SCALABLE MODELING OF NONSTATIONARY COVARIANCE FUNCTIONS WITH NON-FOLDING B-SPLINE DEFORMATIONS

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ABSTRACT

We propose a method for nonstationary covariance function modeling, based on the spatial deformation method of Sampson and Guttorp [1992], but using a low-rank, scalable deformation function written as a linear combination of the tensor product of B-spline basis. This approach addresses two important weaknesses in current computational aspects. First, it allows one to constrain estimated 2D deformations to be non-folding (bijective) in 2D. This requirement of the model has, up to now, been addressed only by arbitrary levels of spatial smoothing. Second, basis functions with compact support enable the application to large datasets of spatial monitoring sites of environmental data. An application to rainfall data in southeastern Brazil illustrates the method.

Keywords Spatial statistics · Nonstationary Gaussian processes · Splines

1 Introduction

Geostatistical methods for spatial and spatio-temporal data are in great demand from fields such as earth and climate sciences, epidemiology and agriculture. A comprehensive overview can be found in Cressie and Wikle [2011]. Spatially stationary processes are commonly used as models in geostatistical applications, but often the assumption of stationarity and isotropic covariance functions are difficult to hold in real applications; see for example, Guttorp et al. [1994], Le and Zidek [2006, pp. 95–101], Damian et al. [2001]. A recent review of methods that allow nonhomogenous covariance models is Schmidt and Guttorp [2020].

We propose a semiparametric method of nonstationary spatial covariance function that expands upon the work of Sampson and Guttorp [1992]. Data observed in a set

2 Spatial Deformation Model (SDM)

Let \( x_1, x_2, \ldots, x_n \) be spatial locations with \( x_i = (x_{1i}, x_{2i})^t \in G \subset \mathbb{R}^2 \) for all \( i \) in a geostatistical domain \( G \), and \( y_1, y_2, \ldots, y_n \), with \( y_i = (y_{1i}, y_{2i})^t \in D \subset \mathbb{R}^2 \) for all \( i \). Moreover, let \( f_\ell : \mathbb{R}^2 \rightarrow \mathbb{R} \), such that \( y_{1i} = f_1(x_{1i}, x_{2i}), y_{2i} = f_2(x_{1i}, x_{2i}) \) for all \( i \) and \( f_\ell \) are bijective, differentiable functions, for \( \ell = 1, 2 \).

Let \( Z \) be a Gaussian random field with spatial covariance function \( C \). For any pair of spatial sites \( x_i, x_{i'} \), we have \( Z_{i,t} = Z(x_i, t), Z_{i',t} = Z(x_{i'}, t) \), with \( \text{Cov}(Z_{i,t}, Z_{i',t}) = C(x_i, x_{i'}) \) given by

\[
C(x_i, x_{i'}) = \sigma^2 \rho(\|y_1 - y_2\|, \Delta);
\]

where \( \sigma^2 > 0 \), and \( \rho \) is a stationary, isotropic correlation function with parameters \( \Delta \). We remark that this model may not be identifiable, since \( C \) is invariant for shifts and rigid rotations in \( f_1, f_2 \). Moreover, scaling \( f_1, f_2 \) by a
constant $\alpha$ will produce the same $C$ if $\phi$ is also scaled by $\alpha$. Nevertheless the model can be used for Kriging and spatial interpolation without issues.

For example, consider $G = [0, 1]^2$ and $D$ given by the swirl transformation shown in Figure 1. We sampled from a spatio-temporal process on a regular grid of $n = 121$ points, with $\mu = 0$ and separable covariance function

$$\text{Cov}(Z(x_1, t_1), Z(x_2, t_2)) = \exp\{-\|y_2 - y_1\|/0.25\} \delta(t_1, t_2),$$

where $y_1 = (f_1(x_1), f_2(x_1))$, $y_2 = (f_1(x_2), f_2(x_2))$ and $\delta(t_1, t_2) = I\{t_1 = t_2\}$. A realization of a random field on a fine mesh grid is also shown in Figure 1 obtained with the RandomFields package [Schlather et al. 2015].

3 Spatial Deformation Estimation

Let

$$2\gamma(y_1, y_2) = \text{Var}(Z(y_1) - Z(y_2)),$$

then $\gamma$ is the semivariogram of the random field $Z$. In particular, for a stationary, isotropic $Z$,

$$2\gamma(y, y + h) = 2C(0) - 2C(||h||) = g(||h||),$$

where $g$ is a positive non-decreasing function of $||h||$. Note valid $g$ functions are conditionally negative definite [Cressie 1993].

If there are ways to obtain a sample covariance matrix, such as temporal replicates, then we can construct a sample variogram as

$$d^2_{ij} = s_{ii} + s_{jj} - 2s_{ij}.$$

If the variogram is isotropic on a set of artificial coordinates $D$, then it must be have form

$$g(||y_i - y_j||) = g(h_{ij}),$$

where $h_{ij} = ||y_i - y_j||_2$. Therefore, the variogram entries can be seen as a dispersion metric, with $g(h_{ij}) \approx d^2_{ij}$.

