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## New Parsimonious Multivariate Spatial Model: Spatial Envelope

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### *Abstract:*

Dimension reduction provides a useful tool for analyzing high dimensional data. The recently developed *Envelope* method is a parsimonious version of the classical multivariate regression model through identifying a minimal reducing subspace of the responses. However, existing envelope methods assume an independent error structure in the model. While the assumption of independence is convenient, it does not address the additional complications associated with spatial or temporal correlations in the data. In this article, we introduce a *Spatial Envelope* method for dimension reduction in the presence of dependencies across space. We study the asymptotic properties of the proposed estimators and show that the asymptotic variance of the estimated regression coefficients under the

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spatial envelope model is smaller than that from the traditional maximum likelihood estimation. Furthermore, we present a computationally efficient approach for inference. The efficacy of the new approach is investigated through simulation studies and an analysis of an Air Quality Standard (AQS) dataset from the Environmental Protection Agency (EPA).

*Key words and phrases:* Dimension reduction, Grassmanian manifold, Matern covariance function, Spatial dependency.

## 1. Introduction

In many research areas, such as health science (Lave, and Seskin, 1973; Liang, Zeger, and Qaqish, 1992), environmental sciences (Guinness et al., 2014), and business (Cooper, Schindler, and Sun, 2003), etc., it is common to observe multiple outcomes simultaneously. The traditional multivariate linear model has proved to be useful in these cases to understand the relationship between response variables and predictors. Mathematically, the model is typically presented as:

$$\mathbf{Y} = \boldsymbol{\alpha} + \boldsymbol{\beta}\mathbf{X} + \boldsymbol{\epsilon}, \quad (1.1)$$

where  $\mathbf{Y} \in \mathbb{R}^r$  denotes the response vector,  $\mathbf{X} \in \mathbb{R}^p$  is a predictor vector,  $\boldsymbol{\alpha} \in \mathbb{R}^r$  denotes the vector of intercept,  $\boldsymbol{\beta} \in \mathbb{R}^{(r \times p)}$  is the matrix of regression coefficients, and  $\boldsymbol{\epsilon} \sim N_r(\mathbf{0}, \boldsymbol{\Sigma})$  is an error vector with  $\boldsymbol{\Sigma} \geq 0$  being

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an unknown covariance matrix (Christensen, 2001). In order to completely specify a multivariate linear model, there are  $r$  unknown intercepts,  $p \times r$  unknown parameters for the matrix of regression coefficients, and  $r(r+1)/2$  unknown parameters to specify an unstructured covariance matrix. Therefore, one must estimate  $r + pr + r(r+1)/2$  parameters which can be large with the increase of either  $r$  or  $p$  or both.

Based on the observation that some linear combinations of  $\mathbf{Y}$  do not depend on any of the predictors in some cases, Cook, Li, and Chiaromonte (2010) proposed the *Envelope* method as a parsimonious version of the classical multivariate linear model. This approach separates the  $\mathbf{Y}$  into material and immaterial parts, thereby allowing gains in estimation efficiency compared to the usual maximum likelihood estimation. The envelope approach constructs a link between the mean function and covariance matrix using a minimal reducing subspace such that the resulting number of parameters will be maximally reduced. Cook, Li, and Chiaromonte (2010) showed that the envelope estimator are at least as efficient as the standard maximum likelihood estimator (MLE). Along the same line, the idea of envelope has been further developed from both theoretical and computational points of view in a series of papers including, but not restricted to, Su and Cook (2011, 2012, 2013), Cook and Zhang (2015), and Cook, Forzani, and Su

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(2016). Furthermore, Li and Zhang (2017) and Zhang and Li (2017) extended the envelope model to the tensor response and tensor covariates, respectively.

