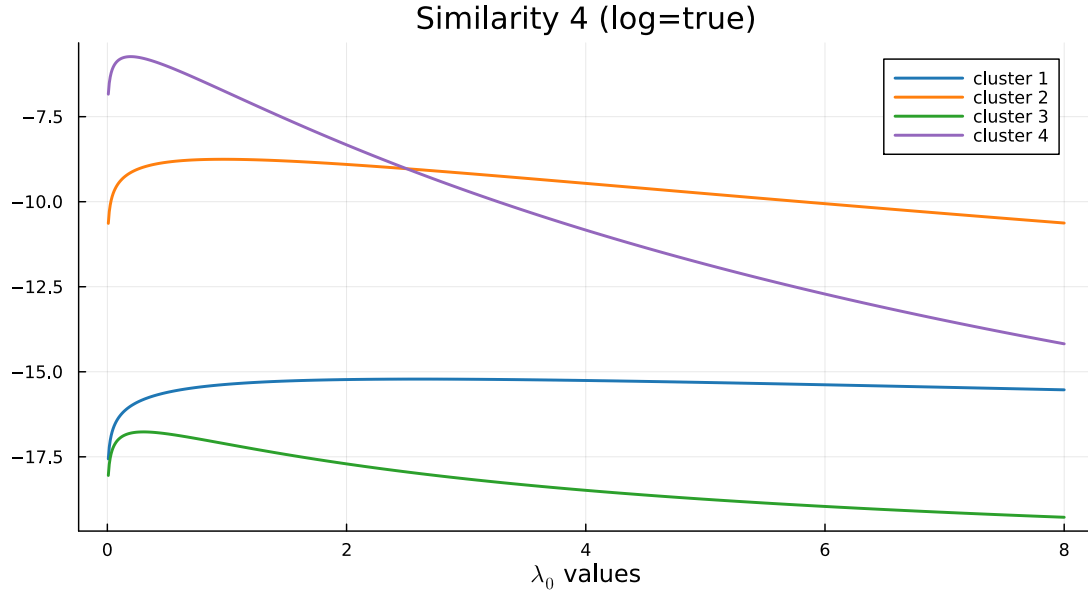


Figure 2.7: Similarity 4 computed on the test case partition, with respect to the different values of its tuning parameter. The other parameters has been set to $\mu_0 = 0$, $a_0 = b_0 = 1$.

All the similarities, except for g_2 , agree to classify the clusters with the purple one being the one with the highest similarity, followed by orange, blue, and green, as we can see from Figures 2.6 and 2.7. Indeed, Figure 2.5 seems to confirm this ranking, by intuitively reasoning about the sparsity of each cluster.

Chapter 3

Implementation and optimizations

To implement our updated model, and to do it efficiently, we decided to opt for the Julia language [Bez+17].

In fact, Julia combines the ease and expressiveness of high-level languages to the efficiency and performance of low-level ones. This balance largely achieved through the just-in-time (JIT) compilation, implemented using the LLVM framework. This design choice allows Julia to be used interactively, in the same fashion to the R, Matlab or Python consoles, while also supporting the more traditional program execution style of statically compiled languages such as C, C++ and Fortran. This solution provides faster development phases, since for examples code sections can be evaluated and tested line by line, and at the same time guarantees efficient implementations. Performances are further enhanced by the use of the optimized BLAS [Law+79] and LAPACK libraries for linear algebra computation, whose operations are often at the core of all scientific applications. Regarding productivity, instead, Julia provides an extensive ecosystem, currently comprised by more than ten thousand packages spanning over almost all branches of scientific computing. Moreover, most of them are already highly tested and optimized, and can therefore reduce the implementation time required to the users. As an example, in this work we employed the `Distributions` [Bes+21] [Lin+19] and `Statistics` packages, while the original C implementation had to write all the statistical functionalities from scratch.

Considering all this, the Julia choice was deemed very natural.

3.1 Optimizations

As we will see in Section 4, even despite the higher complexity of the model we managed to get better performance in Julia compared to the original C implementation. This at the reasonable cost of a smaller increase in the memory requirements.

In fact, one major issue encountered during the earlier stages of designing the fitting function in Julia was controlling the amount of memory and allocations that some functions, structures, or algorithms would require. At the beginning of

the development and testing, where the correctness of the algorithm was the only priority, we saw that most of the execution time was actually spent by the garbage collector of Julia, which had the burden of tracking all the allocated memory and reclaiming the unused one in order to make it available again for new computations.

Together with avoiding useless allocations, or in general managing more finely the memory, another important aspect to focus on to improve performances is ensuring type stability of the function. Luckily, Julia disposes of several tools to inspect and address both problems.

Regarding the first point, there are packages such as **Cthulhu**, or even the simple `@code_warntype` macro, which allow to ensure that a function is type-stable, i.e. that the types of all variables can be correctly predicted by the compiler and stay consistent throughout the execution. Type stability is crucial for performance as it enables the compiler to generate optimized machine code, removing the load derived from dynamic type checks. In fact, Julia is dynamically typed, which means that variables do not have to be necessarily declared with their type, in contrast to fully statically typed languages such as C, and they could change it during execution. For example a variable initialized as an integer could later become a float, or even a string. However, for performance purposes, these dynamicisms should be avoided, and those tools help to ensure that this happens.

Regarding allocations, we relied on profiling suites such as **ProfileCanvas**. This profiler generates a plot, the *flame graph* of Figure 3.1, which depicts the different sections of code with regions whose size is proportional to a certain metric, e.g. the time spent on them during execution or the number (or size) of allocations that was required. This allows to see if the running time is spent on actual useful operations or instead on “bad” ones, such as garbage collection; highlighting therefore the sections of code which could possibly be optimized. All the modelling variables were of course preallocated, but the key has been to refactor the code to make it work more *in place*, passing directly as arguments the variables which would be modified the function, and modify them inside the function, rather than returning some values and then use them on the initial variables.

More in general, **BenchmarkTools** [CR16] had been also a great ally to quickly analyse and compare whole fits or just small sections of code and simple instructions. For example, we can test different versions of equivalent instructions to see which could be the most efficient, as in this case

```
using BenchmarkTools
nh_tmp = rand(100)
@btime nclus_temp = sum($nh_tmp .> 0)
# 168.956 ns (2 allocations: 112 bytes)
@btime nclus_temp = count(x->(x>0), $nh_tmp)
# 11.612 ns (0 allocations: 0 bytes)
```

or this other one

```
n = 100; rho_tmp = rand((1:5),n); k = 1
@btime findall(j -> ($rho_tmp)[j]==$k, 1:n) # with anonymous function
# 272.302 ns (5 allocations: 384 bytes)
@btime findall_faster(j -> ($rho_tmp)[j]==$k, 1:n) # custom implementation
```


models proved to be already optimally performing. The main problem was instead with cohesions 3 and 4, the auxiliary and double dippery, which by nature would involve some linear algebra computations with vectors and matrices.

The first implementation of those cohesions turned out to be really slow, due to the overhead generated by allocating and then freeing, at each call, the memory devoted to all vectors and matrices. This in the end meant that most of the execution time was actually spent by the garbage collector, rather than in the real and useful operations. A first solution was then to resort to a scalar implementation, which would remove the overhead of the more complex memory structures, but in the end we managed to combine the readability of the first idea with the performance of the second one into a final version, as we can see from Listing 1.

Listing 1: Sections of the Julia code for the three implementation cases of the spatial cohesions 3 and 4. The first one has the classical vector computations derived from the mathematical formulation, the second one is the conversion to only have scalar variables, while the third one is the final version, keeping the vector form but improved using static structures.

```
# original vector version
sbar = [mean(s1), mean(s2)]
vtmp = sbar - mu_0
Mtmp = vtmp * vtmp'
Psi_n = Psi + S + (k0*sdim) / (k0+sdim) * Mtmp

# scalar-only version
sbar1 = mean(s1); sbar2 = mean(s2)
vtmp_1 = sbar1 - mu_0[1]
vtmp_2 = sbar2 - mu_0[2]
Mtmp_1 = vtmp_1^2
Mtmp_2 = vtmp_1 * vtmp_2
Mtmp_3 = copy(Mtmp_2)
Mtmp_4 = vtmp_2^2
aux1 = k0 * sdim; aux2 = k0 + sdim
Psi_n_1 = Psi[1] + S1 + aux1 / (aux2) * Mtmp_1
Psi_n_2 = Psi[2] + S2 + aux1 / (aux2) * Mtmp_2
Psi_n_3 = Psi[3] + S3 + aux1 / (aux2) * Mtmp_3
Psi_n_4 = Psi[4] + S4 + aux1 / (aux2) * Mtmp_4

# static improved version
sbar1 = mean(s1); sbar2 = mean(s2)
sbar = SVector((sbar1, sbar2))
vtmp = sbar .- mu_0
Mtmp = vtmp * vtmp'
aux1 = k0 * sdim; aux2 = k0 + sdim
Psi_n = Psi .+ S .+ aux1 / (aux2) .* Mtmp
```

This final version exploits the `StaticArrays` package of Julia, which allows to use vectors and matrices more efficiently if their size is known at compile time; which is the case of the spatial cohesions computation, since working with planar spatial coordinates we will always have 2×1 vectors and 2×2 matrices. The benefits of this final version are that we maintain the natural mathematical form of the first one, improving the clearness of the code, together with the efficiency of the second one, since now with static structures the compiler is able to optimize all memory allocations as it was doing with the simple scalar variables.

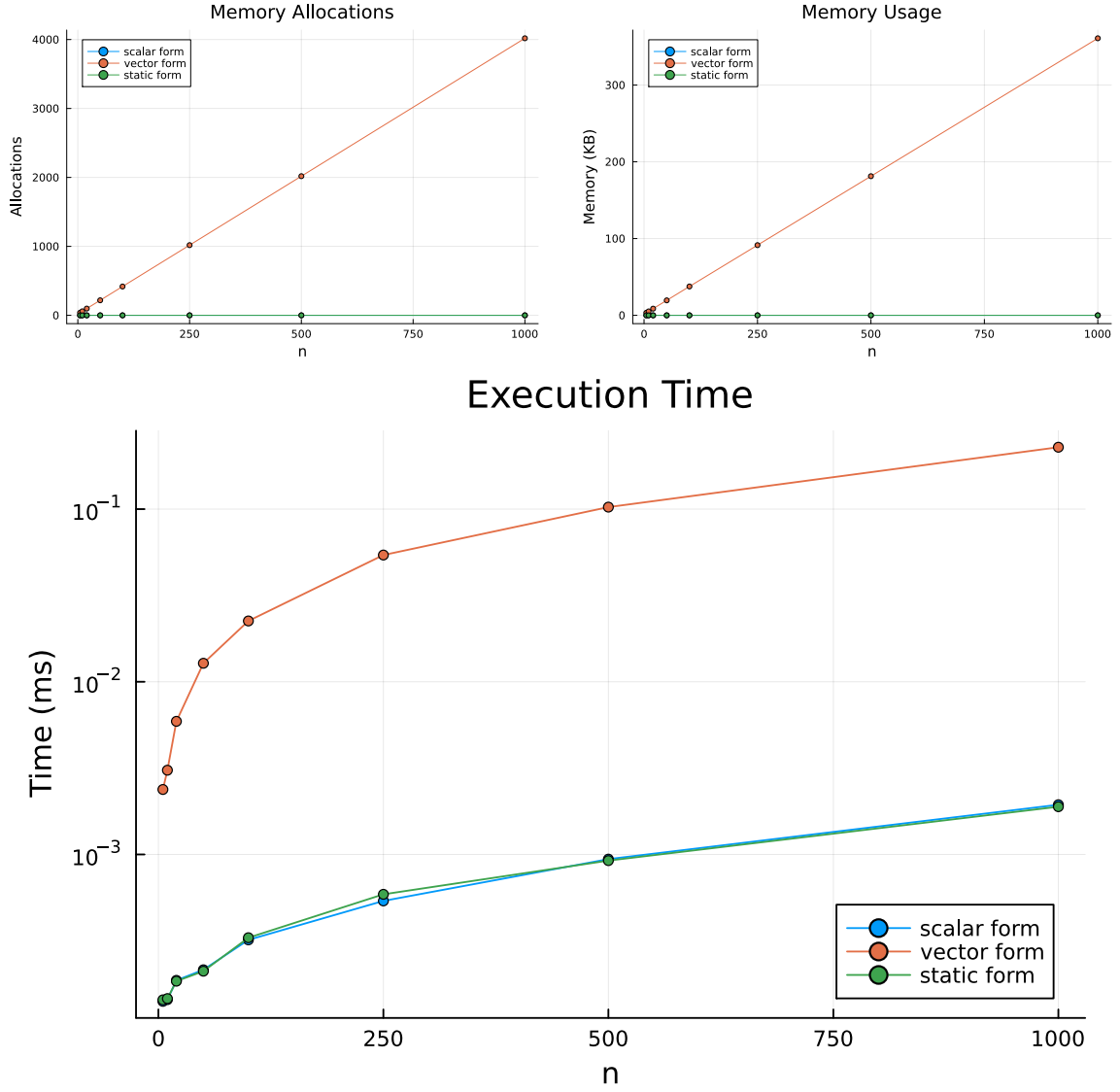


Figure 3.2: Performance comparison between the three versions of the cohesion 4 function. Tests ran through the `BenchmarkTools` package of Julia by randomly generating the spatial coordinates of the various test sizes n , with similar results standing for cohesion 3. The memory allocation and usage plots are constant at zero for both the scalar and vector static cases.

Figure 3.2 shows the comparison of their performances, where we can see how the scalar and static versions indeed perform very similarly.

Noticeably, the C implementation of the model didn't have to worry about all this reasoning, since C can't natively, nor gracefully, work with vectors and matrices.

3.1.2 Optimizing covariates similarities

Another problem was how to speed up the computation of the similarity functions, since those would also be called the possibly millions of times as the cohesion ones, considering also that we could incorporate more than one covariate into the clustering

process, so there would be an additional loop based on p , the number of covariates decided to be included.

As in the previous case, some of the functions didn't show any special need or room for relevant optimizations. The fourth one instead, the auxiliary similarity function, was essential to be optimized; not only being one the most frequent choice among all the similarities, but also because it involves a computationally heavy sum of the squares of the covariate values, as we can see in Listing 2.

Listing 2: Fully equipped version of the similarity 4 function, i.e. with all the optimizing macros. The performance analysis will focus just on that inside loop, since the rest is not negotiable.

```
function similarity4(X_jt::AbstractVector{<:Real}, mu_c::Real, lambda_c::Real,
↳ a_c::Real, b_c::Real, lg::Bool)
    n = length(X_jt)
    nm = n/2
    xbar = mean(X_jt)
    aux2 = 0.
    @inbounds @fastmath @simd for i in eachindex(X_jt)
        aux2 += X_jt[i]^2
    end
    aux1 = b_c + 0.5 * (aux2 - (n*xbar + lambda_c*mu_c)^2/(n+lambda_c) +
↳ lambda_c*mu_c^2 )
    out = -nm*log2pi + 0.5*log(lambda_c/(lambda_c+n)) + lgamma(a_c+nm) -
↳ lgamma(a_c) + a_c*log(b_c) + (-a_c-nm)*log(aux1)
    return lg ? out : exp(out)
end
```

The idea to optimize it has been to annotate the loop with some macros provided by Julia. They are the following:

- `@inbounds` eliminates the array bounds checking within expressions. This allows to skip the checks, at the cost to guarantee, by code design, that no out-of-bounds or wrong accesses will occur in the code and therefore no undefined behaviour will take place. The above loop is indeed very simple and safe, so this assumption is clearly satisfied.
- `@fastmath` executes a transformed version of the expression, which calls functions that may violate strict IEEE semantics¹. For example, its use could make $(a + b) + c \neq a + (b + c)$, but just in very pathological cases. Again, this is not a problem in our case where we are computing $\sum X_i^2$, since it does not have an intrinsically “right order” in which it has to be done.
- `@simd` (single instruction multiple data) annotate a for loop to allow the compiler to take extra liberties to allow loop re-ordering. This is a sort of parallelism technique, but rather than distributing the computational load on more processors we just *vectorize* the loop, i.e. we enable the CPU to

¹Institute of Electrical and Electronics Engineers. The IEEE-754 standard defines floating-point formats, i.e. the ways to represent real numbers in hardware, and the expected behavior of arithmetic operations on them, including precision, rounding, and handling of special values (e.g. NaN (Not a Number) and infinity).

perform that single instruction (summing the square of the i th component to a reduction variable) on multiple data chunks at once, using vector registers, rather than working on each element of the vector individually.

As we can see from Figure 3.3, the actual performance difference basically derives just from the use of `@simd`, with the other two annotations making not much of a difference. For that reason, and to reassure all pure mathematicians, we decided to remove the `@fastmath` annotation, leaving just `@inbounds` and `@simd`.

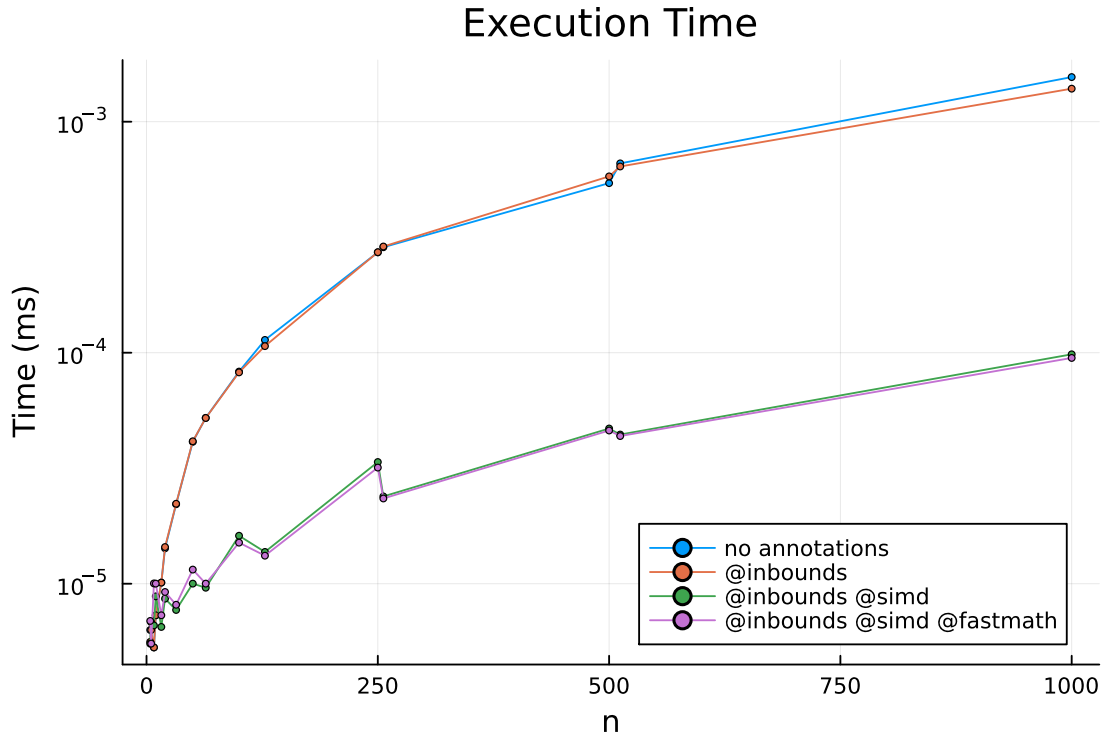


Figure 3.3: Comparison of the performances of the different possible loop annotations in the similarity 4 implementation. Their numerical output results are indeed the same for all cases. There are no memory allocation and usage plots since the analysis has been conducted only to evaluate the performances of the inside loop, which has no memory issues.

We can also notice interestingly how the tests with `@simd` annotation runs quicker in the case of n being a power of two compared to its closest rounded integer (e.g. 256 against 250 or 512 against 500), despite having some more data. This is a proof of the effectiveness of the SIMD paradigm: according to the different architectures, the CPUs can provide different register sizes (e.g. 64, 128, 256 or 512 bits) and therefore the data subdivision can fit perfectly in them when the total memory occupied by the elements is a multiple of that register size (i.e. the number of data values is a power of two). Otherwise there will be some “leftovers chunks”, which will of course be processed, but will also cause, as a consequence of the imperfect fit, a bit of overhead.

Chapter 4

Testing

4.1 Assessing the equivalence of the models

Our model, and the corresponding Julia code, is just an improvement of the original DRPM one with his relative C implementation. These improvements, as described in the previous chapters, refer to the insertion of covariates, both at the clustering and likelihood levels, the handling of missing values in the target variable, and the computational efficiency. In this sense, our updates are just add-ons to the original model, and therefore at a common testing level they should perform similarly by agreeing in the clusters that they produce on a given dataset.

To assess this ideally equivalent behaviour we ran two tests: the first one with only the target values, using generated data, while the second with also spatial information, using a real spatio-temporal dataset. From now on, for the sake of clarity, we will refer to CDRPM as the original model and implementation from [PQD22], while to JDRPM as the updated version derived from this thesis work.

