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A Kronecker-based covariance specification for spatially continuous multivariate data

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Abstract

We propose a covariance specification for modeling spatially continuous multivariate data. This model is based on a reformulation of Kronecker's product of covariance matrices for Gaussian random fields. We illustrate the case with the Matérn function used for specifying marginal covariances. The structure holds for other choices of covariance functions with parameters varying in their usual domains, which makes the estimation process more accessible. The reduced computational time and flexible generalization for increasing number of variables, make it an attractive alternative for modelling spatially continuous data. Theoretical results for the likelihood function and the derivatives of the covariance matrix are presented. The proposed model is fitted to the literature's *soil250* dataset, and adequacy measures, forecast errors and estimation times are compared with the ones obtained based on classical models. Furthermore, the model is fitted to the classic *meuse* dataset to illustrate the model's flexibility in a four-variate analysis. A simulation study is performed considering different parametric scenarios to evaluate the asymptotic properties of the maximum likelihood estimators. The satisfactory results, its simpler structure and the reduced estimation time make the proposed model a candidate approach for multivariate analysis of spatial data.

Keywords: Gaussian random fields, Covariance functions, Geostatistics, Matérn correlation model, Multivariate spatial data

1 Introduction

Multivariate random fields have been of interest from the very early days of the geostatistical literature, with an increasing number of proposed approaches as data sets became richer and the ever-increasing computational power. The specification of the covariance structure is central in the estimation and prediction process. Recent contributions include asymmetric models (Qadir et al, 2021; Alegría et al, 2018), modeling on spheres (Bevilacqua et al, 2020; Emery et al, 2019; Alegría et al, 2019; Emery and Porcu, 2019), on mapping disease (Martinez-Beneito, 2020; MacNab, 2018, 2016), on multinary problems (Teichmann et al, 2021), to name a few.

We are interested in multivariate random fields analysis, in the specific context of spatially continuous data. Possible applications cover a wide range of disciplines, such as climatology, meteorology, geophysics, among others, where spatially referenced data is usually of interest. We consider two illustrative examples, one on chemical soil properties relevant for agriculture and the other on heavy metal concentrations within a study area.

Let $\mathbf{Y}(\mathbf{s}) = \{Y_1(\mathbf{s}), \dots, Y_p(\mathbf{s})\}^\top$, on $\mathbb{R}^d$, $d \geq 1$, a p -dimensional multivariate Gaussian random field with mean vector $\boldsymbol{\mu}(\mathbf{s}) = E[\mathbf{Y}(\mathbf{s})]$ and matrix-valued covariance function:

$$\boldsymbol{\Sigma}(\mathbf{h}) = \text{cov}\{\mathbf{Y}(\mathbf{s}_1), \mathbf{Y}(\mathbf{s}_2)\} = [\Sigma_{ij}(\mathbf{h})]_{i,j=1}^p, \quad (1)$$

where $\mathbf{h} = \mathbf{s}_1 - \mathbf{s}_2 \in \mathbb{R}^d$ is the spatial separation vector. We consider a stationary and isotropic process (Chilès and Delfiner, 2012; Diggle and Ribeiro Jr, 2007; Gneiting, 1999) where $i = j$, the functions $\Sigma_{ii}(\mathbf{h})$ in Eq. (1) describe the spatial variability of the i th process $Y_i(\mathbf{s})$, for $i = 1, \dots, p$, and are referred as the direct- or marginal-covariance functions (Genton and Kleiber, 2015) and, if $i \neq j$, the functions $\Sigma_{ij}(\mathbf{h})$ in Eq. (1) describe the spatial variability between the process $Y_i(\mathbf{s})$ and $Y_j(\mathbf{s})$ and are called as cross-covariance functions. An important condition for (1) is that it must meet the positive definite condition, that is, $\mathbf{a}^\top \boldsymbol{\Sigma} \mathbf{a} > 0$, for any vector $\mathbf{a} \neq \mathbf{0}$.

The main goal is to propose a valid covariance specification for (1) in the case of spatially continuous multivariate data. The model, presented in Section 2, is based on the Kronecker products and it is quite flexible to handle with two or more variables. Furthermore, we present the conditions for the positive definiteness and detail the inferential process of the proposed model.

The literature on covariance functions for multivariate random fields is extensive. A careful review of the main works in the area can be found in Genton and Kleiber (2015) and Salvaña and Genton (2020). An intuitive early

proposal and possibly the most traditional model is the linear model of coregionalization (LMC) (Goulard and Voltz, 1992; Bourgault and Marcotte, 1991; Wackernagel, 2003). The key idea for the LMC is the overlap of spatial processes in order to induce a multivariate field. This approach is widely explored, including under the Bayesian approach for inference and prediction. Finley et al (2015), Banerjee et al (2003), Gelfand et al (2004), Schmidt and Gelfand (2003) and Cecconi et al (2016) are examples where the LMC structure underlies the models.

Another popular structure considers the class of Matérn correlation functions (Matérn, 1986; Guttorp and Gneiting, 2006). For the univariate case, the Matérn class covariance model is defined as $\sigma^2 M(\mathbf{h}|\nu, 1/\phi)$, where $M(\mathbf{h}|\nu, 1/\phi) = \frac{2^{1-\nu}}{\Gamma(\nu)} (|\mathbf{h}|/\phi)^\nu K_\nu(|\mathbf{h}|/\phi)$, is the Matérn spatial correlation at distance $|\mathbf{h}|$, K_ν is the modified Bessel function, $\sigma^2, \nu, \phi > 0$ are the variance, smoothness and scale parameters, respectively. When $\nu = 0.5$, the Matérn model reduces to the exponential covariance function. Gneiting et al (2010) elegantly extended this class for multivariate case considering the Matérn family for the marginal and cross-covariance functions. The authors present conditions for the parameters that lead to a valid covariance structure, the full bivariate Matérn model. For more than two variables the authors presented the parsimonious multivariate Matérn model, which considers common scale and constrained smoothness parameters. Another important specification are the separable models, which considers that the components of the multivariate random field share the same correlation structure (Bevilacqua et al, 2016a; Vallejos et al, 2020) and appears as a parsimonious modeling alternative because it allows a simplification of the more complex models. Bevilacqua and Morales-Oñate (2018) and Vallejos et al (2020) present two simplified structures with Matérn correlation function for bivariate data, the bivariate separable Matérn model and the bivariate Matérn model with constraints. Both models can be estimated by the `Geomodels` package (Bevilacqua and Morales-Oñate, 2018).