Proposed envelope methodology by Cook, Li, and Chiaromonte (2010) assumes observations are taken under identical conditions where independence is assured. While models based on the independence assumption are extremely useful, their use is limited in applications where the data has inherent dependency (Cressie, 1993). For example, in environment monitoring, each station collects data concerning several pollutants such as ozone, carbon monoxide, nitrogen dioxide, etc. These data have a special type of dependency which is called spatial correlation. Myers (1991) and Ver Hoef and Barry (1998) used pseudo cross-variogram to model the multivariate spatial cross-correlation. In addition, Chiles and Delfiner (1999) and Wackernagel (2003) introduced several multivariate covariogram and cross-variogram that results in a nonnegative definite covariance matrix (also called valid spatial covariance function). Linear Coregionalization Models (LCM) is one the most commonly used approaches in the multivariate spatial data analysis. This model assumes that the observed variables are linear combinations of sets of independent underlying variables and they covary jointly over a region. Different methods have been proposed for

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fitting LCM in literatures including, but not restricted to, least square approach (Goulard and Voltz, 1992), expectation-maximization (EM) algorithm (Zhang, 2007), etc. Gneiting, Kleiber, and Schlather (2010) introduced a flexible and interpretable Matern cross-covariance function for multivariate spatial random field. Genton and Kleiber (2015) provided a comprehensive review on common approaches for building a valid spatial cross-covariance models. In this paper, we introduce a *Spatial Envelope* approach for spatially correlated data. This new approach addresses the impact of spatial correlation among observations in the model and thus provides more efficient estimators than the traditional multivariate linear model and linear coregionalization model. Accounting for the intrinsic spatial correlation allows the appropriate inference on aforementioned data.

The rest of the paper is organized as follows: in section 2, we briefly review envelope methodology. The spatial envelope is detailed in Section 3. Section 4 and 5 provides asymptotic variance and prediction properties of the proposed method. Section 6 and 7 contain a simulation study and the analysis of the northeastern United State air pollution data. We conclude the article with a short discussion in Section 8. All technical details are provided in the Supplement.

## 2. Brief Review of envelope

For model (1.1), suppose that we can find an orthogonal matrix  $(\mathbf{\Gamma}_1, \mathbf{\Gamma}_0) \in \mathbb{R}^{r \times r}$  that satisfies the following two conditions: (i)  $\text{span}(\boldsymbol{\beta}) \subseteq \text{span}(\mathbf{\Gamma}_1)$ , and (ii)  $\mathbf{\Gamma}_1^T \mathbf{Y}$  is conditionally independent of  $\mathbf{\Gamma}_0^T \mathbf{Y}$  given  $\mathbf{X}$ . That is,  $\mathbf{\Gamma}_0^T \mathbf{Y}$  is marginally independent of  $\mathbf{X}$  and conditionally independent of  $\mathbf{X}$  given  $\mathbf{\Gamma}_1^T \mathbf{Y}$ . Then, we can rewrite  $\boldsymbol{\Sigma}$  as

$$\boldsymbol{\Sigma} = \mathbf{P}_{\mathbf{\Gamma}_1} \boldsymbol{\Sigma} \mathbf{P}_{\mathbf{\Gamma}_1} + \mathbf{Q}_{\mathbf{\Gamma}_1} \boldsymbol{\Sigma} \mathbf{Q}_{\mathbf{\Gamma}_1}, \quad (2.1)$$

where  $\mathbf{P}_{(\cdot)}$  represents an orthogonal projection operator with respect to the standard inner product and  $\mathbf{Q}_{(\cdot)} = \mathbf{I}_r - \mathbf{P}_{(\cdot)}$  is the projection onto its complement space. Cook, Li, and Chiaromonte (2010) used this idea to construct the unique smallest subspace  $\text{span}(\mathbf{\Gamma}_1)$  that satisfies (2.1) and contains  $\text{span}(\boldsymbol{\beta})$ . In summary, the goal is to find a subspace  $\text{span}(\mathbf{\Gamma}_1) \subseteq \mathbb{R}^r$  such that

$$\mathbf{Q}_{\mathbf{\Gamma}_1} \mathbf{Y} | \mathbf{X} \sim \mathbf{Q}_{\mathbf{\Gamma}_1} \mathbf{Y}, \quad (2.2a)$$

$$\mathbf{Q}_{\mathbf{\Gamma}_1} \mathbf{Y} \perp\!\!\!\perp \mathbf{P}_{\mathbf{\Gamma}_1} \mathbf{Y} | \mathbf{X}. \quad (2.2b)$$

where  $\perp\!\!\!\perp$  means statistical independence. This minimal subspace is called the  $\boldsymbol{\Sigma}$ -envelope of  $\text{span}(\boldsymbol{\beta})$  in full and the envelope for brevity.  $\mathbf{P}_{\mathbf{\Gamma}_1} \mathbf{Y}$  and  $\mathbf{Q}_{\mathbf{\Gamma}_1} \mathbf{Y}$  are referred as material and immaterial parts of  $\mathbf{Y}$ , respectively, where  $u \leq r$ , is referred as the dimension of the envelope subspace.