In the following, we will rely on the ARI index [HA85], which is a correlation index to measure similarities between clusterings. More precisely, given two partitions ρ_1 and ρ_2 , the $\text{ARI}(\rho_1, \rho_2)$ returns a value between $[-1, 1]$, with higher values indicating higher levels of agreement between the two partitions. Its expected value (being a *random* index) is equal 0, which refers to comparing two randomly generated partitions.

We will use this index both to study the time evolution of the clusterings, to see if they show the time dependence that the models implement, and also to check the level of agreement among the different models.

4.1.1 Target variable only

For the first test we generated a dataset of $n = 10$ units and $T = 12$ time instants, and fitted both models collecting 1000 iterates derived from 10000 total iterations, discarding the first 5000 as burnin, and thinning by 5. Those parameters, as well as the generating function, were the same of [PQD22]. The generating function allowed to create data points with temporal dependence which could be

tuned through some dedicated parameters.

Table 4.1: Summary of the comparison between the two fits. The MSE columns refer to the accuracy between the fitted values generated by the models (estimated by taking the mean and the median of the returned 1000 iterates) and the true values of the target variable. Higher LPML and lower WAIC indicate a better fit.

	MSE mean	MSE median	LPML	WAIC	execution time
CDRPM	1.6731	1.5861	-249.61	469.69	4.8s
JDRPM	1.2628	1.2181	-227.83	415.03	2.5s

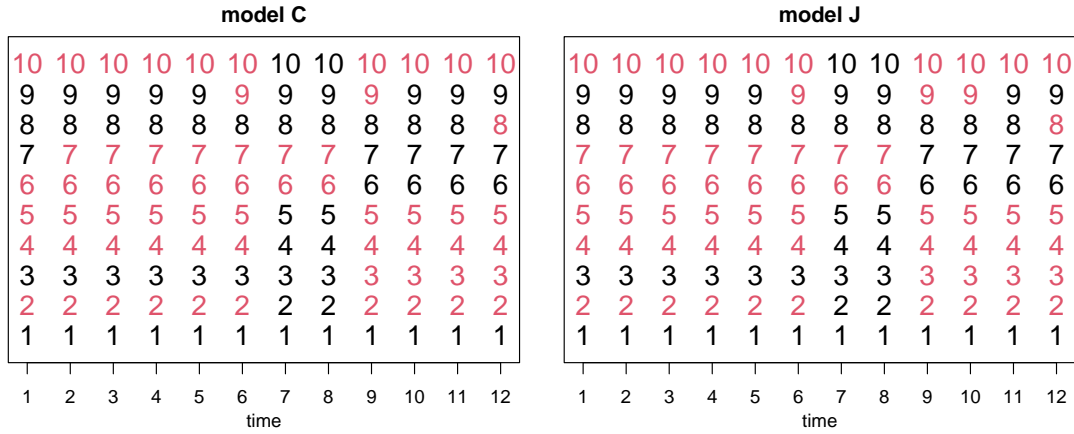


Figure 4.1: Clustering produced by the two models, with time points on the x axis, units indicated vertically by their number, and colors representing the cluster label.

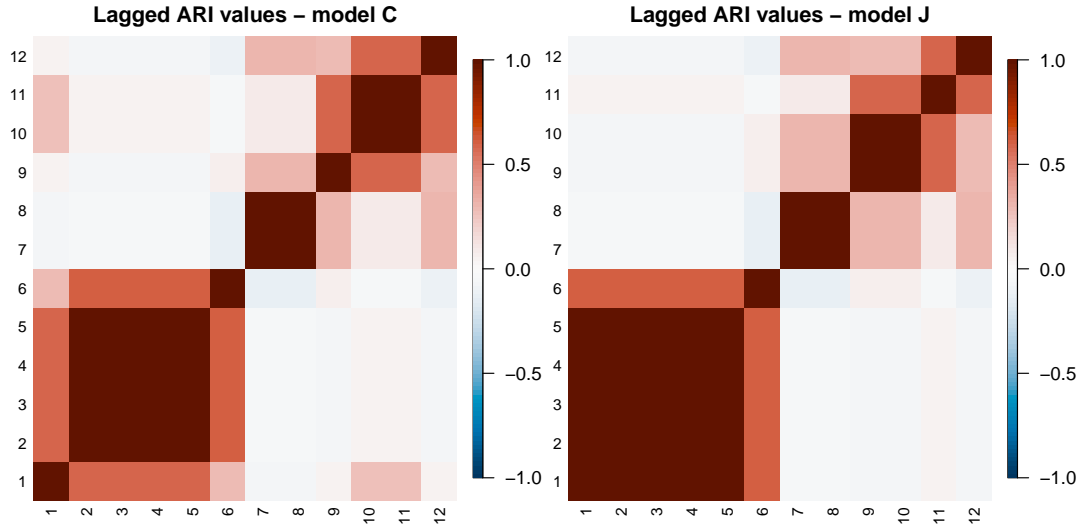


Figure 4.2: Lagged ARI values for the two models, on the fit with target only data. The partitions were estimated using the `salso` function from the corresponding R library.

At this testing stage there was just the target values from Y_{it} to dictate the clusters definition, and both models managed to provide good fits, as we can read from Table 4.1. The JDRPM model had better fit metrics (lower WAIC and higher

LPML) and also faster execution time. Regarding the fitted values, displayed in Figure 4.4 together with the original data, they turned out to be also more precise than the one generated by CDRPM, having lower MSEs.

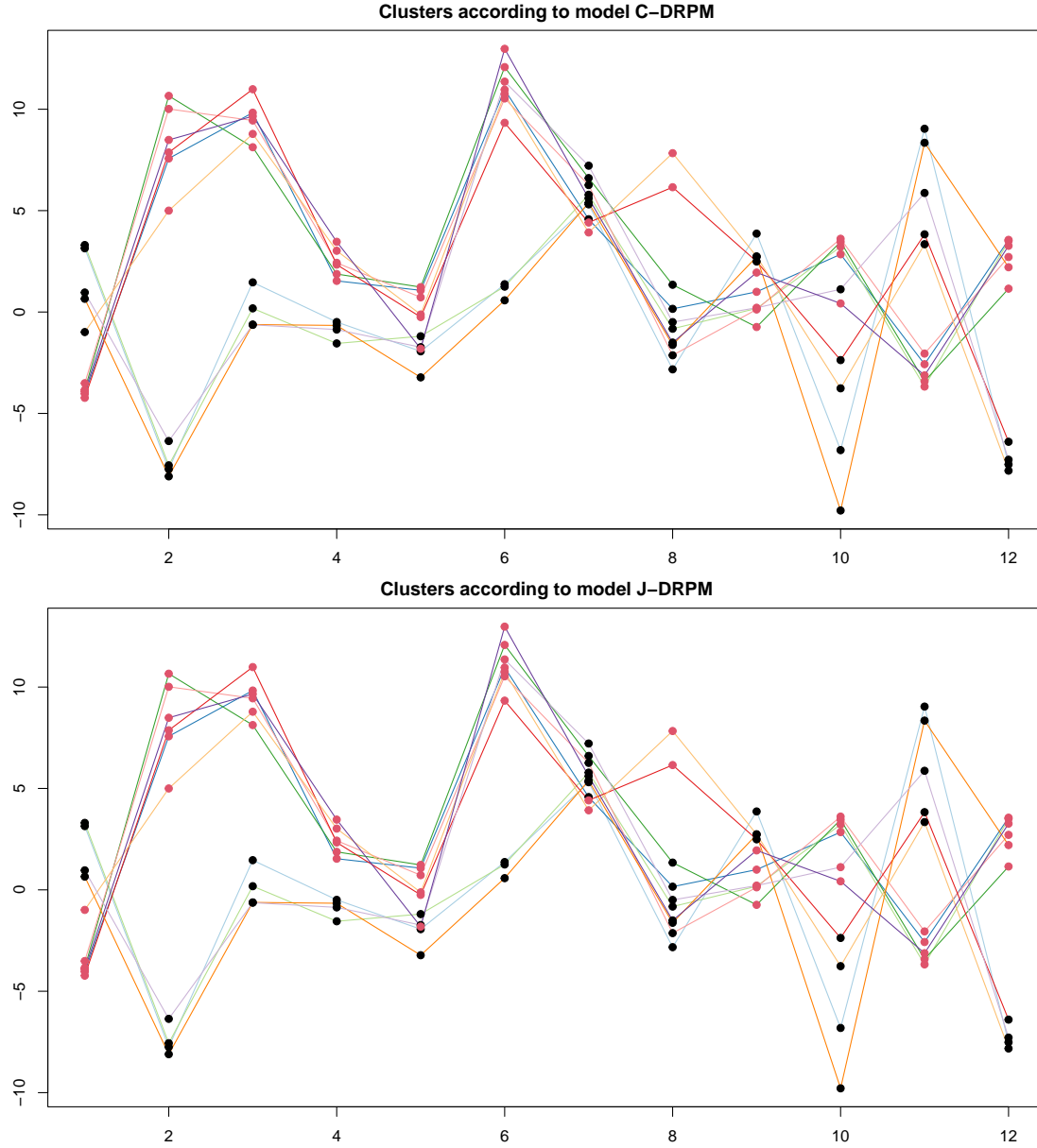


Figure 4.3: Visual representation of the clusters produced by the models, on the fit with target only data, with units' labels represented as colored dots overlaid to the trend of the generated target variable. The only differences occur at times 1 and 10.

The resulting clusters were indeed very similar. Figure 4.2 shows how they manifest the same temporal trend, while Figure 4.1 highlights how the clusters produced are really the same except for two differences occurred at times 1 and 10. By visually inspecting the clusters from Figure 4.3, we can see how at $t = 1$ the JDRPM model assigned a red label to a unit closer to the black pack, to which in fact model CDRPM assigned a black label. However, that same unit in the following time instants would be clearly part of the red cluster, thus making the

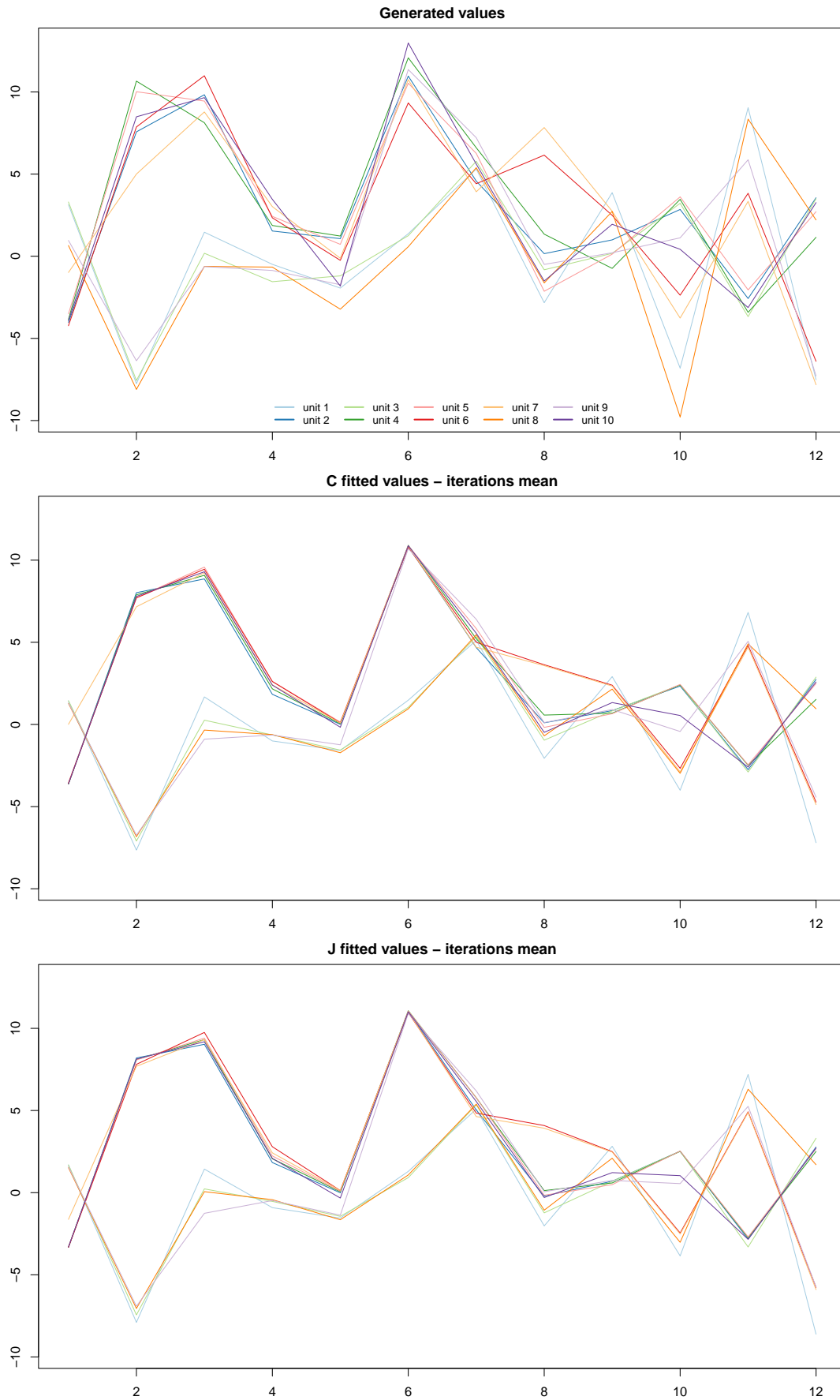


Figure 4.4: Generated target values (top), together with their fitted values estimate trough the mean of the 1000 iterates generated by model CDRPM (middle) and JDRPM (bottom).

JDRPM choice very reasonable. The opposite happens at $t = 10$, where now the CDRPM model seems to give more importance on the temporal trend, assigning a black label to a unit really closer to the red pack but that is destined to enter the black cluster in the following two time instants.

4.1.2 Target variable plus space

We now consider a more realistic scenario in which we fit the models using a spatio-temporal dataset. In particular, we used the AGRIMONIA [Fas+23] data which stores PM_{10} levels, together with many other environmental variables, in the Lombardy region from 2016 to 2021. For the following testing fits, we employed a summary dataset composed by weekly averages of the data from year 2018. We selected all $n = 105$ stations but we limited the time horizon to $T = 12$, which corresponds to a three-month monitoring period, just to reduce the time needed to perform all tests. Convergence was ensured visually by inspecting trace plots and, for the JDRPM model, by numerical diagnostics such as ESS and \hat{R} , which instead the CDRPM model is not able to provide directly from the fit. We collected 4000 iterates, from 110000 total iterates with a burnin of 90000 and thinning by 5.

Table 4.2: Summary of the comparison between the two fits. The MSE columns refer to the accuracy between the fitted values generated by the models (estimated by taking the mean and the median of the returned 4000 iterates) and the true values of the target variable. Higher LPML and lower WAIC indicate a better fit.

	MSE mean	MSE median	LPML	WAIC	execution time
CDRPM	0.0142	0.0149	694.81	-1768.42	1h 38m
JDRPM	0.0131	0.0138	624.91	-1898.05	37m

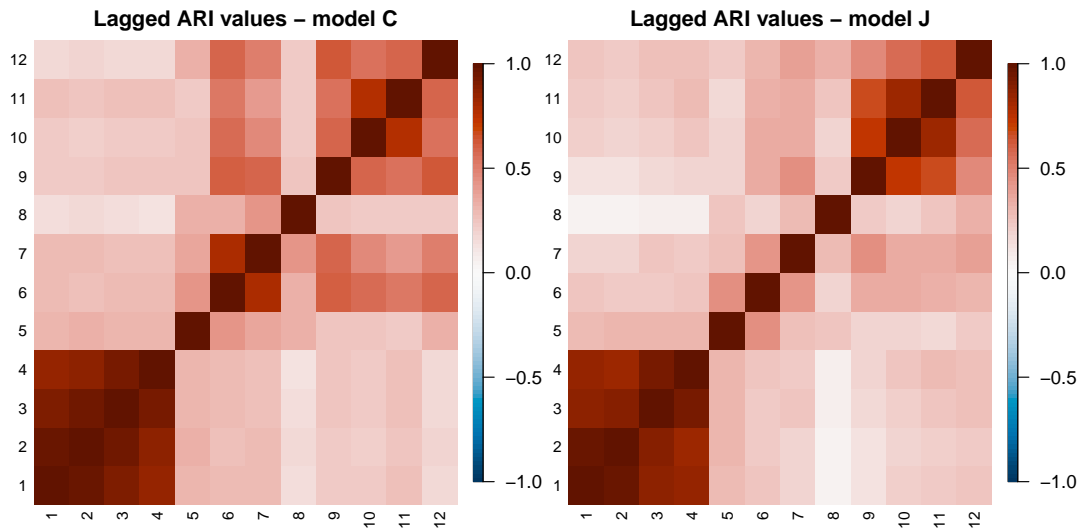


Figure 4.5: Lagged ARI values for the two models, on the fit with target plus space data. The partitions were estimated using the `salso` function from the corresponding R library.

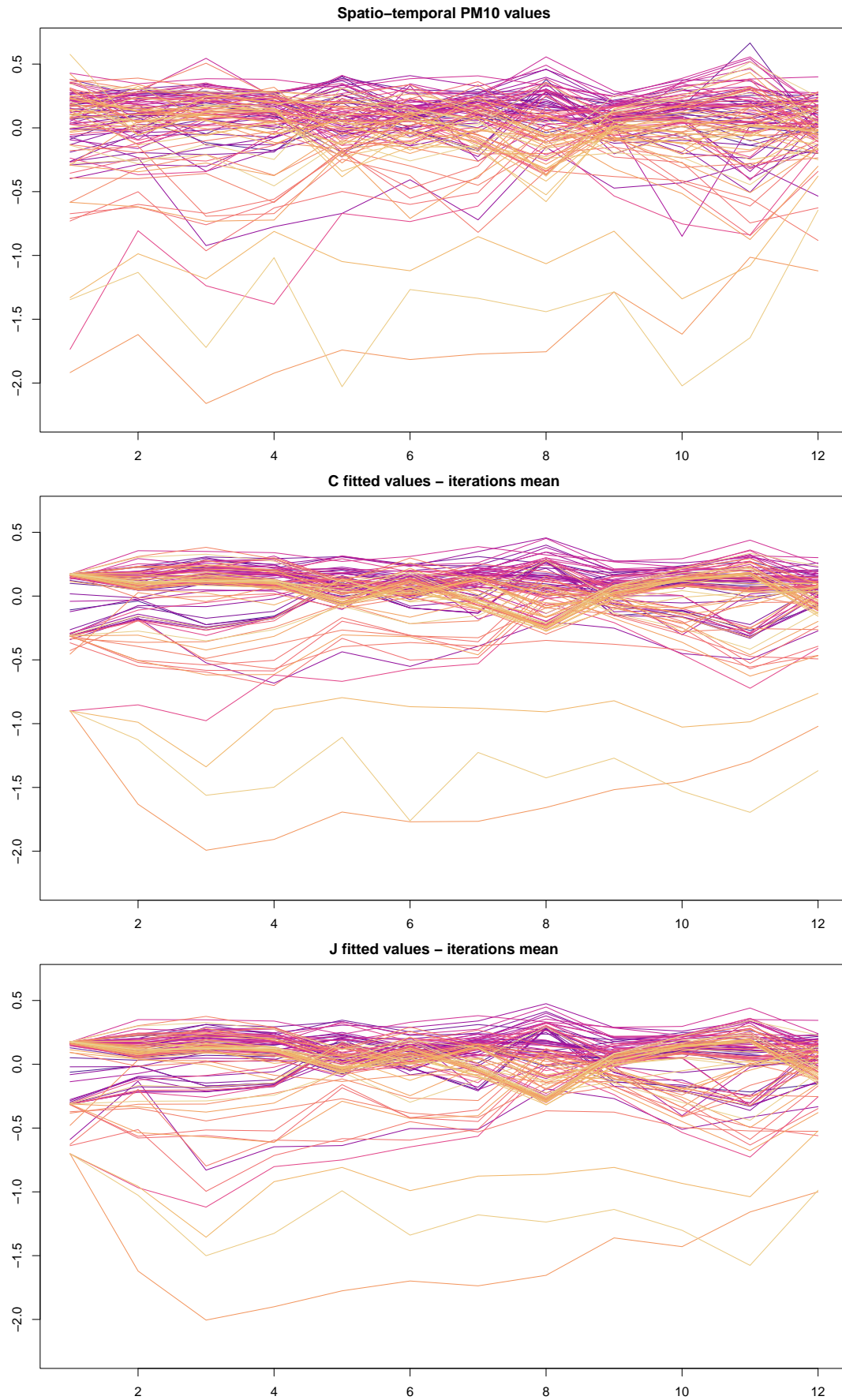


Figure 4.6: Target Y_{it} values (top), together with their fitted values estimate trough the mean of the 4000 iterates generated by model CDRPM (middle) and JDRPM (bottom).