3.1 Non-metric multidimensional scaling

[Sampson and Guttrop 1992] first step is to consider a non-metric multidimensional scaling approach [hereafter, nMDS; see Kruskal 1964; Mardia et al. 1979; Cox and Cox 2000]. From a set of dispersions $d^2_{ij}$, we seek a monotone transformation $\delta(d_{ij}) = \delta_{ij}$ such that

$$\delta(d_{ij}) = \delta_{ij} \approx ||y_i - y_j||.$$
We propose a different approach for the spline smoothing by making use of low rank approximation (finite approximation) for the deformation functions. Specifically, let \( x_1 = (x_{11}, \ldots, x_{1n}) \) and \( x_2 = (x_{21}, \ldots, x_{2n}) \) be a collection of points in \( \mathbb{R}^2 \). Define a map \( f : G \rightarrow D \) such that

\[
f(x) = \sum_{k=1}^{n} \psi_k(x) y_k
\]

where the functions \( \psi_k : G \subset \mathbb{R}^2 \rightarrow \mathbb{R} \) form a partition of unity.

Particularly, suppose that \( \psi_k \) are the B-splines basis functions and there is an integer number \( K < n \) such that a map \( f : G \rightarrow D \) is represented by

\[
f(x) = \sum_{k=1}^{K} \psi_k(x) \theta_k
\]

where \( \theta_k = (\theta_k^{(1)}, \theta_k^{(2)}) \) and \( f(x)^t = (f_1(x), f_2(x)) \). Let \( \psi_k(x) = B_{k_1}(x_1)B_{k_2}(x_2) \) for some index set \( k_1 = 1, \ldots, K_1; k_2 = 1, \ldots, K_2 \) such that \( K = K_1 \times K_2 \). Then the functions \( f_\ell \) are well approximated by

\[
\begin{bmatrix} f_1(x_1, x_2) \\ f_2(x_1, x_2) \end{bmatrix} \approx \begin{bmatrix} \sum_{k_1=1}^{K_1} \sum_{k_2=1}^{K_2} \theta_{k_1, k_2}^{(1)} B_{k_1}(x_1)B_{k_2}(x_2) \\ \sum_{k_1=1}^{K_1} \sum_{k_2=1}^{K_2} \theta_{k_1, k_2}^{(2)} B_{k_1}(x_1)B_{k_2}(x_2) \end{bmatrix}
\]
where $K_1$, $K_2$ are fixed positive integers and $B_{k_1}, B_{k_2}$ are B-spline basis functions [see, e.g., Ramsay and Silverman, 2005].

To guarantee that the functions $f_\ell$ do not fold onto themselves, we must guarantee that $f_\ell$ is locally invertible and differentiable. In fact, a diffeomorphism is desirable [see, e.g., Perrin and Monestiez, 1999]. A necessary condition is that everywhere in the $G$ domain,

$$\Pr = \frac{\partial f_1}{\partial x_1}, \frac{\partial f_2}{\partial x_2} - \frac{\partial f_1}{\partial x_2} \frac{\partial f_2}{\partial x_1} \neq 0,$$

(3)

but in practice such constraint is difficult to implement, requiring the evaluation of the Jacobian $J$ for every pair $(x_1, x_2) \in \mathbb{R}^2$. We will show in Section 4 that such condition can be translated into a condition onto the coefficients $\Theta_\ell = (\theta_{k_1,k_2}^\ell)$, for $\ell = 1, 2$. Note however that it is enough to ensure $|J| > 0$, since a change in signs would imply a discontinuous Jacobian.

### 3.4 Simultaneous estimation of covariance function and deformation

The covariance parameters $\Delta$, as well as the mean vector $\mu$ are estimated by maximizing the profile log-likelihood. Without loss of generality set $\mu = 0$. Thus our proposed B-spline approach can be estimated as

1. Given $\hat{\Theta}_1^{(k)}$, $\hat{\Theta}_2^{(k)}$, solve the optimization problem

$$\hat{\Delta}^{(k)} = \arg \max_{\Delta} Q_1(\Delta|\hat{\Theta}_1^{(k)}, \hat{\Theta}_2^{(k)})$$

where $Q_1(\Delta|\Theta_1, \Theta_2)$ corresponds to the optimization target $Q$ seen as a function of $\Delta$ only, with parameters $\Theta_1, \Theta_2$ fixed.