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Following the envelope idea, model (1.1) can be rewritten as

$$\mathbf{Y} = \boldsymbol{\alpha} + \boldsymbol{\Gamma}_1 \boldsymbol{\eta} \mathbf{X} + \boldsymbol{\epsilon}, \quad (2.3)$$

where  $\boldsymbol{\beta} = \boldsymbol{\Gamma}_1 \boldsymbol{\eta}$ ,  $\boldsymbol{\eta} \in \mathbb{R}^{u \times p}$ , and  $\boldsymbol{\Sigma} = \boldsymbol{\Sigma}_0 + \boldsymbol{\Sigma}_1$  such that  $\boldsymbol{\Sigma}_0 = \mathbf{Q}_{\boldsymbol{\Gamma}_1} \boldsymbol{\Sigma} \mathbf{Q}_{\boldsymbol{\Gamma}_1}^T$  being the variance of the immaterial part of response and  $\boldsymbol{\Sigma}_1 = \mathbf{P}_{\boldsymbol{\Gamma}_1} \boldsymbol{\Sigma} \mathbf{P}_{\boldsymbol{\Gamma}_1}^T$  being the variance of the material part of response. Cook, Li, and Chiaromonte (2010) showed that  $\boldsymbol{\Sigma} = \boldsymbol{\Gamma}_1 \boldsymbol{\Omega}_1 \boldsymbol{\Gamma}_1^T + \boldsymbol{\Gamma}_0 \boldsymbol{\Omega}_0 \boldsymbol{\Gamma}_0^T$  where  $\boldsymbol{\Omega}_1 = \text{var}(\boldsymbol{\Gamma}_1^T \mathbf{Y}) \in \mathbb{R}^{u \times u}$  and  $\boldsymbol{\Omega}_0 = \text{var}(\boldsymbol{\Gamma}_0^T \mathbf{Y}) \in \mathbb{R}^{(r-u) \times (r-u)}$  are unknown positive definite matrices with  $0 < u \leq r$ . Here, one only needs to estimate  $r + pu + r(r+1)/2$  parameters. The difference in the number of parameters between the envelope and classical multivariate regression is  $p(r-u)$ . More details can be found in Cook, Li, and Chiaromonte (2010) and the references therein.

### 3. New Spatial Envelope

In this section, we detail the spatial envelope method. We start with a review of spatial multivariate model, then derive the likelihood function of spatial envelope model, and show the computational steps for the parameter estimation. Let  $\mathbf{Y}(s_i) = (y_1(s_i), \dots, y_r(s_i))^T$  be an  $r$ -variate stochastic spatial response vector along with  $p$  regressors  $\mathbf{X}(s_i) = (x_1(s_i), \dots, x_p(s_i))^T$  observed at locations  $s = \{s_1, s_2, \dots, s_n; s_i \in \mathbb{R}^2; i = 1, 2, \dots, n\}$ . The



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multivariate spatial regression model can be written as:

$$Y(s_i) = \boldsymbol{\alpha} + \boldsymbol{\beta}X(s_i) + \boldsymbol{\epsilon}(s_i), \quad (3.1)$$

where  $Y(s)$  denotes the  $r \times 1$  response vector at location  $s_i$  for  $i = 1, \dots, n$ ,  $X(s)$  is the  $p \times 1$  vector of fixed and nonstochastic covariates. Furthermore,  $\boldsymbol{\alpha}$  denotes the  $r \times 1$  vector of intercept,  $\boldsymbol{\beta}$  is the  $r \times p$  matrix of regression coefficients, and  $\boldsymbol{\epsilon}$  is a multivariate spatial process with mean 0. We assume that the data generating process is second order stationary and the covariance of the response vectors  $Y(s_i)$  and  $Y(s_j)$  at two sites  $s_i$  and  $s_j$  is a function of distance between the two sites. Namely the covariance can be written as:

$$\text{Cov}(Y(s_i), Y(s_j)) = C_{ij}(\mathbf{h}), \quad \mathbf{h} = \|s_i - s_j\|, \quad (3.2)$$