Table 4.2 shows how both model managed to be accurate not only with respect to the fitting metrics of LPML and WAIC, but also in terms of the fitted values. Execution times are also reported, but they are a bit biased since during the fitting I was busy in writing this thesis, meaning that not all the computational resources of my laptop were devoted to the fitting task. According to my calculations, we could expect faster execution times by about 30%, but in any case more accurate performance evaluations on the timings will be conducted in Section 4.4.

From Figure 4.5 we can see how the temporal trend was very similar, confirming the correctness of the JDRPM implementation. Regarding the similarity of the produced clusters, the partition plot as in Figure 4.1 would now be more crowded due to the high number of units. For this reason, in order to still convey that information, we computed $\text{ARI}(\rho_{\text{JDRPM}}(t), \rho_{\text{CDRPM}}(t))$ for all time instants $t = 1, \dots, 12$, and we obtained a mean of 0.80 and a median of 0.86, denoting high levels of agreement in the clusters produced. A visual representation of the clusters is anyway provided in Figure ??.

4.2 Performance with missing values

We now repeat the tests of the previous section on a dataset with missing values, by randomly introducing some NAs into it to see how the JDRPM model reacts to the absence of a full dataset, and to see if it can still perform well. Based on the amount of missing values in the Agrimonia [Fas+23] dataset, used for the spatio-temporal tests, we chose to set to 10% the percentage of values that would be replaced by NAs. To perform such replacements, we randomly drew $nT/10$ indexes from the sets $[1, \dots, n]$ and $[1, \dots, T]$ to get all the pairs (i, t) which would become missing values in the Y_{it} dataset. The treating of NAs was an upgrade of the JDRPM model, so we can't perform these tests with the original CDRPM model, since it cannot handle missing data.

4.2.1 Target variable only (NA case)

The JDRPM seems to exhibit good performance also with missing data. From Table 4.3 we can see how the performances, naturally worse than the fit with the full case, are still good. The MSE is inevitably higher since the model did not have all the data points, and so we get less precise fitted values for the corresponding missing spots in the dataset, but the fitted values of Figure 4.7 are still close the one obtained with the full dataset fit. The WAIC is actually lower, i.e. better, but this could be just due to some randomness of the computation (e.g. the chosen seed).

From Figures 4.9 and 4.8 we can see how we get almost the same temporal trend since indeed the assigned clusters are almost the same. The only difference occurs on a single unit at time 10, where now the JDRPM model does the same thing that CDRPM did in its corresponding fit of Section 4.1.1.

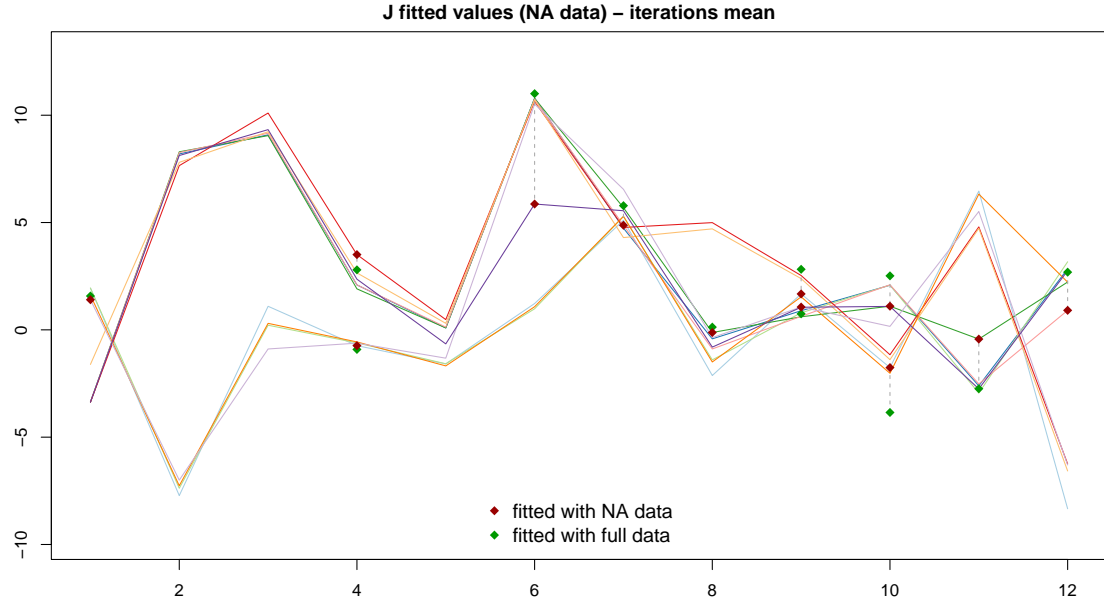


Figure 4.7: Fitted values estimate through the mean of the 1000 iterates generated by model JDRPM. The generated target values were the same of Figure 4.4. Special point markers are used for the data points which were missing, to highlight the gaps between the fitted values on the full dataset (green squares) and the fitted ones on the NA dataset (red squares).

Table 4.3: Summary of the comparison between the two Julia fits on target values only. The MSE columns refer to the accuracy between the fitted values generated by the models (estimated by taking the mean and the median of the returned 1000 iterates) and the true values of the target variable. Higher LPML and lower WAIC indicate a better fit.

<i>JDRPM</i>	MSE mean	MSE median	LPML	WAIC	execution time
NA data	2.1819	1.7876	-239.21	417.21	3.0s
full data	1.2628	1.2181	-227.83	415.03	2.5s

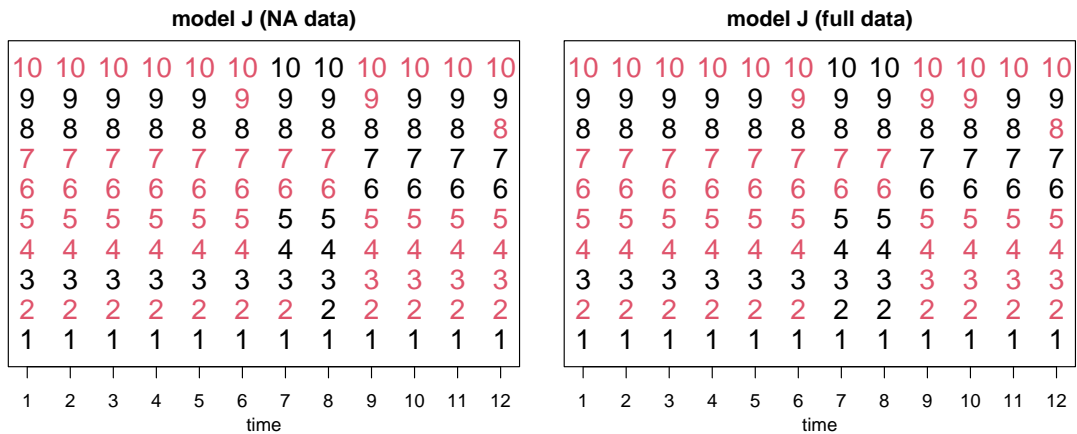


Figure 4.8: Clustering produced by the two tests on the JDRPM model, with time points on the x axis, units indicated vertically by their number, and colors representing the cluster label.

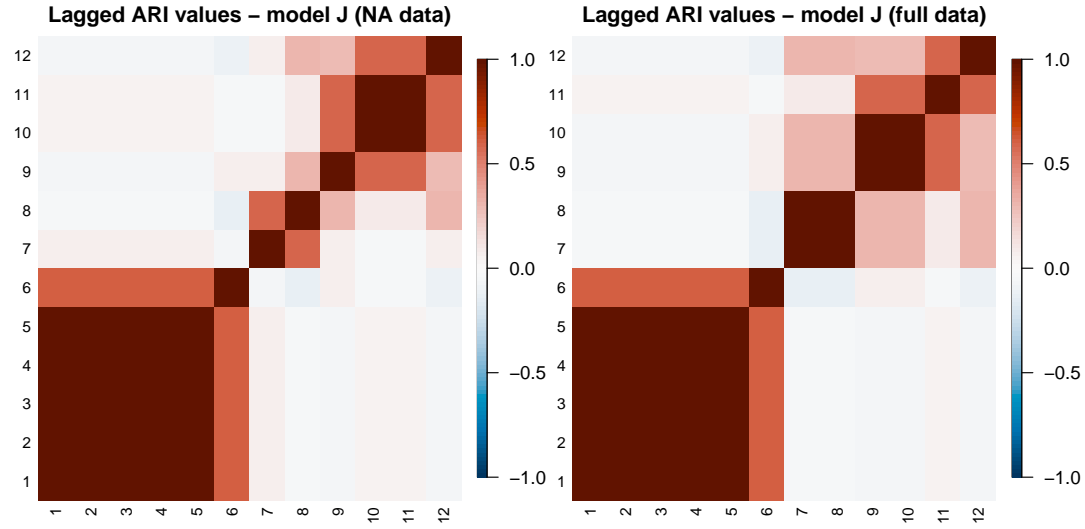


Figure 4.9: Lagged ARI values for the two fits on the JDRPM model with target values only. The partitions were estimated using the `salso` function from the corresponding R library.

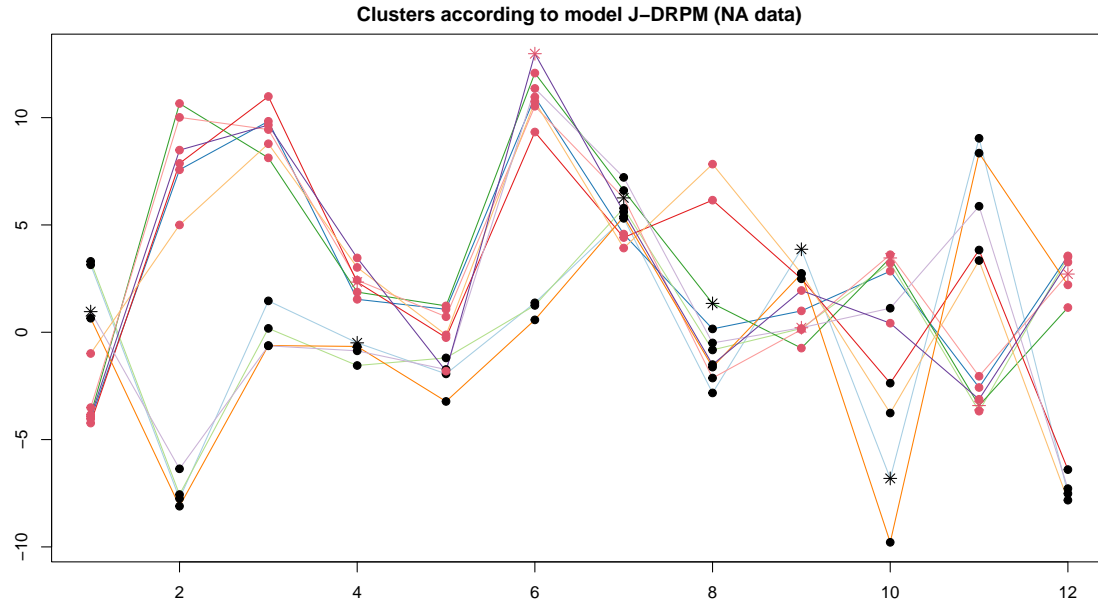


Figure 4.10: Visual representation of the clusters produced by the model, with units' labels represented as colored dots overlaid to the trend of the original generated target variables. Special point markers are used for the data points corresponding to missing values.

4.2.2 Target variable plus space (NA case)

Also in the case with spatial information the JDRPM model is able to perform well. Table 4.4 shows how the accuracy reduces, which is inevitable since we are fitting with missing data, but not drastically: the drops in LPML and WAIC metrics are in fact just of 3.16% and 0.95% respectively.

The temporal trend managed to remain similar, as we can see from Figure 4.11. Regarding the similarity of the produced clusters, we computed, as before having

lots of units, the values $\text{ARI}(\rho_{\text{JDRPM_NA}}(t), \rho_{\text{JDRPM_full}}(t))$ for all time instants $t = 1, \dots, 12$, and we obtained a mean of 0.82 and a median of 0.86, denoting still a relatively high level of agreement despite the loss of quite some data (121 points out of the 1260 of the full dataset).

Table 4.4: Summary of the comparison between the two Julia fits on target plus space values. The MSE columns refer to the accuracy between the fitted values generated by the models (estimated by taking the mean and the median of the returned 4000 iterates) and the true values of the target variable. Higher LPML and lower WAIC indicate a better fit.

<i>JDRPM</i>	MSE mean	MSE median	LPML	WAIC	execution time
NA data	0.0160	0.0170	502.86	-1793.64	48m
full data	0.0131	0.0138	624.91	-1898.05	37m

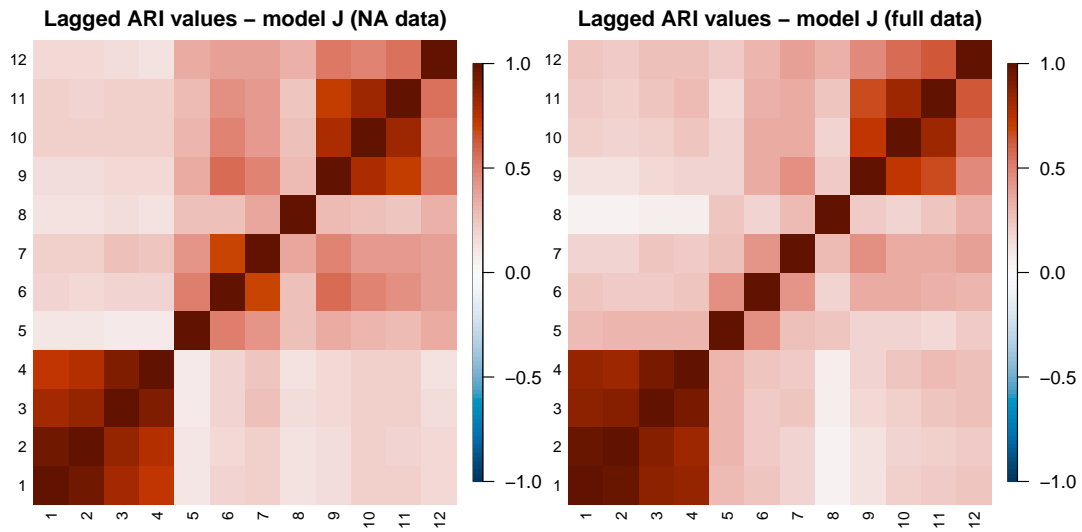


Figure 4.11: Lagged ARI values for the two fits on the JDRPM model with target plus space values. The partitions were estimated using the `salso` function from the corresponding R library.

4.3 Effects of the covariates

4.3.1 Covariates in the likelihood

Picking back the previous section, we can quickly test the case of inserting covariates in the likelihood, to maybe recover some accuracy in the case of missing data. In fact, the addition of the regression parameter β_t had only the main goal of improving the accuracy of the model when estimating the target values Y_{it} . With that in mind, the most natural use case of such parameter would be when fitting with missing values.

Indeed, after including the `Altitude` variable in the likelihood level and repeating the NA fit, under the same conditions apart from this addition, we obtained an LPML of 601.77 and WAIC of -1909.09, which compared to Table 4.4 appears to

be better than the case of just missing data without any “external suggestions”. However, both MSE errors dropped a bit, settling around 0.021 rather than the 0.017 of the original NA test, denoting how maybe the effect of the covariate in the likelihood could have been too strong on the Y_{it} estimation and would therefore require a more careful tuning.

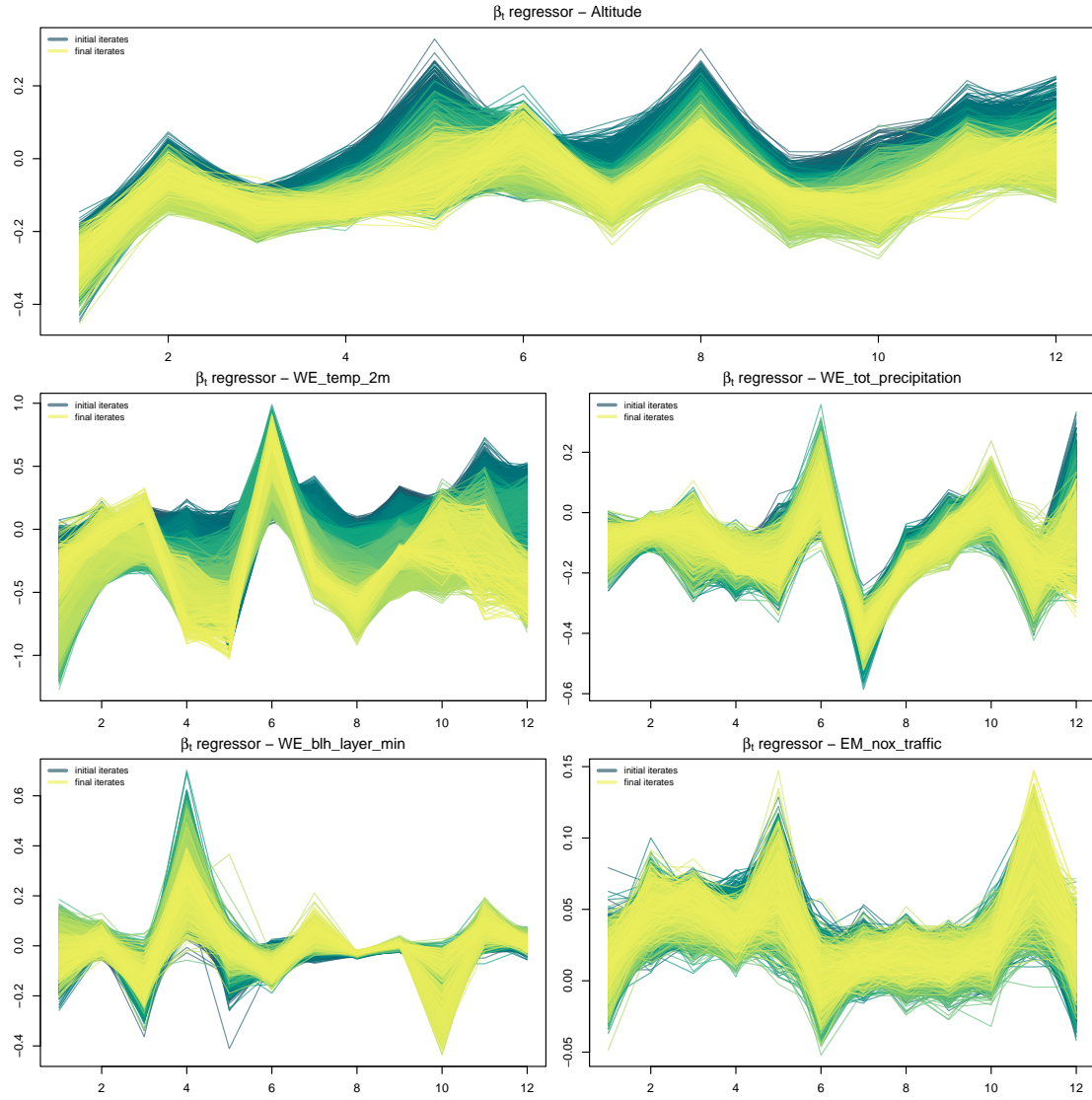


Figure 4.12: Regression vector β_t for the $p = 5$ covariates inserted in the likelihood in the NA data fit test, with time instants $t = 1, \dots, 12$ are on the x axis.

Another tests was ran with multiple covariates in the likelihood and it showed similar results, with again an increase in the fit metrics LMPL and WAIC, being respectively equal to 604.90 and -1805.87, and this time also an improvement in the fitted values accuracy, with the MSEs that now stayed around the same value 0.016 of the original simple NA fit. The sampled values for β_t in this more complex ran are proposed in Figure 4.12.

