A Kronecker-based model for multivariate spatial data

Angélica Maria Tortola Ribeiro
Supervisor: Paulo Justiniano Ribeiro Jr
Wagner Bonat

Introduction

- Context: Multivariate spatial data analysis;

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- Important: Specify an adequate and valid covariance function;
- Literature proposals: LMC, multivariate model Matérn, separable model classes;
- Thus, more robust covariance models for multivariate random fields are still a challenge.

Introduction

- Proposal: a valid covariance specification for spatially continuous multivariate data;

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- Allows different marginal covariance structures;

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- Proposal: a valid covariance specification for spatially continuous multivariate data;
- Flexible to handle with two or more variables;
- Allows different marginal covariance structures;
- Results: theoretical results, simulation studies, estimation times, data analysis;

Bibliometric Study

Bibliometric Analysis:

Bibliometric analysis studies bibliographic behavior in a research area.

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Bibliometric Study

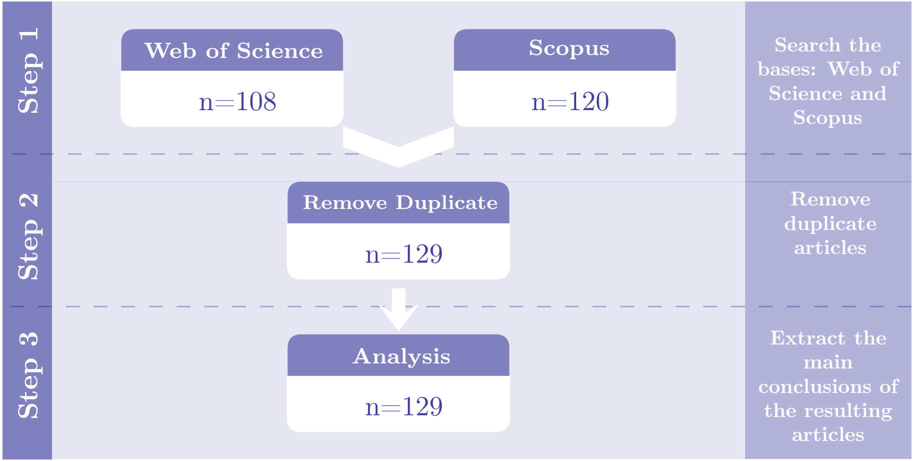

Figure 1: Research steps.

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Bibliometric Analysis

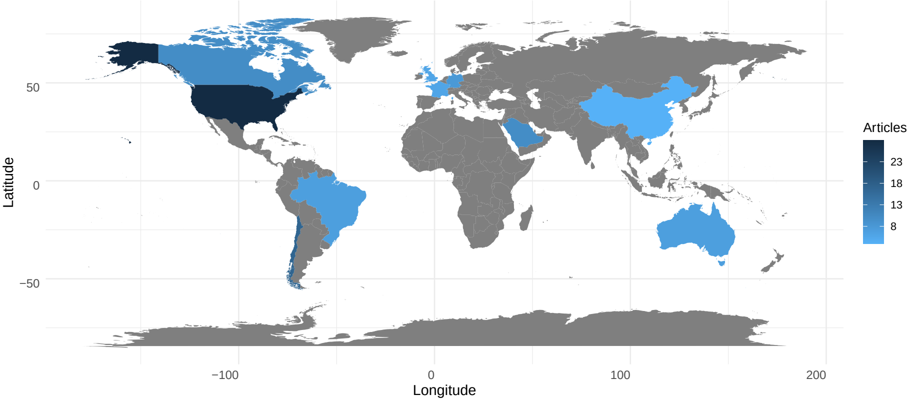


Figure 2: Articles distribution by country of the corresponding author.

Bibliometric Analysis

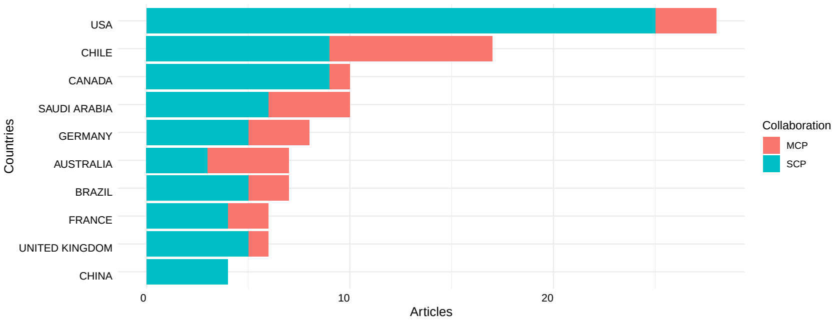


Figure 3: The 10 most productive countries (by corresponding authors).

Bibliometric Analysis

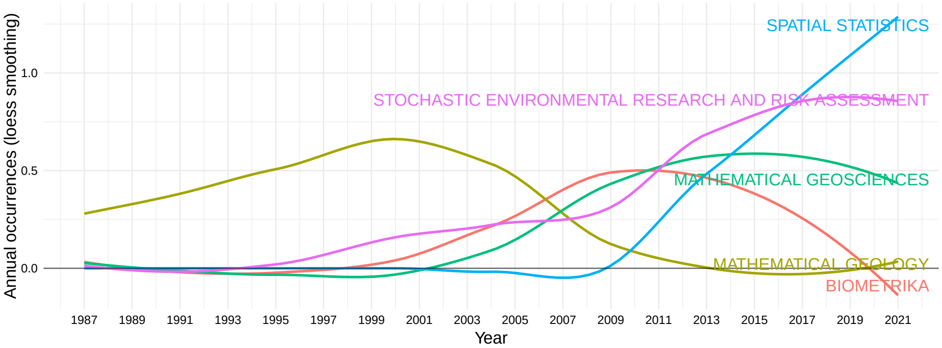


Figure 4: Smoothed behavior of articles production by journal over the years.