where  $\|\cdot\|$  denotes Euclidean distance. The function  $C(\mathbf{h}) = \{C_{ij}(\mathbf{h})\}$  is the multivariate covariogram,  $C_{ij}(\cdot)$  is the direct covariogram for  $i = j$  and cross-covariogram for  $i \neq j$ . By adopting the *proportional correlation model* (Chiles and Delfiner, 1999), the spatial covariance function can be written as

$$C_{ij}(\mathbf{h}) = \mathbf{V}\rho_{ij}(\mathbf{h}), \quad (3.3)$$

where  $\mathbf{V}$  is an  $r \times r$  positive definite matrix and  $\rho_{ij}(\mathbf{h})$  is the spatial correlation between two sites  $s_i$  and  $s_j$  (Wackernagel, 2003). Estimating the

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correlation function solely from the data without any structural assumptions is difficult and sometimes infeasible. Usually, it is assumed that the form of the correlation function is a known function but with unknown parameters  $\boldsymbol{\theta}$ , which control range, smoothness, and other characteristics of the correlation function. Thus instead of  $\rho(\mathbf{h})$ , we use  $\rho(\mathbf{h}, \boldsymbol{\theta})$  to represent unknown parameters  $\boldsymbol{\theta}$  in the correlation function. For simplicity of notation,  $\rho(\mathbf{h}, \boldsymbol{\theta})$  is denoted by  $\rho(\boldsymbol{\theta})$  throughout the rest of the paper.

The matrix form for model (3.1)

$$\mathbf{Y}(s) = \boldsymbol{\alpha}^T \otimes \mathbf{1}_n + \mathbf{X}(s)\boldsymbol{\beta}^T + \boldsymbol{\epsilon}(s), \quad (3.4)$$

where  $\mathbf{Y}(s) = \begin{pmatrix} Y^T(s_1) \\ \vdots \\ Y^T(s_n) \end{pmatrix}$  denotes the  $n \times r$  response matrix  $\mathbf{X}(s)$  is the  $n \times p$

matrix of covariates. Furthermore,  $\otimes$  denotes the Kronecker product and

$\mathbf{1}_n$  is an  $n \times 1$  column vector with 1 at each entry. From the envelope idea,

$\mathbf{V}$  can be written as  $\mathbf{V}_0 + \mathbf{V}_1$  where  $\mathbf{V}_0 = \mathbf{Q}_{\mathbf{\Gamma}_1} \mathbf{V} \mathbf{Q}_{\mathbf{\Gamma}_1}$  denotes the covariance matrix associated with the immaterial part of response and  $\mathbf{V}_1 = \mathbf{P}_{\mathbf{\Gamma}_1} \mathbf{V} \mathbf{P}_{\mathbf{\Gamma}_1}$

denotes the covariance matrix associated with the material part where  $\mathbf{\Gamma}_1$

is the semi-orthogonal basis of  $\text{span}(\mathbf{V}_1)$ . Hence, the spatial covariance

matrix of  $C_{ij}(\mathbf{h})$  can be written as follows:

$$C_{ij}(\mathbf{h}) = \mathbf{V} \rho_{ij}(\boldsymbol{\theta})$$

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$$= (\mathbf{V}_0 + \mathbf{V}_1)\rho_{ij}(\boldsymbol{\theta}) \quad (3.5)$$

Let  $0 < u \leq r$  denotes the structural dimension of the envelope, where  $u$  can be selected using a modified information criterion such as modified BIC (Li and Zhang (2017)), model free dimension selection such as full Grassmanian (FG; Zhang and Mai, 2017) and the 1-D algorithm (Cook and Zhang, 2016), or cross-validation. More details can be found in (Zhang and Mai, 2017; Zhang, Wang, and Wu, 2018) and the references therein.