The aforementioned models are widely assessed in the geostatistical literature. Cressie (1993), Gneiting et al (2010), Goovaerts et al (1997), Porcu et al (2013), Bevilacqua et al (2016b) noticed some difficulties to handling with the LMC due, for example, to its lack of flexibility and difficulty in recovering the smoothness of latent processes. Separable models are not capable to capture the different scales and smoothness for the variables under study (Bevilacqua et al, 2016a, 2015). The bivariate Matérn model presents some restrictions in the parametric space. Vallejos et al (2020) note that variation of the colocated correlation parameter is constrained by the values of the scale and smoothness parameters, resulting in difficulties for the estimation process and parameter interpretation.

The covariance specification presented here emerges as an additional modeling alternative for multivariate random fields that can be more flexible to deal with two or more variables, as it allows the model parameters to vary freely in their usual parametric domains. With a simple construction, the computational implementation has no major difficulties for a number of variables and

sampling location points, with a parsimonious estimation computational time, especially for small sample sizes. Furthermore, unlike the separable models, our proposal allows different marginal correlation structures, making it able to capture the structure of each variable.

The article is organized as follows. In Section 2 we present our covariance specification for multivariate spatial data and discuss the maximum likelihood estimation for model parameters. The dataset analyses are presented in Section 3. In Section 4, through a simulation study, we evaluate the asymptotic properties of the proposed model estimators. Finally, the main conclusions are summarized in Section 5. The model implementation and reported analysis are performed using the computational statistical software R (R Core Team, 2021).

2 Model specification

This section presents our proposed covariance specification for multivariate Gaussian random fields, which is based upon Martinez-Beneito (2013). We present the proof of its validity and discuss how to obtain the maximum likelihood estimates of the model parameters.

In Martinez's proposal, the results are presented for modeling multivariate mapping diseases problems based on Gaussian Markov random fields (GMRF), which are discretely indexed, following a Gaussian multivariate distribution with the additional restriction of conditional independence (Rue and Held, 2005).

Our proposal extends Martinez's approach to construct a covariance function for Gaussian random fields that are continuously indexed, with several applications in geostatistical problems.

We present a simple construction that allows its generalization to larger dimensions more easily. The idea is to write the cross-covariance matrix as a product of matrices that induce variability within processes and between processes, and it is built upon the Kronecker products reformulation of covariance matrices. The resulting construction will be always positive definite for any parameter values in their usual domains.

Consider a symmetric correlation matrix Σ_b , with dimension $p \times p$, induces a spatial correlation between the processes, while the marginal-covariance functions Σ_{ii} , for $i = 1, \dots, p$, model the variability within each process. We specify the covariance matrix for the $\mathbf{Y}$ process considering the generalized Kronecker product, presented in Martinez-Beneito (2013). Thus, for the Gaussian random fields continuously indexed, the matrix-valued covariance function is defined by:

$$\Sigma(\mathbf{h}) = B_{\text{diag}} \left(\tilde{\Sigma}_{11}, \tilde{\Sigma}_{22}, \dots, \tilde{\Sigma}_{pp} \right) (\Sigma_b \otimes \mathbf{I}) B_{\text{diag}} \left(\tilde{\Sigma}_{11}^{\top}, \tilde{\Sigma}_{22}^{\top}, \dots, \tilde{\Sigma}_{pp}^{\top} \right), \quad (2)$$

where, $\tilde{\Sigma}_{ii}$ is the lower triangular matrix of the Cholesky decomposition of the matrix Σ_{ii} , B_{diag} represents the matrix in diagonal blocks of the matrices $\tilde{\Sigma}_{11}$, $\tilde{\Sigma}_{22}$, $\dots$, $\tilde{\Sigma}_{pp}$ and $\mathbf{I}$ is the identity matrix. The structure defined in (2) is very flexible, allowing different marginal-covariance functions for Σ_{ii} and different correlation structures for Σ_b .

Without loss of generality, we will consider that the spatial correlation between the processes will be induced by the correlation matrix:

$$\Sigma_b = \begin{pmatrix} 1 & \rho_{12} & \dots & \rho_{1p} \\ \rho_{12} & 1 & \dots & \rho_{2p} \\ \dots & \dots & \dots & \dots \\ \rho_{1p} & \rho_{2p} & \dots & 1 \end{pmatrix}, \quad (3)$$

where ρ_{ij} , $ij = 1, \dots, p$, is the correlation parameter between the variables i and j .

To quantify the variability within each process we will use, in this work, the Matérn covariance function, that is,

$$\Sigma_{ii}(\mathbf{h}) = \sigma_i^2 M(\mathbf{h}|\nu_i, 1/\phi_i), \quad \text{for } i = 1, 2, \dots, p. \quad (4)$$

The structure specified by (2), (3) and (4) will be called as *simpler multivariate Matérn* (MatSimpler) model. It accepts different marginal behaviors and is able to handle with different smoothness and scale parameters for each variable. The *simpler multivariate exponential* (ExpSimpler) model is a particular case when the exponential correlation function is used. [Ribeiro et al \(2021\)](#) illustrates the ExpSimpler model in bivariate analysis of meteorological data.

In Theorem 2.1, below, we prove the validity of our covariance specification for modeling multivariate spatial data.