Bibliometric Analysis

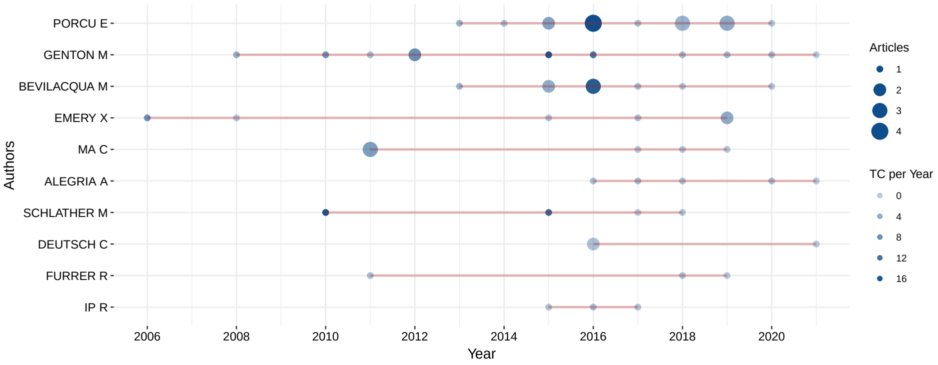


Figure 5: The most relevant authors over the years.

Bibliometric Analysis

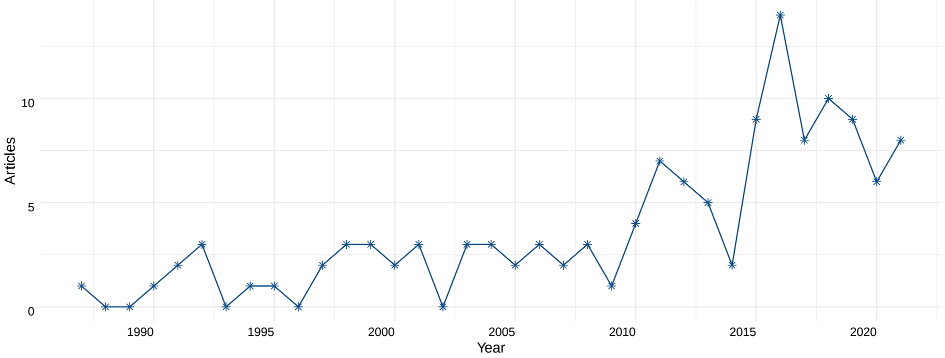


Figure 6: Annual scientific production.

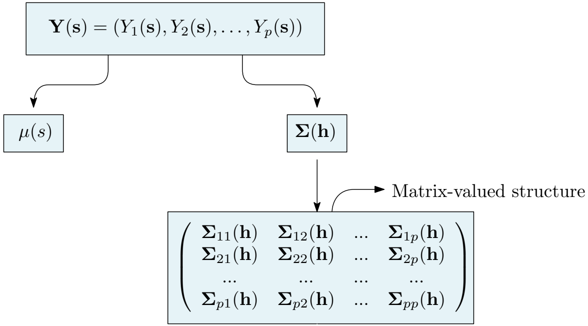
Covariance Models

$$\boxed{\mathbf{Y}(\mathbf{s}) = (Y_1(\mathbf{s}), Y_2(\mathbf{s}), \ldots, Y_p(\mathbf{s}))}$$

Covariance Models

$$
\begin{tikzcd}
 & \boxed{\mathbf{Y}(\mathbf{s}) = (Y_1(\mathbf{s}), Y_2(\mathbf{s}), \ldots, Y_p(\mathbf{s}))} \arrow[dl] \arrow[dr] & \\
\boxed{\mu(s)} & & \boxed{\boldsymbol{\Sigma}(\mathbf{h})}
\end{tikzcd}
$$

Covariance Models



Covariance Models

$$\mathbf{Y}(\mathbf{s}) = (Y_1(\mathbf{s}), Y_2(\mathbf{s}), \dots, Y_p(\mathbf{s}))$$

$$\mu(s)$$

$$\boldsymbol{\Sigma}(\mathbf{h})$$

Matrix-valued structure

$$\begin{pmatrix} \boldsymbol{\Sigma}_{11}(\mathbf{h}) & \boldsymbol{\Sigma}_{12}(\mathbf{h}) & \dots & \boldsymbol{\Sigma}_{1p}(\mathbf{h}) \\ \boldsymbol{\Sigma}_{21}(\mathbf{h}) & \boldsymbol{\Sigma}_{22}(\mathbf{h}) & \dots & \boldsymbol{\Sigma}_{2p}(\mathbf{h}) \\ \dots & \dots & \dots & \dots \\ \boldsymbol{\Sigma}_{p1}(\mathbf{h}) & \boldsymbol{\Sigma}_{p2}(\mathbf{h}) & \dots & \boldsymbol{\Sigma}_{pp}(\mathbf{h}) \end{pmatrix}$$

$$\boldsymbol{\Sigma}_{ij}(\mathbf{h}) = E[Y_i(\mathbf{s}) - \mu_i(\mathbf{s})][Y_j(s+\mathbf{h}) - \mu_j(s+\mathbf{h})]$$

Cross-covariance function

Linear model of co-regionalization (LMC)

- Linear combination of independent univariate processes;
- Thus, the resulting covariance function takes the form:

$$\boldsymbol{\Sigma}_{ij}(\mathbf{h}) = \sum_{k=1}^{r} a_{ik} a_{jk} R_k(\mathbf{h}), \quad \text{with} \quad 1 \leq r \leq p,$$

where $R_k(.)$ are valid correlation functions and $\mathbf{A} = [a_{ij}]_{p \times r}$ is a full rank matrix.

Matérn covariance model

Full bivariate Matérn model

Matérn covariance model

Full bivariate Matérn model

$$\mathbf{\Sigma}_{ii} = \sigma_i^2 M(\mathbf{h}|\nu_i, 1/\phi_i)$$
$$\mathbf{\Sigma}_{12} = \mathbf{\Sigma}_{21} = \rho_{12}\sigma_1\sigma_2 M(\mathbf{h}|\nu_{12}, 1/\phi_{12})$$

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Matérn covariance model

Full bivariate Matérn model

$$\mathbf{\Sigma}_{ii} = \sigma_i^2 M(\mathbf{h}|\nu_i, 1/\phi_i)$$

$$\mathbf{\Sigma}_{12} = \mathbf{\Sigma}_{21} = \rho_{12}\sigma_1\sigma_2 M(\mathbf{h}|\nu_{12}, 1/\phi_{12})$$