To illustrate the estimation, we use a *vec* operator on the response matrix. That is, let  $\mathbb{Y}(s) = \text{vec}(\mathbf{Y}(s))$  be an  $nr \times 1$  vector for the vectorized response variable, and  $\mathbb{X}(s) = \mathbf{I}_r \otimes \mathbf{X}(s)$  be an  $nr \times pr$  block diagonal matrix having  $\mathbf{X}_i(s)$  as blocks. Thus, the vectorized version of the multivariate spatial linear model can be written as:

$$\mathbb{Y}(s) = \boldsymbol{\alpha} \otimes \mathbf{1}_n + \mathbb{X}(s)\boldsymbol{\beta}^* + \boldsymbol{\epsilon}^*(s). \quad (3.6)$$

where  $\boldsymbol{\alpha}$  is an  $r \times 1$  vector of intercept,  $\boldsymbol{\beta}^* = \text{vec}(\boldsymbol{\beta}^T)$  shows an  $pr \times 1$  vector of regression coefficients, and  $\boldsymbol{\epsilon}^*(s)$  is an  $nr \times 1$  vector of spatial errors with mean 0. With the use of proportional covariance model and the vectorization of the response matrix, the  $nr \times nr$  covariance matrix of the response variables  $\boldsymbol{\Sigma}_{\mathbb{Y}}$ , can be written as  $\mathbf{V} \otimes \boldsymbol{\rho}(\boldsymbol{\theta})$ .

The likelihood function of model (3.6) is:

$$L(\boldsymbol{\alpha}, \boldsymbol{\beta}^*, \mathbf{V}, \boldsymbol{\theta}) = [\det(\mathbf{V} \otimes \boldsymbol{\rho}(\boldsymbol{\theta}))]^{-\frac{1}{2}} \times \exp \left\{ -\frac{1}{2} (\mathbb{Y}(s) - \boldsymbol{\alpha} \otimes \mathbf{1}_n - \mathbb{X}(s)\boldsymbol{\beta}^*)^T (\mathbf{V} \otimes \boldsymbol{\rho}(\boldsymbol{\theta}))^{-1} (\mathbb{Y}(s) - \boldsymbol{\alpha} \otimes \mathbf{1}_n - \mathbb{X}(s)\boldsymbol{\beta}^*) \right\}, \quad (3.7)$$

where  $\det(\cdot)$  denotes the determinant of the matrix. Suppose the response vector can be decomposed into the material and immaterial part,  $\mathbb{Y}_1 = (\mathbf{I}_r \otimes \mathbf{P}_{\mathbf{r}_1})\mathbb{Y}(s)$  and  $\mathbb{Y}_0 = (\mathbf{I}_r \otimes \mathbf{Q}_{\mathbf{r}_1})\mathbb{Y}(s)$ , respectively. From (3.5), the covariance matrix of  $\mathbb{Y}(s)$  can be written as follows:

$$\begin{aligned} \boldsymbol{\Sigma}_{\mathbb{Y}} &= \mathbf{V} \otimes \boldsymbol{\rho}(\boldsymbol{\theta}) \\ &= \mathbf{V}_0 \otimes \boldsymbol{\rho}(\boldsymbol{\theta}) + \mathbf{V}_1 \otimes \boldsymbol{\rho}(\boldsymbol{\theta}). \end{aligned} \quad (3.8)$$

Combining (3.7) and (3.8), we have

$$L^u(\boldsymbol{\alpha}, \boldsymbol{\beta}^*, \mathbf{V}_0, \mathbf{V}_1, \boldsymbol{\theta}) = L_1^u(\boldsymbol{\alpha}, \boldsymbol{\beta}^*, \mathbf{V}_1, \boldsymbol{\theta}) \times L_2^u(\boldsymbol{\alpha}, \mathbf{V}_0, \boldsymbol{\theta}), \quad (3.9)$$

with

$$\begin{aligned} L_1^u(\boldsymbol{\alpha}, \boldsymbol{\beta}^*, \mathbf{V}_1, \boldsymbol{\theta}) &= [\det_0(\mathbf{V}_1)]^{-\frac{n}{2}} [\det(\boldsymbol{\rho}(\boldsymbol{\theta}))]^{-\frac{r}{2}} \\ &\times \exp \left\{ -\frac{1}{2} (\mathbb{Y}(s) - \boldsymbol{\alpha} \otimes \mathbf{1}_n - \mathbb{X}(s)\boldsymbol{\beta}^*)^T \left( \mathbf{V}_1^\dagger \otimes \boldsymbol{\rho}^{-1}(\boldsymbol{\theta}) \right) (\mathbb{Y}(s) - \boldsymbol{\alpha} \otimes \mathbf{1}_n - \mathbb{X}(s)\boldsymbol{\beta}^*) \right\}, \\ L_2^u(\boldsymbol{\alpha}, \mathbf{V}_0, \boldsymbol{\theta}) &= [\det_0(\mathbf{V}_0)]^{-\frac{n}{2}} [\det(\boldsymbol{\rho}(\boldsymbol{\theta}))]^{-\frac{r}{2}} \\ &\times \exp \left\{ -\frac{1}{2} (\mathbb{Y}(s) - \boldsymbol{\alpha} \otimes \mathbf{1}_n)^T \left( \mathbf{V}_0^\dagger \otimes \boldsymbol{\rho}^{-1}(\boldsymbol{\theta}) \right) (\mathbb{Y}(s) - \boldsymbol{\alpha} \otimes \mathbf{1}_n) \right\}, \end{aligned} \quad (3.10)$$