2. Given $\hat{\Delta}^{(k)}$, obtain $\hat{\Theta}_1^{(k+1)}$, $\hat{\Theta}_2^{(k+1)}$ such that

$$\arg \min_{\Theta_1, \Theta_2} \text{tr}(R^TR)$$

s.t. $\text{vec}(\Theta_1)^t A_{i,j} \text{vec}(\Theta_2) > 0$, for $i = 2, \ldots, K$, $j = 2, \ldots, K$

where $R_{n \times 2} = Y - (W \text{vec}(\Theta_1), W \text{vec}(\Theta_2))$, $W_{n \times K_1 K_2} = b_2(x_{i,2}) \otimes b_1(x_{i,1})$, $b_1, b_2$ are the row vector of basis functions and $\otimes$ is the Kronecker product, and for some choice of $A_{i,j}$ such that $|J| > 0$ if $\text{vec}(\Theta_1)^t A_{i,j} \text{vec}(\Theta_2) > 0$.

3. Repeat steps 1 and 2 until convergence.

We remark that the matrices $W$ are sparse when using B-splines, therefore solutions to step 2 are scalable. To evaluate the inequality $|J| > 0$, consider the following: write

$$f_\ell(x_1, x_2) = (B_1(x_1) \cdots B_K)(\theta_{1,1}^{\ell} \cdots \theta_{1,K_2}^{\ell}) (B_1(x_2) \cdots B_K(x_2)),$$

or simply $f_\ell = b_1^{\ell}(\Theta_1) b_2$, where $b_1$ is a $K_1 \times 1$ vector of B-spline basis functions evaluated at $x_1$, similarly $b_2$ is a $K_2 \times 1$ vector of B-spline basis evaluated at $x_2$, and $\theta_\ell$ is a $K_1 \times K_2$ matrix of spline coefficients for the tensor product approximation of the $\ell$-th function $f_\ell$. Similarly,

$$\frac{\partial}{\partial x_1} f_\ell(x_1, x_2) = (B_1'(x_1) \cdots B_K')(\theta_{1,1}^{\ell} \cdots \theta_{1,K_2}^{\ell}) (B_1(x_2) \cdots B_K(x_2)),$$
is the partial derivative of $f_i$ with respect to $x_1$, and if we write $b'_k = (B'_1(x_k) \cdots B'_{K_i}(x_k))$, $k = 1, 2$, then
\[
\frac{\partial f_i}{\partial x_1} = (b'_1)^t \Theta b_2.
\]
This allows us to see that
\[
|J| = ((b'_1)^t \Theta b_2) \cdot (b'_1^t \Theta b_2) - (b'_1 \Theta b_2)^2 \cdot ((b'_1)^t \Theta b_2)
\]
\[
= \left[ (b_2 \otimes b_1)^t \text{vec} (\Theta_1) \right] \left[ (b_2 \otimes b_1)^t \text{vec} (\Theta_2) \right] - \left[ (b_2 \otimes b_1)^t \text{vec} (\Theta_1) \right] \left[ (b_2 \otimes b_1)^t \text{vec} (\Theta_2) \right]
\]
\[
= \text{vec} (\Theta_1)^t \left[ (b_2 \otimes b_1)^t (b_2 \otimes b_1)^t - (b_2 \otimes b_1) (b_2 \otimes b_1)^t \right] \text{vec} (\Theta_2)
\]
\[
= \text{vec} (\Theta_1)^t A(x_1, x_2) \text{vec} (\Theta_2)
\]
so the determinant of the Jacobian $J$ as a function of $x_1, x_2$ is an inner product of $\text{vec} (\Theta_1)$, $\text{vec} (\Theta_2)$, weighted by the skew-Symmetric matrix $A(x_1, x_2)$. Ensuring the inequality $|J| > 0$ for all values of $x_1, x_2$ remains a difficult task, but we can choose a set of basis for which $A(x_1, x_2)$ does not depend on $x_1, x_2$.

4 Constrained spatial deformation estimation

We will use an approach similar to [Muse et al., 2001]. Consider B-splines of degree 1 on $[0, T]$. Assume that there are $K - 2$ equally spaced inner knots, where $0 < \tau_1 < \ldots < \tau_{K-2} < T$. Since the knots are equally spaced, they can be written as $0 < \tau < 2\tau < \ldots < (K-2)\tau < T$, where $\tau = T/(K-1)$. In this case, the $K$ B-spline bases are given by

\[
B_1(x) = \begin{cases} 1 - \frac{x}{\tau} & \text{if } x \in [0, \tau], \\ 0 & \text{otherwise}, \end{cases}
\]
\[
B_2(x) = \begin{cases} \frac{x}{\tau} & \text{if } x \in [0, \tau], \\ 2 - \frac{x}{\tau} & \text{if } x \in [\tau, 2\tau], \\ 0 & \text{otherwise}, \end{cases}
\]
\[
B_k(x) = B_2(x - (k - 2)\tau), \quad k = 3, \ldots, K - 1.
\]
\[
B_K(x) = B_1(K - 1 - x),
\]
with derivatives

\[
B'_1(x) = \begin{cases} -\frac{1}{\tau} & \text{if } x \in [0, \tau], \\ 0 & \text{otherwise}, \end{cases}
\]
\[
B'_2(x) = \begin{cases} \frac{1}{\tau} & \text{if } x \in [0, \tau], \\ -\frac{1}{\tau} & \text{if } x \in [\tau, 2\tau], \\ 0 & \text{otherwise}, \end{cases}
\]