Notation

$M(\mathbf{h}|\nu, 1/\phi) = \dfrac{2^{1-\nu}}{\Gamma(\nu)} \left(|\mathbf{h}|/\phi\right)^{\nu} K_{\nu}\left(|\mathbf{h}|/\phi\right) \rightarrow$ Matern correlation function

$\sigma, \nu, \phi > 0 \rightarrow$ standard deviation, smoothness and scale parameters

$\rho_{12} \rightarrow$ correlation parameter

Separable models

Separable models

Separable models

Separable models

$\downarrow$

$$\boldsymbol{\Sigma}(\mathbf{h}) = [\rho_{ij}\sigma_i\sigma_j R(\mathbf{h}|\boldsymbol{\Psi})]_{i,j=1}^{p}, \quad \rho_{ii} = 1$$

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Separable models

Separable models

$$\boldsymbol{\Sigma}(\mathbf{h}) = [\rho_{ij}\sigma_i\sigma_j R(\mathbf{h}|\boldsymbol{\Psi})]_{i,j=1}^{p}\,, \quad \rho_{ii} = 1$$

Notation

$R(\mathbf{h}|\boldsymbol{\Psi}) \rightarrow$ Univariate correlation model

$\sigma^2 > 0 \rightarrow$ marginal variances

$\rho_{12} \rightarrow$ correlation parameter

Matern model simplifications

Matérn model simplifications

Matern model simplifications

Matérn model simplifications

Separable Matérn model
(MatSep)

$$\phi_1 = \phi_2 = \phi_{12} = \phi$$

$$\nu_1 = \nu_2 = \nu_{12} = \nu$$

Matern model simplifications

Matérn model simplifications

Separable Matérn model (MatSep)

$$\phi_1 = \phi_2 = \phi_{12} = \phi$$

$$\nu_1 = \nu_2 = \nu_{12} = \nu$$

Constrained Matérn model (MatConstr)

$$\phi_{12} = \frac{\phi_1 + \phi_2}{2} \qquad \nu_{12} = \frac{\nu_1 + \nu_2}{2}$$

Literature models considered

- Linear model of coregionalization (LMC): with exponential correlation function;
- Separable Matérn model (MatSep); with Matérn correlation function;
- Constrained Matérn model (MatConstr); with Matérn correlation function;
- Independent Matérn model (MatInd); with Matérn correlation function;

All these models are implemented in GeoModels package for bivariate data.

Literature discussions

LMC:

"... the lack of flexibility of the LMC and related models for multivariate spatial random fields has been noted by various authors, including Cressie (1993, p. 141), Goovaerts (1997, p. 123), and recently Jun, Knutti, and Nychka (2008, p. 945) ..." - Gneiting et al. (2010)

"... the linear model of coregionalization [LMC, see Wackernagel (2003)] has been criticized for having a number of drawbacks, and we refer the reader to Porcu et al. (2013), Gneiting et al. (2010) and Genton and Kleiber (2015) among others." - Bevilacqua et al. (2016)

"... One major shortcoming of this model is that it lacks flexibility as it bestows on all variables the smoothness of the roughest underlying univariate spatial process" - Salvaña and Genton (2020)

Literature discussions

Full bivariate Matérn:

"Note that this condition shrinks the range of validity of ρ_{12}. In general, considering the nonseparable construction, leads to restrictions on the upper and lower bound of the colocated parameter than can be more or less severe depending on the scale and smoothness parameters."
- (Vallejos et al., 2020, p. 50)

Separable models:

Bevilacqua et al. (2016), Vallejos et al. (2020), noticed that this model is not able to capture the different scales and smoothness of the components.

Model specification

$$\boldsymbol{\Sigma}(\mathbf{h}) = B_{\text{diag}}\left(\tilde{\boldsymbol{\Sigma}}_{11}, \tilde{\boldsymbol{\Sigma}}_{22}, \ldots, \tilde{\boldsymbol{\Sigma}}_{pp}\right)\left(\boldsymbol{\Sigma}_b \otimes \mathbf{I}\right) B_{\text{diag}}\left(\tilde{\boldsymbol{\Sigma}}_{11}^{\top}, \tilde{\boldsymbol{\Sigma}}_{22}^{\top}, \ldots, \tilde{\boldsymbol{\Sigma}}_{pp}^{\top}\right)$$

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Model specification

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$\tilde{\boldsymbol{\Sigma}}_{ii} \rightarrow$ Cholesky decomposition of $\boldsymbol{\Sigma}_{ii}$
$B_{diag} \rightarrow$ Matrix in diagonal blocks of $\tilde{\boldsymbol{\Sigma}}_{ii}$
$\mathbf{I}_n \rightarrow$ Identity matrix

Model specification

$$\boldsymbol{\Sigma}(\mathbf{h}) = B_{\text{diag}}\left(\tilde{\boldsymbol{\Sigma}}_{11}, \tilde{\boldsymbol{\Sigma}}_{22}, \ldots, \tilde{\boldsymbol{\Sigma}}_{pp}\right)(\boldsymbol{\Sigma}_b \otimes \mathbf{I})\, B_{\text{diag}}\left(\tilde{\boldsymbol{\Sigma}}_{11}^\top, \tilde{\boldsymbol{\Sigma}}_{22}^\top, \ldots, \tilde{\boldsymbol{\Sigma}}_{pp}^\top\right)$$

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$$\boldsymbol{\Sigma}_b = \begin{pmatrix} 1 & \rho_{12} & \ldots & \rho_{1p} \\ \rho_{12} & 1 & \ldots & \rho_{2p} \\ \ldots & \ldots & \ldots & \ldots \\ \rho_{1p} & \rho_{2p} & \ldots & 1 \end{pmatrix}$$

Model specification

Notation

$$\boldsymbol{\Sigma}(\mathbf{h}) = B_{\text{diag}}\left(\tilde{\boldsymbol{\Sigma}}_{11}, \tilde{\boldsymbol{\Sigma}}_{22}, \dots, \tilde{\boldsymbol{\Sigma}}_{pp}\right)(\boldsymbol{\Sigma}_b \otimes \mathbf{I})\, B_{\text{diag}}\left(\tilde{\boldsymbol{\Sigma}}_{11}^\top, \tilde{\boldsymbol{\Sigma}}_{22}^\top, \dots, \tilde{\boldsymbol{\Sigma}}_{pp}^\top\right)$$

