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Semiparametric Modeling with Nonseparable and Nonstationary Spatio-Temporal Covariance Functions and Its Inference

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Abstract

In this paper, we develop a new semiparametric approach to modeling geostatistical data repeatedly taken over time and drawing inference about the parameters and components of the underlying spatio-temporal process. Dependence in time and across space is modeled semiparametrically, giving rise to a class of nonseparable and nonstationary spatio-temporal covariance functions. A two-step procedure is devised to estimate the model parameters based on likelihood for detrended data, and the computational algorithm is efficient due to dimension reduction. Extensions

to spatio-temporal processes with general mean trends are also considered. Further, the asymptotic properties of our proposed method are established including consistency and asymptotic normality. A simulation study shows sound finite-sample properties of the proposed method and a real data example illustrates our method in comparison with alternative approaches.

Keywords: Geostatistics, semiparametric methods, spatio-temporal processes

1 Introduction

As the real-time monitoring technologies continue to advance, data over space and time are becoming more abundant. Collectively known as spatio-temporal data, these data arise in many scientific fields with different data formats and goals to address. To analyze various types of spatio-temporal data, different statistical models and methods have been developed, such as varying coefficents models (Lu et al., 2009), hierarchial dynamic spatial models (Zhang et al., 2003; Johannesson et al., 2007; Ghosh et al., 2010), filtering and dimensional reduction (Huang and Cressie, 1996; Cressie et al., 2010; Brynjarsdóttir and Berliner, 2014). For more details about spatio-temporal statistics, see Cressie and Wikle (2011). In this paper, we focus on spatio-temporal data such that the individual units are spatial sampling locations and at a given sampling location, repeated measures are taken over time. We propose a class of semiparametric models with nonseparable and nonstationary spatio-temporal covariance functions. We develop new methodology for inferences that balance model flexibility and computational feasibility, as well as establish

the corresponding asymptotic properties.

For modeling spatio-temporal data, it is generally important to incorporate spatio-temporal covariance. Separablility, such that the spatio-temporal covariance function is assumed to be a product of spatial covariance and temporal covariance, is a convenient assumption, but can be overly restrictive in many applications. Thus, various nonseparable spatio-temporal covariance functions have been proposed. For example, Cressie and Huang (1999) and Gneiting (2002) constructed nonseparable spatio-temporal covariance functions by Fourier inversion and completely monotone functions, respectively. While the above approaches allow spatio-temporal nonseparablility, the spatio-temporal processes are assumed to be stationary. To relax the stationarity assumption, Stein (2005) considered asymmetric models, that is, the covariance function is spatially isotropic but not symmetric spatio-temporally. Fuentes et al. (2008) and Rodrigues and Diggle (2010) developed nonstationary and nonseparable models via spectral representation and convolution, respectively. While the above methods concern covariance model building for spatio-temporal data, it is not always clear how model estimation and statistical inference are to be carried out. There is a clear need for further development of statistical methodology for the analysis of spatio-temporal data taken at regular or irregular sampling locations.

Nonparametric approaches are increasingly used for spatio-temporal modeling, which tend to be robust against covariance function misspecification. For example, extending the work of Gneiting (2002), Choi et al. (2013) proposed a nonparametric approxima-

tion of completely monotone functions in the construction of spatial and spatio-temporal covariance structures. Nonparametric methods may also alleviate computational burden in the estimation of spatio-temporal covariance functions. With an originally parametric covariance function, Zhang et al. (2015) proposed a nonparametric full scale approximation, which applies reduced rank techniques and sparse matrix algorithms to enhance computational efficiency, although theoretical backing is not given. We believe that there is considerable value to further develop nonparametric or semiparametric methods and explore their theoretical properties in spatio-temporal statistics. Here, we adopt a semiparametric approach to modeling and drawing inferences about the spatio-temporal mean function and covariance function. Moreover, the theoretical properties of our new methods are established, which seem to be still rare in semiparametric spatio-temporal statistics.

In particular, we model dependence over space and time by a Karhunen-Loève type expansion which results in nonseparable and nonstationary spatio-temporal covariance functions. The model parameters are estimated by a two-step procedure based on likelihood and the computational feasibility is further enhanced by dimension reduction. Extensions to spatio-temporal models with a general mean function (or, trend) are also considered. Further, the asymptotic properties of our proposed method, such as consistency and asymptotic normality, are investigated and established. These theoretical results are, to the best of our knowledge, first of its kind for semiparametric methods to infer about spatio-tempral models with nonseparable and nonstationary covariance functions. A simulation study shows sound finite-sample properties of the estimates and a real

data example illustrates our method in comparison with some of the existing approaches. Our model may also be regarded as spatially correlated functional data, although without replicates at each sampling location (Paul and Peng, 2011; Gromenko et al., 2012; Hörmann and Kokoszka, 2013). However, Gromenko et al. (2012) did not establish the theoretical properties of their method, whereas Paul and Peng (2011) and Hörmann and Kokoszka (2013) restricted attention to, respectively, separable models and the consistency of sample means and empirical covariance operators only (see also Horváth and Kokoszka (2012)).

The remainder of the paper is organized as follows. We propose a nonseparable and nonstationary spatio-temporal covariance model in Section 2. We develop an estimation procedure for the detrended spatio-temporal data in Section 3.1, and in Section 4.1, we extend the results to spatio-temporal data with a general mean trend. The theoretical properties of our methodology are established as theorems in Sections 3.2 and 4.2. Numerical examples using simulated and real data are given in Section 5. The technical details including theorem proofs are provided as supplementary materials.

2 Semiparametric Spatio-Temporal Model Formulation

Let $\mathcal{R}$ denote a spatial domain of interest in $\mathbb{R}^d$ with $d \geq 1$, and let $[0, T]$ denote the time interval of interest with $0 < T < \infty$. Taking into account possible spatio-temporal

correlation and measurement error, we model the spatio-temporal response variable $y(s,t)$ by

$$y(s,t) = \mu(s,t) + \varepsilon(s,t) + \upsilon(s,t), \tag{1}$$

where $\mu(s,t) = E\{y(s,t)\}$ is a fixed spatio-temporal mean function, $\varepsilon(s,t)$ is a zero-mean spatio-temporal random process, and $\upsilon(s,t)$ is a zero-mean measurement error, where $s \in \mathcal{R}$ and $t \in [0,T]$. For the spatial domain of interest $\mathcal{R}$, our method allows some irregularity such as non-convexity, but the domain needs to be continuous. In this and the following sections, we will assume a zero-mean function $\mu(s,t) = 0$ and consider more general mean functions in Section 4. We also assume that the measurement error $\upsilon(s,t)$ follows iid Gaussian distribution with mean 0 and variance σ^2, independent of $\varepsilon(s,t)$.