The JDRPM fitting function also includes a `beta_update_threshold` argument, defaulted to zero, to set after which iteration the algorithm should start to update

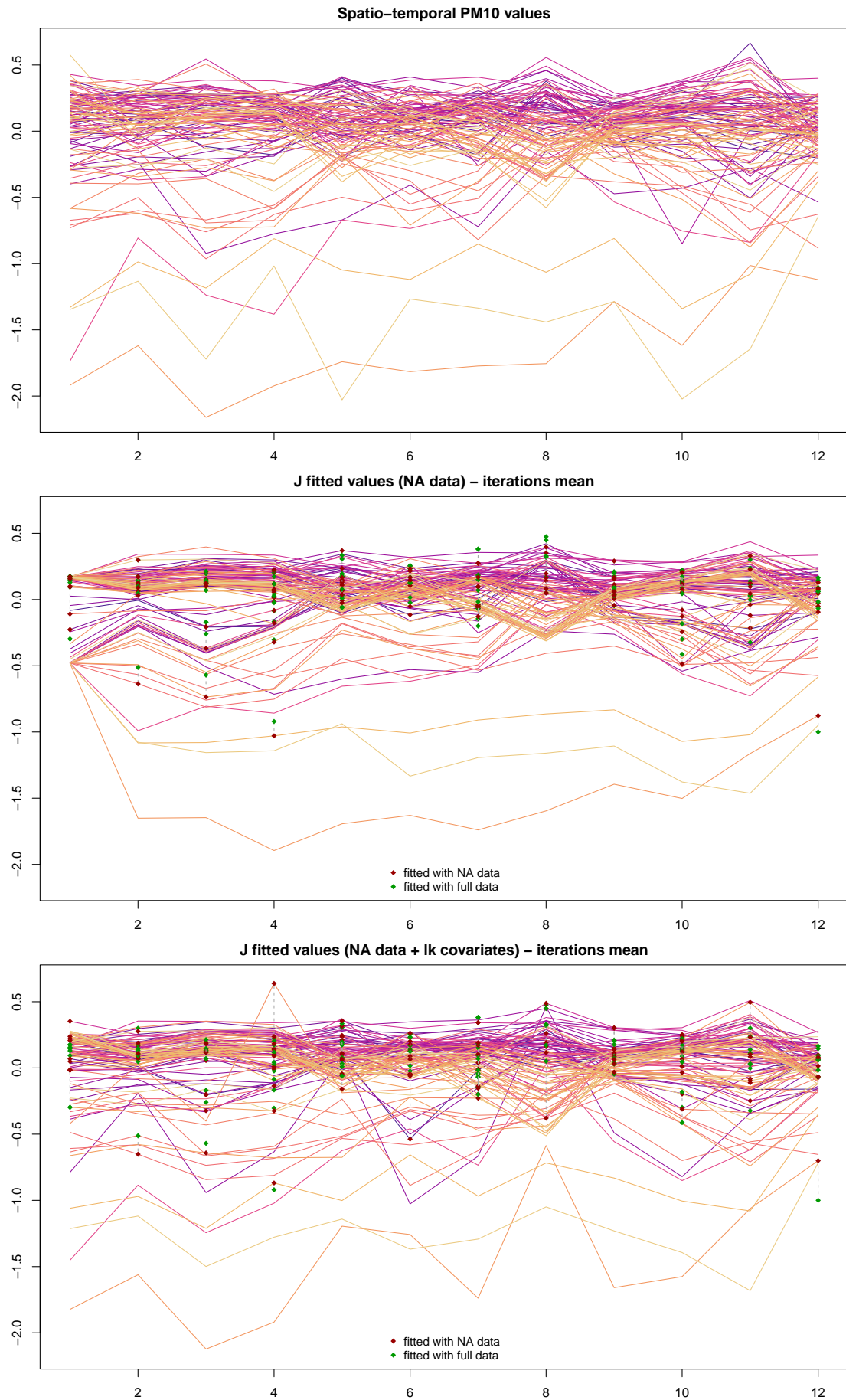


Figure 4.13: Target and fitted values of the JDRPM fits with target plus space values, on the NA dataset, to compare the simple fit to the one with covariates in the likelihood.

the β_t parameter. This was an harmless and simple addition, which was considered useful to firstly let the model update and improve the more delicate and relevant parameters for the clustering, such as μ_{jt}^* and σ_{jt}^{2*} , and secondly tune also the less impactful β_t . Otherwise, maybe, the initial development of the model parameters and clusterings could be biased by early inaccurate samples of the likelihood regressor.

Finally, Figure 4.13 compares the fitted values of this final ran, with multiple covariates in the likelihood, to the fitted values of the simple NA fit without any “seasonings”. We can now indeed, or at least visually, the fitted values from the seasoned fit managed to resemble more accurately the original PM₁₀ values, denoting how the addition of this regression parameter β_t could be beneficial to recover more accurate results, if well tuned and refined, especially in the case of fits missing data.

4.3.2 Covariates in the clustering

4.4 Scaling performances

To really assess if the goal of faster fits was reached, we setup several tests to compare the two models and the different information levels at which they could be called. The original CDRPM allowed to perform clustering using just the target values or by also including spatial information. In addition to them, the options introduced by JDRPM are the inclusion of covariates at clustering and/or likelihood levels.

Apart, of course, from the target values, all the other information levels are indeed independent: one could perform the fit ignoring space and accounting just for covariates, for example; but with an additive perspective in mind we decide to perform incremental tests, adding new layers on top of the base ones. Therefore, in what follows, we will see comparisons of fits using just the target values, then those plus space, then those two plus covariates in the clustering, and finally all those plus covariates in the likelihood.

As it appeared from Section 3, the Julia implementation seemed to be a little more eager for memory than the C one. This meant that when we ran the larger tests my system could have ran out of RAM memory, resulting in some data needing to be stored in the slower swap space on the disk, and therefore losing performance. However, on newer or just more technical-oriented machines than my simple laptop, this memory limitation should not be an issue.

Accounting all this, in what follows we should consider really accurate just the intermediate-values tests, i.e. the ones with n or T being 10, 50 or 100, and take with a pinch of salt the extreme one of 250, for which my laptop hardware limitations could have concealed the true results. Nonetheless, the analysis is really encouraging for the JDRPM model.

The tests were conducted on randomly generated values, according to n and T , for the target data Y_{it} and the spatial coordinates \mathbf{s}_i . In this way, we produced a sort of “mesh” of possible fitting parameters, ranging from small number of units and

time horizons to larger ones. To record the expected execution time per iteration of each case we ran each fit with a number of iterations inversely proportional to the size of the test, e.g. 10000 iterations for the case $(n, T) = (10, 10)$ and 16 iterations for $(n, T) = (250, 250)$. This ensured that each fit lasted approximately the same time. Each fit was ran four times, to then save the minimum time observed during those multiple runs. Such practice, common in benchmarking, helps to eliminate bias from the results due to the system computational demands and fluctuations, filtering in this way just the “ideal” execution time in which all the system performance are devoted to that task.

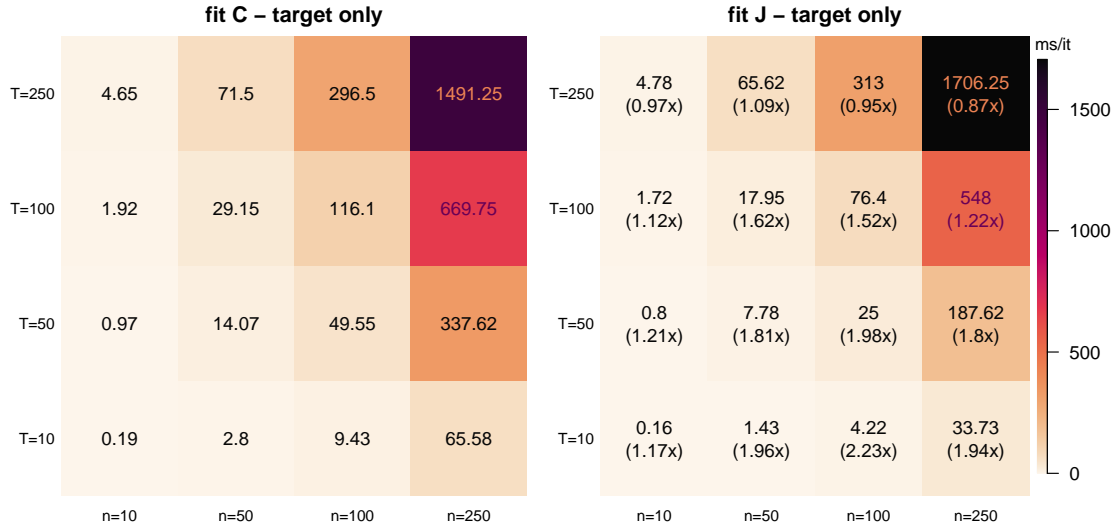


Figure 4.14: Execution times, measured in milliseconds per iteration, when fitting the models using just the target values to generate the clusters. On the JDRPM plot (on the right), in brackets, are reported the speedups relative to the CDRPM timings (on the left), where higher values indicate better performance.

From Figure 4.14 we can see how the basic fit, with just the target values, perform very quickly in Julia, with peaks even around a 2x speedup. Similar improvements appeared in the case of fits including also the spatial information, as Figure 4.15 shows. Therefore, especially looking at the more reliable non-extreme tests, we can confidently claim that the JDRPM implementation is faster than the CDRPM one.

Regarding fits with covariates, we also generated them randomly by creating matrices of dimensions $n \times p \times T$. For these tests, we avoided to treat different values of p : the previous figures summarizing the fits up to spatial information were in fact projection of 3d information (n , T , and execution time), while if we extended the mesh to also account for p , the number of covariates, we would have ended up with 4d information, or even 5d if we considered separately clustering and likelihood covariates. Therefore, to keep things tidy and understandable, we just fixed $p = 5$ for both cases.

Figure 4.16 shows how fits including covariates saw a drop of performance, which was inevitable due to the additional work to perform, but they still remain at a good performance level. Indeed, Figure 4.17 will point out how some of the fits

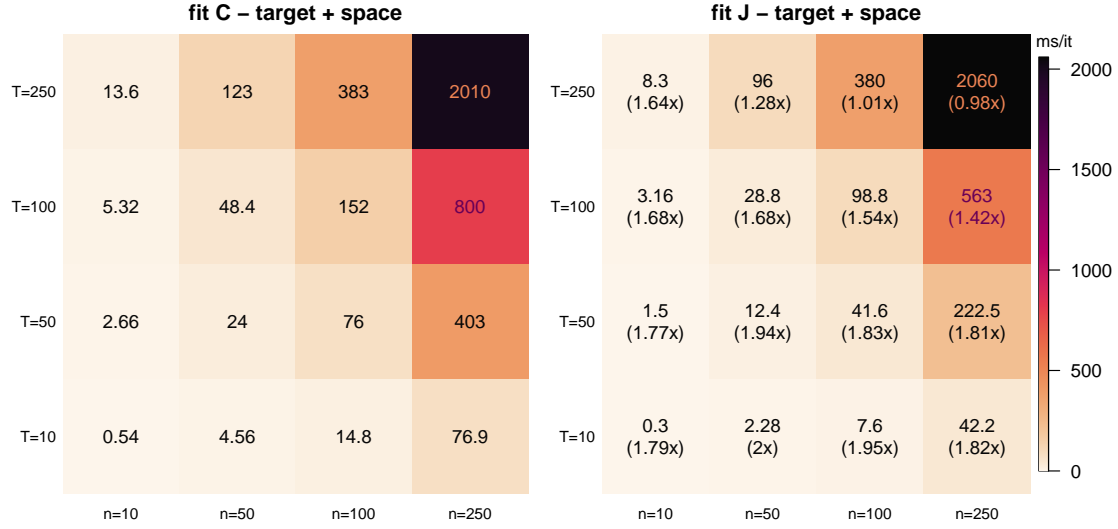


Figure 4.15: Execution times, measured in milliseconds per iteration, when fitting the models using the target values plus the spatial information to generate the clusters. On the JDRPM plot (on the right), in brackets, are reported the speedups relative to the CDRPM timings (on the left), where higher values indicate better performance.

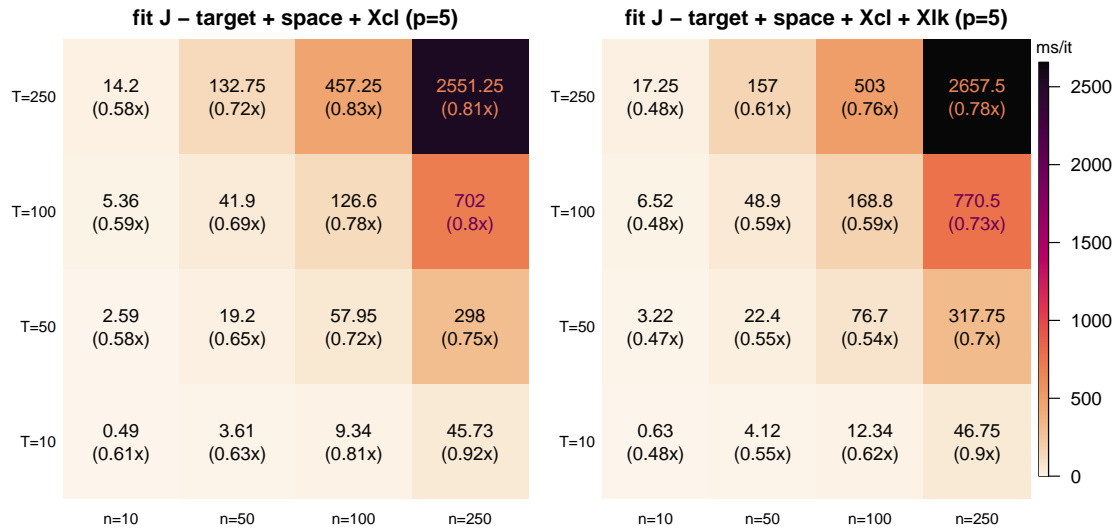


Figure 4.16: Execution times, measured in milliseconds per iteration, when fitting the JDRPM model using target values, spatial information, covariates in the clustering level (left), and covariates in both clustering and likelihood levels (right). In brackets are reported the speedups relative to the JDRPM timings of the fitting with target and space, with higher values still indicating better performance.

with all information levels in Julia were actually faster than the basic fits in C.

We can also notice how with larger fits the performance drop reduces to just around 0.8x, rather than the 0.6x of the small cases: this indicates that on fits with heavy n and T the bottleneck is no more the algorithm complexity, meaning the choice of which information levels to include in the clusters generation, but rather the available hardware resources.

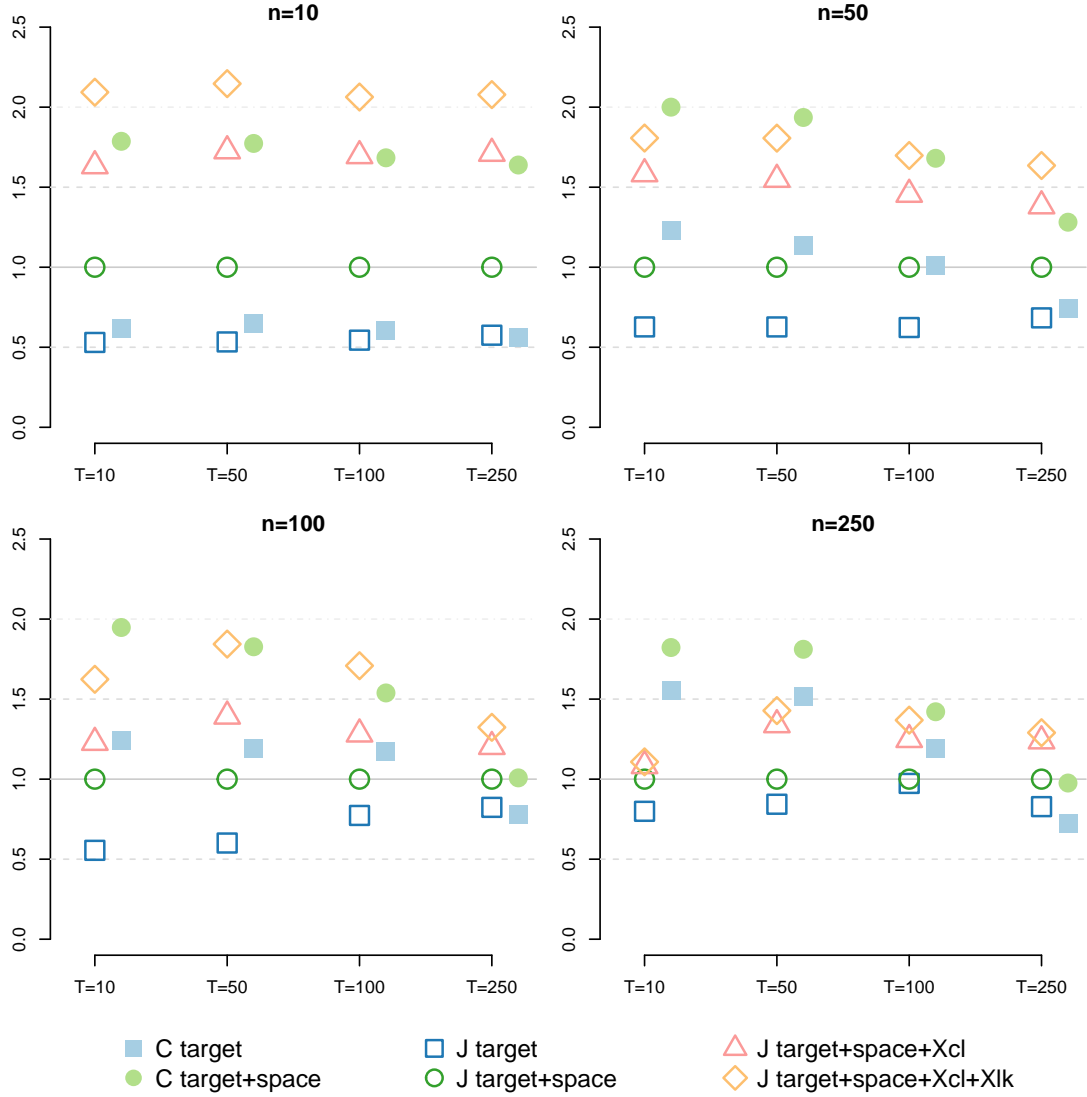


Figure 4.17: Visual representation of the performance of all the fits, for all the n and T cases, relatively to the JDRPM fit using target values and spatial information. Namely, the execution time per iteration metric of that fit has been taken as a reference, to which then all other fits have been compared to derive their speedup (or slowdown) factor. Points above the reference line indicate slower fits, while points below denote faster fits.

Chapter 5

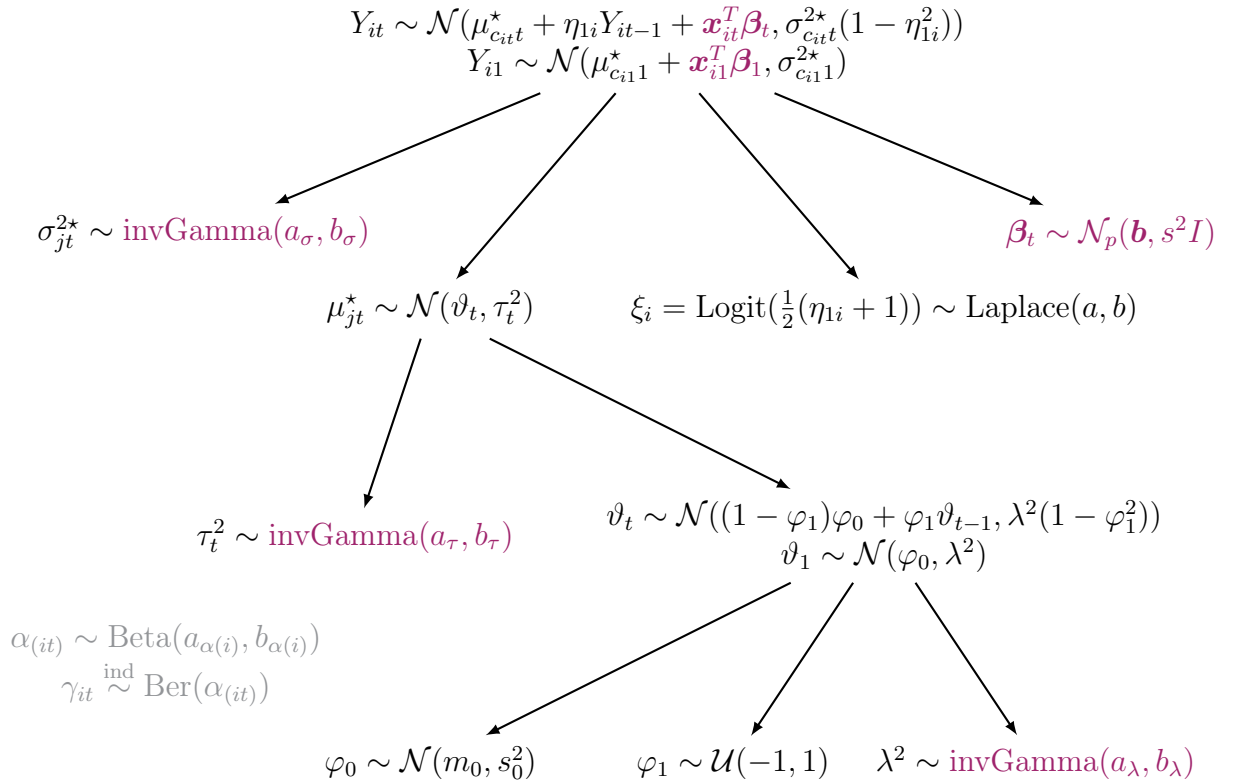
Conclusion

Appendix A

Theoretical details

A.1 Extended computations of the full conditionals

We propose here the extended computations which allowed to extract the full conditionals presented in Chapter 2. We report also the model graph to make it quickly accessible as a reference for the laws involved in the following computations.