Theorem 2.1 *Let Σ_{ii} , for $i = 1, \dots, p$, the marginal covariance functions of dimension $n \times n$, Σ_b a valid spatial correlation function of dimension $p \times p$ and $\mathbf{I}$ the identity matrix of dimension $n \times n$, then the covariance function defined in (2) is a valid and full rank np specification for multivariate spatial data modeling.*

Proof Since the marginal covariance functions, Σ_{ii} , for $i = 1, \dots, p$, are symmetric positive definite matrix, the matrices $\tilde{\Sigma}_{ii}$, resulting from the Cholesky decomposition, are lower triangular with positive diagonal elements and therefore, full rank ([Banerjee and Roy, 2014](#)). Let's denote by $R_{\tilde{\Sigma}_{ii}}$, the rank of $\tilde{\Sigma}_{ii}$. Thus, $\text{rank}(\tilde{\Sigma}_{ii}) = R_{\tilde{\Sigma}_{ii}} = n$, for all i , and from the rank properties of the block-diagonal matrix, the rank of any block-diagonal matrix is the sum of the ranks of its diagonal blocks ([Banerjee and Roy, 2014](#)), that is:

$$\text{rank} \left[B_{\text{diag}} \left(\tilde{\Sigma}_{11}^\top, \tilde{\Sigma}_{22}^\top, \dots, \tilde{\Sigma}_{pp}^\top \right) \right] = \sum_{i=1}^p R_{\tilde{\Sigma}_{ii}} = np,$$

therefore, $B_{\text{diag}} \left(\tilde{\Sigma}_{11}^\top, \tilde{\Sigma}_{22}^\top, \dots, \tilde{\Sigma}_{pp}^\top \right)$ is a full np rank matrix.

On the other hand, since Σ_b and $\mathbf{I}$ are positive definite matrices, it follows by the kronecker product properties that $(\Sigma_b \otimes \mathbf{I})$ is also a positive definite matrix (Hardy and Steeb, 2019). With Σ_b of dimension p and $\mathbf{I}$ of dimension n , the resulting kronecker product between them will be a positive definite matrix of dimension np .

Now, for simplicity of notation, let's denote by $\mathbf{A}$ and $\mathbf{B}$ the respective $(\Sigma_b \otimes \mathbf{I})$ and $B_{\text{diag}}(\tilde{\Sigma}_{11}^\top, \tilde{\Sigma}_{22}^\top, \dots, \tilde{\Sigma}_{pp}^\top)$ matrices. Since $\mathbf{A}$ is a positive definite matrix and $\mathbf{B}$ is a full rank matrix, follows that $\mathbf{B}^\top \mathbf{A} \mathbf{B}$ preserves not only the rank but also the positive definiteness (Gentle, 2017; Petersen et al, 2008). To visualize this, let $\mathbf{a} \neq \mathbf{0}$, any vector of dimension np , and let $\mathbf{z} = \mathbf{B}\mathbf{a}$, where $\mathbf{z} \neq \mathbf{0}$, because $\mathbf{B}$ is a full rank matrix. Using the positive definite matrix definition, follows:

$$\begin{aligned} \mathbf{a}^\top (\mathbf{B}^\top \mathbf{A} \mathbf{B}) \mathbf{a} &= (\mathbf{a}\mathbf{B})^\top \mathbf{A} (\mathbf{B}\mathbf{a}) \\ &= \mathbf{z}^\top \mathbf{A} \mathbf{z} \\ &> 0 \end{aligned}$$

□

The result holds if variables are observed in different numbers of sample locations, since the incomplete data can be treated as missing information and this does not imply any additional complexity and the proof of theorem 2.1 remains valid.

The dimensions of the resulting covariance matrix will depend on the number of sample locations for each variable considered in the analysis. If we consider marginal covariance functions with dimension n_i , for $i = 1, \dots, p$, the resulting covariance matrix will have dimension $N = \sum_{i=1}^p n_i$.

Considering that Σ is a valid covariance specification for any valid choice of marginal-covariance and correlation functions, the proposed model allows its smoothing parameters, scale, correlation and variance to vary in their usual domains, favoring the inferential process and allowing the model parameters to be more easily interpreted.

To illustrate the behavior of the proposed model, we simulate a bivariate MatSimpler model on a regular unit grid. We set the parameter values as $\sigma_1 = 0.5$, $\sigma_2 = 1.0$, $\nu_1 = 0.5$, $\nu_2 = 0.8$, $\phi_1 = 0.1$, $\phi_2 = 0.2$ and $\rho_{12} = -0.7$ or 0.7 , aiming to illustrate different smoothness and variability in the data and situations with positive and negative correlations between the variables. Fig. 1 shows the corresponding simulations with the corresponding code available in the on-line supplementary material.

2.1 Estimation and inference

For the estimation process, let $N = np$ and $\mathbf{Y} = \{\mathbf{Y}_1^\top, \dots, \mathbf{Y}_p^\top\}^\top$, be the $N \times 1$ stacked vector of response variables, with $N \times 1$ mean-vector $\boldsymbol{\mu} = \{\boldsymbol{\mu}_1^\top, \dots, \boldsymbol{\mu}_p^\top\}^\top$, where $\boldsymbol{\mu}_i = \mathbf{X}_i \boldsymbol{\beta}_i$ denotes the $n \times 1$ vector of expected values for the response variable $\mathbf{Y}_i$, $i = 1, \dots, p$, with $\mathbf{X}_i$ being a $n \times k_i$ design matrix composed of k_i covariates and, consequently, $\boldsymbol{\beta}_i$ denotes a $k_i \times 1$ regression parameter vector.