To model the spatio-temporal random process $\varepsilon(s,t)$, we assume that it is a zero-mean Gaussian process with a Karhunen-Loève (KL) type expansion (Ghanem and Spanos, 1991). That is, $\varepsilon(s,t) = \sum_{j=1}^{\infty} \xi_j(s)\varphi_j(t)$, where $\{\xi_j(s) : s \in \mathcal{R}\}_{j=1}^{\infty}$ is assumed to be a sequence of independent Gaussian processes, and $\{\varphi_j(t)\}_{j=1}^{\infty}$ is a sequence of eigenfunctions. Thus, (1) can be rewritten as

$$y(s,t) = \mu(s,t) + \sum_{j=1}^{\infty} \xi_j(s)\varphi_j(t) + \upsilon(s,t). \tag{2}$$

In general, we may assume that, for a given $s \in \mathcal{R}$, $\varepsilon(s,t) \in L^2[0,T]$ is a square integrable random function and is modeled by a stochastic (not necessarily Gaussian) process with mean zero and a spatio-temporal covariance function denoted as

$$\gamma(t,s;t',s') = \mathrm{cov}\{\varepsilon(s,t), \varepsilon(s',t')\}, \qquad s,s' \in \mathcal{R}, \quad t,t' \in [0,T].$$

We also assume that, for two locations $s \neq s'$, the two curves $\varepsilon(s,t)$ and $\varepsilon(s',t')$ have the same (possibly nonstationary) temporal covariance function $\gamma_0(t,t')$ (see, e.g., Gromenko et al., 2012; Hörmann and Kokoszka, 2013). Sufficient conditions to establish (2) are given in Appendix A of the supplementary materials. Let $\lambda_j = \text{var}\{\xi_j(s)\}$ denote the jth eigenvalue of the covariance function $\gamma_0(t,t')$. We further assume $\text{cov}\{\xi_j(s), \xi_{j'}(s')\} = 0$ for $j \neq j'$, which ensures positive definiteness of the covariance function $\gamma(t,s;t',s')$ and enhances the computational feasibility (Gromenko and Kokoszka, 2013). From the KL expansion, we can write the spatio-temporal covariance function as

$$\gamma(t,s;t',s') = \sum_{j=1}^{\infty} \text{cov}\{\xi_j(s), \xi_j(s')\}\varphi_j(t)\varphi_j(t'). \tag{3}$$

In spatio-temporal statistics, it is a common practice to assume that the spatio-temporal process $\varepsilon(s,t)$ in model (1) is stationary over space and time, whereas $\varepsilon(s,t)$ formulated here via the KL expansion encompasses spatio-temporal covariances functions that are nonstationary. Specifically, from (3), it is clear that $\varepsilon(s,t)$ does not need to be stationary in space or time, but can be stationary in space if $\xi_j(s)$ is a stationary spatial process for all j (Cressie, 1993). The spatio-temporal covariance function in (3) also does not need to be separable in space and time (Cressie and Huang, 1999; Fuentes et al., 2008), but is separable if $\lambda_j = 0$ for $j \geq 2$. Moreover, if any $\xi_j(s)$ is a nonstationary spatial process, $\varepsilon(s,t)$ is nonstationary in both space and time.

Next, we approximate (2) by the first J components; that is, we assume

$$y(s,t) = \mu(s,t) + \xi(s)^T\varphi(t) + \upsilon(s,t), \tag{4}$$

where $\xi(s) = (\xi_1(s), \ldots, \xi_J(s))^T$ and $\varphi(t) = (\varphi_1(t), \ldots, \varphi_J(t))^T$ for $s \in \mathcal{R}$ and $t \in [0, T]$. We further assume that the spatial covariance function of $\xi_j(s)$ is $\lambda_j \rho_j(\|s - s'\|; \theta_j)$, where $\rho_j(\cdot; \theta_j)$ is a spatial correlation function in the Matérn family with a q_i-dimensional vector of correlation parameters θ_j (Cressie, 1993). While there are multiple ways to model a spatial process, we have chosen the Matérn family because it is theoretically sound and is a popular choice in practice. That is, the spatio-temporal covariance structure specified in (4) is semiparametric.

3 Covariance Estimation and Theoretical Properties

3.1 A Two-step Estimation Procedure

We now turn to the estimation of the covariance function in (4) assuming that $\mu(s, t)$ is known. We will relax this assumption and consider a general mean trend in Section 4.

Suppose data are observed at n sampling locations $s_1, \ldots, s_n$, and at sampling location s_i, $y(s_i, t)$ is observed at m_i time points $t_{i1}, \ldots, t_{im_i}$. Let $y_{s_i} = (y(s_i, t_{i1}), \ldots, y(s_i, t_{im_i}))^T$ denote the observed data at sampling location s_i, $y = (y_{s_1}^T, \ldots, y_{s_n}^T)^T$ denote the observed data at all the sampling locations, $\breve{y}_{s_i} = (y(s_i, t_{i1}) - \mu(s_i, t_{i1}), \ldots, y(s_i, t_{im_i}) - \mu(s_i, t_{im_i}))^T$ denote the detrended data at sampling location s_i, $\breve{y} = (\breve{y}_{s_1}^T, \ldots, \breve{y}_{s_n}^T)^T$ denote the detrended data at all the sampling locations, and $N = \sum_{i=1}^n m_i$ denote the total number of observations. Further, let $\Phi_i = (\varphi(t_{i1}), \ldots, \varphi(t_{im_i}))$ denote a $J \times m_i$ matrix of eigenfunctions at sampling location s_i, $\Phi = \text{diag}\{\Phi_1, \ldots, \Phi_n\}$ denote a block diagonal ma-

trix of eigenfunctions at all the sampling locations, $\Lambda_{i,i'} = (\mathrm{cov}\{\xi_j(s_i), \xi_{j'}(s_{i'})\})_{j,j'=1}^{J} = \mathrm{diag}\{\lambda_1\rho_1(\|s_i - s_{i'}\|;\theta_1), \ldots, \lambda_J\rho_J(\|s_i - s_{i'}\|;\theta_J)\}$ denote a $J \times J$ diagonal matrix for the covariance between sampling locations s_i and $s_{i'}$, and $\Lambda = [\Lambda_{i,i'}]_{i,i'=1}^{n}$ denote an $n \times n$ block matrix for covariances between all pairs of sampling locations. It follows that the variance-covariance matrix of y is

$$\mathrm{cov}(y) = \Sigma = \Phi^T \Lambda \Phi + \sigma^2 I_N,$$

where recall from (1) that σ^2 is the measurement error variance, and I_N is the identity matrix with rank N.