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$$\boldsymbol{\Sigma}_{ii}(\mathbf{h}) = \sigma_i^2 R\left(\mathbf{h} | \boldsymbol{\Psi}_i\right)$$

Model specification

Notation

$$\boldsymbol{\Sigma}(\mathbf{h}) = B_{\text{diag}}\left(\tilde{\boldsymbol{\Sigma}}_{11}, \tilde{\boldsymbol{\Sigma}}_{22}, \ldots, \tilde{\boldsymbol{\Sigma}}_{pp}\right)(\boldsymbol{\Sigma}_b \otimes \mathbf{I})\, B_{\text{diag}}\left(\tilde{\boldsymbol{\Sigma}}_{11}^{\top}, \tilde{\boldsymbol{\Sigma}}_{22}^{\top}, \ldots, \tilde{\boldsymbol{\Sigma}}_{pp}^{\top}\right)$$

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$$\boldsymbol{\Sigma}_{ii}(\mathbf{h}) = \sigma_i^2 R\left(\mathbf{h}|\boldsymbol{\Psi}_i\right)$$

ExpSimpler

$$\boldsymbol{\Sigma}_{ii}(\mathbf{h}) = \sigma_i^2 \exp\left(-\frac{\mathbf{h}}{\phi_i}\right)$$

$\sigma_i, \phi_i > 0$

MatSimpler

$$\boldsymbol{\Sigma}_{ii}(\mathbf{h}) = \sigma_i^2 \frac{2^{1-\nu_i}}{\Gamma(\nu_i)}\left(\frac{\mathbf{h}}{\phi_i}\right)^{\nu_i} K_{\nu_i}\left(\frac{\mathbf{h}}{\phi_i}\right)$$

$\sigma_i, \phi_i, \nu_i > 0$

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Model specification

Theorem

Let $\boldsymbol{\Sigma}_{ii}$, for $i = 1, \ldots, p$, the marginal covariance functions, $\boldsymbol{\Sigma}_b$ a valid spatial correlation function and $\mathbf{I}$ the identity matrix, then the proposed covariance function is a valid and full rank specification for multivariate spatial data modeling.

Model specification

$$\boxed{\boldsymbol{\Sigma}(\mathbf{h}) = B_{\text{diag}}\left(\tilde{\boldsymbol{\Sigma}}_{11}, \tilde{\boldsymbol{\Sigma}}_{22}, \ldots, \tilde{\boldsymbol{\Sigma}}_{pp}\right)(\boldsymbol{\Sigma}_b \otimes \mathbf{I})\, B_{\text{diag}}\left(\tilde{\boldsymbol{\Sigma}}_{11}^\top, \tilde{\boldsymbol{\Sigma}}_{22}^\top, \ldots, \tilde{\boldsymbol{\Sigma}}_{pp}^\top\right)}$$

Model specification

$$\boldsymbol{\Sigma}(\mathbf{h}) = B_{\text{diag}}\left(\tilde{\boldsymbol{\Sigma}}_{11}, \tilde{\boldsymbol{\Sigma}}_{22}, \ldots, \tilde{\boldsymbol{\Sigma}}_{pp}\right)(\boldsymbol{\Sigma}_b \otimes \mathbf{I})\, B_{\text{diag}}\left(\tilde{\boldsymbol{\Sigma}}_{11}^\top, \tilde{\boldsymbol{\Sigma}}_{22}^\top, \ldots, \tilde{\boldsymbol{\Sigma}}_{pp}^\top\right)$$

$$\downarrow$$

$$\begin{pmatrix} \tilde{\boldsymbol{\Sigma}}_{11} & \mathbf{0} & \ldots & \mathbf{0} \\ \mathbf{0} & \tilde{\boldsymbol{\Sigma}}_{22} & \ldots & \mathbf{0} \\ \ldots & \ldots & \ldots & \ldots \\ \mathbf{0} & \mathbf{0} & \ldots & \tilde{\boldsymbol{\Sigma}}_{pp} \end{pmatrix} \begin{pmatrix} \mathbf{I} & \rho_{12}\mathbf{I} & \ldots & \rho_{1p}\mathbf{I} \\ \rho_{12}\mathbf{I} & \mathbf{I} & \ldots & \rho_{2p}\mathbf{I} \\ \ldots & \ldots & \ldots & \ldots \\ \rho_{1p}\mathbf{I} & \rho_{2p}\mathbf{I} & \ldots & \mathbf{I} \end{pmatrix} \begin{pmatrix} \tilde{\boldsymbol{\Sigma}}_{11}^\top & \mathbf{0} & \ldots & \mathbf{0} \\ \mathbf{0} & \tilde{\boldsymbol{\Sigma}}_{22}^\top & \ldots & \mathbf{0} \\ \ldots & \ldots & \ldots & \ldots \\ \mathbf{0} & \mathbf{0} & \ldots & \tilde{\boldsymbol{\Sigma}}_{pp}^\top \end{pmatrix}$$

Model specification

$$\boldsymbol{\Sigma}(\mathbf{h}) = B_{\text{diag}}\left(\tilde{\boldsymbol{\Sigma}}_{11}, \tilde{\boldsymbol{\Sigma}}_{22}, \dots, \tilde{\boldsymbol{\Sigma}}_{pp}\right)(\boldsymbol{\Sigma}_b \otimes \mathbf{I})\, B_{\text{diag}}\left(\tilde{\boldsymbol{\Sigma}}_{11}^\top, \tilde{\boldsymbol{\Sigma}}_{22}^\top, \dots, \tilde{\boldsymbol{\Sigma}}_{pp}^\top\right)$$