Fig. 1 Simulation of a bivariate MatSimpler model with (A) $\sigma_1 = 0.5$, $\sigma_2 = 1.0$, $\nu_1 = 0.5$, $\nu_2 = 0.8$, $\phi_1 = 0.1$, $\phi_2 = 0.2$ and $\rho_{12} = 0.7$ and (B) $\sigma_1 = 0.5$, $\sigma_2 = 1.0$, $\nu_1 = 0.5$, $\nu_2 = 0.8$, $\phi_1 = 0.1$, $\phi_2 = 0.2$ and $\rho_{12} = -0.7$

We will denote the set of parameters to be estimated by $\boldsymbol{\theta} = (\boldsymbol{\beta}^\top, \boldsymbol{\lambda}^\top)^\top$, where $\boldsymbol{\beta} = (\boldsymbol{\beta}_1^\top, \dots, \boldsymbol{\beta}_p^\top)^\top$ denotes the regression parameters vector and $\boldsymbol{\lambda} =$

$(\rho_1, \dots, \rho_{p(p-1)/2}, \sigma_1, \dots, \sigma_p, \nu_1, \dots, \nu_p, \phi_1, \dots, \phi_p)^\top$ is the covariance specification parameters vector. Considering $\mathbf{y}$ the stacked vector of observed values, the log-likelihood function for $\boldsymbol{\theta}$ is given by:

$$\mathcal{L}(\boldsymbol{\theta}; \mathbf{y}) = -\frac{1}{2} [N \ln(2\pi) + \ln|\boldsymbol{\Sigma}(\boldsymbol{\lambda})| + (\mathbf{y} - \boldsymbol{\mu}(\boldsymbol{\beta}))^\top \boldsymbol{\Sigma}(\boldsymbol{\lambda})^{-1} (\mathbf{y} - \boldsymbol{\mu}(\boldsymbol{\beta}))]. \quad (5)$$

The vector of expected values, $\boldsymbol{\mu}(\boldsymbol{\beta})$, depends on the regression parameters while the covariance specification $\boldsymbol{\Sigma}(\boldsymbol{\lambda})$ depends on the covariance parameters vector, $\boldsymbol{\lambda}$. We obtain the maximum likelihood estimators by maximizing the function in (5) with respect to the $\boldsymbol{\theta}$ parameter vector.

Based on matrix properties (Wand, 2002; Bonat et al, 2020), the score functions with respect to the $\boldsymbol{\beta}$ and $\boldsymbol{\lambda}$ parameters, are given, respectively, by:

$$\begin{aligned} \mathcal{U}_{\boldsymbol{\beta}} &= \mathbf{D}^\top \boldsymbol{\Sigma}(\boldsymbol{\lambda})^{-1} \mathbf{r}(\boldsymbol{\beta}), \\ \mathcal{U}_{\boldsymbol{\lambda}} &= -\frac{1}{2} \left\{ \boldsymbol{\Sigma}(\boldsymbol{\lambda})^{-1} - \boldsymbol{\Sigma}(\boldsymbol{\lambda})^{-1} \mathbf{r}(\boldsymbol{\beta}) \mathbf{r}(\boldsymbol{\beta})^\top \boldsymbol{\Sigma}(\boldsymbol{\lambda})^{-1} \right\} \frac{\partial \boldsymbol{\Sigma}(\boldsymbol{\lambda})}{\partial \boldsymbol{\lambda}}, \end{aligned} \quad (6)$$

with $\mathbf{r}(\boldsymbol{\beta}) = (\mathbf{y} - \boldsymbol{\mu}(\boldsymbol{\beta}))$ and $\mathbf{D} = \frac{\partial \boldsymbol{\mu}(\boldsymbol{\beta})}{\partial \boldsymbol{\beta}} = \text{Bdiag}(\mathbf{X}_1, \dots, \mathbf{X}_p)$.

We achieve the maximum likelihood estimator of $\boldsymbol{\beta}$ by solving $\mathcal{U}_{\boldsymbol{\beta}}$, which results in:

$$\hat{\boldsymbol{\beta}} = (\mathbf{D}^\top \boldsymbol{\Sigma}(\boldsymbol{\lambda})^{-1} \mathbf{D})^{-1} (\mathbf{D}^\top \boldsymbol{\Sigma}(\boldsymbol{\lambda})^{-1} \mathbf{y}).$$

Making similar calculations, we find the Fisher information matrix which, for $\boldsymbol{\beta}$, is given by:

$$\mathcal{F}_{\boldsymbol{\beta}} = \mathbf{D}^\top \boldsymbol{\Sigma}(\boldsymbol{\lambda})^{-1} \mathbf{D}.$$

For $\boldsymbol{\lambda}$, the $(i, j)^{th}$ entry of the Fisher information matrix, is given by:

$$[\mathcal{F}_{\boldsymbol{\lambda}}]_{ij} = \frac{1}{2} \text{tr} [\mathbf{W}_{\lambda_i} \boldsymbol{\Sigma}(\boldsymbol{\lambda}) \mathbf{W}_{\lambda_j} \boldsymbol{\Sigma}(\boldsymbol{\lambda})],$$

where $\mathbf{W}_{\lambda_i} = -\partial \boldsymbol{\Sigma}(\boldsymbol{\lambda})^{-1} / \partial \lambda_i$.

Considering $\hat{\boldsymbol{\theta}} = (\hat{\boldsymbol{\beta}}^\top, \hat{\boldsymbol{\lambda}}^\top)^\top$ the maximum likelihood estimator of $\boldsymbol{\theta}$ parameter, we have that its asymptotic distribution is $\hat{\boldsymbol{\theta}} \sim N(\boldsymbol{\theta}, \mathcal{F}_{\boldsymbol{\theta}}^{-1})$, where $\mathcal{F}_{\boldsymbol{\theta}} = \begin{pmatrix} \mathcal{F}_{\boldsymbol{\beta}} & \mathbf{0} \\ \mathbf{0} & \mathcal{F}_{\boldsymbol{\lambda}} \end{pmatrix}$ denotes the Fisher information matrix of $\boldsymbol{\theta}$.