Thus, the negative log-likelihood function of the parameters in (4) is

$$\ell(\lambda, \varphi(t), \theta_j, \sigma^2) = \frac{1}{2}\breve{y}^T\Sigma^{-1}\breve{y} + \frac{1}{2}\log\{\det(\Sigma)\} + \frac{N}{2}\log(2\pi), \tag{5}$$

where $\lambda = (\lambda_1, \ldots, \lambda_J)^T$ and recall from (4) that $\varphi(t) = (\varphi_1(t), \ldots, \varphi_J(t))^T$. Maximizing (5) would give the maximum likelihood estimates of the eigenvalues λ, eigenfunctions $\varphi(t)$, q_i-dimensional correlation parameters θ_j, and measurement error variance σ^2. However, such computation is intensive if not infeasible, since there are $J + \sum_{j=1}^{J} q_j + 1$ unknown parameters and J unknown functions involved. To overcome this challenge, we develop a two-step procedure that is likelihood-based but computationally more feasible than the maximum likelihood estimation. The theoretical properties of the resulting estimates will be established in Section 3.2.

In Step I of the estimation procedure, with

$$\widehat{\gamma}_0(t, t') = n^{-1}\sum_{i=1}^{n}\breve{y}(s_i, t)\breve{y}(s_i, t')$$

where $\breve{y}(s_i,t) = y(s_i,t) - \mu(s_i,t)$, we estimate λ and $\varphi(t)$ as follows. First, let $\widetilde{\varphi}_1(t)$ be the maximizer of

$$\max_{\|f(t)\|_\alpha=1} \int_0^T \int_0^T f(t)\widehat{\gamma}_0(t,t')f(t')dtdt' \tag{6}$$

where $\|f\|_\alpha = (f,f)_\alpha^{1/2}$ and $(f,g)_\alpha = \int_0^T f(t)g(t)dt + \alpha \int_0^T f''(t)g''(t)dt$ is an inner product, and $\alpha > 0$ controls the smoothness of the resulting maximizer. When $\alpha = 0$, we denote $\|f\| = (f,f)^{1/2}$ and $(f,g) = \int_0^T f(t)g(t)dt$. Consequently, the standardized $\widetilde{\varphi}_1(t)$, defined as $\widehat{\varphi}_1(t) = \widetilde{\varphi}_1(t)/||\widetilde{\varphi}_1(t)||$, provides an estimate of $\varphi_1(t)$. For $j > 2$, let $\widetilde{\varphi}_j(t)$ be the maximizer of (6) subject to the constraints $(f,\widetilde{\varphi}_k)_\alpha = 0$ for $k < j$. Similarly, define $\widehat{\varphi}_j(t) = \widetilde{\varphi}_j(t)/\|\widetilde{\varphi}_j(t)\|$ to be the estimate of $\varphi_j(t)$. Next, given $\widetilde{\varphi}_j(t)$, the estimate of λ_j is

$$\widehat{\lambda}_j = \int_0^T \int_0^T \widetilde{\varphi}_j(t)\widehat{\gamma}_0(t,t')\widetilde{\varphi}_j(t')dtdt', \quad j = 1,\ldots,J.$$

The computation in Step I above can be carried out by an algorithm for smoothed functional principal component analysis via a basis expansion (Silverman, 1996). Although this algorithm is fast to compute and the consistency of the resulting estimates is well-established when data are drawn independently from a stochastic process, its applicability and the estimation properties for spatio-temporal data have not been adequately studied before. We will pursue this in Section 3.2.

In Step II of the estimation procedure, we estimate θ_j and σ^2 by minimizing the negative log-likelihood function (5) given $\varphi(t) = \widehat{\varphi}(t)$ and $\lambda = \widehat{\lambda}$ as follows.

$$\ell(\theta_j, \sigma^2|\widehat{\lambda}, \widehat{\varphi}(t)) = \frac{1}{2}\breve{y}^T\Sigma^{-1}\breve{y} + \frac{1}{2}\log\{\det(\Sigma)\} + \frac{N}{2}\log(2\pi).$$

The resulting estimates are denoted as $\widehat{\theta}_j$ and $\widehat{\sigma}^2$. The computational complexity is of

order $\mathcal{O}(N^3)$, where N is the total number of observations, due to the inversion and determinant calculation of an $N \times N$ matrix Σ which is still intensive for large N. Thus, we further improve the computational efficiency by Sherman-Morrison-Woodbury formula and Sylvester's determinant theorem (Harville, 2008)

$$\Sigma^{-1} = (\Phi^T \Lambda \Phi + \sigma^2 I_N)^{-1} = \sigma^{-2} I_N - \sigma^{-2} \Phi^T \{\Phi \Phi^T + \sigma^2 \Lambda^{-1}\}^{-1} \Phi,$$

$$\det(\Sigma) = \det(\Phi^T \Lambda \Phi + \sigma^2 I_N) = \sigma^{2N} \det(\Lambda) \det(\Phi \Phi^T / \sigma^2 + \Lambda^{-1}),$$

which reduce the computational complexity to a smaller order of $\mathcal{O}(J^3 n^3)$, where n is the number of sampling locations. A similar approach has been taken by Nychka et al. (2015), although our method is semiparametric for spatio-temporal processes, and theirs is nonparametric for spatial-only processes.

3.2 Theoretical Properties

We now investigate the asymptotic properties of the estimates obtained from the proposed two-step procedure in Section 3.1. Let $\xrightarrow{P}$ denote convergence in probability and $\xrightarrow{D}$ denote convergence in distribution. We consider the increasing domain asymptotics such that the distance between any two sampling sites is greater than a constant. We assume the following regularity conditions for Theorem 1. Let $\mathcal{R}_{n^*}$ denote the spatial domain $\mathcal{R}$ at the n^*-th stage of the asymptotics.

(A.1) The eigenvalues of $\gamma_0(t, t')$ satisfy $\lambda_1 > \lambda_2 > \cdots > 0$.

(A.2) The smoothness parameter satisfies $\alpha \to 0$ as $n \to \infty$.

(A.3) $\sum_{i=1}^{n}\sum_{i'=1}^{n}\sum_{j=1}^{\infty}\sum_{j'=1}^{\infty} E\{\xi_j(s_i)\xi_j(s_{i'})\}E\{\xi_{j'}(s_i)\xi_{j'}(s_{i'})\} = o(n^2)$ as $n \to \infty$.

(A.4) $\sum_{i=1}^{n}\sum_{i'=1}^{n}\sum_{j=1}^{\infty}[E\{\xi_j(s_i)\xi_j(s_{i'})\}]^2 = o(n^2)$ as $n \to \infty$.

Conditions (A.1) and (A.2) have been assumed to establish consistency of $\hat{\lambda}_j$ and $\hat{\varphi}_j(t)$ for functional data analysis (Silverman, 1996) and are assumed here for spatio-temporal data. For a spatio-temporal separable covariance function with $J = 1$, Condition (A.1) can be relaxed to $\lambda_1 > \lambda_2 > \cdots \lambda_M > 0, \lambda_{M+1} = \ldots = 0$, for some $M > 0$. Conditions (A.3) and (A.4) are about the covariance function of the spatial random process $\xi_j(s)$ and hold for commonly used spatial covariance functions, some of which are shown in the supplementary materials.