$$\downarrow$$

$$\begin{pmatrix} \tilde{\boldsymbol{\Sigma}}_{11} & \mathbf{0} & \dots & \mathbf{0} \\ \mathbf{0} & \tilde{\boldsymbol{\Sigma}}_{22} & \dots & \mathbf{0} \\ \dots & \dots & \dots & \dots \\ \mathbf{0} & \mathbf{0} & \dots & \tilde{\boldsymbol{\Sigma}}_{pp} \end{pmatrix} \begin{pmatrix} \mathbf{I} & \rho_{12}\mathbf{I} & \dots & \rho_{1p}\mathbf{I} \\ \rho_{12}\mathbf{I} & \mathbf{I} & \dots & \rho_{2p}\mathbf{I} \\ \dots & \dots & \dots & \dots \\ \rho_{1p}\mathbf{I} & \rho_{2p}\mathbf{I} & \dots & \mathbf{I} \end{pmatrix} \begin{pmatrix} \tilde{\boldsymbol{\Sigma}}_{11}^\top & \mathbf{0} & \dots & \mathbf{0} \\ \mathbf{0} & \tilde{\boldsymbol{\Sigma}}_{22}^\top & \dots & \mathbf{0} \\ \dots & \dots & \dots & \dots \\ \mathbf{0} & \mathbf{0} & \dots & \tilde{\boldsymbol{\Sigma}}_{pp}^\top \end{pmatrix}$$

$$\downarrow$$

$$\begin{pmatrix} \tilde{\boldsymbol{\Sigma}}_{11}\tilde{\boldsymbol{\Sigma}}_{11}^\top & \rho_{12}\tilde{\boldsymbol{\Sigma}}_{11}\tilde{\boldsymbol{\Sigma}}_{22}^\top & \dots & \rho_{1p}\tilde{\boldsymbol{\Sigma}}_{11}\tilde{\boldsymbol{\Sigma}}_{pp}^\top \\ \rho_{12}\tilde{\boldsymbol{\Sigma}}_{22}\tilde{\boldsymbol{\Sigma}}_{11}^\top & \tilde{\boldsymbol{\Sigma}}_{22}\tilde{\boldsymbol{\Sigma}}_{22}^\top & \dots & \rho_{2p}\tilde{\boldsymbol{\Sigma}}_{22}\tilde{\boldsymbol{\Sigma}}_{pp}^\top \\ \dots & \dots & \dots & \dots \\ \rho_{1p}\tilde{\boldsymbol{\Sigma}}_{pp}\tilde{\boldsymbol{\Sigma}}_{11}^\top & \rho_{2p}\tilde{\boldsymbol{\Sigma}}_{pp}\tilde{\boldsymbol{\Sigma}}_{22}^\top & \dots & \tilde{\boldsymbol{\Sigma}}_{pp}\tilde{\boldsymbol{\Sigma}}_{pp}^\top \end{pmatrix}$$

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$$\boldsymbol{\Sigma}(\mathbf{h}) = B_{\text{diag}}\left(\tilde{\boldsymbol{\Sigma}}_{11}, \tilde{\boldsymbol{\Sigma}}_{22}, \ldots, \tilde{\boldsymbol{\Sigma}}_{pp}\right)(\boldsymbol{\Sigma}_b \otimes \mathbf{I})\, B_{\text{diag}}\left(\tilde{\boldsymbol{\Sigma}}_{11}^\top, \tilde{\boldsymbol{\Sigma}}_{22}^\top, \ldots, \tilde{\boldsymbol{\Sigma}}_{pp}^\top\right)$$

$$\downarrow$$

$$\begin{pmatrix} \tilde{\boldsymbol{\Sigma}}_{11} & \mathbf{0} & \ldots & \mathbf{0} \\ \mathbf{0} & \tilde{\boldsymbol{\Sigma}}_{22} & \ldots & \mathbf{0} \\ \ldots & \ldots & \ldots & \ldots \\ \mathbf{0} & \mathbf{0} & \ldots & \tilde{\boldsymbol{\Sigma}}_{pp} \end{pmatrix} \begin{pmatrix} \mathbf{I} & \rho_{12}\mathbf{I} & \ldots & \rho_{1p}\mathbf{I} \\ \rho_{12}\mathbf{I} & \mathbf{I} & \ldots & \rho_{2p}\mathbf{I} \\ \ldots & \ldots & \ldots & \ldots \\ \rho_{1p}\mathbf{I} & \rho_{2p}\mathbf{I} & \ldots & \mathbf{I} \end{pmatrix} \begin{pmatrix} \tilde{\boldsymbol{\Sigma}}_{11}^\top & \mathbf{0} & \ldots & \mathbf{0} \\ \mathbf{0} & \tilde{\boldsymbol{\Sigma}}_{22}^\top & \ldots & \mathbf{0} \\ \ldots & \ldots & \ldots & \ldots \\ \mathbf{0} & \mathbf{0} & \ldots & \tilde{\boldsymbol{\Sigma}}_{pp}^\top \end{pmatrix}$$

$$\downarrow$$

$$\begin{pmatrix} \tilde{\boldsymbol{\Sigma}}_{11}\tilde{\boldsymbol{\Sigma}}_{11}^\top & \rho_{12}\tilde{\boldsymbol{\Sigma}}_{11}\tilde{\boldsymbol{\Sigma}}_{22}^\top & \ldots & \rho_{1p}\tilde{\boldsymbol{\Sigma}}_{11}\tilde{\boldsymbol{\Sigma}}_{pp}^\top \\ \rho_{12}\tilde{\boldsymbol{\Sigma}}_{22}\tilde{\boldsymbol{\Sigma}}_{11}^\top & \tilde{\boldsymbol{\Sigma}}_{22}\tilde{\boldsymbol{\Sigma}}_{22}^\top & \ldots & \rho_{2p}\tilde{\boldsymbol{\Sigma}}_{22}\tilde{\boldsymbol{\Sigma}}_{pp}^\top \\ \ldots & \ldots & \ldots & \ldots \\ \rho_{1p}\tilde{\boldsymbol{\Sigma}}_{pp}\tilde{\boldsymbol{\Sigma}}_{11}^\top & \rho_{2p}\tilde{\boldsymbol{\Sigma}}_{pp}\tilde{\boldsymbol{\Sigma}}_{22}^\top & \ldots & \tilde{\boldsymbol{\Sigma}}_{pp}\tilde{\boldsymbol{\Sigma}}_{pp}^\top \end{pmatrix}$$

$$\downarrow$$

$$\boldsymbol{\Sigma}_{ij}(\mathbf{h}) = \rho_{ij}\tilde{\boldsymbol{\Sigma}}_{ii}\tilde{\boldsymbol{\Sigma}}_{jj}^\top, \quad \rho_{ii} = 1$$

Model specification

Theorem

Let $Y_1(\mathbf{s}), Y_2(\mathbf{s}), \ldots, Y_p(\mathbf{s})$ a p-dimensional random field with the same spatial dependence structure for all $Y_i(\mathbf{s})$, $i = 1, \ldots, p$, then the simpler covariance model is reduced to the class of separable models.