Consider $(x_1, x_2) \in [\tau_{i-1}, \tau_i] \times [\tau_{j-1}, \tau_j]$, where $i$ and $j$ is between 1 and $K - 1$ (where $\tau_0 = 0$ and $\tau_{K-1} = T$). Then there are only 4 bases that evaluate to non-zero values, indexed by $i-1, i, j-1$ and $j$, so

\[
b_2 \otimes b_1^t = \begin{pmatrix} \tau^t x_2 - (j - 1)\tau^2 \\ -\tau^t x_2 - (j - 1)\tau^2 \end{pmatrix} = \begin{pmatrix} 0 \tau^t x_2 - (j - 2)\tau^2 \\ -\tau^t x_2 - (j - 2)\tau^2 \end{pmatrix}
\]
\[
b_2' \otimes b_1 = \begin{pmatrix} \tau^t x_1 - (i - 1)\tau^2 \\ -\tau^t x_1 - (i - 1)\tau^2 \end{pmatrix} = \begin{pmatrix} 0 \tau^t x_1 - (i - 2)\tau^2 \\ -\tau^t x_1 - (i - 2)\tau^2 \end{pmatrix}
\]

and therefore, looking only at the non-zero pairs $(i-1, j-1), (i, j-1), (i-1, j), (i, j)$, we have

\[
A_{(i-1);i,(j-1);j}(x_1, x_2) = \frac{1}{\tau^4} \begin{pmatrix} 0 & a & b & c \\ -a & 0 & d & e \\ -b & -d & 0 & f \\ -c & -e & -f & 0 \end{pmatrix}
\]

where

\[ a = -\tau (x_2 - (j-1)\tau) \]
\[ b = \tau (x_1 - (i-1)\tau) \]
\[ c = \tau (x_2 - x_1 - \tau(j-i)) \]
\[ d = -\tau(x_1 + x_2 - \tau(i+j-3)) \]
\[ e = \tau(x_1 - (i-2)\tau) \]
\[ f = -\tau(x_2 - (j-2)\tau) \]

note \( \text{vec}(\Theta_1)^T A(x_1, x_2) \text{vec}(\Theta_2) \) is therefore proportional to

\[ = (x_1 - (i-1)\tau) \left( \theta_{i-1,j-1}^{(2)} - \theta_{i-1,j-1}^{(1)} - \theta_{i-1,j-1}^{(1)} - \theta_{i-1,j-1}^{(2)} \right) \]
\[ + (x_1 - (i-2)\tau) \left( \theta_{i-1,j}^{(1)} - \theta_{i-1,j}^{(2)} - \theta_{i-1,j}^{(2)} - \theta_{i-1,j}^{(1)} \right) \]
\[ + (x_2 - (j-1)\tau) \left( \theta_{i-1,j-1}^{(2)} - \theta_{i-1,j-1}^{(1)} - \theta_{i-1,j-1}^{(1)} - \theta_{i-1,j-1}^{(2)} \right) \]
\[ + (x_2 - (j-2)\tau) \left( \theta_{i-1,j}^{(1)} - \theta_{i-1,j}^{(2)} - \theta_{i-1,j}^{(2)} - \theta_{i-1,j}^{(1)} \right) \]

The above equations describe a plane in \( x_1, x_2 \) with coefficients depending on \( \Theta_1, \Theta_2 \). Now, since \( x_1 \in [\tau_{i-1}, \tau_i] \) and \( x_2 \in [\tau_{j-1}, \tau_j] \), where \( \tau_i = i\tau, i = 1, 2, \ldots, K - 1 \) (and similarly for \( j \)), we have four restrictions to consider:

- When \( x_1 = (i-1)\tau \) and \( x_2 = (j-1)\tau \),
  \[ |J| = \tau \left( \theta_{i-1,j}^{(1)}(\theta_{i-1,j}^{(2)} - \theta_{i-1,j}^{(1)}) - \theta_{i-1,j}^{(1)}(\theta_{i-1,j}^{(2)} - \theta_{i-1,j}^{(1)}) \right) + \theta_{i-1,j}^{(1)}(\theta_{i-1,j}^{(2)} - \theta_{i-1,j}^{(1)}) - \theta_{i-1,j}^{(1)}(\theta_{i-1,j}^{(2)} - \theta_{i-1,j}^{(1)}) \]