In the following Theorem 1, we establish the consistency for the estimated eigenvalues $\widehat{\lambda}_j$ and the estimated eigenfunctions $\widehat{\varphi}_j$, obtained from Step I of the two-step procedure given in Section 3.1.

Theorem 1. *Under (2) and (A.1)–(A.4), for each j, we have*

$$\widehat{\lambda}_j \xrightarrow{P} \lambda_j, \quad (\widehat{\varphi}_j, \varphi_j)^2 \xrightarrow{P} 1,$$

as $n \to \infty$, where $(\widehat{\varphi}_j, \varphi_j) = \int_0^T \widehat{\varphi}_j(t)\varphi_j(t)dt$.

Theorem 1 is under the assumption that the mean function is known, which will be relaxed in Theorem 3.

Next, we establish the asymptotic properties for the estimates of the spatial parameters θ_j from Step II, given λ, $\varphi_j(t)$, and σ^2. For an $n \times n$ matrix A, let $\mu_i(A)$ denote the ith

largest eigenvalue of A and $\|A\|_2 = \max_{i=1,\ldots,n}\{\mu_i(A^TA)\}^{1/2}$ denote the spectral norm of A. Define

$$\Lambda_j = \left[\mathrm{cov}\{\xi_j(s_i), \xi_j(s_{i'})\}\right]_{i,i'=1}^n = \left[\lambda_j \rho_j(\|s_i - s_{i'}\|; \theta_j)\right]_{i,i'=1}^n,$$

whose (i, i')th component is the $((i-1)m + j, (i'-1)m + j)$th component of Λ. With $q = \sum_{j=1}^J q_j$, let $\vartheta = (\theta_1^T, \ldots, \theta_J^T)^T$ denote a q-dimensional vector and define $\vartheta_0 = (\theta_{10}^T, \ldots, \theta_{J0}^T)^T$, where θ_{j0} denotes the true value of the correlation parameter in $\rho_j(\cdot; \theta_j)$. Moreover, define $D_k\Lambda_j = \partial\Lambda_j/\partial\theta_{j,k}$, $D_{kk'}\Lambda_j = \partial^2\Lambda_j/\partial\theta_{j,k}\partial\theta_{j,k'}$, $w_{j,kk'} = \mathrm{tr}\{(\Lambda_j+\sigma^2 I_n)^{-1}(D_k\Lambda_j)(\Lambda_j+\sigma^2 I_n)^{-1}(D_{k'}\Lambda_j)\}$, for $k, k' = 1, \ldots, q_j$ and $j = 1, \ldots, J$. Finally, with ϑ_l denoting the lth component of ϑ, define $D_l\Sigma = \partial\Sigma/\partial\vartheta_l$, $D_{ll'}\Sigma = \partial^2\Sigma/\partial\vartheta_l\partial\vartheta_{l'}$, $D_l\Lambda = \partial\Lambda/\partial\vartheta_l$, $D_{ll'}\Lambda = \partial^2\Lambda/\partial\vartheta_l\partial\vartheta_{l'}$, and $t^*_{ll'} = \mathrm{tr}\{\Sigma^{-1}(D_l\Sigma)\Sigma^{-1}(D_{l'}\Sigma)\}$, for $l, l' = 1, \ldots, q$.

The regularity conditions for Theorem 2 are as follows.

(A.5) The correlation function $\rho_j(\cdot, \cdot; \theta_j)$ is twice differentiable, with respect to θ_j, with continuous second-order derivatives for $\theta_j \in \Omega_j$, where Ω_j is an open set.

(A.6) As $n \to \infty$, $\|\Lambda_j\|_2 = \mathcal{O}(1)$, $\|D_k\Lambda_j\|_2 = \mathcal{O}(1)$, $\|D_{kk'}\Lambda_j\|_2 = \mathcal{O}(1)$ for $k, k' = 1, \ldots, q_j$ and $j = 1, \ldots, J$.

(A.7) For some $\delta > 0$, there exist positive constants C_k such that $\|D_k\Lambda_j\|_F^{-2} \le C_k n^{-1/2-\delta}$ for $k = 1, \ldots, q_j$ and $j = 1, \ldots, J$.

(A.8) For any $k, k' = 1, \ldots, q_j$, $a_{j,kk'} = \lim_{n\to\infty}\{w_{j,kk'}(w_{j,kk}w_{j,k'k'})^{-1/2}\}$ exists and $A_j = [a_{j,kk'}]_{k,k'=1}^q$ is nonsingular, for $j = 1, \ldots, J$.

(A.9) There exists a positive constant c_0, such that $\|\Lambda_j^{-1}\|_2 < c_0 < \infty$, for $j = 1, \ldots, J$.

(A.10) As $n \to \infty$, $m_i = \mathcal{O}(1)$ and $\Phi_i^T \Phi_i = m_i I_{m_i}$.

Conditions (A.5)–(A.9) are standard assumptions made about Gaussian random fields in spatial linear models to ensure smoothness, growth and convergence of the information matrix (Mardia and Marshall, 1984). For spatio-temporal data, we assume (A.5)–(A.9) for $\xi_j(s)$, a spatial Gaussian process, in the Karhunen-Loève type expansion. Condition (A.10) is based on the orthonormality of eigenfunctions $\varphi_j(t)$, that is, $\int_0^T \varphi_j(t)\varphi_{j'}(t)dt = 1$ if $j = j'$ and 0 otherwise. Together with (A.5)–(A.9), (A.10) ensures smoothness, growth and convergence of the information matrix for spatio-temporal data (Sweeting, 1980).

Let $\ell''(\vartheta, \vartheta) = \frac{\partial^2 \ell(\lambda, \varphi(t), \theta_j, \sigma^2)}{\partial \vartheta \, \partial \vartheta^T}$ be the second-order derivatives of $\ell(\lambda, \varphi(t), \theta_j, \sigma^2)$ with respect to ϑ. Under (A.5)–(A.10), the asymptotic normality of $\widehat{\theta}_j$ is established in the following theorem.

Theorem 2. *Under (4) and (A.5)–(A.10), we have*

$$H(\vartheta_0)^{1/2}(\widehat{\vartheta} - \vartheta_0) \xrightarrow{D} N(0, I_q),$$

as $n \to \infty$, *where* $q = \sum_{j=1}^{J} q_j$, $\widehat{\vartheta} = (\widehat{\theta}_1^T, \ldots, \widehat{\theta}_J^T)^T$, *and* $H(\vartheta_0) = E\{-\ell''(\vartheta_0, \vartheta_0)\}$ *is the information matrix for* ϑ.

Although Theorems 1 and 2 give consistency and asymptotic normality of the parameter estimates, they are established for detrended spatio-temporal data — an assumption we will relax in Section 4.