Proof.

$$
\begin{aligned}
\boldsymbol{\Sigma}_{ij}(\mathbf{h}) &= \rho_{ij}\tilde{\boldsymbol{\Sigma}}_{ii}(\mathbf{h})\tilde{\boldsymbol{\Sigma}}_{jj}(\mathbf{h})^\top \\
&= \rho_{ij}\sigma_i\tilde{R}(\mathbf{h}|\boldsymbol{\Psi})\sigma_j\tilde{R}(\mathbf{h}|\boldsymbol{\Psi})^\top \\
&= \rho_{ij}\sigma_i\sigma_j\tilde{R}(\mathbf{h}|\boldsymbol{\Psi})\tilde{R}(\mathbf{h}|\boldsymbol{\Psi})^\top \\
&= \rho_{ij}\sigma_i\sigma_j R(\mathbf{h}|\boldsymbol{\Psi}), \quad \text{for} \quad i,j = 1, \ldots, p \quad \text{and} \quad \rho_{ii} = 1,
\end{aligned}
$$

$\square$

Model specification

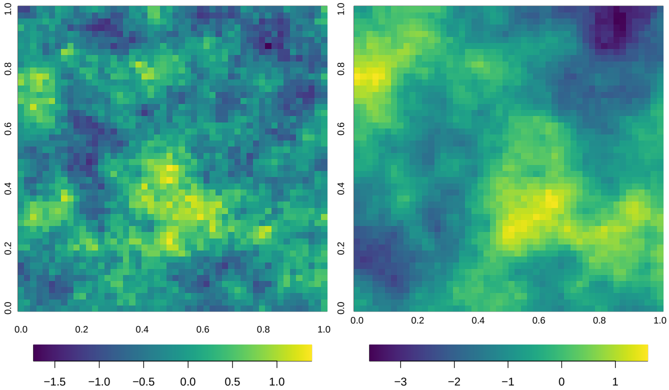


Figure 7: Simulation of a bivariate MatSimpler model

Estimation and Inference

- Let $\mathbf{Y} = \{\mathbf{Y}_1^\top, \dots, \mathbf{Y}_p^\top\}^\top$, be the stacked vector of variables (We suppress the spatial indexes for convenience);
- With mean-vector $\boldsymbol{\mu} = \{\boldsymbol{\mu}_1^\top, \dots, \boldsymbol{\mu}_p^\top\}^\top$, where $\boldsymbol{\mu}_i = \mathbf{X}_i \boldsymbol{\beta}_i$ and covariance matrix $\boldsymbol{\Sigma}(\boldsymbol{\lambda})$;
- Let $\boldsymbol{\theta} = (\boldsymbol{\beta}^\top, \boldsymbol{\lambda}^\top)^\top$ the set of parameters to be estimated;
- The log-likelihood function for $\boldsymbol{\theta}$ is given by:

$$\mathcal{L}(\boldsymbol{\theta}; \mathbf{y}) = -\frac{1}{2}\left[N \ln(2\pi) + \ln|\boldsymbol{\Sigma}(\boldsymbol{\lambda})| + \mathbf{r}(\boldsymbol{\beta})^\top \boldsymbol{\Sigma}(\boldsymbol{\lambda})^{-1}\mathbf{r}(\boldsymbol{\beta})\right],$$

with $\mathbf{r}(\boldsymbol{\beta}) = (\mathbf{y} - \boldsymbol{\mu}(\boldsymbol{\beta}))$.

Computational Resources

- `Matrix` Bates and Maechler (2021) package: `chol`, `bdiag` function;
- `geoR` Ribeiro Jr et al. (2020) package: `matern` function;
- `mvnfast` package Fasiolo (2016): `dmvn` function, `rmvn` function;
- Other functions: `kronecker`, `crossprod` and `tcrossprod`, `optim`
- R codes available at:

  https://angelicamariatortola.github.io/academic/thesis.html

Simulation study

Table 1: Parameter values for each simulated scenario

Scenarios	Situation	Parameters						
		ϕ_1	ϕ_2	ν_1	ν_2	σ_1	σ_2	ρ_{12}
1	Less smoothness and less variability	0.05	0.1	0.3	0.4	0.5	1.0	-0.7 -0.4 0.0 0.4 0.7
2	Less smoothness and greater variability	0.05	0.1	0.3	0.4	1.5	2.0	
3	Greater smoothness and less variability	0.05	0.1	0.7	1.0	0.5	1.0	

Simulation study

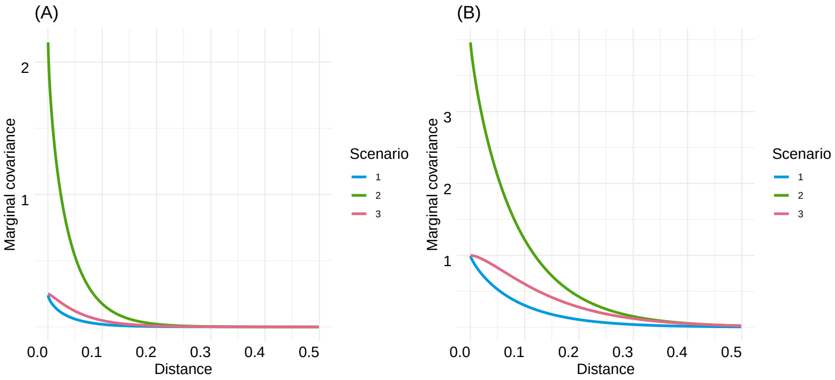
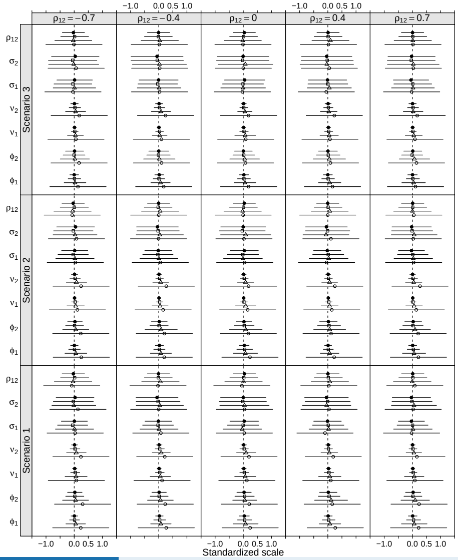