- update σ_{jt}^{2*}

for $t = 1$:

$$f(\sigma_{jt}^{2*} | -) \propto f(\sigma_{jt}^{2*}) f(\{Y_{it} : c_{it} = j\} | \sigma_{jt}^{2*}, -)$$

$$\begin{aligned}
&= \mathcal{L}_{\text{invGamma}(a_\sigma, b_\sigma)}(\sigma_{jt}^{2*}) \prod_{i \in S_{jt}} \mathcal{L}_{\mathcal{N}(\mu_{c_{it}t}^* + \mathbf{x}_{it}^T \boldsymbol{\beta}_t, \sigma_{c_{it}1}^{2*})}(Y_{it}) \\
&\propto \left[\left(\frac{1}{\sigma_{jt}^{2*}} \right)^{a_\sigma + 1} \exp \left\{ -\frac{1}{\sigma_{jt}^{2*}} b \right\} \right] \\
&\cdot \left[\prod_{i \in S_{jt}} \left(\frac{1}{\sigma_{jt}^{2*}} \right)^{1/2} \exp \left\{ -\frac{1}{2\sigma_{jt}^{2*}} (Y_{it} - \mu_{jt}^* - \mathbf{x}_{it}^T \boldsymbol{\beta}_t)^2 \right\} \right] \\
&\propto \left(\frac{1}{\sigma_{jt}^{2*}} \right)^{(a_\sigma + |S_{jt}|/2) + 1} \exp \left\{ -\frac{1}{\sigma_{jt}^{2*}} \left(b_\sigma + \frac{1}{2} \sum_{i \in S_{jt}} (Y_{it} - \mu_{jt}^* - \mathbf{x}_{it}^T \boldsymbol{\beta}_t)^2 \right) \right\} \\
\Rightarrow f(\sigma_{jt}^{2*} | -) &\propto \text{kernel of a invGamma}(a_{\sigma(\text{post})}, b_{\sigma(\text{post})}) \text{ with} \\
a_{\tau(\text{post})} &= a_\sigma + \frac{|S_{jt}|}{2} \\
b_{\tau(\text{post})} &= b_\sigma + \frac{1}{2} \sum_{i \in S_{jt}} (Y_{it} - \mu_{jt}^* - \mathbf{x}_{it}^T \boldsymbol{\beta}_t)^2 \tag{A.1}
\end{aligned}$$

for $t > 1$:

$$\begin{aligned}
f(\sigma_{jt}^{2*} | -) &\propto f(\sigma_{jt}^{2*}) f(\{Y_{it} : c_{it} = j\} | \sigma_{jt}^{2*}, -) \\
&= \mathcal{L}_{\text{invGamma}(a_\sigma, b_\sigma)}(\sigma_{jt}^{2*}) \prod_{i \in S_{jt}} \mathcal{L}_{\mathcal{N}(\mu_{c_{it}t}^* + \eta_{1i} Y_{it-1} + \mathbf{x}_{it}^T \boldsymbol{\beta}_t, \sigma_{c_{it}1}^{2*})}(Y_{it}) \\
&\propto \left[\left(\frac{1}{\sigma_{jt}^{2*}} \right)^{a_\sigma + 1} \exp \left\{ -\frac{1}{\sigma_{jt}^{2*}} b \right\} \right] \\
&\cdot \left[\prod_{i \in S_{jt}} \left(\frac{1}{\sigma_{jt}^{2*}} \right)^{1/2} \exp \left\{ -\frac{1}{2\sigma_{jt}^{2*}} (Y_{it} - \mu_{jt}^* - \eta_{1i} Y_{it-1} - \mathbf{x}_{it}^T \boldsymbol{\beta}_t)^2 \right\} \right] \\
&\propto \left(\frac{1}{\sigma_{jt}^{2*}} \right)^{(a_\sigma + |S_{jt}|/2) + 1} \\
&\cdot \exp \left\{ -\frac{1}{\sigma_{jt}^{2*}} \left(b_\sigma + \frac{1}{2} \sum_{i \in S_{jt}} (Y_{it} - \eta_{1i} Y_{it-1} - \mu_{jt}^* - \mathbf{x}_{it}^T \boldsymbol{\beta}_t)^2 \right) \right\} \\
\Rightarrow f(\sigma_{jt}^{2*} | -) &\propto \text{kernel of a invGamma}(a_{\sigma(\text{post})}, b_{\sigma(\text{post})}) \text{ with} \\
a_{\tau(\text{post})} &= a_\sigma + \frac{|S_{jt}|}{2} \\
b_{\tau(\text{post})} &= b_\sigma + \frac{1}{2} \sum_{i \in S_{jt}} (Y_{it} - \mu_{jt}^* - \eta_{1i} Y_{it-1} - \mathbf{x}_{it}^T \boldsymbol{\beta}_t)^2 \tag{A.2}
\end{aligned}$$

- update μ_{jt}^*

for $t = 1$:

$$f(\mu_{jt}^* | -) \propto f(\mu_{jt}^*) f(\{Y_{it} : c_{it} = j\} | \mu_{jt}^*, -)$$

$$\begin{aligned}
&= \mathcal{L}_{\mathcal{N}(\vartheta_t, \tau_t^2)}(\mu_{jt}^*) \prod_{i \in S_{jt}} \mathcal{L}_{\mathcal{N}(\mu_{jt}^*, \sigma_{jt}^{2*})}(Y_{it}) \\
&\propto \exp \left\{ -\frac{1}{2\tau_t^2} (\mu_{jt}^* - \vartheta_t)^2 \right\} \exp \left\{ -\frac{1}{2\sigma_{jt}^{2*}} \left(\sum_{i \in S_{jt}} (\mu_{jt}^* - Y_{i1})^2 \right) \right\} \\
&\propto \exp \left\{ -\frac{1}{2\tau_t^2} (\mu_{jt}^* - \vartheta_t)^2 \right\} \exp \left\{ -\frac{|S_{jt}|}{2\sigma_{jt}^{2*}} \left(\mu_{jt}^* - \frac{\text{SUM}_y}{|S_{jt}|} \right)^2 \right\} \\
&\text{where } \text{SUM}_y = \sum_{i \in S_{jt}} Y_{i1} \\
&\implies f(\mu_{jt}^* | -) \propto \text{kernel of a } \mathcal{N}(\mu_{\mu_{jt}^*}^*(\text{post}), \sigma_{\mu_{jt}^*}^2(\text{post})) \text{ with} \\
&\sigma_{\mu_{jt}^*}^2(\text{post}) = \frac{1}{\frac{1}{\tau_t^2} + \frac{|S_{jt}|}{\sigma_{jt}^{2*}}} \\
&\mu_{\mu_{jt}^*}^*(\text{post}) = \sigma_{\mu_{jt}^*}^2(\text{post}) \left(\frac{\vartheta_t}{\tau_t^2} + \frac{\text{SUM}_y}{\sigma_{jt}^{2*}} \right) \tag{A.3}
\end{aligned}$$

for $t > 1$:

$$\begin{aligned}
&f(\mu_{jt}^* | -) \propto f(\mu_{jt}^*) f(\{Y_{it} : c_{it} = j\} | \mu_{jt}^*, -) \\
&= \mathcal{L}_{\mathcal{N}(\vartheta_1, \tau_1^2)}(\mu_{jt}^*) \prod_{i \in S_{jt}} \mathcal{L}_{\mathcal{N}(\mu_{jt}^* + \eta_{1i} Y_{i,t-1}, \sigma_{jt}^{2*}(1 - \eta_{1i}^2))}(Y_{it}) \\
&\propto \exp \left\{ -\frac{1}{2\tau_t^2} (\mu_{jt}^* - \vartheta_t)^2 \right\} \\
&\cdot \exp \left\{ -\frac{1}{2\sigma_{jt}^{2*}} \left(\sum_{i \in S_{jt}} \frac{1}{1 - \eta_{1i}^2} (\mu_{jt}^* - (Y_{it} - \eta_{1i} Y_{i,t-1}))^2 \right) \right\} \\
&\propto \exp \left\{ -\frac{1}{2\tau_t^2} (\mu_{jt}^* - \vartheta_t)^2 \right\} \exp \left\{ -\frac{\text{SUM}_{e2}}{2\sigma_{jt}^{2*}} \left(\mu_{jt}^* - \frac{\text{SUM}_y}{\text{SUM}_{e2}} \right)^2 \right\} \\
&\text{where } \text{SUM}_y = \sum_{i \in S_{jt}} \frac{Y_{it} - \eta_{1i} Y_{i,t-1}}{1 - \eta_{1i}^2}, \text{SUM}_{e2} = \sum_{i \in S_{jt}} \frac{1}{1 - \eta_{1i}^2} \\
&\implies f(\mu_{jt}^* | -) \propto \text{kernel of a } \mathcal{N}(\mu_{\mu_{jt}^*}^*(\text{post}), \sigma_{\mu_{jt}^*}^2(\text{post})) \text{ with} \\
&\sigma_{\mu_{jt}^*}^2(\text{post}) = \frac{1}{\frac{1}{\tau_t^2} + \frac{\text{SUM}_{e2}}{\sigma_{jt}^{2*}}} \\
&\mu_{\mu_{jt}^*}^*(\text{post}) = \sigma_{\mu_{jt}^*}^2(\text{post}) \left(\frac{\vartheta_t}{\tau_t^2} + \frac{\text{SUM}_y}{\sigma_{jt}^{2*}} \right) \tag{A.4}
\end{aligned}$$

- update β_t

for $t = 1$:

$$\begin{aligned}
&f(\beta_t | -) \propto f(\beta_t) f(\{Y_{1t}, \dots, Y_{nt}\} | \beta_t, -) \\
&= \mathcal{L}_{\mathcal{N}(\mathbf{b}, s^2 I)}(\beta_t) \prod_{i=1}^n \mathcal{L}_{\mathcal{N}(\mu_{c_{it}}^* + \mathbf{x}_{it}^T \beta_t, \sigma_{c_{it}}^{2*})}(Y_{it})
\end{aligned}$$

$$\begin{aligned}
& \propto \exp \left\{ -\frac{1}{2} \left[(\boldsymbol{\beta}_t^T - \mathbf{b})^T \frac{1}{s^2} (\boldsymbol{\beta}_t - \mathbf{b}) \right] \right\} \exp \left\{ -\frac{1}{2} \sum_{i=1}^n (Y_{it} - \mu_{c_{it}}^* - \mathbf{x}_{it}^T \boldsymbol{\beta}_t)^2 \right\} \\
& \propto \exp \left\{ -\frac{1}{2} \left[\boldsymbol{\beta}_t^T \left(\frac{1}{s^2} I + \sum_{i=1}^n \frac{\mathbf{x}_{it} \mathbf{x}_{it}^T}{\sigma_{c_{it}}^{2*}} \right) \boldsymbol{\beta}_t \right. \right. \\
& \quad \left. \left. - 2 \left(\frac{\mathbf{b}}{s^2} + \sum_{i=1}^n \frac{(Y_{it} - \mu_{c_{it}}^*) \mathbf{x}_{it}}{\sigma_{c_{it}}^{2*}} \right) \cdot \boldsymbol{\beta}_t \right] \right\} \\
& \implies f(\boldsymbol{\beta}_t | -) \propto \text{kernel of a } \mathcal{N}(\mathbf{b}_{(\text{post})}, A_{(\text{post})}) \text{ with} \\
& \quad A_{(\text{post})} = \left(\frac{1}{s^2} I + \sum_{i=1}^n \frac{\mathbf{x}_{it} \mathbf{x}_{it}^T}{\sigma_{c_{it}}^{2*}} \right)^{-1} \\
& \quad \mathbf{b}_{(\text{post})} = A_{(\text{post})} \left(\frac{\mathbf{b}}{s^2} + \sum_{i=1}^n \frac{(Y_{it} - \mu_{c_{it}}^*) \mathbf{x}_{it}}{\sigma_{c_{it}}^{2*}} \right) \\
& \iff f(\boldsymbol{\beta}_t | -) \propto \text{kernel of a } \mathcal{N}\text{Canon}(\mathbf{h}_{(\text{post})}, J_{(\text{post})}) \text{ with} \\
& \quad \mathbf{h}_{(\text{post})} = \left(\frac{\mathbf{b}}{s^2} + \sum_{i=1}^n \frac{(Y_{it} - \mu_{c_{it}}^*) \mathbf{x}_{it}}{\sigma_{c_{it}}^{2*}} \right) \\
& \quad J_{(\text{post})} = \left(\frac{1}{s^2} I + \sum_{i=1}^n \frac{\mathbf{x}_{it} \mathbf{x}_{it}^T}{\sigma_{c_{it}}^{2*}} \right) \tag{A.5}
\end{aligned}$$

for $t > 1$:

$$\begin{aligned}
& f(\boldsymbol{\beta}_t | -) \propto f(\boldsymbol{\beta}_t) f(\{Y_{1t}, \dots, Y_{nt}\} | \boldsymbol{\beta}_t, -) \\
& = \mathcal{L}_{\mathcal{N}(\mathbf{b}, s^2 I)}(\boldsymbol{\beta}_t) \prod_{i=1}^n \mathcal{L}_{\mathcal{N}(\mu_{c_{it}}^* + \eta_{1i} Y_{it-1} + \mathbf{x}_{it}^T \boldsymbol{\beta}_t, \sigma_{c_{it}}^{2*})}(Y_{it}) \\
& \propto \exp \left\{ -\frac{1}{2} \left[(\boldsymbol{\beta}_t^T - \mathbf{b})^T \frac{1}{s^2} (\boldsymbol{\beta}_t - \mathbf{b}) \right] \right\} \\
& \quad \cdot \exp \left\{ -\frac{1}{2} \sum_{i=1}^n (Y_{it} - \mu_{c_{it}}^* - \eta_{1i} Y_{it-1} - \mathbf{x}_{it}^T \boldsymbol{\beta}_t)^2 \right\} \\
& \propto \exp \left\{ -\frac{1}{2} \left[\boldsymbol{\beta}_t^T \left(\frac{1}{s^2} I + \sum_{i=1}^n \frac{\mathbf{x}_{it} \mathbf{x}_{it}^T}{\sigma_{c_{it}}^{2*}} \right) \boldsymbol{\beta}_t \right. \right. \\
& \quad \left. \left. - 2 \left(\frac{\mathbf{b}}{s^2} + \sum_{i=1}^n \frac{(Y_{it} - \mu_{c_{it}}^* - \eta_{1i} Y_{it-1}) \mathbf{x}_{it}}{\sigma_{c_{it}}^{2*}} \right) \cdot \boldsymbol{\beta}_t \right] \right\} \\
& \implies f(\boldsymbol{\beta}_t | -) \propto \text{kernel of a } \mathcal{N}(\mathbf{b}_{(\text{post})}, A_{(\text{post})}) \text{ with} \\
& \quad A_{(\text{post})} = \left(\frac{1}{s^2} I + \sum_{i=1}^n \frac{\mathbf{x}_{it} \mathbf{x}_{it}^T}{\sigma_{c_{it}}^{2*}} \right)^{-1} \\
& \quad \mathbf{b}_{(\text{post})} = A_{(\text{post})} \left(\frac{\mathbf{b}}{s^2} + \sum_{i=1}^n \frac{(Y_{it} - \mu_{c_{it}}^* - \eta_{1i} Y_{it-1}) \mathbf{x}_{it}}{\sigma_{c_{it}}^{2*}} \right) \\
& \iff f(\boldsymbol{\beta}_t | -) \propto \text{kernel of a } \mathcal{N}\text{Canon}(\mathbf{h}_{(\text{post})}, J_{(\text{post})}) \text{ with}
\end{aligned}$$

$$\begin{aligned}
\mathbf{h}_{(\text{post})} &= \left(\frac{\mathbf{b}}{s^2} + \sum_{i=1}^n \frac{(Y_{it} - \mu_{c_{it}}^* - \eta_{1i} Y_{it-1}) \mathbf{x}_{it}}{\sigma_{c_{it}}^{2*}} \right) \\
J_{(\text{post})} &= \left(\frac{1}{s^2} I + \sum_{i=1}^n \frac{\mathbf{x}_{it} \mathbf{x}_{it}^T}{\sigma_{c_{it}}^{2*}} \right)
\end{aligned} \tag{A.6}$$

- update τ_t^2

$$\begin{aligned}
f(\tau_t^2 | -) &\propto f(\tau_t^2) f((\mu_{1t}^*, \dots, \mu_{k_{tt}}^*) | \tau_t^2, -) \\
&= \mathcal{L}_{\text{invGamma}(a_\tau, b_\tau)}(\tau_t^2) \prod_{j=1}^{k_t} \mathcal{L}_{\mathcal{N}(\vartheta_t, \tau_t^2)}(\mu_{jt}^*) \\
&\propto \left[\left(\frac{1}{\tau_t^2} \right)^{a_\tau+1} \exp \left\{ -\frac{b_\tau}{\tau_t^2} \right\} \right] \left[\prod_{j=1}^{k_t} \left(\frac{1}{\tau_t^2} \right)^{1/2} \exp \left\{ -\frac{1}{2\tau_t^2} (\mu_{jt}^* - \vartheta_t)^2 \right\} \right] \\
&\propto \left(\frac{1}{\tau_t^2} \right)^{\left(\frac{k_t}{2} + a_\tau \right) + 1} \exp \left\{ -\frac{1}{\tau_t^2} \left(\frac{\sum_{j=1}^{k_t} (\mu_{jt}^* - \vartheta_t)^2}{2} + b_\tau \right) \right\} \\
\Rightarrow f(\tau_t^2 | -) &\propto \text{kernel of a invGamma}(a_{\tau(\text{post})}, b_{\tau(\text{post})}) \text{ with} \\
a_{\tau(\text{post})} &= \frac{k_t}{2} + a_\tau \\
b_{\tau(\text{post})} &= \frac{\sum_{j=1}^{k_t} (\mu_{jt}^* - \vartheta_t)^2}{2} + b_\tau
\end{aligned} \tag{A.7}$$

- update ϑ_t

for $t = T$:

$$\begin{aligned}
f(\vartheta_t | -) &\propto f(\vartheta_t) f((\mu_{1t}^*, \dots, \mu_{k_{tt}}^*) | \vartheta_t, -) \\
&= \mathcal{L}_{\mathcal{N}((1-\varphi_1)\varphi_0 + \varphi_1 \vartheta_{t-1}, \lambda^2(1-\varphi_1^2))}(\vartheta_t) \prod_{j=1}^{k_t} \mathcal{L}_{\mathcal{N}(\vartheta_t, \tau_t^2)}(\mu_{jt}^*) \\
&\propto \exp \left\{ -\frac{1}{2(\lambda^2(1-\varphi_1^2))} \left(\vartheta_t - ((1-\varphi_1)\varphi_0 + \varphi_1 \vartheta_{t-1}) \right)^2 \right\} \\
&\quad \cdot \exp \left\{ -\frac{k_t}{2\tau_t^2} \left(\vartheta_t - \frac{\sum_{j=1}^{k_t} \mu_{jt}^*}{k_t} \right)^2 \right\} \\
\Rightarrow f(\vartheta_t | -) &\propto \text{kernel of a } \mathcal{N}(\mu_{\vartheta_t(\text{post})}, \sigma_{\vartheta_t(\text{post})}^2) \text{ with} \\
\sigma_{\vartheta_t(\text{post})}^2 &= \frac{1}{\frac{1}{\lambda^2(1-\varphi_1^2)} + \frac{k_t}{\tau_t^2}} \\
\mu_{\vartheta_t(\text{post})} &= \sigma_{\vartheta_t(\text{post})}^2 \left(\frac{\sum_{j=1}^{k_t} \mu_{jt}^*}{\tau_t^2} + \frac{(1-\varphi_1)\varphi_0 + \varphi_1 \vartheta_{t-1}}{\lambda^2(1-\varphi_1^2)} \right)
\end{aligned} \tag{A.8}$$

for $1 < t < T$:

$$f(\vartheta_t | -) \propto \underbrace{f(\vartheta_t) f((\mu_{1t}^*, \dots, \mu_{k_{tt}}^*) | \vartheta_t, -)}_{\text{as in the case } t = T} f(\vartheta_{t+1} | \vartheta_t, -)$$

$$\begin{aligned}
&= \mathcal{L}_{\mathcal{N}(\mu_{\vartheta_t(\text{post})}, \sigma_{\vartheta_t(\text{post})}^2)}(\vartheta_t) \mathcal{L}_{\mathcal{N}((1-\varphi_1)\varphi_0 + \varphi_1\vartheta_t, \lambda^2(1-\varphi_1^2))}(\vartheta_{t+1}) \\
&\propto \exp \left\{ -\frac{1}{2\sigma_{\vartheta_t(\text{post})}^2} (\vartheta_t - \mu_{\vartheta_t(\text{post})})^2 \right\} \\
&\quad \cdot \exp \left\{ -\frac{1}{2\frac{\lambda^2(1-\varphi_1^2)}{\varphi_1^2}} \left(\vartheta_t - \frac{\vartheta_{t+1} - (1-\varphi_1)\varphi_0}{\varphi_1} \right)^2 \right\} \\
&\Rightarrow f(\vartheta_t|-) \propto \text{kernel of a } \mathcal{N}(\mu_{\vartheta_t(\text{post})}, \sigma_{\vartheta_t(\text{post})}^2) \text{ with} \\
&\quad \sigma_{\vartheta_t(\text{post})}^2 = \frac{1}{\frac{1+\varphi_1^2}{\lambda^2(1-\varphi_1^2)} + \frac{k_t}{\tau_t^2}} \\
&\quad \mu_{\vartheta_t(\text{post})} = \sigma_{\vartheta_t(\text{post})}^2 \left(\frac{\sum_{j=1}^{k_t} \mu_{jt}^*}{\tau_t^2} + \frac{\varphi_1(\vartheta_{t-1} + \vartheta_{t+1}) + \varphi_0(1-\varphi_1)^2}{\lambda^2(1-\varphi_1^2)} \right) \quad (\text{A.9})
\end{aligned}$$

for $t = 1$:

$$\begin{aligned}
&f(\vartheta_t|-) \propto f(\vartheta_t)f(\vartheta_{t+1}|\vartheta_t, -)f(\boldsymbol{\mu}_{jt}^*|\vartheta_t, -) \\
&= \mathcal{L}_{\mathcal{N}(\varphi_0, \lambda^2)}(\vartheta_t) \mathcal{L}_{\mathcal{N}((1-\varphi_1)\varphi_0 + \varphi_1\vartheta_{t-1}, \lambda^2(1-\varphi_1^2))}(\vartheta_{t+1}) \prod_{j=1}^{k_t} \mathcal{L}_{\mathcal{N}(\vartheta_t, \tau_t^2)}(\mu_{jt}^*) \\
&\propto \exp \left\{ -\frac{1}{2\lambda^2} (\vartheta_t - \varphi_0)^2 \right\} \\
&\quad \cdot \exp \left\{ -\frac{1}{2\frac{\lambda^2(1-\varphi_1^2)}{\varphi_1^2}} \left(\vartheta_t - \frac{\vartheta_{t+1} - (1-\varphi_1)\varphi_0}{\varphi_1} \right)^2 \right\} \\
&\quad \cdot \exp \left\{ -\frac{k_t}{2\tau_t^2} \left(\vartheta_t - \frac{\sum_{j=1}^{k_t} \mu_{jt}^*}{k_t} \right)^2 \right\} \\
&\Rightarrow f(\vartheta_t|-) \propto \text{kernel of a } \mathcal{N}(\mu_{\vartheta_t(\text{post})}, \sigma_{\vartheta_t(\text{post})}^2) \text{ with} \\
&\quad \sigma_{\vartheta_t(\text{post})}^2 = \frac{1}{\frac{1}{\lambda^2} + \frac{\varphi_1^2}{\lambda^2(1-\varphi_1^2)} + \frac{k_t}{\tau_t^2}} \\
&\quad \mu_{\vartheta_t(\text{post})} = \sigma_{\vartheta_t(\text{post})}^2 \left(\frac{\varphi_0}{\lambda^2} + \frac{\varphi_1(\vartheta_{t+1} - (1-\varphi_1)\varphi_0)}{\lambda^2(1-\varphi_1^2)} + \frac{\sum_{j=1}^{k_t} \mu_{jt}^*}{\tau_t^2} \right) \quad (\text{A.10})
\end{aligned}$$