4 Extensions to Spatio-Temporal Data with Trend

4.1 A Modified Two-step Estimation Procedure

In geostatistics, the mean function tends to vary over space and thus $\mu(s,t) = E\{y(s,t)\}$ depends on location s. In addition, $\mu(s,t)$ is generally unknown and needs to be estimated. There are various methods to estimate $\mu(s,t)$ such as kernel smoothing which often yields consistent estimates (Altman, 1990). Here, we let $\bar{\mu}(s,t)$ denote an estimated mean trend and $\bar{y}_s(t) = y(s,t) - \bar{\mu}(s,t)$ denote the detrended process. Further, let $\bar{y}_{s_i} = (y(s_i,t_{i1}) - \bar{\mu}(s_i,t_{i1}), \ldots, y(s_i,t_{im_i}) - \bar{\mu}(s_i,t_{im_i}))^T$ denote the detrended data, and $\bar{y} = (\bar{y}_{s_1}^T, \ldots, \bar{y}_{s_n}^T)^T$ denote the detrended data at all the sampling locations. The two-step estimation procedure developed in Section 3.1 for detrended data can be applied here by replacing $\breve{y}(s,t)$, $\breve{y}_{s_i}$ and $\breve{y}$ with $\bar{y}(s,t)$, $\bar{y}_{s_i}$ and $\bar{y}$, respectively.

Specifically, in Step I of the modified two-step procedure, let $\bar{\gamma}_0(t,t') = n^{-1}\sum_{i=1}^n \bar{y}(s_i,t)\bar{y}(s_i,t')$. For $j=1$, let $\widetilde{\varphi}_1(t)$ be the maximizer of

$$\max_{\|f(t)\|_\alpha=1} \int_0^T \int_0^T f(t)\bar{\gamma}_0(t,t')f(t')dtdt' \tag{7}$$

For $j > 2$, let $\widetilde{\varphi}_j(t)$ be the maximizer of (7) subject to the constraints $(f, \widetilde{\varphi}_k)_\alpha = 0$ for $k < j$. After standardization, $\widehat{\varphi}_j(t) = \widetilde{\varphi}_j(t)/\|\widetilde{\varphi}_j(t)\|$ becomes the estimate of $\varphi_j(t)$. The estimate of λ_j is

$$\widehat{\lambda}_j = \int_0^T \int_0^T \widetilde{\varphi}_j(t)\bar{\gamma}_0(t,t')\widetilde{\varphi}_j(t')dtdt', \quad j = 1, \ldots, J.$$

In Step II of the modified two-step procedure, the negative log-likelihood function (5)

with a plug-in estimated mean function takes on the form

$$\ell(\lambda, \varphi(t), \theta_j, \sigma^2) = \frac{1}{2}\bar{y}^T\Sigma^{-1}\bar{y} + \frac{1}{2}\log\{\det(\Sigma)\} + \frac{N}{2}\log(2\pi),$$

and is minimized with $\varphi(t) = \widehat{\varphi}(t)$ and $\lambda = \widehat{\lambda}$ held fixed. The resulting estimates are denoted as $\widehat{\theta}_j$ and $\widehat{\sigma}^2$.

Next, we consider a linear regression for the mean function, $\mu(s,t) = x(s,t)^T\beta$, where $x(s,t) = (x_1(s,t), \ldots, x_p(s,t))^T$ denotes p covariate functions at location s and time t, $\beta = (\beta_1, \ldots, \beta_p)^T$ denotes a p-dimensional vector of regression coefficients. The model (4) becomes

$$y(s,t) = x(s,t)^T\beta + \sum_{j=1}^{J}\xi_j(s)\varphi_j(t) + \upsilon(s,t). \tag{8}$$

Let $X(s_i) = (x(s_i, t_{i1}), \ldots, x(s_i, t_{im_i}))^T$ denote an $m_i \times p$ design matrix at sampling location s_i and $X = (X(s_1)^T, \ldots, X(s_n)^T)^T$ denote an $N \times p$ design matrix. Thus, the negative log-likelihood function of the parameters in model (4) is

$$\ell(\lambda, \varphi(t), \beta, \theta_j, \sigma^2) \;=\; (y - X\beta)^T\Sigma^{-1}(y - X\beta)/2 + (1/2)\log\{\det(\Sigma)\} + (N/2)\log(2\pi). \tag{9}$$

A practical choice of $\bar{\mu}(s,t)$ is $\bar{\mu}(s,t) = x(s,t)^T\bar{\beta}_{\text{ols}}$, where $\bar{\beta}_{\text{ols}} = (X^TX)^{-1}X^Ty$ is the least squares estimate of β. Then, Step I of the modified two-step estimation procedure can be carried out as before. In Step II, however, we minimize the negative log-likelihood function (9) with respect to β, θ_j, and σ^2, with $\varphi(t) = \widehat{\varphi}(t)$ and $\lambda = \widehat{\lambda}$ held fixed. The resulting estimates are denoted as $\widehat{\beta}$, $\widehat{\theta}_j$, and $\widehat{\sigma}^2$.

4.2 Theoretical Properties

Now, we consider the asymptotic properties of the parameter estimates obtained from the modified two-step procedure above under additional regularity conditions. First, we assume the following about the fourth moment of the estimated mean function.

(A.11) As $n \to \infty$, there exists a sequence $c_n \to 0$, such that $E\{\bar{\mu}(s,t) - \mu(s,t)\}^4 \leq c_n$ for $t \in [0,T]$, where c_n does not depend on s.

For kernel smoothing estimate $\bar{\mu}(s,t)$, (A.11) can be verified to hold under certain conditions (El Machkouri, 2007).

The following Theorem 3 establishes the consistency for the parameter estimates in Step I of the modified estimation procedure, in the case of an unknown mean function $\mu(s,t)$.

Theorem 3. *Under the assumptions of Theorem 1 and (A.11), we have*

$$\widehat{\lambda}_j \xrightarrow{P} \lambda_j, \quad (\widehat{\varphi}_j, \varphi_j)^2 \xrightarrow{P} 1,$$

as $n \to \infty$.

For model (8), we establish the asymptotic properties of $\widehat{\beta}$ and $\widehat{\theta}_j$ from Step II, given λ, $\varphi_j(t)$, and σ^2. An additional regularity condition is assumed about the design matrix, which is standard for spatial linear models (Mardia and Marshall, 1984).

(A.12) The design matrix X has full rank p and is uniformly bounded in max norm with $\lim_{n\to\infty}(X^T X)^{-1} = 0$.

Let $\ell''(\beta,\beta) = \frac{\partial^2 \ell(\lambda,\varphi(t),\beta,\theta_j,\sigma^2)}{\partial\beta\ \partial\beta^T}$ be the second-order derivatives of $\ell(\lambda,\varphi(t),\beta,\theta_j,\sigma^2)$ with respect to β. The asymptotic normality of $\widehat{\beta}$ and $\widehat{\theta}_j$ are established in Theorem 4.