Figure 8: Marginal covariances for (A) first and (B) second variable for each scenario

Simulation study



Comparing estimation times

Situation 1:

- Simulation and estimation times of MatSimpler model;
- p: 2 to 6, $n = (100, 225, 400, 625, 900)$;
- We set $\phi_i = 0.2$, $\nu_i = 0.5$, $\sigma_i = 0.3$, for all $i = 1, \ldots, p$;
- Correlation parameters between -0.7 and 0.7;

Situation 2:

- Simulation bivariate data of MatConstr model;
- We set $\phi_i = 0.2$, $\nu_i = 0.5$, $\sigma_i = 0.3$, for $i = 1, 2$, and $\rho_{12} = 0.8$;
- The MatConstr, MatSep and LMC models were estimated by `GeoModels` package;

Estimation times - Situation 1

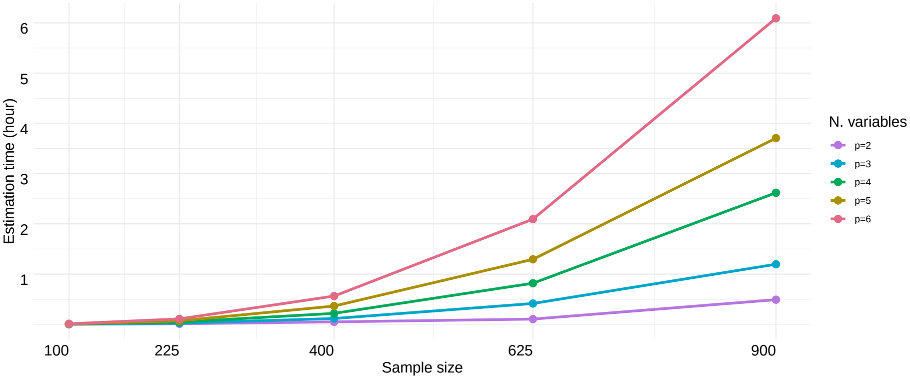


Figure 9: Estimation times for MatSimpler model for different sample sizes and number of variables

Estimation times - Situation 2

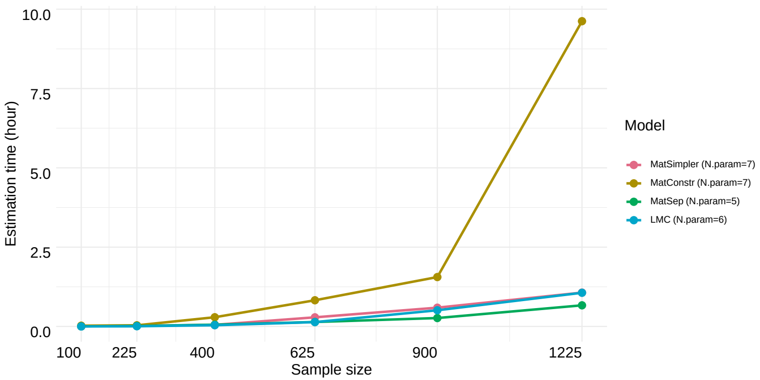


Figure 10: Estimation times for the MatSimpler, MatConstr, MatSep and LMC models

Simulation summary

- Good fit;
- Flexible for more than two variables;
- Low computing time.

Soil data

- *soil250* dataset from geoR package Ribeiro Jr et al. (2020): soil chemistry properties measured on a regular grid;

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- *soil250* dataset from geoR package Ribeiro Jr et al. (2020): soil chemistry properties measured on a regular grid;
- Relation between: Hydrogen content and CTC;
- The sample correlation between the variables was 0.68;
- Considered models: MatSimpler, MatConstr, MatInd, LMC and MatSep;

Soil data

Table 2: Parameter estimates of each model for soil250 data.

Estimates	Models				
	MatSimpler	MatConstr	MatInd	LMC	MatSep
a_{11}	-	-	-	0.615	-
a_{12}	-	-	-	-0.067	-
a_{22}	-	-	-	0.544	-
a_{21}	-	-	-	0.608	-
$\hat{\phi}_1$	1.077	1.415	1.849	1.156	1.978
$\hat{\phi}_2$	1.994	1.483	2.340	2.816	
ν_1	0.543	0.509	0.398	-	0.495
ν_2	0.513	0.562	0.422	-	
$\hat{\sigma}_1$	0.627	0.671	0.648	-	0.774
$\hat{\sigma}_2$	0.920	0.850	0.848	-	0.891
$\hat{\rho}_{12}$	0.823	0.811	-	-	0.816
LL	-161.551	-166.143	-301.813	-164.688	-166.298
AIC	337.103	346.285	615.626	341.376	342.595
BIC	361.753	375.787	640.914	366.663	363.668

Soil data

- Likelihood ratio test comparing the separable and MatSimpler model;
- Test statistic: $\lambda_0 = 9.494$
- p-value $= 0.008$;
- Evidence against the separable model.

Soil data

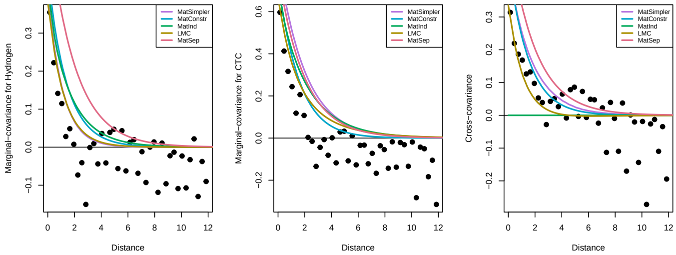

Figure 11: Empirical and estimated covariance functions.

"... disagreements between empirical and theoretical fits are typically observed in practice, and it can be associated to biases in the empirical estimators." - Alegría et al. (2019)

Soil data

- Cross-validation study;
- Select 200 locations (80% of the data) and estimate the models;
- Prediction for the 50 remaining locations (20% of the data);
- Calculate the mean absolute error (MAE), the root mean square error (RMSE) and the normalized mean square error (NMSE);
- Repeated the same process 150 times, calculating the log-likelihood, MAE_i, RMSE_i and NMSE_i values.