- update φ_0

$$\begin{aligned}
&f(\varphi_0|-) \propto f(\varphi_0)f((\vartheta_1, \dots, \vartheta_T)|\varphi_0, -) \\
&= \mathcal{L}_{\mathcal{N}(m_0, s_0^2)}(\varphi_0) \mathcal{L}_{\mathcal{N}(\varphi_0, \lambda^2)}(\vartheta_1) \prod_{t=2}^T \mathcal{L}_{\mathcal{N}((1-\varphi_1)\varphi_0 + \varphi_1\vartheta_{t-1}, \lambda^2(1-\varphi_1^2))}(\vartheta_t) \\
&\propto \exp \left\{ \left\{ -\frac{1}{2s_0^2} (\varphi_0 - m_0)^2 \right\} \right\} \exp \left\{ \left\{ -\frac{1}{2\lambda^2} (\varphi_0 - \vartheta_1)^2 \right\} \right\} \\
&\quad \cdot \exp \left\{ \left\{ -\frac{1}{2\frac{\lambda^2(1-\varphi_1^2)}{(T-1)(1-\varphi_1)^2}} \left(\varphi_0 - \frac{(1-\varphi_1)(\text{SUM}_t)}{(T-1)(1-\varphi_1)^2} \right)^2 \right\} \right\}
\end{aligned}$$

$$\begin{aligned}
& \text{where } \text{SUM}_t = \sum_{t=2}^T (\vartheta_t - \varphi_1 \vartheta_{t-1}) \\
& \implies f(\varphi_0 | -) \propto \text{kernel of a } \mathcal{N}(\mu_{\varphi_0(\text{post})}, \sigma_{\varphi_0(\text{post})}^2) \text{ with} \\
& \sigma_{\varphi_0(\text{post})}^2 = \frac{1}{\frac{1}{s_0^2} + \frac{1}{\lambda^2} + \frac{(T-1)(1-\varphi_1)^2}{\lambda^2(1-\varphi_1^2)}} \\
& \mu_{\varphi_0(\text{post})} = \sigma_{\varphi_0(\text{post})}^2 \left(\frac{m_0}{s_0^2} + \frac{\vartheta_1}{\lambda^2} + \frac{1-\varphi_1}{\lambda^2(1-\varphi_1^2)} \text{SUM}_t \right) \tag{A.11}
\end{aligned}$$

- update λ^2

$$\begin{aligned}
& f(\lambda^2 | -) \propto f(\lambda^2) f(\vartheta_1, \dots, \vartheta_T | \lambda^2, -) \\
& = \mathcal{L}_{\text{invGamma}(a_\lambda, b_\lambda)}(\lambda^2) \mathcal{L}_{\mathcal{N}(\varphi_0, \lambda^2)}(\vartheta_1) \prod_{t=2}^T \mathcal{L}_{\mathcal{N}((1-\varphi_1)\varphi_0 + \varphi_1 \vartheta_{t-1}, \lambda^2(1-\varphi_1^2))}(\vartheta_t) \\
& \propto \left[\left(\frac{1}{\lambda_t^2} \right)^{a_\lambda+1} \exp \left\{ -\frac{b_\lambda}{\lambda^2} \right\} \right] \left[\left(\frac{1}{\lambda^2} \right)^{1/2} \exp \left\{ -\frac{1}{2\lambda^2} (\vartheta_1 - \varphi_0)^2 \right\} \right] \\
& \cdot \left[\prod_{t=2}^T \left(\frac{1}{\lambda^2} \right)^{1/2} \exp \left\{ -\frac{1}{2\lambda^2} (\vartheta_t - (1-\varphi_1)\varphi_0 - \varphi_1 \vartheta_{t-1})^2 \right\} \right] \\
& \propto \left(\frac{1}{\lambda^2} \right)^{\left(\frac{T}{2} + a_\lambda\right) + 1} \\
& \cdot \exp \left\{ -\frac{1}{\lambda^2} \left(\frac{(\vartheta_1 - \varphi_0)^2}{2} + \sum_{t=2}^T \frac{(\vartheta_t - (1-\varphi_1)\varphi_0 - \varphi_1 \vartheta_{t-1})^2}{2} + b_\lambda \right) \right\} \\
& \implies f(\lambda^2 | -) \propto \text{kernel of a } \text{invGamma}(a_{\lambda(\text{post})}, b_{\lambda(\text{post})}) \text{ with} \\
& a_{\lambda(\text{post})} = \frac{T}{2} + a_\lambda \\
& b_{\lambda(\text{post})} = \frac{(\vartheta_1 - \varphi_0)^2}{2} + \sum_{t=2}^T \frac{(\vartheta_t - (1-\varphi_1)\varphi_0 - \varphi_1 \vartheta_{t-1})^2}{2} + b_\lambda \tag{A.12}
\end{aligned}$$

- update α

$$\begin{aligned}
& \text{if global } \alpha: \text{ prior is } \alpha \sim \text{Beta}(a_\alpha, b_\alpha) \\
& f(\alpha | -) \propto f(\alpha) f((\gamma_{11}, \dots, \gamma_{1T}, \dots, \gamma_{n1}, \dots, \gamma_{nT}) | \alpha) \\
& \propto \alpha^{a_\alpha-1} (1-\alpha)^{b_\alpha-1} \prod_{i=1}^n \prod_{t=1}^T \alpha^{\gamma_{it}} (1-\alpha)^{1-\gamma_{it}} \\
& = \alpha^{(a_\alpha + \sum_{i=1}^n \sum_{t=1}^T \gamma_{it})-1} (1-\alpha)^{(b_\alpha + nT - \sum_{i=1}^n \sum_{t=1}^T \gamma_{it})-1} \\
& \implies f(\alpha | -) \propto \text{kernel of a } \text{Beta}(a_{\alpha(\text{post})}, b_{\alpha(\text{post})}) \text{ with} \\
& a_{\alpha(\text{post})} = a_\alpha + \sum_{i=1}^n \sum_{t=1}^T \gamma_{it} \quad b_{\alpha(\text{post})} = b_\alpha + nT - \sum_{i=1}^n \sum_{t=1}^T \gamma_{it} \tag{A.13}
\end{aligned}$$

if time specific α : prior is $\alpha_t \sim \text{Beta}(a_\alpha, b_\alpha)$

$$\begin{aligned}
f(\alpha_t|-) &\propto f(\alpha_t)f((\gamma_{1t}, \dots, \gamma_{nt})|\alpha_t) \\
&\propto \alpha_t^{a_\alpha-1}(1-\alpha_t)^{b_\alpha-1} \prod_{i=1}^n \alpha_t^{\gamma_{it}}(1-\alpha_t)^{1-\gamma_{it}} \\
&= \alpha_t^{(a_\alpha+\sum_{i=1}^n \gamma_{it})-1}(1-\alpha_t)^{(b_\alpha+n-\sum_{i=1}^n \gamma_{it})-1} \\
\Rightarrow f(\alpha_t|-) &\propto \text{kernel of a Beta}(a_{\alpha(\text{post})}, b_{\alpha(\text{post})}) \text{ with} \\
a_{\alpha(\text{post})} &= a_\alpha + \sum_{i=1}^n \gamma_{it} \quad b_{\alpha(\text{post})} = b_\alpha + n - \sum_{i=1}^n \gamma_{it} \quad (\text{A.14})
\end{aligned}$$

if unit specific α : prior is $\alpha_i \sim \text{Beta}(a_{\alpha i}, b_{\alpha i})$

$$\begin{aligned}
f(\alpha_i|-) &\propto f(\alpha_i)f((\gamma_{i1}, \dots, \gamma_{iT})|\alpha_i) \\
&\propto \alpha_i^{a_{\alpha i}-1}(1-\alpha_i)^{b_{\alpha i}-1} \prod_{t=1}^T \alpha_i^{\gamma_{it}}(1-\alpha_i)^{1-\gamma_{it}} \\
&= \alpha_{it}^{(a_{\alpha i}+\sum_{t=1}^T \gamma_{it})-1}(1-\alpha_{it})^{(b_{\alpha i}+T-\sum_{t=1}^T \gamma_{it})-1} \\
\Rightarrow f(\alpha_i|-) &\propto \text{kernel of a Beta}(a_{\alpha(\text{post})}, b_{\alpha(\text{post})}) \text{ with} \\
a_{\alpha(\text{post})} &= a_{\alpha i} + \sum_{t=1}^T \gamma_{it} \quad b_{\alpha(\text{post})} = b_{\alpha i} + T - \sum_{t=1}^T \gamma_{it} \quad (\text{A.15})
\end{aligned}$$

if time and unit specific α : prior is $\alpha_{it} \sim \text{Beta}(a_{\alpha i}, b_{\alpha i})$

$$\begin{aligned}
f(\alpha_{it}|-) &\propto f(\alpha_{it})f(\gamma_{it}|\alpha_{it}) \\
&\propto \alpha_{it}^{a-1}(1-\alpha_{it})^{b-1} \alpha_{it}^{\gamma_{it}}(1-\alpha_{it})^{1-\gamma_{it}} \\
&= \alpha_i^{(a+\gamma_{it})-1}(1-\alpha_i)^{(b+1+\gamma_{it})-1} \\
\Rightarrow f(\alpha_{it}|-) &\propto \text{kernel of a Beta}(a_{\alpha(\text{post})}, b_{\alpha(\text{post})}) \text{ with} \\
a_{\alpha(\text{post})} &= a_{\alpha i} + \gamma_{it} \quad b_{\alpha(\text{post})} = b_{\alpha i} + 1 - \gamma_{it} \quad (\text{A.16})
\end{aligned}$$

- update a missing observation Y_{it}

for $t = 1$:

$$\begin{aligned}
f(Y_{it}|-) &\propto f(Y_{it})f(Y_{it+1}|Y_{it}, -) \\
&= \mathcal{L}_{\mathcal{N}(\mu_{c_{it}t}^* + \mathbf{x}_{it}^T \boldsymbol{\beta}_t, \sigma_{c_{it}t}^{2*})}(Y_{it}) \\
&\cdot \mathcal{L}_{\mathcal{N}(\mu_{c_{it+1}t+1}^* + \eta_{1i} Y_{it} + \mathbf{x}_{it+1}^T \boldsymbol{\beta}_{t+1}, \sigma_{c_{it+1}t+1}^{2*}(1-\eta_{1i}^2))}(Y_{it+1}) \\
&\propto \exp \left\{ -\frac{1}{2\sigma_{c_{it}t}^{2*}} (Y_{it} - \mu_{c_{it}t}^* - \mathbf{x}_{it}^T \boldsymbol{\beta}_t)^2 \right\} \\
&\cdot \exp \left\{ -\frac{1}{2\sigma_{c_{it+1}t+1}^{2*}(1-\eta_{1i}^2)} (Y_{it+1} - \mu_{c_{it+1}t+1}^* - \eta_{1i} Y_{it} - \mathbf{x}_{it+1}^T \boldsymbol{\beta}_{t+1})^2 \right\} \\
&= \exp \left\{ -\frac{1}{2\sigma_{c_{it}t}^{2*}} (Y_{it} - (\mu_{c_{it}t}^* + \mathbf{x}_{it}^T \boldsymbol{\beta}_t))^2 \right\} \\
&\cdot \exp \left\{ -\frac{\eta_{1i}^2}{2\sigma_{c_{it+1}t+1}^{2*}(1-\eta_{1i}^2)} \left(Y_{it} - \frac{Y_{it+1} - \mu_{c_{it+1}t+1}^* - \mathbf{x}_{it+1}^T \boldsymbol{\beta}_{t+1}}{\eta_{1i}} \right)^2 \right\}
\end{aligned}$$

$$\begin{aligned}
&\Rightarrow f(Y_{it}|-) \propto \text{kernel of a } \mathcal{N}(\mu_{Y_{it}(\text{post})}, \sigma_{Y_{it}(\text{post})}^2) \text{ with} \\
&\sigma_{Y_{it}(\text{post})}^2 = \frac{1}{\frac{1}{\sigma_{c_{it}t}^{2*}} + \frac{\eta_{1i}^2}{2\sigma_{c_{it+1}t+1}^{2*}(1-\eta_{1i}^2)}} \\
&\mu_{Y_{it}(\text{post})} = \sigma_{Y_{it}(\text{post})}^2 \left(\frac{\mu_{c_{it}t}^* + \mathbf{x}_{it}^T \boldsymbol{\beta}_t}{\sigma_{c_{it}t}^{2*}} + \frac{\eta_{1i}(Y_{it+1} - \mu_{c_{it+1}t+1}^* - \mathbf{x}_{it+1}^T \boldsymbol{\beta}_{t+1})}{\sigma_{c_{it+1}t+1}^{2*}(1-\eta_{1i}^2)} \right)
\end{aligned} \tag{A.17}$$

for $1 < t < T$:

$$\begin{aligned}
&f(Y_{it}|-) \propto f(Y_{it})f(Y_{it+1}|Y_{it}, -) \\
&= \mathcal{L}_{\mathcal{N}(\mu_{c_{it}t}^* + \eta_{1i}Y_{it-1} + \mathbf{x}_{it}^T \boldsymbol{\beta}_t, \sigma_{c_{it}t}^{2*})}(Y_{it}) \\
&\cdot \mathcal{L}_{\mathcal{N}(\mu_{c_{it+1}t+1}^* + \eta_{1i}Y_{it} + \mathbf{x}_{it+1}^T \boldsymbol{\beta}_{t+1}, \sigma_{c_{it+1}t+1}^{2*}(1-\eta_{1i}^2))}(Y_{it+1}) \\
&\propto \exp \left\{ -\frac{1}{2\sigma_{c_{it}t}^{2*}(1-\eta_{1i}^2)} (Y_{it} - \mu_{c_{it}t}^* - \eta_{1i}Y_{it-1} - \mathbf{x}_{it}^T \boldsymbol{\beta}_t)^2 \right\} \\
&\cdot \exp \left\{ -\frac{1}{2\sigma_{c_{it+1}t+1}^{2*}(1-\eta_{1i}^2)} (Y_{it+1} - \mu_{c_{it+1}t+1}^* - \eta_{1i}Y_{it} - \mathbf{x}_{it+1}^T \boldsymbol{\beta}_{t+1})^2 \right\} \\
&= \exp \left\{ -\frac{1}{2\sigma_{c_{it}t}^{2*}(1-\eta_{1i}^2)} (Y_{it} - (\mu_{c_{it}t}^* + \eta_{1i}Y_{it-1} + \mathbf{x}_{it}^T \boldsymbol{\beta}_t))^2 \right\} \\
&\cdot \exp \left\{ -\frac{\eta_{1i}^2}{2\sigma_{c_{it+1}t+1}^{2*}(1-\eta_{1i}^2)} \left(Y_{it} - \frac{Y_{it+1} - \mu_{c_{it+1}t+1}^* - \mathbf{x}_{it+1}^T \boldsymbol{\beta}_{t+1}}{\eta_{1i}} \right)^2 \right\} \\
&\Rightarrow f(Y_{it}|-) \propto \text{kernel of a } \mathcal{N}(\mu_{Y_{it}(\text{post})}, \sigma_{Y_{it}(\text{post})}^2) \text{ with}
\end{aligned}$$

$$\begin{aligned}
&\sigma_{Y_{it}(\text{post})}^2 = \frac{1 - \eta_{1i}^2}{\frac{1}{\sigma_{c_{it}t}^{2*}} + \frac{\eta_{1i}^2}{\sigma_{c_{it+1}t+1}^{2*}}} \\
&\mu_{Y_{it}(\text{post})} = \sigma_{Y_{it}(\text{post})}^2 \left(\frac{\mu_{c_{it}t}^* + \eta_{1i}Y_{it-1} + \mathbf{x}_{it}^T \boldsymbol{\beta}_t}{\sigma_{c_{it}t}^{2*}(1-\eta_{1i}^2)} + \frac{\eta_{1i}(Y_{it+1} - \mu_{c_{it+1}t+1}^* - \mathbf{x}_{it+1}^T \boldsymbol{\beta}_{t+1})}{\sigma_{c_{it+1}t+1}^{2*}(1-\eta_{1i}^2)} \right)
\end{aligned} \tag{A.18}$$

for $t = T$:

$$\begin{aligned}
&f(Y_{it}|-) \propto f(Y_{it}) \\
&= \mathcal{L}_{\mathcal{N}(\mu_{c_{it}t}^* + \eta_{1i}Y_{it-1} + \mathbf{x}_{it}^T \boldsymbol{\beta}_t, \sigma_{c_{it}t}^{2*}(1-\eta_{1i}^2))}(Y_{it}) \\
&\Rightarrow f(Y_{it}|-) \text{ is just the likelihood of } Y_{it}
\end{aligned} \tag{A.19}$$

Appendix B

Computational details

B.1 Fitting algorithm code

We report here the full code of the `MCMC_fit` function, which implements the updated DRPM model described in this work. We include it to let the readers appreciate the ease, clarity and even elegance of the Julia language in translating the mathematical formulation into code. Especially compared to the original C implementation, Julia is not only more readable and efficient, being still a compiled language, but also faster in the testing and development phase, thanks to the possibility of her interactive use trough the Julia REPL, similar to the one of the R console. Moreover, Julia’s extensive ecosystem provides users flexibility and all the supports they could need, thanks to the vast documentation or even an online active forum¹ (where I wrote myself some questions during the development of the thesis). For example, packages like `Distributions` and `Statistics` came in very handy for this work; while the C implementation had to write all the statistical functionalities from scratch.

All this with the the hope for Julia to become the new natural choice in the statistical, or in general scientific, computing field, giving to it a refreshing approach.