Theorem 4. *Under the assumptions of Theorem 2 and (A.12), we have*

$$\begin{pmatrix} H(\beta_0)^{1/2} & O_{p\times q} \\ O_{q\times p} & H(\vartheta_0)^{1/2} \end{pmatrix} \left\{ \begin{pmatrix} \widehat{\beta} \\ \widehat{\vartheta} \end{pmatrix} - \begin{pmatrix} \beta_0 \\ \vartheta_0 \end{pmatrix} \right\} \xrightarrow{D} N(0, I_{p+q}),$$

as $n \to \infty$, where $H(\beta_0) = E\{-\ell''(\beta_0,\beta_0)\}$ is the information matrix for β, and $O_{p\times q}$ denotes a $p \times q$ zero matrix.

The proof of the proposition and theorems above are given as supplementary materials. The Gaussian assumption can be readily relaxed in Theorems 1 and 3, but it does not appear to be the case for Theorems 2 and 4.

5 Numerical Examples

5.1 Simulation Study

A simulation study is conducted to investigate the finite-sample properties of our spatio-temporal semiparametric covariance (SemiCov) method developed in Sections 2–4. First, the covariates $x(s,t)$ are generated from the standard normal distributions with a cross-covariate correlation of 0.5, and the regression coefficients are set to be $\beta = (4,3,2,1,0,0,0)^T$. Each covariate is standardized to have sample mean 0 and sample variance 1 and the response has a sample mean 0. Thus, there is no intercept in this model. The spatio-temporal process is defined as $\varepsilon_1(s,t) = \xi_1(s)\varphi_1(t) + \xi_2(s)\varphi_2(t)$, where $\xi_1(s)$ and $\xi_2(s)$

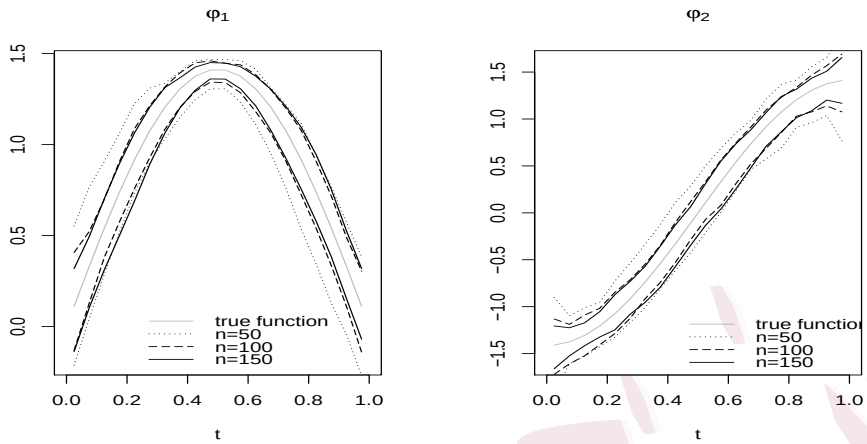

Figure 1: *The* 95% *pointwise simulation intervals for* $\varphi_1(t)$ *(left) and* $\varphi_2(t)$ *(right) using our method. The true* $\varphi_1(t)$ *and* $\varphi_2(t)$ *are drawn in gray solid line. The pointwise simulation intervals for* $n = 50$, 100 *and* 150 *are drawn by black dotted, dashed and solid lines, respectively.*

are two independent zero-mean stationary and isotropic Gaussian processes with an exponential covariance function $\lambda_1 \exp(-d/r_1)$ and $\lambda_2 \exp(-d/r_2)$ for spatial distance d, respectively, with $\lambda_1 = 2.5$, $r_1 = 0.5$, $\lambda_2 = 0.5$ and $r_2 = 0.3$. Moreover, $\varphi_1(t) = c_1 \cos(\pi t)$ and $\varphi_2(t) = c_2 \sin(\pi t)$ are two orthonormal functions on $[0, 1]$ with normalization constants c_1 and c_2. The number of sampling locations is set to be $n = 50$, 100 and 150 and the locations are randomly distributed within the spatial domain $\mathcal{R} = [0, l] \times [0, l]$, where $l = 2^{-1} n^{1/2}$. At each sampling location, twenty time points are set at $t_i = (2i - 1)/(2m)$ for $i = 1, \ldots, m$ and $m = 20$. For each sample size n, 100 data sets are simulated.

For each simulated data set, our method is applied to estimate the regression coefficients β, the spatial parameters (r_1, r_2), the eigenvalues (λ_1, λ_2), the eigenfunctions $(\varphi_1(t), \varphi_2(t))$, and the measurement error variance σ^2. Our method is compared with two alternative methods, namely, the ordinary least squares which ignores both spatial and

temporal dependence (denoted as ALT_1) and the functional data analysis that accounts for temporal but not spatial dependence (denoted as ALT_2). Moreover, the prediction in space and time is performed using all these three approaches.

n	Method	β_1	β_2	β_3	β_4	β_5	β_6	β_7	MSPE_1	MSPE_2
	True Values	4.000	3.000	2.000	1.000	0.000	0.000	0.000	–	–
50	SemiCov	4.001	3.000	1.997	0.996	0.006	-0.006	0.009	2.667	1.112
	SD	0.043	0.044	0.045	0.048	0.042	0.043	0.041	1.006	0.177
	SDm	0.045	0.045	0.045	0.045	0.045	0.045	0.045	–	–
	ALT_1	4.005	3.005	1.996	0.992	0.006	-0.005	0.009	3.927	3.768
	SD	0.086	0.077	0.087	0.076	0.081	0.082	0.076	1.703	0.744
	ALT_2	4.001	3.000	1.997	0.996	0.006	-0.007	0.009	3.917	1.114
	SD	0.043	0.044	0.045	0.049	0.043	0.043	0.041	1.704	0.177
100	SemiCov	4.001	2.992	1.998	1.007	0.002	0.000	-0.001	2.610	1.106
	SD	0.031	0.030	0.029	0.031	0.033	0.027	0.030	0.715	0.108
	SDm	0.031	0.031	0.031	0.031	0.031	0.031	0.031	–	–
	ALT_1	3.996	2.991	2.001	1.011	0.005	-0.005	0.004	3.720	3.775
	SD	0.053	0.055	0.054	0.058	0.056	0.053	0.057	1.130	0.453
	ALT_2	4.001	2.992	1.998	1.007	0.002	0.000	-0.001	3.715	1.109
	SD	0.031	0.030	0.029	0.032	0.033	0.027	0.030	1.133	0.108
150	SemiCov	4.001	3.004	1.997	0.997	-0.001	0.000	0.002	2.616	1.093
	SD	0.027	0.026	0.025	0.027	0.032	0.024	0.027	0.600	0.105
	SDm	0.025	0.025	0.025	0.025	0.025	0.025	0.026	–	–
	ALT_1	4.005	3.007	1.991	1.001	-0.001	-0.007	0.005	3.836	3.847
	SD	0.043	0.054	0.051	0.048	0.049	0.045	0.045	0.914	0.414
	ALT_2	4.001	3.004	1.997	0.997	0.000	0.000	0.002	3.830	1.095
	SD	0.027	0.026	0.025	0.027	0.032	0.023	0.027	0.912	0.105