The maximum likelihood estimates of $\boldsymbol{\lambda}$ can be found through Newton's scoring iterative algorithm (Bonat et al, 2020):

$$\boldsymbol{\lambda}^{i+1} = \boldsymbol{\lambda}^i - \alpha \mathcal{F}_{\boldsymbol{\lambda}}^{-1} \mathcal{U}_{\boldsymbol{\lambda}}(\tilde{\boldsymbol{\theta}}; \mathbf{y}),$$

where $\tilde{\boldsymbol{\theta}} = (\hat{\boldsymbol{\beta}}^\top, \boldsymbol{\lambda}^\top)^\top$ and α controls the step length.

In Section 4 through a simulation study we evaluate the asymptotic properties of the maximum likelihood estimators for the model in a finite sample scenario.

2.2 Derivatives of the covariance matrix

We present in this subsection the derivative of matrix Σ used in calculations of (6). Let ρ_r , for $r = 1, \dots, p(p-1)/2$, denoting the correlation parameters of Σ_b , σ_i^2 , ϕ_i and ν_i , denoting the variance, scale and smoothness parameters of the marginal-covariance matrix, Σ_{ii} , for $i = 1, \dots, p$.

The partial derivative of the matrix-valued covariance function Σ , with respect to each correlation parameter, ρ_r , is given by:

$$\frac{\partial \Sigma}{\partial \rho_r} = B_{\text{diag}} \left(\tilde{\Sigma}_{11}, \tilde{\Sigma}_{22}, \dots, \tilde{\Sigma}_{pp} \right) \left(\frac{\partial \Sigma_b}{\partial \rho_r} \otimes \mathbf{I} \right) B_{\text{diag}} \left(\tilde{\Sigma}_{11}^\top, \tilde{\Sigma}_{22}^\top, \dots, \tilde{\Sigma}_{pp}^\top \right).$$

To obtain the partial derivative with respect to variance parameter, σ_i^2 , we will use matrix properties, that is,

$$\begin{aligned} \frac{\partial \Sigma}{\partial \sigma_i^2} = & B_{\text{diag}} \left(\mathbf{0}, \dots, \frac{\partial \tilde{\Sigma}_{ii}}{\partial \sigma_i^2}, \dots, \mathbf{0} \right) (\Sigma_b \otimes \mathbf{I}) B_{\text{diag}} \left(\tilde{\Sigma}_{11}^\top, \tilde{\Sigma}_{22}^\top, \dots, \tilde{\Sigma}_{pp}^\top \right) \\ & + B_{\text{diag}} \left(\tilde{\Sigma}_{11}, \tilde{\Sigma}_{22}, \dots, \tilde{\Sigma}_{pp} \right) (\Sigma_b \otimes \mathbf{I}) B_{\text{diag}} \left(\mathbf{0}, \dots, \frac{\partial \tilde{\Sigma}_{ii}^\top}{\partial \sigma_i^2}, \dots, \mathbf{0} \right). \end{aligned} \quad (7)$$

An analogous procedure to the Eq. (7) can be used to obtain the derivatives with respect to ϕ_i and ν_i . Thus, to obtain the derivatives of Σ with respect to each parameter, we must calculate the partial derivatives in (7). Using the result of partial derivatives of Cholesky's factorization ([Särkkä, 2013](#); [Bonat and Jørgensen, 2016](#)), follows:

$$\begin{aligned} \frac{\partial \tilde{\Sigma}_{ii}}{\partial \sigma_i^2} &= \tilde{\Sigma}_{ii} \Phi \left(\tilde{\Sigma}_{ii}^{-1} \frac{\partial \Sigma_{ii}}{\partial \sigma_i^2} \tilde{\Sigma}_{ii}^{-1} \right), \\ \frac{\partial \tilde{\Sigma}_{ii}}{\partial \phi_i} &= \tilde{\Sigma}_{ii} \Phi \left(\tilde{\Sigma}_{ii}^{-1} \frac{\partial \Sigma_{ii}}{\partial \phi_i} \tilde{\Sigma}_{ii}^{-1} \right), \\ \frac{\partial \tilde{\Sigma}_{ii}}{\partial \nu_i} &= \tilde{\Sigma}_{ii} \Phi \left(\tilde{\Sigma}_{ii}^{-1} \frac{\partial \Sigma_{ii}}{\partial \nu_i} \tilde{\Sigma}_{ii}^{-1} \right), \end{aligned}$$

where $\Phi(\cdot)$ is the strictly lower triangular part of the argument and half of its diagonal.

2.3 Computational results

As already mentioned, the MatSimpler model can be extended for more than two variables with relative ease. The computational time estimation will depend on the number of variables and sample locations considered in the analysis. To illustrate the computational time spent on estimation, we implement the generic model for p variables and n sample locations and simulate scenarios of the MatSimpler model considering different sample sizes and variable numbers. To make the simulation process easier, we set $\phi_i = 0.2$, $\nu_i = 0.5$, $\sigma_i = 0.3$, for all $i = 1, \dots, p$. The correlation parameters were chosen between -0.7 to 0.7 such that the resulting Σ_b was a valid structure. We consider the number of variables, p , ranging from 2 to 6 and the number of sample locations, $n = (100, 225, 400, 625, 900)$, taken in a unit square grid.

The results, presented in Appendix A (Fig. 8) shows that the estimation computational time increases with the number of variables and sample locations, which is due to the Cholesky decompositions of the marginal-covariance matrices. These calculations are necessary to obtain the proposed specification.

We also compare the estimation computational times for the bivariate case of the MatSimpler model with three other literature models, the *bivariate Matérn model with constraints* (MatConstr), the *bivariate separable Matérn model* (MatSep) and the LMC model. The data were simulated from the 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, in which we consider the standard likelihood function. For all models we used the Nelder-Mead optimizer and convergence was successful in all scenarios. Fig. 9 in Appendix A illustrates the comparisons between models.