Listing 3: Julia code which implements the fitting model algorithm. We report here just the “functional” part, i.e. not all the previous setup lines regarding the function definition, variable preallocations, input arguments checks, etc.

```
##### start MCMC algorithm #####
println("Starting MCMC algorithm")

t_start = now()
progresso = Progress(round{Int64}(draws)),
    showspeed=true,
    output=stdout, # not stderr, to make it work nicer on R
    dt=1, # every how many seconds update the feedback
    barlen=0 # no progress bar, just time feedback
)

for i in 1:draws
```

¹<https://discourse.julialang.org/>

```

##### sample the missing values #####
# from the "update rho" section onwards also the Y[j,t] will be needed (to
↪ compute weights, update laws, etc)
# so we need now to simulate the values (from their full conditional) for the
↪ data which are missing
if Y_has_NA
  # we have to use the missing_idxes to remember which units and at which
  ↪ times had a missing value,
  # in order to simulate just them and instead use the given value for the
  ↪ other units and times
  for (j,t) in missing_idxes
    # What if when filling a NA we occur in another NA value? eg when we
    ↪ also need Y[j,t+1]?
    # I decided here to set that value to 0, if occurs, since anyway target
    ↪ should be centered
    # so it seems a reasonable patch, and I think there was no other
    ↪ solution

    c_it = Si_iter[j,t]
    Xlk_term_t = (lk_xPPM ? dot(view(Xlk_covariates,j,:,t), beta_iter[t]) :
    ↪ 0)
    aux1 = eta1_iter[j]^2

    if t==1
      c_itp1 = Si_iter[j,t+1]
      Xlk_term_tp1 = (lk_xPPM ? dot(view(Xlk_covariates,j,:,t+1),
      ↪ beta_iter[t+1]) : 0)

      sig2_post = 1 / (1/sig2h_iter[c_it,t] +
      ↪ aux1/(sig2h_iter[c_itp1,t+1]*(1-aux1)))
      mu_post = sig2_post * (
        (1/sig2h_iter[c_it,t])*(muh_iter[c_it,t] + Xlk_term_t) +
        (eta1_iter[j]/(sig2h_iter[c_itp1,t+1]*(1-aux1)))*((ismissing(Y[j,t+1])
        ↪ ? 0 : Y[j,t+1]) - muh_iter[c_itp1,t+1] - Xlk_term_tp1)
      )

      Y[j,t] = rand(Normal(mu_post,sqrt(sig2_post)))

    elseif 1<t<T
      c_itp1 = Si_iter[j,t+1]
      Xlk_term_tp1 = (lk_xPPM ? dot(view(Xlk_covariates,j,:,t+1),
      ↪ beta_iter[t+1]) : 0)

      sig2_post = (1-aux1) / (1/sig2h_iter[c_it,t] +
      ↪ aux1/sig2h_iter[c_itp1,t+1])
      mu_post = sig2_post * (
        (1/(sig2h_iter[c_it,t]*(1-aux1)))*(muh_iter[c_it,t] +
        ↪ eta1_iter[j]*(ismissing(Y[j,t-1]) ? 0 : Y[j,t-1]) +
        ↪ Xlk_term_t) +
        (eta1_iter[j]/(sig2h_iter[c_itp1,t+1]*(1-aux1)))*((ismissing(Y[j,t+1])
        ↪ ? 0 : Y[j,t+1]) - muh_iter[c_itp1,t+1] - Xlk_term_tp1)
      )

      Y[j,t] = rand(Normal(mu_post,sqrt(sig2_post)))

    else # t==T
      Y[j,t] = rand(Normal(
        muh_iter[c_it,t] + eta1_iter[j]*(ismissing(Y[j,t-1]) ? 0 :
        ↪ Y[j,t-1]) + Xlk_term_t,
        sqrt(sig2h_iter[c_it,t]*(1-aux1))
      ))
    end
  end
end

```

```

end
end

for t in 1:T
##### update gamma #####
for j in 1:n
    if t==1
        gamma_iter[j,t] = 0
        # at the first time units get reallocated
    else
        # we want to find  $\rho_t^{R_t(-j)}$  ...
        indexes = findall_faster(jj -> jj != j && gamma_iter[jj, t] == 1,
            ↪ 1:n)
        Si_red = Si_iter[indexes, t]
        copy!(Si_red1, Si_red)
        push!(Si_red1, Si_iter[j,t]) # ... and  $\rho_t^{R_t(+j)}$ 

        # get also the reduced spatial info if sPPM model
        if sPPM
            sp1_red = @view sp1[indexes]
            sp2_red = @view sp2[indexes]
        end
        # and the reduced covariates info if cl_xPPM model
        if cl_xPPM
            Xcl_covariates_red = @view Xcl_covariates[indexes,:,t]
        end

        # compute n_red's and nclus_red's and relabel
        n_red = length(Si_red) # = "n" relative to here, i.e. the
            ↪ sub-partition size
        n_red1 = length(Si_red1)
        relabel!(Si_red, n_red)
        relabel!(Si_red1, n_red1)
        nclus_red = isempty(Si_red) ? 0 : maximum(Si_red) # = number of
            ↪ clusters
        nclus_red1 = maximum(Si_red1)

        # save the label of the current working-on unit j
        j_label = Si_red1[end]

        # compute also nh_red's
        nh_red .= 0
        nh_red1 .= 0
        for jj in 1:n_red
            nh_red[Si_red[jj]] += 1 # = numerosities for each cluster label
            nh_red1[Si_red1[jj]] += 1
        end
        nh_red1[Si_red1[end]] += 1 # account for the last added unit j, not
            ↪ included in the above loop

        # start computing weights
        lg_weights .= 0

        # unit j can enter an existing cluster...
        for k in 1:nclus_red
            aux_idx = findall(Si_red .== k) # fast
            lC .= 0.
            if sPPM
                # filter the spatial coordinates of the units of label k
                copy!(s1o, sp1_red[aux_idx])
                copy!(s2o, sp2_red[aux_idx])
            end
        end
    end
end
end

```

```

    copy!(s1n,s1o); push!(s1n, sp1[j])
    copy!(s2n,s2o); push!(s2n, sp2[j])
    spatial_cohesion!(spatial_cohesion_idx, s1o, s2o,
        ↪ sp_params_struct, true, M_dp, S, 1, false, lC)
    spatial_cohesion!(spatial_cohesion_idx, s1n, s2n,
        ↪ sp_params_struct, true, M_dp, S, 2, false, lC)
end
lS .= 0.
if cl_xPPM
    # and the covariates of the units of label k
    for p in 1:p_cl
        copy!(Xo, @view Xcl_covariates_red[aux_idx,p])
        copy!(Xn, Xo); push!(Xn,Xcl_covariates[j,p,t])
        covariate_similarity!(covariate_similarity_idx, Xo,
            ↪ cv_params, true, 1, true, lS)
        covariate_similarity!(covariate_similarity_idx, Xn,
            ↪ cv_params, true, 2, true, lS)
    end
end
lg_weights[k] = log(nh_red[k]) + lC[2] - lC[1] + lS[2] - lS[1]
end
# ... or unit j can create a singleton
lC .= 0.
if sPPM
    spatial_cohesion!(spatial_cohesion_idx, SVector(sp1[j]),
        ↪ SVector(sp2[j]), sp_params_struct, true, M_dp, S, 2, false,
        ↪ lC)
end
lS .= 0.
if cl_xPPM
    for p in 1:p_cl
        covariate_similarity!(covariate_similarity_idx,
            ↪ SVector(Xcl_covariates[j,p,t]), cv_params, true, 2, true,
            ↪ lS)
    end
end
lg_weights[nclus_red+1] = log_Mdp + lC[2] + lS[2]

# now use the weights towards sampling the new gamma_jt
max_ph = maximum(@view lg_weights[1:(nclus_red+1)])
sum_ph = 0.0
# exponentiate...
for k in 1:(nclus_red+1)
    # for numerical purposes we subtract max_ph
    lg_weights[k] = exp(lg_weights[k] - max_ph)
    sum_ph += lg_weights[k]
end
# ... and normalize
lg_weights ./= sum_ph

# compute probh
probh = 0.0
if time_specific_alpha==false && unit_specific_alpha==false
    probh = alpha_iter / (alpha_iter + (1 - alpha_iter) *
        ↪ lg_weights[j_label])
elseif time_specific_alpha==true && unit_specific_alpha==false
    probh = alpha_iter[t] / (alpha_iter[t] + (1 - alpha_iter[t]) *
        ↪ lg_weights[j_label])
elseif time_specific_alpha==false && unit_specific_alpha==true
    probh = alpha_iter[j] / (alpha_iter[j] + (1 - alpha_iter[j]) *
        ↪ lg_weights[j_label])
elseif time_specific_alpha==true && unit_specific_alpha==true

```

```

        probh = alpha_iter[j,t] / (alpha_iter[j,t] + (1 -
        ↪ alpha_iter[j,t]) * lg_weights[j_label])
    end

    # compatibility check for gamma transition
    if gamma_iter[j, t] == 0
        # we want to find  $\rho_{(t-1)}^{\{R_t(+j)\}}$  ...
        indexes = findall_faster(jj -> jj==j gamma_iter[jj, t]==1, 1:n)
        Si_comp1 = @view Si_iter[indexes, t-1]
        Si_comp2 = @view Si_iter[indexes, t] # ... and  $\rho_{t-1}^{R_t(+j)}$ 

        rho_comp = compatibility(Si_comp1, Si_comp2)
        if rho_comp == 0
            probh = 0.0
        end
    end
    # sample the new gamma
    gt = rand(Bernoulli(probh))
    gamma_iter[j, t] = gt
end
end # for j in 1:n

##### update rho #####
# we only update the partition for the units which can move (i.e. with
↪ gamma_jt=0)
movable_units = findall(gamma_iter[:,t] .== 0)

for j in movable_units
    # remove unit j from the cluster she is currently in

    if nh[Si_iter[j,t],t] > 1 # unit j does not belong to a singleton
        ↪ cluster
        nh[Si_iter[j,t],t] -= 1
        # no nclus_iter[t] change since j's cluster is still alive
    else # unit j belongs to a singleton cluster
        j_label = Si_iter[j,t]
        last_label = nclus_iter[t]

        if j_label < last_label
            # here we enter if j_label is not the last label, so we need to
            # relabel clusters in order to then remove j's cluster
            # eg: units 1 2 3 4 5 j 7 -> units 1 2 3 4 5 j 7
            #      label 1 1 2 2 2 3 4      label 1 1 2 2 2 4 3

            # swap cluster labels...
            for jj in 1:n
                if Si_iter[jj, t] == last_label
                    Si_iter[jj, t] = j_label
                end
            end
            Si_iter[j, t] = last_label
            # ... and cluster-specific parameters
            sig2h_iter[j_label, t], sig2h_iter[last_label, t] =
            ↪ sig2h_iter[last_label, t], sig2h_iter[j_label, t]
            muh_iter[j_label, t], muh_iter[last_label, t] =
            ↪ muh_iter[last_label, t], muh_iter[j_label, t]
            nh[j_label, t] = nh[last_label, t]
            nh[last_label, t] = 1
        end

        # remove the j-th observation and the last cluster (being j in a
        ↪ singleton)
    end
end

```

```

    nh[last_label, t] -= 1
    nclus_iter[t] -= 1
end

# setup probability weights towards the sampling of rho_jt
ph .= 0.0
resize!(ph, nclus_iter[t]+1)
copy!(rho_tmp, @view Si_iter[:,t])

# compute nh_tmp (numerosities for each cluster label)
copy!(nh_tmp, @view nh[:,t])
# unit j contribute is already absent from the change we did above
nclus_temp = 0

# we now simulate the unit j to be assigned to one of the existing
↳ clusters...
for k in 1:nclus_iter[t]
    rho_tmp[j] = k
    indexes = findall(gamma_iter[:,t+1] .== 1)
    # we check the compatibility between rho_t^{h=k, R_(t+1)} ...
    Si_comp1 = @view rho_tmp[indexes]
    Si_comp2 = @view Si_iter[indexes,t+1] # and rho_(t+1)^{R_(t+1)}
    rho_comp = compatibility(Si_comp1, Si_comp2)

    if rho_comp != 1
        ph[k] = log(0) # assignment to cluster k is not compatible
    else
        # update params for "rho_jt = k" simulation
        nh_tmp[k] += 1
        nclus_temp = count(a->(a>0), nh_tmp)

        lPP .= 0.
        for kk in 1:nclus_temp
            aux_idx = findall(rho_tmp .== kk)
            if sPPM
                copy!(s1n, @view sp1[aux_idx])
                copy!(s2n, @view sp2[aux_idx])
                spatial_cohesion!(spatial_cohesion_idx, s1n, s2n,
                    ↳ sp_params_struct, true, M_dp, S, 1, true, lPP)
            end
            if cl_xPPM
                for p in 1:p_cl
                    Xn_view = @view Xcl_covariates[aux_idx,p,t]
                    covariate_similarity!(covariate_similarity_idx, Xn_view,
                        ↳ cv_params, true, 1, true, lPP)
                end
            end
            lPP[1] += log_Mdp + lgamma(nh_tmp[kk])
        end

        if t==1
            ph[k] = loglikelihood(Normal(
                muh_iter[k,t] + (lk_xPPM ? dot(view(Xlk_covariates,j,:,t),
                    ↳ beta_iter[t]) : 0),
                sqrt(sig2h_iter[k,t])),
                Y[j,t]) + lPP[1]
        else
            ph[k] = loglikelihood(Normal(
                muh_iter[k,t] + eta1_iter[j]*Y[j,t-1] + (lk_xPPM ?
                    ↳ dot(view(Xlk_covariates,j,:,t), beta_iter[t]) : 0),
                sqrt(sig2h_iter[k,t]*(1-eta1_iter[j]^2))),
                Y[j,t]) + lPP[1]
        end
    end
end

```



```

        end

        # restore params after "rho_jt = k" simulation
        nh_tmp[k] -= 1
    end
end
# ... plus the case of being assigned to a new (singleton for now)
↪ cluster
k = nclus_iter[t]+1
rho_tmp[j] = k
# declare (for later scope accessibility) the new params here
muh_draw = 0.0; sig2h_draw = 0.0

indexes = findall(gamma_iter[:,t+1] .== 1)
Si_comp1 = @view rho_tmp[indexes]
Si_comp2 = @view Si_iter[indexes,t+1]
rho_comp = compatibility(Si_comp1, Si_comp2)

if rho_comp != 1
    ph[k] = log(0) # assignment to a new cluster is not compatible
else
    # sample new params for this new cluster
    muh_draw = rand(Normal(theta_iter[t], sqrt(tau2_iter[t])))
    sig2h_draw = rand(InverseGamma(sig2h_priors[1], sig2h_priors[2]))

    # update params for "rho_jt = k" simulation
    nh_tmp[k] += 1
    nclus_temp = count(a->(a>0), nh_tmp)

    lPP .= 0.
    for kk in 1:nclus_temp
        aux_idx = findall(rho_tmp .== kk)
        if sPPM
            copy!(s1n, @view sp1[aux_idx])
            copy!(s2n, @view sp2[aux_idx])
            spatial_cohesion!(spatial_cohesion_idx, s1n, s2n,
                ↪ sp_params_struct, true, M_dp, S, 1, true, lPP)
        end
        if cl_xPPM
            for p in 1:p_cl
                Xn_view = @view Xcl_covariates[aux_idx,p,t]
                covariate_similarity!(covariate_similarity_idx, Xn_view,
                    ↪ cv_params, true, 1, true, lPP)
            end
        end
        lPP[1] += log_Mdp + lgamma(nh_tmp[kk])
    end

    if t==1
        ph[k] = loglikelihood(Normal(
            muh_draw + (lk_xPPM ? dot(view(Xlk_covariates,j,:),t),
                ↪ beta_iter[t]) : 0),
            sqrt(sig2h_draw)),
            Y[j,t]) + lPP[1]
    else
        ph[k] = loglikelihood(Normal(
            muh_draw + eta1_iter[j]*Y[j,t-1] + (lk_xPPM ?
                ↪ dot(view(Xlk_covariates,j,:),t), beta_iter[t]) : 0),
            sqrt(sig2h_draw*(1-eta1_iter[j]^2))),
            Y[j,t]) + lPP[1]
    end
end

```

```

    # restore params after "rho_jt = k" simulation
    nh_tmp[k] -= 1
end

# now exponentiate the weights...
max_ph = maximum(ph)
sum_ph = 0.0
for k in eachindex(ph)
    # for numerical purposes we subtract max_ph
    ph[k] = exp(ph[k] - max_ph)
    sum_ph += ph[k]
end
# ... and normalize them
ph ./= sum_ph

# now sample the new label Si_iter[j,t]
u = rand(Uniform(0,1))
cph = cumsum(ph)
cph[end] = 1 # fix numerical problems of having sums like 0.999999etc
new_label = 0
for k in eachindex(ph)
    if u <= cph[k]
        new_label = k
        break
    end
end

if new_label <= nclus_iter[t]
    # we enter an existing cluster
    Si_iter[j, t] = new_label
    nh[new_label, t] += 1
else
    # we create a new singleton cluster
    nclus_iter[t] += 1
    cl_new = nclus_iter[t]
    Si_iter[j, t] = cl_new
    nh[cl_new, t] = 1
    muh_iter[cl_new, t] = muh_draw
    sig2h_iter[cl_new, t] = sig2h_draw
end

# now we need to relabel after the possible mess created by the
#   ↪ sampling
# eg: (before sampling)    (after sampling)
#   units j 2 3 4 5 -> units j 2 3 4 5
#   labels 1 1 1 2 2    labels 3 1 1 2 2
# the after case has to be relabelled
Si_tmp = @view Si_iter[:,t]

relabel_full!(Si_tmp, n, Si_relab, nh_reorder, old_lab)
# - Si_relab gives the relabelled partition
# - nh_reorder gives the numerosities of the relabelled partition, ie
#   ↪ "nh_reorder[k] = #(units of new cluster k)"
# - old_lab tells "the index in position i (which before was cluster i)"
#   ↪ is now called cluster old_lab[i]"
# eg:
#       Original labels (Si): 4 2 1 1 1 3 1 4 5
#       Relabeled groups (Si_relab): 1 2 3 3 3 4 3 1 5
#       Reordered cluster sizes (nh_reorder): 2 1 4 1 1 0 0 0 0
#       Old labels (old_lab): 4 2 1 3 5 0 0 0 0

# now fix everything (morally permute params)
Si_iter[:,t] = Si_relab

```

```

copy!(muh_iter_copy, muh_iter)
copy!(sig2h_iter_copy, sig2h_iter)
len = findlast(x -> x != 0, nh_reorder)
for k in 1:nclus_iter[t]
    muh_iter[k,t] = muh_iter_copy[old_lab[k],t]
    sig2h_iter[k,t] = sig2h_iter_copy[old_lab[k],t]
    nh[k,t] = nh_reorder[k]
end

end # for j in movable_units

##### update muh #####
if t==1
    for k in 1:nclus_iter[t]
        sum_Y = 0.0
        for j in 1:n
            if Si_iter[j,t]==k
                sum_Y += Y[j,t] - (lk_xPPM ? dot(view(Xlk_covariates,j,:,t),
                    ↪ beta_iter[t]) : 0.0)
            end
        end
        sig2_star = 1 / (1/tau2_iter[t] + nh[k,t]/sig2h_iter[k,t])
        mu_star = sig2_star * (theta_iter[t]/tau2_iter[t] +
            ↪ sum_Y/sig2h_iter[k,t])

        muh_iter[k,t] = rand(Normal(mu_star,sqrt(sig2_star)))
    end
else # t>1
    for k in 1:nclus_iter[t]
        sum_Y = 0.0
        sum_e2 = 0.0
        for j in 1:n
            if Si_iter[j,t]==k
                aux1 = 1 / (1-eta1_iter[j]^2)
                sum_e2 += aux1
                sum_Y += (Y[j,t] - eta1_iter[j]*Y[j,t-1] - (lk_xPPM ?
                    ↪ dot(view(Xlk_covariates,j,:,t), beta_iter[t]) : 0.0)) *
                    ↪ aux1
            end
        end
        sig2_star = 1 / (1/tau2_iter[t] + sum_e2/sig2h_iter[k,t])
        mu_star = sig2_star * (theta_iter[t]/tau2_iter[t] +
            ↪ sum_Y/sig2h_iter[k,t])

        muh_iter[k,t] = rand(Normal(mu_star,sqrt(sig2_star)))
    end
end

##### update sigma2h #####
if t==1
    for k in 1:nclus_iter[t]
        a_star = sig2h_priors[1] + nh[k,t]/2
        sum_Y = 0.0
        S_kt = findall(Si_iter[:,t] .== k)
        for j in S_kt
            sum_Y += (Y[j,t] - muh_iter[k,t] - (lk_xPPM ?
                ↪ dot(view(Xlk_covariates,j,:,t), beta_iter[t]) : 0.0))^2
        end
    end
end