- When \( x_1 = i\tau \) and \( x_2 = (j-1)\tau \),
  \[ |J| = \tau \left( \theta_{i-1,j}^{(1)}(\theta_{i-1,j}^{(2)} - \theta_{i-1,j}^{(1)}) - \theta_{i-1,j}^{(1)}(\theta_{i-1,j}^{(2)} - \theta_{i-1,j}^{(1)}) \right) + \theta_{i-1,j}^{(1)}(\theta_{i-1,j}^{(2)} - \theta_{i-1,j}^{(1)}) - \theta_{i-1,j}^{(1)}(\theta_{i-1,j}^{(2)} - \theta_{i-1,j}^{(1)}) \]

- When \( x_1 = (i-1)\tau \) and \( x_2 = j\tau \),
  \[ |J| = \tau \left( \theta_{i-1,j}^{(1)}(\theta_{i-1,j}^{(2)} - \theta_{i-1,j}^{(1)}) - \theta_{i-1,j}^{(1)}(\theta_{i-1,j}^{(2)} - \theta_{i-1,j}^{(1)}) \right) + \theta_{i-1,j}^{(1)}(\theta_{i-1,j}^{(2)} - \theta_{i-1,j}^{(1)}) - \theta_{i-1,j}^{(1)}(\theta_{i-1,j}^{(2)} - \theta_{i-1,j}^{(1)}) \]

- When \( x_1 = i\tau \) and \( x_2 = j\tau \),
  \[ |J| = \tau \left( \theta_{i-1,j}^{(1)}(\theta_{i-1,j}^{(2)} - \theta_{i-1,j}^{(1)}) - \theta_{i-1,j}^{(1)}(\theta_{i-1,j}^{(2)} - \theta_{i-1,j}^{(1)}) \right) + \theta_{i-1,j}^{(1)}(\theta_{i-1,j}^{(2)} - \theta_{i-1,j}^{(1)}) - \theta_{i-1,j}^{(1)}(\theta_{i-1,j}^{(2)} - \theta_{i-1,j}^{(1)}) \]

This collection of constraints, for \( i = 1, \ldots, K - 1 \) and \( j = 1, \ldots, K - 1 \) together imply in a non-folding deformation map, and can be enforced with constrained optimization routines. We have employed [Svanberg [2002]] constrained optimization algorithm, available in the nlopt package [Johnson [2020]]. The code is available as an R package in [https://github.com/guiludwig/beplinedef](https://github.com/guiludwig/beplinedef).
Figure 2: Comparison of estimated deformation functions for simulated data. The upper row corresponds to the proposed regularized B-spline approach with $K = 4, 6$ and $8$, respectively. The bottom row corresponds to the Sampson and Guttrop [1992] method with $\lambda = 30, 7.5$ and $3.2$, which are equivalent in degrees of freedom to the upper cases.

5 Simulation study

To evaluate the performance of the algorithm, we conducted a simulation study based on the swirl function shown in Figure 5. Each sample has $n = 121$ spatial points on a regular grid in the geographical domain $G = [0, 1] \times [0, 1]$. We simulated from a Gaussian random field with mean function $\mu(x) = 0$ and covariance function $C(x_1, x_2) = \sigma^2 e^{-\|x_1 - x_2\|/\phi}$, with parameters $\sigma^2 = 1$, and $\phi = 0.25$. First, consider a single realization of the spatial random field. The estimated deformation maps are shown in Figure 2. We have obtained the constrained B-spline deformations (hereafter, bdef) with $K \times K = 4^2, 6^2$ and $8^2$ basis functions. The estimated deformation function does not fold, even though the true deformation function is difficult to be recovered. The case when $K = 8$ performs better than $K = 4$ or $K = 6$, indicating that there are features in the deformation map that need a large number of degrees of freedom to be estimated. On the other hand, the functions using Sampson and Guttrop [1992] (SG) method have smoothing parameters $\lambda = 30, 7.5$ and $3.2$, set to match the bdef approach. They start showing folding at $\lambda = 3.2$, and cannot recover deformation maps that require a number of degrees of freedom larger than $8^2$. Note that the SG maps were stretched or shrunk to fit the plot area, but the bdef maps did not require this step.

The comparison of estimated covariance matrices allow us to overlook the identifiability issues with rotations, shifts and scaling of the estimated maps. In Figure 3 we show a scatterplot of the upper-diagonal entries of the estimated covariance matrices for the data, versus the true covariance matrices. We remark that the bdef method shows no apparent bias and becomes more accurate as the number of degrees of freedom increase. On the other hand, SG has good performance at a small number of degrees of freedom (more smoothing), but tends to overestimate matrix entries as the number of degrees of freedom for the thin-plate spline increases.

6 Case study: Rainfall data in southeastern Brazil

The dataset we use to illustrate our method comes from meteorological surveys conducted by INMET – Instituto Nacional de Meteorologia, Brazil. The measurements are made at every 15 minutes, and daily accumulated values are made available. Following Rozante et al. [2010], we grouped the rainfall data in periods of 10 days.