Based on the simulations carried out, we see that the MatSimpler model, with 7 parameters, presents estimation times much lower than the MatConstr model which have the same number of parameters. Furthermore, our model presents estimation times very close to the MatSep model (with 5 parameters), especially for sample locations less than 400, and to the LMC (with 6 parameters). The R codes and the simulation results presented in Figures 8 and 9 are available in the supplementary material.

2.4 Prediction

For the case of multivariate spatial data, spatial prediction is a generalization of the univariate case that consists of predicting $\mathbf{Y}$ at some unknown location, $\mathbf{s}_0$, based on other sample information, $\mathbf{s}_i$, for $i = 1, \dots, n$ (Ver Hoef and Cressie, 1993; Bivand et al, 2008; Pebesma, 2004).

Let $\Sigma_{\mathbf{Y}_1}$ be the covariance matrix of $\mathbf{Y}_1 = \mathbf{Y}(\mathbf{s}_i)$, for $i = 1, \dots, n$, $\Sigma_{\mathbf{Y}_0}$ be the covariance matrix of $\mathbf{Y}_0 = \mathbf{Y}(\mathbf{s}_0)$, $\Sigma_{\mathbf{Y}_1\mathbf{Y}_0}$ be the covariance matrix between $\mathbf{Y}_1$ and $\mathbf{Y}_0$ and $\mathbf{d}_0 = \text{Bdiag}(\mathbf{x}_1(\mathbf{s}_0), \dots, \mathbf{x}_p(\mathbf{s}_0))$. Then, the best linear unbiased predictor for $\mathbf{Y}_0$ is:

$$E(\mathbf{Y}_0|\mathbf{Y}_1) = E(\mathbf{Y}_0) + \Sigma_{\mathbf{Y}_1\mathbf{Y}_0}^\top \Sigma_{\mathbf{Y}_1}^{-1}(\mathbf{Y}_1 - E(\mathbf{Y}_1)),$$

with prediction covariance matrix:

$$\text{Cov}(\mathbf{Y}_0|\mathbf{Y}_1) = \Sigma_{\mathbf{Y}_0} - \Sigma_{\mathbf{Y}_1\mathbf{Y}_0}^\top \Sigma_{\mathbf{Y}_1}^{-1} \Sigma_{\mathbf{Y}_1\mathbf{Y}_0}.$$

We can replace the unknown parameters of the model by their respective maximum likelihood estimators (Martins et al, 2016) and, with this, we obtain the stacked vector prediction for the p variables in the $\mathbf{s}_0$ unobserved locations.

2.5 Computational resources

In our computational implementation, we used the R statistical software (R Core Team, 2021) for the estimation, simulation and prediction procedures. For the implementation of the proposed covariance matrix specification, we used the `kronecker` function, basic to R, which enables the calculation of the kronecker product between the matrices Σ_b and $\mathbf{I}$. We use the `Matrix` (Bates and Maechler, 2021) package to perform matrix operations more efficiently, such as the Cholesky decomposition of the marginal-covariance matrices, through the `chol` function, and the construction of the diagonal block matrix $B_{\text{diag}}(\tilde{\Sigma}_{11}, \tilde{\Sigma}_{22}, \dots, \tilde{\Sigma}_{pp})$, through the `bdiag` function.

To calculate the marginal-covariance functions, we use the `matern` function from `geoR` (Ribeiro Jr et al, 2020) package. Furthermore, the `crossprod` and `tcrossprod` functions allowed a more efficient calculation of products between matrices. To calculate the log-likelihood function, used in the estimation process, we use the `dmvn` function and for simulations we use the `rmvn` function, both from `mvnfast` package (Fasiolo, 2016) that provides computationally efficient methods related to the multivariate normal and Student's t distributions. For the log-likelihood function optimization, we use `optim` function. R codes are available in on-line supplementary material.

3 Data analysis

This section illustrates the application of the proposed model in two datasets. For the first one, the `soill` dataset, aim is to model the hydrogen content and the cation exchange capability (CTC). We compare results obtained fitting the `MatSimpler` and other models. The second one, a dataset on heavy metal concentration, is used to illustrate the model's flexibility by fitting a four-variate dataset.

3.1 Example 1: Soil data

The `soil250` dataset from `geoR` package (Ribeiro Jr et al, 2020) contains some soil chemistry properties measured on a regular grid with 10×25 points spaced by 5 meters. We study the relation between the hydrogen content and the cation exchange capability (CTC). These data illustrate a scenario with strong

correlation between the variables under study. Fig. 2 shows circle plots of the hydrogen (left panel) and CTC (right panel) data separately. The coordinates are divided by a constant to easy the visualizations.

Fig. 3 shows the histograms of each variable. Scatterplots of each variable against each spatial coordinate in Fig. 4 are used to check for spatial trends. We proceed with the residuals of a linear regression with constant trend as a realization of a zero-mean bivariate isotropic stationary Gaussian random field. The sample correlation between the variables was 0.68. Standard deviations are 0.60 for hydrogen content and 0.77 for the CTC.

The models considered in the estimation step are the MatSimpler, LMC, MatConstr, MatInd and MatSep. For MatSimpler and MatConstr the vector of parameters to be estimated is $\lambda = (\phi_1, \phi_2, \nu_1, \nu_2, \sigma_1, \sigma_2, \rho_{12})$, for the separable model, MatSep, we have $\phi_1 = \phi_2$ and $\nu_1 = \nu_2$ and for the independent model we have $\rho_{12} = 0$. The LMC model is parameterized by $\lambda = (a_{11}, a_{12}, a_{22}, a_{21}, \phi_1, \phi_2)$, where a_{11}, a_{12}, a_{22} and a_{21} are elements of the correlogramization matrix and ϕ_1 and ϕ_2 are parameters of the exponential correlation model. Table 1 presents the parameter estimates, the maximized log-likelihood (LL), the Akaike information criterion (AIC) and the Bayesian information criterion (BIC) values considering each model. The MatConstr, MatInd, LMC and MatSep models are estimated using the `GeoFit` function from the `GeoModels` package (Bevilacqua and Morales-Oñate, 2018) for which the standard likelihood function and the Euclidean distance were considered. The Nelder-Mead optimizer is the algorithm of choice for all model fits. Table 2 presents the estimation times. The R codes for the Tables 1-2 are available in the supplementary material.