Soil data

Table 3: Mean and standard deviation (sd) for log-likelihood and prediction errors considering 150 splits of data into training (80%) and test (20%) for each model and each variable for soil250 data

Models		LL	MAE_H	$RMSE_H$	$NMSE_H$	MAE_{CTC}	$RMSE_{CTC}$	$NMSE_{CTC}$
MatSimpler	Mean	-144.267	0.278	0.369	0.166	0.315	0.417	0.187
	sd	7.632	0.031	0.045	0.021	0.033	0.050	0.024
MatConstr	Mean	-148.533	0.271	0.364	0.163	0.308	0.411	0.184
	sd	7.549	0.032	0.047	0.022	0.034	0.052	0.025
MatInd	Mean	-255.602	0.272	0.364	0.163	0.309	0.412	0.185
	sd	11.186	0.031	0.045	0.021	0.034	0.052	0.025
LMC	Mean	-147.542	0.272	0.363	0.163	0.307	0.410	0.184
	sd	7.319	0.032	0.046	0.021	0.034	0.052	0.025
MatSep	Mean	-148.916	0.270	0.364	0.163	0.307	0.410	0.184
	sd	7.538	0.032	0.047	0.022	0.034	0.053	0.025

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Meuse data

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  $\hat{\rho}_{23} = 0.6970$, $\hat{\rho}_{24} = 0.7466$, $\hat{\rho}_{34} = 0.9392$;

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- Sample standard deviations:
  $\hat{s}_1 = 0.8627$, $\hat{s}_2 = 0.3343$, $\hat{s}_3 = 0.4625$ and $\hat{s}_4 = 0.4339$.

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Meuse data

Table 4: Parameter estimates for meuse data

LL = -89.28	Estimates					
	$\hat{\phi}_1$	$\hat{\phi}_2$	$\hat{\phi}_3$	$\hat{\phi}_4$	$\hat{\nu}_1$	$\hat{\nu}_2$
Value	0.4260	0.4449	0.4098	0.3401	0.1021	0.1952
sd	0.2925	0.2258	0.1983	0.1557	0.0506	0.0591
	$\hat{\nu}_3$	$\hat{\nu}_4$	$\hat{s}_1$	$\hat{s}_2$	$\hat{s}_3$	$\hat{s}_4$
Value	0.2063	0.2409	0.8897	0.3610	0.4786	0.4596
sd	0.0555	0.0656	0.0595	0.0288	0.0378	0.0348
	$\hat{\rho}_{12}$	$\hat{\rho}_{13}$	$\hat{\rho}_{14}$	$\hat{\rho}_{23}$	$\hat{\rho}_{24}$	$\hat{\rho}_{34}$
Value	0.6701	0.6242	0.7260	0.6728	0.7530	0.9376
sd	0.0447	0.0495	0.0384	0.0444	0.0351	0.0098

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Meuse data

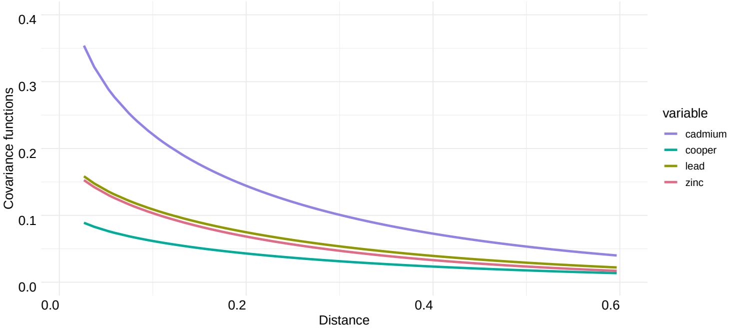

Figure 12: Marginal covariance functions of each variable for meuse data

Data analysis summary

Soil data - Bivariate analysis:

- Good fit;
- Highest likelihood value;
- Lower estimation times;
- Equivalent results in terms of predictive capacity.

Meuse data - Four-variate analysis:

- Illustration in a 4-variate data;
- Estimates close to sample values;
- The model was able to capture individual behaviors.

General models summary

Models \ Charac.	Complexity[1]	ρ_{ij}	Different correlations[2]	Different models[3]	Cross-cov. from marginal-cov.[4]	One model by variable[5]	Time[6]
Separable model		X		X	X		6,92%
LMC			X	X			11,03%
Simpler model		X	X	X	X	X	11,09%
Matérn with Constr.	X	X	X				100%

(1) Constraints in parametric space

(2) Different correlation structures for each variable (considering the Matérn model)

(3) Supports different correlation families: Matérn, Spherical, Cauchy, ...

(4) Cross-covariance function specified from the marginal-covariance functions

(5) Allows different variables to be represented by different correlation families

(6) Proportion of estimation times with respect to maximum time (Figure 20 - Ap. C) for n=1225.

Conclusions

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- We presented a covariance specification for multivariate random fields for continuously indexed data;
- Our proposal: compact and flexible, allowing different correlation and marginal-covariance functions;
- Allows its parameters to vary in their usual parametric domains;

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Conclusions

- We presented a covariance specification for multivariate random fields for continuously indexed data;
- Our proposal: compact and flexible, allowing different correlation and marginal-covariance functions;
- Allows its parameters to vary in their usual parametric domains;
- Computational cost: Cholesky decomposition, which depends on the number of sample locations and response variables;
- For bivariate case: MatSimpler $<$ MatConstr time, being a competitive model.

Conclusions

"... The most fundamental question is the theoretical characterization of the allowable classes of multivariate covariances. For instance, given two marginal covariances, what is the valid class of possible cross-covariances that still results in a non-negative definite structure? Such a characterization is an unsolved problem." - (Genton and Kleiber, 2015).

Future directions

- Explore distinct correlation functions for each variable;
- The organization of an R package that involves the proposed approach;
- Context of non-Gaussian modeling and asymmetric data for multivariate spatial problems;
- Covariance function to accommodate non-stationarity and anisotropies;
- Estimation methods.

Thank you!

e-mail: angelicaribeiro@utfpr.edu.br

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