Since we seek temporally stationary data, we decided to restrain the data collection to 2018-01-01 to 2018-03-30 (rainfall season), for a total of 9 time periods (period 1: 2018-01-01 to 2018-01-10, ..., period 9: 2018-03-22 to 2018-03-31).
Figure 3: Comparison of upper-diagonal entries for the estimated covariance matrix of the simulated data, versus the true covariance matrix. The upper row corresponds to the proposed regularized B-spline approach with $K = 4, 6$ and $8$, respectively. The bottom row corresponds to the Sampson and Guttorp [1992] method with $\lambda = 30, 7.5$ and $3.2$, which are equivalent in degrees of freedom to the upper cases.

Figure 4: Left panel: map of meteorological stations located in southeastern Brazil. Right panel: estimated deformation functions using $K \times K = 16$ B-spline basis.

We selected the 50 stations of the southeastern region of Brazil that had complete observations available during the period. The stations are shown in the left panel of Figure 4. Data can be obtained at [http://www.inmet.gov.br/portal/index.php?r=bdmep/bdmep](http://www.inmet.gov.br/portal/index.php?r=bdmep/bdmep).

In the right panel of Figure 4, we show the estimated deformation map, using $K \times K = 16$ B-spline basis functions. The estimated deformation map reveals topographical features shown in the left panel of the same Figure. Weather stations located in northwestern flat lands of Minas Gerais are treated as closer to each other than stations near the rough coast of Rio de Janeiro and São Paulo states, where elevation changes are abrupt.
In Figure 5, we perform conditional simulation of the Gaussian random field (Kriging) for the 10-day periods starting in 2018–01–01 and 2018–01–11, showing the resulting prediction maps.

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A Derivation of the non-folding constraint

We can derive the constraint presented in Section 4 as follows: Observe that

\[
\begin{align*}
    b_2 \otimes b'_1 &= (0^t \quad B_{j-1}(x_2)B'_{i-1}(x_1) \quad B_j(x_2)B'_i(x_1) \quad 0^t \quad B_j(x_2)B'_i(x_1) \quad 0^t) \quad t \\
    b'_2 \otimes b_1 &= (0^t \quad B'_{j-1}(x_2)B_{i-1}(x_1) \quad B'_j(x_2)B_{i-1}(x_1) \quad 0^t \quad B'_j(x_2)B_{i-1}(x_1) \quad 0^t) \quad t
\end{align*}
\]

or

\[
\begin{align*}
    b_2 \otimes b'_1 &= \left(0^t \quad -\left(2 - \frac{x_2 - (j - 3)\tau}{\tau}\right) \frac{1}{\tau} \quad \left(2 - \frac{x_2 - (j - 3)\tau}{\tau}\right) \frac{1}{\tau} \quad 0^t \quad 0^t \right) \quad t \\
    b'_2 \otimes b_1 &= \left(0^t \quad -\left(2 - \frac{x_2 - (j - 2)\tau}{\tau}\right) \frac{1}{\tau} \quad \left(2 - \frac{x_2 - (j - 2)\tau}{\tau}\right) \frac{1}{\tau} \quad 0^t \quad 0^t \right) \quad t
\end{align*}
\]

Further simplifying leads to

\[
\begin{align*}
    b_2 \otimes b'_1 &= \left(0^t \quad \frac{x_2 - (j - 1)\tau}{\tau^2} \quad -\frac{x_2 - (j - 1)\tau}{\tau^2} \quad \frac{x_2 - (j - 2)\tau}{\tau^2} \quad \frac{x_2 - (j - 2)\tau}{\tau^2} \quad 0^t \quad 0^t \right) \quad t \\
    b'_2 \otimes b_1 &= \left(0^t \quad \frac{x_1 - (i - 1)\tau}{\tau^2} \quad -\frac{x_1 - (i - 1)\tau}{\tau^2} \quad \frac{x_1 - (i - 2)\tau}{\tau^2} \quad \frac{x_1 - (i - 2)\tau}{\tau^2} \quad 0^t \quad 0^t \right) \quad t
\end{align*}
\]

and therefore, looking only at the non-zero pairs \((i-1, j-1), (i, j-1), (i-1, j), (i, j)\), we have

\[
A_{(i-1):i,(j-1):j}(x_1, x_2) = \frac{1}{\tau^4} \begin{pmatrix}
0 & a & b & c \\
-a & 0 & d & e \\
-b & -d & 0 & f \\
-c & -e & -f & 0
\end{pmatrix}
\]

where

\[
\begin{align*}
    a &= -\tau(x_2 - (j - 1)\tau) \\
    b &= \tau(x_1 - (i - 1)\tau) \\
    c &= \tau(x_2 - x_1 - \tau(j - i)) \\
    d &= -\tau(x_1 + x_2 - \tau(i + j - 3)) \\
    e &= \tau(x_1 - (i - 2)\tau) \\
    f &= -\tau(x_2 - (j - 2)\tau)
\end{align*}
\]