Fig. 2 Circle plot of the (A) Hydrogen content and (B) CTC for soil250 data

Fig. 3 Histogram of (A) Hydrogen content and (B) CTC for soil250 data

Fig. 4 Scatterplots of (A) Hydrogen content and (B) CTC against the coordinates for soil250 data

The predictive behavior was assessed by a random training selection of 200 locations (80% of the data), from which we estimate the models under study and compute the mean absolute error (MAE), the root mean square error (RMSE) and the normalized mean square error (NMSE) for each model using cokriging predictor for the 50 remaining locations (20% of the data). These

Table 1 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

Table 2 Estimation times for each model for soil250 data

Estimates	Models				
	MatSimpler	MatConstr	MatInd	LMC	MatSep
User	109.918	405.609	169.595	96.770	113.649
System	0.442	0.588	0.120	0.253	0.124
Elapsed	59.301	406.421	169.630	97.002	113.752
N. Param	7	7	6	6	5

measures are defined as,

$$\text{MAE}_i = \frac{1}{50} \sum_{k=1}^{50} |X_i(\mathbf{s}_k) - \hat{X}_i(\mathbf{s}_k)|,$$

$$\text{RMSE}_i = \sqrt{\frac{1}{50} \sum_{k=1}^{50} (X_i(\mathbf{s}_k) - \hat{X}_i(\mathbf{s}_k))^2},$$

$$\text{NMSE}_i = \frac{\text{RMSE}_i}{\max(\hat{X}_i(\mathbf{s}_k)) - \min(\hat{X}_i(\mathbf{s}_k))},$$

where $\hat{X}_i(\mathbf{s}_k)$ is the cokriging predictor of the variable $X_i(\mathbf{s}_k)$, with $i = \text{H, CTC}$, representing hydrogen content and CTC, respectively. We repeated the same process 150 times, calculating the values of the MAE_i , RMSE_i and NMSE_i , for each variable each time. Table 3 presents the mean and standard

deviation for the prediction errors considering each model estimated for each variable.

The MatSimpler model showed a better fit when compared to the other models with respect to log-likelihood, AIC and BIC values. The estimation times of the MatSimpler model were also lower, especially when compared to the MatConstr model which has the same number of parameters. Thus, we observe that the proposed MatSimpler model is a competitive model with the classical models in the literature.

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

Models		MAE _H	RMSE _H	NMSE _H	MAE _{CTC}	RMSE _{CTC}	NMSE _{CTC}
MatSimpler	Mean	0.277	0.367	0.215	0.314	0.416	0.151
	sd	0.032	0.045	0.032	0.032	0.049	0.023
MatConstr	Mean	0.271	0.364	0.204	0.307	0.410	0.150
	sd	0.032	0.046	0.030	0.034	0.052	0.024
MatInd	Mean	0.271	0.363	0.210	0.308	0.411	0.156
	sd	0.032	0.045	0.029	0.034	0.051	0.024
LMC	Mean	0.271	0.363	0.208	0.307	0.409	0.153
	sd	0.032	0.046	0.030	0.034	0.051	0.025
MatSep	Mean	0.270	0.363	0.202	0.307	0.409	0.152
	sd	0.033	0.047	0.030	0.034	0.052	0.024

3.2 Example 2: Heavy metal concentration data

To illustrate the application of the MatSimpler model to a 4-variate set, we consider the data *meuse* dataset from the `sp` package, which contains topsoil heavy metal concentrations, collected in a plain flood of the river Meuse an area of approximately 15m x 15m. We studied the relationship between the variables cadmium, copper, lead, zinc, which have a strong sample correlation with each other. Fig. 5 shows the concentrations of each metal along the region under study.

One of the important predictors of heavy metal concentrations is the distance to the Meuse river. Thus, we consider such trend we take residuals from a linear fit of the metal concentrations on such distance. Considering $\hat{\rho}_{ij}$ the sample correlation between the variables i and j , for $i, j = 1, \dots, 4$, the correlations between them are: $\hat{\rho}_{12} = 0.6510$, $\hat{\rho}_{13} = 0.6165$, $\hat{\rho}_{14} = 0.6585$, $\hat{\rho}_{23} = 0.6970$, $\hat{\rho}_{24} = 0.7466$, $\hat{\rho}_{34} = 0.9392$, with standard deviations: $\hat{s}_1 = 0.8627$, $\hat{s}_2 = 0.3343$, $\hat{s}_3 = 0.4625$ and $\hat{s}_4 = 0.4339$. The histograms of each quantity are shown in Fig. 6.

The parametric estimates as well as the standard errors for the MatSimpler model are presented in Table 4. The model was able to capture the individual variability of each variable as well as the estimated correlations between them.

Fig. 5 Circle plot of (A) cadmium, (B) copper, (C) lead and (D) zinc concentration for meuse data

4 Simulation study

This section presents a simulation study to evaluate the behavior of the maximum likelihood estimators for the model parameters of the MatSimpler model. We explored a bivariate random field in three different scenarios to illustrate different situations that could occur in practice, exemplifying the flexibility of the proposed model in each case. Table 5 summarizes the simulated scenarios.