```

```

        b_star = sig2h_priors[2] + sum_Y/2
        sig2h_iter[k,t] = rand(InverseGamma(a_star, b_star))
    end

else # t>1
    for k in 1:nclus_iter[t]
        a_star = sig2h_priors[1] + nh[k,t]/2
        sum_Y = 0.0
        S_kt = findall(Si_iter[:,t] .== k)
        for j in S_kt
            sum_Y += (Y[j,t] - muh_iter[k,t] - eta1_iter[j]*Y[j,t-1] -
                ↪ (lk_xPPM ? dot(view(Xlk_covariates,j,:,t), beta_iter[t]) :
                ↪ 0.0))^2
        end

        b_star = sig2h_priors[2] + sum_Y/2
        sig2h_iter[k,t] = rand(InverseGamma(a_star, b_star))
    end
end

##### update beta #####
# if lk_xPPM && i>=beta_update_threshold # conditional update version
if lk_xPPM
    if t==1
        sum_Y = zeros(p_lk)
        A_star = I(p_lk)/s2_beta
        for j in 1:n
            X_jt = @view Xlk_covariates[j,:,t]
            sum_Y += (Y[j,t] - muh_iter[Si_iter[j,t],t]) * X_jt /
                ↪ sig2h_iter[Si_iter[j,t],t]
            A_star += (X_jt * X_jt') / sig2h_iter[Si_iter[j,t],t]
        end
        b_star = beta0/s2_beta + sum_Y
        A_star = Symmetric(A_star)
        # Symmetric is needed for numerical problems
        # but A_star is indeed symm and pos def (by construction) so there
        ↪ is no problem
        beta_iter[t] = rand(MvNormalCanon(b_star, A_star)) # quicker and
        ↪ more accurate method
        # old method with the MvNormal and the inversion required
        # beta_iter[t] = rand(MvNormal(inv(Symmetric(A_star))*b_star,
        ↪ inv(Symmetric(A_star))))
    else
        sum_Y = zeros(p_lk)
        A_star = I(p_lk)/s2_beta
        for j in 1:n
            X_jt = @view Xlk_covariates[j,:,t]
            sum_Y += (Y[j,t] - muh_iter[Si_iter[j,t],t] -
                ↪ eta1_iter[j]*Y[j,t-1]) * X_jt / sig2h_iter[Si_iter[j,t],t]
            A_star += (X_jt * X_jt') / sig2h_iter[Si_iter[j,t],t]
        end
        b_star = beta0/s2_beta + sum_Y
        A_star = Symmetric(A_star)
        beta_iter[t] = rand(MvNormalCanon(b_star, A_star)) # quicker and
        ↪ more accurate method
        # old method with the MvNormal and the inversion required
        # beta_iter[t] = rand(MvNormal(inv(Symmetric(A_star))*b_star,
        ↪ inv(Symmetric(A_star))))
    end
end
end

```

```

##### update theta #####
aux1 = 1 / (lambda2_iter*(1-phi1_iter^2))
kt = nclus_iter[t]
sum_mu = 0.0
for k in 1:kt
    sum_mu += muh_iter[k,t]
end

if t==1
    sig2_post = 1 / (1/lambda2_iter + phi1_iter^2*aux1 + kt/tau2_iter[t])
    mu_post = sig2_post * (phi0_iter/lambda2_iter + sum_mu/tau2_iter[t] +
        ↪ (phi1_iter*(theta_iter[t+1] - (1-phi1_iter)*phi0_iter))*aux1)

    theta_iter[t] = rand(Normal(mu_post, sqrt(sig2_post)))

elseif t==T
    sig2_post = 1 / (aux1 + kt/tau2_iter[t])
    mu_post = sig2_post * (sum_mu/tau2_iter[t] + ((1- phi1_iter)*phi0_iter
        ↪ + phi1_iter*theta_iter[t-1])*aux1)

    theta_iter[t] = rand(Normal(mu_post, sqrt(sig2_post)))

else # 1<t<T
    sig2_post = 1 / ((1+phi1_iter^2)*aux1 + kt/tau2_iter[t])
    mu_post = sig2_post * (sum_mu/tau2_iter[t] +
        ↪ (phi1_iter*(theta_iter[t-1]+theta_iter[t+1]) +
        ↪ phi0_iter*(1-phi1_iter)^2)*aux1)

    theta_iter[t] = rand(Normal(mu_post, sqrt(sig2_post)))
end

##### update tau2 #####
kt = nclus_iter[t]
aux1 = 0.0
for k in 1:kt
    aux1 += (muh_iter[k,t] - theta_iter[t])^2
end
a_star = tau2_priors[1] + kt/2
b_star = tau2_priors[2] + aux1/2
tau2_iter[t] = rand(InverseGamma(a_star, b_star))

end # for t in 1:T

##### update eta1 #####
# the input argument eta1_priors[2] is already the std dev
if update_eta1
    for j in 1:n
        eta1_old = eta1_iter[j]
        eta1_new = rand(Normal(eta1_old, eta1_priors[2])) # proposal value

        if (-1 <= eta1_new <= 1)
            ll_old = 0.0
            ll_new = 0.0
            for t in 2:T
                # likelihood contribution
                ll_old += loglikelihood(Normal(
                    muh_iter[Si_iter[j,t],t] + eta1_old*Y[j,t-1] + (lk_xPPM ?
                    ↪ dot(view(Xlk_covariates,j,:,t), beta_iter[t]) : 0),
                    sqrt(sig2h_iter[Si_iter[j,t],t]*(1-eta1_old^2))
                ))
            end
            ll_new += loglikelihood(Normal(
                muh_iter[Si_iter[j,t],t] + eta1_new*Y[j,t-1] + (lk_xPPM ?
                ↪ dot(view(Xlk_covariates,j,:,t), beta_iter[t]) : 0),
                sqrt(sig2h_iter[Si_iter[j,t],t]*(1-eta1_new^2))
            ))
        end
    end
end

```

```

    ), Y[j,t])
    ll_new += loglikelihood(Normal(
        muh_iter[Si_iter[j,t],t] + eta1_new*Y[j,t-1] + (lk_xPPM ?
        ↪ dot(view(Xlk_covariates,j,:,t), beta_iter[t]) : 0),
        sqrt(sig2h_iter[Si_iter[j,t],t]*(1-eta1_new^2))
    ), Y[j,t])
end
logit_old = aux_logit(eta1_old)
logit_new = aux_logit(eta1_new)

# prior contribution
ll_old += -log(2*eta1_priors[1]) -1/eta1_priors[1]*abs(logit_old)
ll_new += -log(2*eta1_priors[1]) -1/eta1_priors[1]*abs(logit_new)

ll_ratio = ll_new-ll_old
u = rand(Uniform(0,1))
if (ll_ratio > log(u))
    eta1_iter[j] = eta1_new # accept the candidate
    acceptance_ratio_eta1 += 1
end
end
end
end

##### update alpha #####
if update_alpha
    if time_specific_alpha==false && unit_specific_alpha==false
        # a scalar
        sumg = sum(@view gamma_iter[:,1:T])
        a_star = alpha_priors[1] + sumg
        b_star = alpha_priors[2] + n*T - sumg
        alpha_iter = rand(Beta(a_star, b_star))

    elseif time_specific_alpha==true && unit_specific_alpha==false
        # a vector in time
        for t in 1:T
            sumg = sum(@view gamma_iter[:,t])
            a_star = alpha_priors[1] + sumg
            b_star = alpha_priors[2] + n - sumg
            alpha_iter[t] = rand(Beta(a_star, b_star))
        end

    elseif time_specific_alpha==false && unit_specific_alpha==true
        # a vector in units
        for j in 1:n
            sumg = sum(@view gamma_iter[j,1:T])
            a_star = alpha_priors[1,j] + sumg
            b_star = alpha_priors[2,j] + T - sumg
            alpha_iter[j] = rand(Beta(a_star, b_star))
        end

    elseif time_specific_alpha==true && unit_specific_alpha==true
        # a matrix
        for j in 1:n
            for t in 1:T
                sumg = gamma_iter[j,t] # nothing to sum in this case
                a_star = alpha_priors[1,j] + sumg
                b_star = alpha_priors[2,j] + 1 - sumg
                alpha_iter[j,t] = rand(Beta(a_star, b_star))
            end
        end
    end
end
end

```

```

end

##### update phi0 #####
aux1 = 1/lambda2_iter
aux2 = 0.0
for t in 2:T
    aux2 += theta_iter[t] - phi1_iter*theta_iter[t-1]
end
sig2_post = 1 / ( 1/phi0_priors[2] + aux1 * (1 +
    ↪ (T-1)*(1-phi1_iter)/(1+phi1_iter)) )
mu_post = sig2_post * ( phi0_priors[1]/phi0_priors[2] + theta_iter[1]*aux1 +
    ↪ aux1/(1+phi1_iter)*aux2 )
phi0_iter = rand(Normal(mu_post, sqrt(sig2_post)))

##### update phi1 #####
# the input argument phi_priors is already the std dev
if update_phi1
    phi1_old = phi1_iter
    phi1_new = rand(Normal(phi1_old, phi1_priors)) # proposal value

    if (-1 <= phi1_new <= 1)
        ll_old = 0.0; ll_new = 0.0
        for t in 2:T
            # likelihood contribution
            ll_old += loglikelihood(Normal(
                (1-phi1_old)*phi0_iter + phi1_old*theta_iter[t-1],
                sqrt(lambda2_iter*(1-phi1_old^2))
            ), theta_iter[t])
            ll_new += loglikelihood(Normal(
                (1-phi1_new)*phi0_iter + phi1_new*theta_iter[t-1],
                sqrt(lambda2_iter*(1-phi1_new^2))
            ), theta_iter[t])
        end

        # prior contribution
        ll_old += loglikelihood(Uniform(-1,1), phi1_old)
        ll_new += loglikelihood(Uniform(-1,1), phi1_new)

        ll_ratio = ll_new-ll_old
        u = rand(Uniform(0,1))
        if (ll_ratio > log(u))
            phi1_iter = phi1_new # accept the candidate
            acceptance_ratio_phi1 += 1
        end
    end
end

##### update lambda2 #####
aux1 = 0.0
for t in 2:T
    aux1 += (theta_iter[t] - (1-phi1_iter)*phi0_iter -
    ↪ phi1_iter*theta_iter[t-1])^2
end
a_star = lambda2_priors[1] + T/2
b_star = lambda2_priors[2] + ((theta_iter[1] - phi0_iter)^2 + aux1) / 2
lambda2_iter = rand(InverseGamma(a_star,b_star))

##### save MCMC iterates #####

```

```

if i>burnin && i%thin==0
  Si_out[:, :, i_out] = Si_iter[:, 1:T]
  gamma_out[:, :, i_out] = gamma_iter[:, 1:T]
  if time_specific_alpha==false && unit_specific_alpha==false
    # for each iterate, a scalar
    alpha_out[i_out] = alpha_iter
  elseif time_specific_alpha==true && unit_specific_alpha==false
    # for each iterate, a vector in time
    alpha_out[:, i_out] = alpha_iter[1:T]
  elseif time_specific_alpha==false && unit_specific_alpha==true
    # for each iterate, a vector in units
    alpha_out[:, i_out] = alpha_iter
  elseif time_specific_alpha==true && unit_specific_alpha==true
    # for each iterate, a matrix
    alpha_out[:, :, i_out] = alpha_iter[:, 1:T]
  end
  for t in 1:T
    for j in 1:n
      sigma2h_out[j, t, i_out] = sig2h_iter[Si_iter[j, t], t]
      muh_out[j, t, i_out] = muh_iter[Si_iter[j, t], t]
    end
  end
  eta1_out[:, i_out] = eta1_iter
  if lk_xPPM
    for t in 1:T
      beta_out[t, :, i_out] = beta_iter[t]
    end
  end
  theta_out[:, i_out] = theta_iter[1:T]
  tau2_out[:, i_out] = tau2_iter[1:T]
  phi0_out[i_out] = phi0_iter
  phi1_out[i_out] = phi1_iter
  lambda2_out[i_out] = lambda2_iter

##### save fitted values and metrics #####
for j in 1:n
  for t in 1:T
    muh_jt = muh_iter[Si_iter[j, t], t]
    sig2h_jt = sig2h_iter[Si_iter[j, t], t]
    X_lk_term = lk_xPPM ? dot(view(Xlk_covariates, j, :, t), beta_iter[t])
    ↪ : 0.0

    if t==1
      llike[j, t, i_out] = logpdf(Normal(
        muh_jt + X_lk_term,
        sqrt(sig2h_jt)
      ), Y[j, t])
      fitted[j, t, i_out] = muh_jt + X_lk_term
    else # t>1
      llike[j, t, i_out] = logpdf(Normal(
        muh_jt + eta1_iter[j]*Y[j, t-1] + X_lk_term,
        sqrt(sig2h_jt*(1-eta1_iter[j]^2))
      ), Y[j, t])
      fitted[j, t, i_out] = muh_jt + eta1_iter[j]*Y[j, t-1] + X_lk_term
    end

    mean_likelhd[j, t] += exp(llike[j, t, i_out])
    mean_loglikelhd[j, t] += llike[j, t, i_out]
    CPO[j, t] += exp(-llike[j, t, i_out])
  end
end
end

```



```

        i_out += 1
    end

next!(progresso)

end # for i in 1:draws

println("\ndone!")
t_end = now()
println("Elapsed time: ",
    ↪ Dates.canonicalize(Dates.CompoundPeriod(t_end-t_start)))

##### compute LPML and WAIC #####
for j in 1:n
    for t in 1:T
        LPML += log(CPO[j,t])
    end
end
LPML -= n*T*log(nout) # scaling factor
LPML = -LPML # fix sign
println("LPML: ", LPML, " (the higher the better)")

# adjust mean variables
mean_likelhd ./= nout
mean_loglikelhd ./= nout
for j in 1:n
    for t in 1:T
        WAIC += 2*mean_loglikelhd[j,t] - log(mean_likelhd[j,t])
    end
end
WAIC *= -2
println("WAIC: ", WAIC, " (the lower the better)")

if update_eta1 @printf "acceptance ratio eta1: %.2f%%\n"
    ↪ acceptance_ratio_eta1/(n*draws)*100 end
if update_phi1 @printf "acceptance ratio phi1: %.2f%%"
    ↪ acceptance_ratio_phi1/draws*100 end
println()

if perform_diagnostics
    chn = Chains(
        hcat(lambda2_out,phi0_out,tau2_out',theta_out',eta1_out',alpha_out'),
        ["lambda2","phi0",
        [string("tau2_t", i) for i in 1:T]...,
        [string("theta_t", i) for i in 1:T]...,
        [string("eta1_j", i) for i in 1:n]...,
        [string("alpha_t", i) for i in 1:T]...,
        ]
    )
    ss = DataFrame(summarystats(chn))
    println("\nDiagnostics:")
    @show ss[!, [1,4,5,6,7]];
    if logging CSV.write(log_file,ss[!, [1,4,5,6,7]]) end
end

if logging
    close(log_file)
end

if simple_return
    return Si_out, LPML, WAIC
end

```

```

else
  return Si_out, Int.(gamma_out), alpha_out, sigma2h_out, muh_out, include_eta1
  ↪ ? eta1_out : NaN, lk_xPPM ? beta_out : NaN, theta_out, tau2_out,
  ↪ phi0_out, include_phi1 ? phi1_out : NaN, lambda2_out, fitted, llike,
  ↪ LPML, WAIC
end

```

B.2 Interface

Now some more technical details about the whole implementation design. The fitting code was written in Julia, but its main intended use is from R. This choice was made because R is currently the best language for statistical purposes, or at least the most spread; in fact all other models “competitors” to the DRPM are available through some R package. Therefore we thought that letting our work be also accessible from R, and not only from Julia, would have eased the possibilities of testing and comparisons with other models or datasets.

To do so, we relied on the `JuliaConnector` library [LHB22] on R, which allows the interaction between the two languages. In this sense, we can load in R the Julia package `JDRPM`, which stores the Julia project (i.e. all codes and packages dependencies) about the improved version of the DRPM model, and call it using data and arguments from R. The output produced by the Julia functions has then to be converted back into R structures, which is done automatically through a dedicated function of the package. The structure of this workflow is summarized in Listing 4.

Listing 4: Instructions on how to use the JDRPM model from R.

```

##### Requirements #####
# install the required package
install.packages("JuliaConnector")

##### Setup #####
# load the package
library(JuliaConnector)
# check it returns TRUE
juliaSetupOk()

# load the Package manager on Julia
juliaEval("using Pkg")
# enter into the JDRPM project
juliaEval("Pkg.activate("<path/to/where/you/stored/JDRPM>")")

# downloads and install, only once, all the dependencies
juliaEval("Pkg.instantiate()")
# now, as a check, this should print the list of packages that JDRPM uses,
# such as Distributions, Statistics, LinearAlgebra, SpecialFunctions, etc.
juliaEval("Pkg.status()")

# locate the "main" file
module = normalizePath("<path/to/where/you/stored/JDRPM>/src/JDRPM.jl")
# load the "main" file into a callable R object
module_JDRPM = juliaImport(juliaCall("include", module))

```

```

# trigger the compilation of the function, otherwise all first runs
# will be slow since the function still would have to be compiled
module_JDRPM$trigger_compilation()
# it runs a small fit, so it's also a test to ensure that everything works

##### Fit #####
# perform the fit
out = module_JDRPM$MCMC_fit(...)

# convert the output to R structures
rout = juliaGet(out)
names(rout) = c("Si", "gamma", "alpha", "sigma2h", "muh", "eta1", "beta", "theta",
  ↪ "tau2", "phi0", "phi1", "lambda2", "fitted", "llike", "lpml", "waic")

# and reshape it to uniform to the DRPM output form
rout$Si = aperm(rout$Si, c(2, 1, 3))
rout$gamma = aperm(rout$gamma, c(2, 1, 3))
rout$sigma2h = aperm(rout$sigma2h, c(2, 1, 3))
rout$muh = aperm(rout$muh, c(2, 1, 3))
rout$fitted = aperm(rout$fitted, c(2, 1, 3))
rout$llike = aperm(rout$llike, c(2, 1, 3))
rout$alpha = aperm(rout$alpha, c(2, 1))
rout$theta = aperm(rout$theta, c(2, 1))
rout$tau2 = aperm(rout$tau2, c(2, 1))
rout$eta1 = aperm(rout$eta1, c(2, 1))
rout$phi0 = matrix(rout$phi0, ncol = 1)
rout$phi1 = matrix(rout$phi1, ncol = 1)
rout$lambda2 = matrix(rout$lambda2, ncol = 1)
# this reshape works in the case of full model fit, but in the case of special
# fitting options (e.g. unit_specific_alpha=true) it needs to be adjusted

```

Regarding instead the visual interface, in the sense of the feedback provided by the function, we decided to make it more user-friendly, and possibly informative, than the original C implementation. The most relevant add-ons are the possibility to perform diagnostics, on part of the sampled values, and the real-time progress monitoring, which updates itself every second to show the estimated remaining time for completing the fit. As a further proof of the ease of this language, these features were a simple insertion of few lines of code thanks to the Julia packages `MCMCChains` and `ProgressMeter` respectively.

Listing 5: Feedback from the JDRPM implementation.

```

# if verbose=true this initial section is also print
Parameters:
sig2h ~ invGamma(0.01, 0.01)
Logit(1/2(eta1+1)) ~ Laplace(0, 0.9)
tau2 ~ invGamma(1.9, 0.4)
phi0 ~ Normal( $\mu=0.0$ ,  $\sigma=10.0$ )
lambda2 ~ invGamma(1.9, 0.4)
alpha ~ Beta(2.0, 2.0)

- using seed 113.0 -
fitting 100000 total iterates (with burnin=80000, thinning=5)
thus producing 4000 valid iterates in the end

```

```
on n=105 subjects
for T=12 time instants
```

```
[✓] with space? true
[✗] with covariates in the likelihood? false
[✗] with covariates in the clustering process? false
[✗] are there missing data in Y? false
```

```
2024-10-14 09:33:11
Starting MCMC algorithm
Progress: 100% Time: 0:25:39 (15.40 ms/it)
```

```
done!
Elapsed time: 25 minutes, 39 seconds, 569 milliseconds
LPML: 517.182456879369 (the higher the better)
WAIC: -1283.8930457498177 (the lower the better)
acceptance ratio etal: 74.66%
```

```
# if perform_diagnostics=true this final section is also print
Diagnostics:
```

```
ss[!, [1, 4, 5, 6, 7]] = 143×5 DataFrame
```

Row	parameters	mcse	ess_bulk	ess_tail	rhat
	Symbol	Float64	Float64	Float64	Float64
1	lambda2	0.000817173	4243.04	3970.25	0.999769
2	phi0	0.00218706	3533.95	3675.99	1.00018
3	tau2_t1	0.00540064	3716.56	3645.99	0.999968
	⋮				
14	tau2_t12	0.00259168	3965.77	3655.55	0.999951
15	theta_t1	0.00404988	3603.34	3765.78	0.999834
	⋮				
26	theta_t12	0.00337843	3588.83	3907.13	0.999866
27	etal_j1	0.0112187	451.588	1107.96	1.00163
	⋮				
131	etal_j105	0.00328424	1539.36	2194.83	1.00002
132	alpha_t1	0.000213087	3774.24	3920.48	1.00044
	⋮				
143	alpha_t12	0.00266005	541.427	1867.54	1.0084

Appendix C

Further plots

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“This is to be my haven for many long years, my niche which I enter with such a mistrustful, such a painful sensation... And who knows? Maybe when I come to leave it many years hence I may regret it!”

— Fëdor Dostoevskij, *The House of the Dead*

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“Ecco il mio ponte d’approdo per molti lunghi anni, il mio angoletto, nel quale faccio il mio ingresso con una sensazione così diffidente, così morbosa... Ma chi lo sa? Forse, quando tra molti anni mi toccherà abbandonarlo, magari potrei anche rimpiangerlo!”

— Fëdor Dostoevskij, *Memorie da una casa di morti*