Note \(\text{vec}(\Theta_1)^t A(x_1, x_2) \text{vec}(\Theta_2)\) is therefore proportional to

\[
\frac{1}{\tau} \begin{pmatrix}
\theta_{(1)}^{(1)}_{i-1,j-1} & \theta_{(1)}^{(1)}_{i,j-1} & \theta_{(1)}^{(1)}_{i-1,j} & \theta_{(1)}^{(1)}_{i,j} \\
-a & 0 & d & e \\
-b & -d & 0 & f \\
-c & -e & -f & 0
\end{pmatrix} \begin{pmatrix}
\theta_{(2)}^{(1)}_{i-1,j-1} & \theta_{(2)}^{(1)}_{i,j-1} & \theta_{(2)}^{(1)}_{i-1,j} & \theta_{(2)}^{(1)}_{i,j} \\
\theta_{(2)}^{(1)}_{i+1,j-1} & \theta_{(2)}^{(1)}_{i+1,j} & \theta_{(2)}^{(1)}_{i,j+1} & \theta_{(2)}^{(1)}_{i,j}
\end{pmatrix}
\]

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\[
\theta^{(1),t} \left( \begin{array}{c}
-(x_2 - (j - 1) \tau)\theta_{1,j-1}^{(2)} + (x_1 - (i - 1) \tau)\theta_{1,j}^{(2)} + (x_2 - x_1 - \tau(j - i))\theta_{i,j}^{(2)} \\
(x_2 - (j - 1)\tau)\theta_{1,j}^{(2)} - (x_1 + x_2 - \tau(i + j - 3))\theta_{i,j}^{(2)} + (x_1 - (i - 2)\tau)\theta_{i,j}^{(2)} \\
-(x_1 - (i - 1)\tau)\theta_{i,j}^{(2)} - (x_1 + x_2 - \tau(i + j - 3))\theta_{i,j-1}^{(2)} - (x_2 - (j - 2)\tau)\theta_{i,j}^{(2)} \\
-(x_2 - x_1 - \tau(j - i))\theta_{i,j-1}^{(2)} - (x_1 - (i - 2)\tau)\theta_{i,j-1}^{(2)} + (x_2 - (j - 2)\tau)\theta_{i,j}^{(2)} \\
\end{array} \right)
\]

where \( \theta^{(1),t} = \text{vec}(\Theta_1)^t_{(i-1),j,(j-1):j} \), and

\[
\theta^{(1),t} \left( \begin{array}{c}
-(x_2 - (j - 1)\tau)(\theta_{1,j-1}^{(2)} - \theta_{1,j-1}^{(1)}) + (x_2 - (j - 1)\tau)(\theta_{1,j}^{(2)} - \theta_{1,j-1}^{(2)}) \\
(x_1 - (i - 2)\tau)(\theta_{i,j}^{(2)} - \theta_{i,j-1}^{(2)}) - (x_2 - (j - 1)\tau)(\theta_{i,j-1}^{(2)} - \theta_{i,j-1}^{(1)}) \\
(x_1 - (i - 1)\tau)(\theta_{i,j}^{(2)} - \theta_{i,j-1}^{(2)}) - (x_2 - (j - 1)\tau)(\theta_{i,j-1}^{(2)} - \theta_{i,j-1}^{(1)}) \\
-(x_1 - (i - 2)\tau)(\theta_{i,j}^{(2)} - \theta_{i,j-1}^{(2)}) + (x_2 - (j - 2)\tau)(\theta_{i,j}^{(2)} - \theta_{i,j-1}^{(2)}) \\
\end{array} \right)
\]

\[
= (x_1 - (i - 1)\tau) \left( \begin{array}{c}
\theta_{1,j-1}^{(2)} - \theta_{1,j-1}^{(1)} - \theta_{1,j-1}^{(1)} - \theta_{1,j-1}^{(2)} \\
\theta_{1,j}^{(2)} - \theta_{1,j-1}^{(2)} - \theta_{1,j}^{(1)} - \theta_{1,j-1}^{(1)} \\
\theta_{i,j}^{(2)} - \theta_{i,j-1}^{(2)} - \theta_{i,j}^{(1)} - \theta_{i,j-1}^{(1)} \\
\theta_{i,j}^{(2)} - \theta_{i,j}^{(1)} - \theta_{i,j}^{(2)} - \theta_{i,j}^{(1)} \\
\end{array} \right)
\]

The above equations describe a plane in \( x_1, x_2 \) with coefficients depending on \( \Theta_1, \Theta_2 \). Now, since \( x_1 \in [\tau_i, 1] \) and \( x_2 \in [\tau_j, 1] \), where \( \tau_i = i\tau, i = 1, 2, \ldots, K - 1 \) (and similarly for \( j \)), we have four restrictions to consider:

- **When** \( x_1 = (i - 1)\tau \) and \( x_2 = (j - 1)\tau \),

\[
|J| = \tau \left( \begin{array}{c}
\theta_{1,j-1}^{(1)}(\theta_{1,j}^{(2)} - \theta_{1,j-1}^{(2)}) - \theta_{1,j}^{(1)}(\theta_{1,j}^{(2)} - \theta_{1,j-1}^{(2)}) \\
\theta_{i,j}^{(1)}(\theta_{i,j}^{(2)} - \theta_{i,j-1}^{(2)}) - \theta_{i,j}^{(1)}(\theta_{i,j}^{(2)} - \theta_{i,j-1}^{(2)}) \\
\theta_{i,j}^{(1)}(\theta_{i,j}^{(2)} - \theta_{i,j}^{(2)}) - \theta_{i,j}^{(1)}(\theta_{i,j}^{(2)} - \theta_{i,j}^{(2)}) \\
\theta_{i,j}^{(1)}(\theta_{i,j}^{(2)} - \theta_{i,j}^{(2)}) - \theta_{i,j}^{(1)}(\theta_{i,j}^{(2)} - \theta_{i,j}^{(2)}) \\
\end{array} \right)
\]

- **When** \( x_1 = i\tau \) and \( x_2 = (j - 1)\tau \),

\[
|J| = \tau \left( \begin{array}{c}
\theta_{1,j-1}^{(1)}(\theta_{1,j}^{(2)} - \theta_{1,j-1}^{(2)}) - \theta_{1,j}^{(1)}(\theta_{1,j}^{(2)} - \theta_{1,j-1}^{(2)}) \\
\theta_{i,j}^{(1)}(\theta_{i,j}^{(2)} - \theta_{i,j-1}^{(2)}) - \theta_{i,j}^{(1)}(\theta_{i,j}^{(2)} - \theta_{i,j-1}^{(2)}) \\
\theta_{i,j}^{(1)}(\theta_{i,j}^{(2)} - \theta_{i,j}^{(2)}) - \theta_{i,j}^{(1)}(\theta_{i,j}^{(2)} - \theta_{i,j}^{(2)}) \\
\theta_{i,j}^{(1)}(\theta_{i,j}^{(2)} - \theta_{i,j}^{(2)}) - \theta_{i,j}^{(1)}(\theta_{i,j}^{(2)} - \theta_{i,j}^{(2)}) \\
\end{array} \right)
\]

- **When** \( x_1 = (i - 1)\tau \) and \( x_2 = j\tau \),

\[
|J| = \tau \left( \begin{array}{c}
\theta_{1,j-1}^{(1)}(\theta_{1,j}^{(2)} - \theta_{1,j-1}^{(2)}) - \theta_{1,j}^{(1)}(\theta_{1,j}^{(2)} - \theta_{1,j-1}^{(2)}) \\
\theta_{i,j}^{(1)}(\theta_{i,j}^{(2)} - \theta_{i,j-1}^{(2)}) - \theta_{i,j}^{(1)}(\theta_{i,j}^{(2)} - \theta_{i,j-1}^{(2)}) \\
\theta_{i,j}^{(1)}(\theta_{i,j}^{(2)} - \theta_{i,j}^{(2)}) - \theta_{i,j}^{(1)}(\theta_{i,j}^{(2)} - \theta_{i,j}^{(2)}) \\
\theta_{i,j}^{(1)}(\theta_{i,j}^{(2)} - \theta_{i,j}^{(2)}) - \theta_{i,j}^{(1)}(\theta_{i,j}^{(2)} - \theta_{i,j}^{(2)}) \\
\end{array} \right)
\]

- **When** \( x_1 = i\tau \) and \( x_2 = j\tau \),

\[
|J| = \tau \left( \begin{array}{c}
\theta_{1,j-1}^{(1)}(\theta_{1,j}^{(2)} - \theta_{1,j-1}^{(2)}) - \theta_{1,j}^{(1)}(\theta_{1,j}^{(2)} - \theta_{1,j-1}^{(2)}) \\
\theta_{i,j}^{(1)}(\theta_{i,j}^{(2)} - \theta_{i,j-1}^{(2)}) - \theta_{i,j}^{(1)}(\theta_{i,j}^{(2)} - \theta_{i,j-1}^{(2)}) \\
\theta_{i,j}^{(1)}(\theta_{i,j}^{(2)} - \theta_{i,j}^{(2)}) - \theta_{i,j}^{(1)}(\theta_{i,j}^{(2)} - \theta_{i,j}^{(2)}) \\
\theta_{i,j}^{(1)}(\theta_{i,j}^{(2)} - \theta_{i,j}^{(2)}) - \theta_{i,j}^{(1)}(\theta_{i,j}^{(2)} - \theta_{i,j}^{(2)}) \\
\end{array} \right)
\]