Scenario 1 considers the variables have smaller variability, for which we consider relatively small values for the variance parameters: $\sigma_1^2 = 0.25$ and

Fig. 6 Histogram of the residuals after removing tendencies with respect to distance of (A) cadmium, (B) copper, (C) lead and (D) zinc concentration

Table 4 Parameter estimates for meuse dataset

	Estimates					
	$\hat{\phi}_1$	$\hat{\phi}_2$	$\hat{\phi}_3$	$\hat{\phi}_4$	$\hat{\nu}_1$	$\hat{\nu}_2$
Value	0.3953	0.8337	0.3959	0.3948	0.0699	0.0917
sd	0.2351	0.4761	0.1529	0.1663	0.0386	0.0417
	$\hat{\nu}_3$	$\hat{\nu}_4$	$\hat{s}_1$	$\hat{s}_2$	$\hat{s}_3$	$\hat{s}_4$
Value	0.1407	0.1486	0.8650	0.3590	0.4369	0.4250
sd	0.0452	0.0508	0.0524	0.0274	0.0275	0.0273
	$\hat{\rho}_{12}$	$\hat{\rho}_{13}$	$\hat{\rho}_{14}$	$\hat{\rho}_{23}$	$\hat{\rho}_{24}$	$\hat{\rho}_{34}$
Value	0.6888	0.6167	0.7270	0.6745	0.7724	0.9296
sd	0.0433	0.0495	0.0374	0.0445	0.0322	0.0112

Table 5 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
2	Less smoothness and greater variability	0.05	0.1	0.3	0.4	1.5	2.0	0.0
								0.4
3	Greater smoothness and less variability	0.05	0.1	0.7	1.0	0.5	1.0	0.7

$\sigma_2^2 = 1.0$. Also in this scenario, we consider smaller smoothness for the variables, with values equal to $\nu_1 = 0.3$ and $\nu_2 = 0.4$. When $\nu = 0.5$ the Matérn correlation function reduces to the exponential correlation function. Thus, this scenario represents lesser smoothness marginal behavior for the variables when compared to the exponential correlation model.

Scenario 2 keeps $\nu_1 = 0.3$ and $\nu_2 = 0.4$, and considers a greater variability with variances values equal to $\sigma_1^2 = 2.25$ and $\sigma_2^2 = 4.00$.

Scenario 3 considers a situation of smaller variability, with variance values fixed at $\sigma_1^2 = 0.25$ and $\sigma_2^2 = 1.0$, and considers higher smoothness values for variables: $\nu_1 = 0.7$ and $\nu_2 = 1.0$. In this scenario, we have marginal behaviors that are smoother in comparison with the exponential correlation model.

In all scenarios, we set the scale parameters values in $\phi_1 = 0.05$ and $\phi_2 = 0.1$. For the correlation parameter between the variables the values considered are $\rho_{12} = (-0.7, -0.4, 0.0, 0.4, 0.7)$, aiming to illustrate different correlation structures that could occur in practice between the variables, with values ranging from a strong negative correlation ($\rho_{12} = -0.7$) to a strong positive correlation ($\rho_{12} = 0.7$) and including the no correlation case where $\rho_{12} = 0$.

For each scenario, 500 samples of a bivariate stationary isotropic Gaussian random field, of sizes 100, 225, 400 and 625, for each variable, were simulated in a regular unit grid. Fig. 7 illustrates the results of the simulated scenarios showing the expected bias plus and minus the expected standard error for estimators of the model for each scenario.

To facilitate the visualization we follow [Bonat and Jørgensen \(2016\)](#) and [Petterle et al \(2019\)](#), considering, for each parameter, standardized scales with respect to the standard error of the sample size 100, that is, for each parameter, the expected bias and the limits of the confidence intervals are divided by the standard error obtained on the sample of size 100. Standard errors and biases gets closer to zero as the sample size increases for the considered scenarios. In all scenarios, there appears to be a small overestimate for the smoothness and scale parameters, especially for smaller samples.

For the R implementation, we use the **Matrix** package (Bates and Maechler, 2021) which provides efficient linear algebra calculations and the **geoR** package (Ribeiro Jr et al, 2020) for the Matérn correlation function. The **mvnfast** package (Fasiolo, 2016) was used for the simulation of the Gaussian process.

Fig. 7 Expected bias and confidence interval on a standardized scale for each scenario and sample size ($\circ$, 100; $\triangle$, 225; $\square$, 400; $\bullet$, 625) for the parameters of the MatSimpler model

5 Discussion

We presented a covariance structure for multivariate random fields given by the product of matrices for continuously indexed data. The model is simple whilst flexible, allowing for different correlation structures and marginal-covariance functions. Its structure facilitates the specification, estimation, computation and generalization for more than two variables.

The analysis of the two data-sets illustrate the ability to deal with different covariance structures, allowing for different variability, smoothness and scales parameters. It also highlights the reduced computational times in comparison with other models. A simulation study with different combinations of model parameters suggests maximum likelihood estimators are asymptotically unbiased and consistent.

The major computational burden is the Cholesky decomposition, depending on the number of sample locations and response variables considered in the analysis. We illustrate the growth of computational time for up to six response variables and 900 sample locations. In this scenario, estimation time was approximately six hours (Fig. 8). Precise times will be hardware dependent. However, comparing it with some literature models for the bivariate case (Fig. 9), our proposal was competitive, presenting smaller estimation times, specially when compared to the MatConstr model, which has the same number of parameters.

Future directions include the study of estimation methods for the proposed approach that are more efficient, so that the estimation times will not be so penalized by the increase in variables and sampling locations. The organization and construction of an R package that involves the proposed approach shall be considered. Furthermore, the presented proposal opens options for future research in the context of non-Gaussian modeling and asymmetric data for multivariate spatial problems.

Supplementary materials. Supplementary materials for this article are available at: <https://angelicamariatortola.github.io/academic/MatSimpler2021.html>.

A Appendix. Computational results

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Fig. 8 Estimation time for MatSimpler model considering different sample sizes and number of variables

Fig. 9 Estimation times for the MatSimpler, MatConstr, MatSep and LMC models, considering simulated data from the MatConstr model for different sample sizes

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