Table 1: *The mean, standard deviation (SD) of regression coefficient estimates and mean square prediction errors under the proposed SemiCov method, ALT_1 and ALT_2, as well as the mean estimated standard deviation (SDm) under the SemiCov method for sample size $n = 50$, 100 and 150.*

Figure 1 gives the 95% pointwise simulation intervals for the eigenfunctions $\varphi_j(t)$,

defined as

$$\left[(1/2)\left\{\widehat{\varphi}_j^{(97)}(t)+\widehat{\varphi}_j^{(98)}(t)\right\},(1/2)\left\{\widehat{\varphi}_j^{(2)}(t)+\widehat{\varphi}_j^{(3)}(t)\right\}\right],$$

where $\widehat{\varphi}_j^{(i)}(t)$ is the ith largest value of $\{\widehat{\varphi}_j^i(t) : i = 1, \ldots, 100\}$, and $\widehat{\varphi}_j^i(t)$ is the estimate for $\varphi_j(t)$ from the ith simulated data set. The results show that the true eigenfunctions are captured by the 95% pointwise simulation intervals. Moreover, the pointwise simulation intervals become narrower as the number of sampling locations n increases, which supports the theory that the estimates of $\varphi_1(t)$ and $\varphi_2(t)$ are consistent.

Table 1 reports the mean and standard deviation of regression coefficient estimates from 100 simulated data sets using the three approaches. The regression coefficient estimates have lower bias and the standard deviations become smaller as the number of sampling locations n increases. Moreover, both our SemiCov method and the functional data analysis outperform ordinary least squares in terms of smaller standard deviations. This suggests that incorporating spatio-temporal structures can greatly improve the estimation of regression coefficients.

The standard errors of the regression coefficients, eigenvalues, and spatial parameter estimates can be obtained using the information matrix in Theorem 4. That is, for each simulated data set, define $\mathrm{sd}\{\widehat{\beta}\} = \mathrm{diag}\{H(\widehat{\beta})^{-1}\}^{1/2}$, $\mathrm{sd}\{\widehat{\lambda}\} = \mathrm{diag}\{H(\widehat{\lambda})^{-1}\}^{1/2}$, and $\mathrm{sd}\{\widehat{\vartheta}\} = \mathrm{diag}\{H(\widehat{\vartheta})^{-1}\}^{1/2}$, where $\widehat{\beta}$, $\widehat{\lambda}$ and $\widehat{\vartheta}$ are the estimates from the simulated data set, $H(\beta)$, $H(\lambda) = E\{-\ell''(\lambda, \lambda)\}$ and $H(\vartheta)$ are the information matrix for β, λ and ϑ, respectively. From the 100 simulated data sets, the mean of the standard errors (SDm) is computed for our SemiCov method and presented in Table 1. The results show that these

means are close to nominal true standard deviations of regression coefficient estimates.

For prediction, we consider two scenarios. In Scenario 1, prediction is carried out for multiple time points $t_{01}, \ldots, t_{0m}$ at an unsampled location s_0. It is straightforward to show that the best linear unbiased prediction (BLUP) of $y(s_0, t_0)$ is

$$\widetilde{y}(s_0, t_0) = x(s_0, t_0)^T \widetilde{\beta} + c_0^T \Sigma^{-1}(y - X\widetilde{\beta}),$$

where c_0 is an N-dimensional vector whose ith element is $\mathrm{cov}\{y(s_0, t_0), y_i\}$, y_i is the ith element of y, $\Sigma = \mathrm{cov}(y)$, and $\widetilde{\beta} = (X^T\Sigma^{-1}X)^{-1}X^T\Sigma^{-1}y$ (Cressie, 1993). Since Σ and c_0 are usually unknown, the estimates of Σ and c_0 are plugged in and an empirical best linear unbiased prediction is obtained.

To quantify the prediction error for the curve at locations s_0, a mean integral squared error,

$$\mathrm{MISE}(s_0) = \int_0^T \{\widetilde{y}(s_0, t) - y(s_0, t)\}^2 dt,$$

is used. In the simulation study, $T = 1$ and t_i are evenly distributed and thus, $\mathrm{MISE}(s_0)$ is estimated by $m^{-1}\sum_{i=1}^m \{\widetilde{y}(s_0, t_{0i}) - y(s_0, t_{0i})\}^2$. Moreover, we generate 5, 10, and 15 additional curves for sample size $n = 50$, 100, and 150, respectively, and set them aside for prediction. In the end, for M unsampled curves at $s_{01}, \ldots, s_{0M}$, we define the first mean squared prediction error (MSPE_1) as $M^{-1}\sum_{i=1}^M \mathrm{MISE}(s_{0i})$.

In Scenario 2, prediction is made about time points that are missing at a sampling location s_i for $i = 1, \ldots, n$. For m unsampled time points $t_{0i} = (t_{0i,1}, \ldots, t_{0i,m})^T$ at each location s_i, we define a second mean squared prediction error (MSPE_2) as

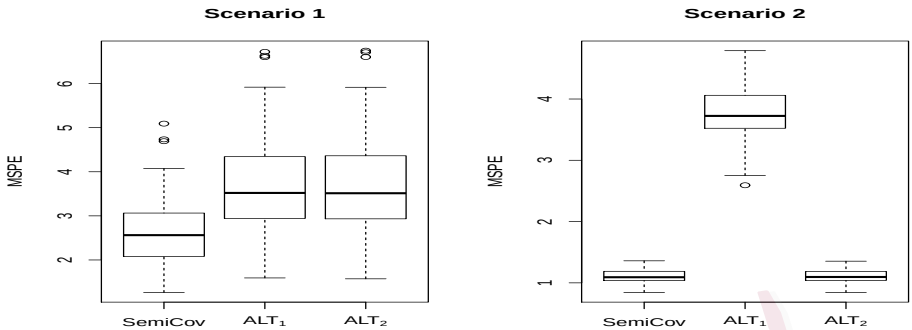

Figure 2: *The mean squared prediction error (MSPE) for Scenario 1 (left) and Scenario 2 (right) under our method (SemiCov) and two alternative approaches (ALT_1 and ALT_2).*

$(mn)^{-1}\sum_{i=1}^{n}\sum_{k=1}^{m}\{\widetilde{y}(s_i,t_{0i,k})-y(s_i,t_{0i,k})\}^2$. For the simulation, predictions are made at $\{(s_i,t_{0i}) : t_{0i}=(0.25,0.75)^T, i=1,\ldots,n\}$.

The prediction performance for different sample sizes are given in Table 1 and the box plots of them for $n = 100$ are given in Figure 2. The results in Scenario 1 show that ALT_2 performs better than ALT_1, while our SemiCov method outperforms both ALT_1 and ALT_2, which provides empirical evidence that incorporating spatial correlation between different locations can substantially improve prediction at unsampled locations. In Scenario 2, our SemiCov method and ALT_2 both outperform ALT_1, and our SemiCov method is slightly better than ALT_2 for prediction at sampled locations with missing time points.

Finally, Table 2 reports the mean, the standard deviation (SD), the mean standard error (SDm) of the estimates for spatio-temporal parameters. The means of the spatio-temporal parameter estimates approach the true values and the standard deviations become smaller as the sample size increases. Moreover, the mean standard error of the

n	Method	λ_1	r_1	λ_2	r_2	σ^2
	True Values	2.50	0.50	0.50	0.30	1.00
50	SemiCov	2.32	0.46	0.48	0.29	1.03
	SD	0.63	0.20	0.10	0.11	0.08
	SDm	0.65	0.18	0.12	0.12	0.05
100	SemiCov	2.31	0.47	0.52	0.32	1.02
	SD	0.45	0.14	0.09	0.11	0.05
	SDm	0.46	0.13	0.10	0.09	0.03
150	SemiCov	2.43	0.48	0.53	0.31	1.01
	SD	0.36	0.10	0.08	0.07	0.03
	SDm	0.41	0.11	0.08	0.07	0.03

Table 2: *The mean, standard deviation (SD) of spatial-temporal coefficients estimates under our method (SemiCov) for sample size* $n = 50$, 100 *and* 150.

spatio-temporal parameter estimates is fairly close to the nominal true standard deviation. For our SemiCov method, the simulated data sets are fitted with the number of eigenfunctions $J = 2$.

5.2 Data Example

The data consists of precipitation (in inches per 24-hour period) from January to December on the log-scale from 259 weather stations in Colorado (Reich and Davis, 2008; Chu et al., 2011), as shown in the left-hand panel of Figure 3. There are ten covariates of interest, including elevation, slope, aspect, and seven spectral bands from a satellite imagery (B1M through B7M). For model fitting, precipitation of 10 months (excluding precipitation of March and October) at 240 weather stations are used. Two types of prediction are considered. First, prediction is made at the remainder 19 weather stations and the prediction results are summarized by MSPE_1. Second, the March and October

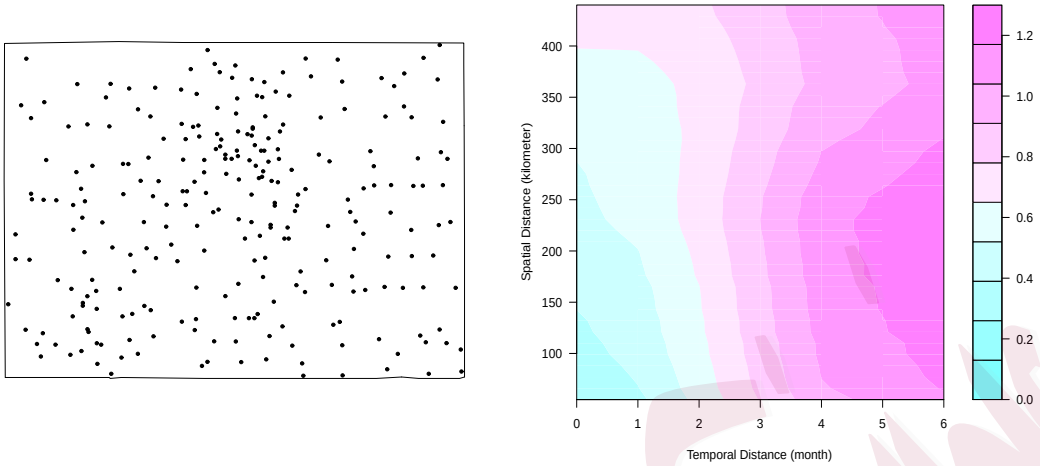

Figure 3: Map of locations of 259 weather stations in the Colorado precipitation data (left), and the empirical variogram over spatial and temporal lags (right).

precipitation for the 240 weather striations are predicted and the results are summarized by MSPE_2.

In the right-hand panel of Figure 3, the empirical variogram over spatial and temporal lags is presented, and suggests that there is a spatio-temporal dependence for Colorado precipitation data. Data analysis is performed by our SemiCov method and two alternative approaches. For our SemiCov method, we choose the number of components $J = 2$ such that $\sum_{j=1}^{J} \widehat{\lambda}_j / \sum_{j=1}^{n} \widehat{\lambda}_j \geq 80\%$, as suggested by Zhu et al. (2014). Furthermore, since there is multicollinearity among the covariates, a forward selection through AIC is applied. The resulting model contains two covariates elevation and B4M. The results without forward selection are reported in Table 3, while the results with forward selection are reported in Table 4. With SemiCov method, there is strong evidence of an elevation and B4M effect, while there is moderate evidence of an effect of B1M. For prediction of all

Method	Elevation	Slope	Aspect	B1M	B2M	B3M	B4M	B5M
SemiCov	0.190	0.003	0.006	0.091	0.006	0.032	-0.208	0.019
SE	0.019	0.010	0.009	0.062	0.026	0.043	0.072	0.037
ALT_1	0.046	0.047	0.010	-0.142	-0.079	0.052	-0.083	0.110
ALT_2	0.101	0.026	0.018	-0.145	-0.031	0.091	-0.077	0.004

	B6M	B7M	$MSPE_1$	$MSPE_2$
SemiCov	0.016	-0.002	0.143	0.085
SE	0.046	0.040	–	–
ALT_1	-0.011	-0.009	0.474	0.137
ALT_2	0.115	-0.047	0.473	0.077

Table 3: *Precipitation data example without forward selection: Regression coefficient estimates and mean squared prediction errors under our method (SemiCov) and two alternative approaches (ALT_1 and ALT_2), along with the standard errors (SE) for our SemiCov method.*

Method	Elevation	B4M	$MSPE_1$	$MSPE_2$
SemiCov	0.203	-0.059	0.140	0.085
SE	0.018	0.013	–	–
ALT_1	0.054	-0.173	0.469	0.140
ALT_2	0.101	-0.102	0.464	0.077

Table 4: *Precipitation data example with forward selection: Regression coefficient estimates and mean squared prediction errors under our method (SemiCov) and two alternative approaches (ALT_1 and ALT_2), along with the standard errors (SE) for our SemiCov method.*

time points at unsampled locations, our SemiCov method outperforms the two alternative methods. On the other hand, for prediction at the two time points set aside at sampling locations, both our method and the functional data analysis outperform the ordinary least squares method, while the functional data analysis is slightly better than our method in this case.

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Supplementary Materials

The supplementary materials contain proofs of Proposition 1 and Theorem 1–4, and additional numerical studies.

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