where  $\dagger$  denotes the Moore-Penrose inverse and  $\det_0(\mathbf{A})$  denotes the product of non-zero eigenvalues of a non-zero symmetric matrix  $\mathbf{A}$ . The likelihood in equation (3.7) can be factorized as equation (3.9) from  $\text{span}(\boldsymbol{\beta}) \subseteq \text{span}(\mathbf{V}_1)$ , and  $(\mathbf{V}_0^\dagger \otimes \boldsymbol{\rho}^{-1}(\boldsymbol{\theta}))\mathbb{X}\boldsymbol{\beta}^* = \mathbf{0}$ . This factorization is detailed in the Supplement, section S2.

The objective is to maximize the likelihood in (3.9) over  $\boldsymbol{\beta}^*, \mathbf{V}_0, \mathbf{V}_1$ , and  $\boldsymbol{\theta}$  subject to the constraints:

$$\begin{aligned} \text{span}(\boldsymbol{\beta}) &\subseteq \text{span}(\mathbf{V}_1), \\ \mathbf{V}_0 \mathbf{V}_1 &= \mathbf{0}. \end{aligned} \tag{3.11}$$

Thus, the multivariate spatial model in (3.6) can be written as

$$\begin{aligned} \mathbb{Y}(s) &= \boldsymbol{\alpha} \otimes \mathbf{1}_n + \mathbb{X}(s) \text{vec}(\boldsymbol{\eta}^T \boldsymbol{\Gamma}_1^T) + \boldsymbol{\epsilon}^*(s), \\ \boldsymbol{\Sigma} &= (\boldsymbol{\Gamma}_1 \boldsymbol{\Omega}_1 \boldsymbol{\Gamma}_1^T + \boldsymbol{\Gamma}_0 \boldsymbol{\Omega}_0 \boldsymbol{\Gamma}_0^T) \otimes \boldsymbol{\rho}(\boldsymbol{\theta}), \end{aligned} \tag{3.12}$$

where  $\boldsymbol{\Gamma}_1$  denotes the semi-orthogonal basis for  $\text{span}(\mathbf{V}_1)$ ,  $\boldsymbol{\Gamma}_0$  denotes the semi-orthogonal basis for the orthogonal complement space of  $\text{span}(\mathbf{V}_1)$ ,  $\boldsymbol{\Omega}_1$  denotes the covariance of the material part of response,  $\boldsymbol{\Omega}_2$  denotes the covariance of the immaterial part of response, and  $\boldsymbol{\eta} \in \mathbb{R}^{u \times r}$  is chosen such that  $\boldsymbol{\beta}^* = \text{vec}(\boldsymbol{\eta}^T \boldsymbol{\Gamma}_1^T)$ .

As mentioned by Cook, Li, and Chiaromonte (2010), the gradient-based algorithms for Grassmann optimization (Edelman, Arias, and Smith, 1998) require a coordinate version of the objective function which must have con-

tinuous directional derivatives. The optimization depends on minimizing the logarithm of  $\mathbf{D}$  over the Grassmann manifold  $\mathbb{G}^{r \times u}$ , where

$$\mathbf{D} = \det(\mathbf{P}_{\mathbf{V}_1} \hat{\Sigma}_{\text{res}} \mathbf{P}_{\mathbf{V}_1} + \mathbf{Q}_{\mathbf{V}_1} \hat{\Sigma}_{\mathbb{Y}} \mathbf{Q}_{\mathbf{V}_1}),$$

and  $\mathbf{D}$  is the partially maximized likelihood function. The derivation of  $\mathbf{D}$  is detailed in the Supplement, section S3. Let  $\hat{\Gamma}_1$  be the semi-orthogonal basis for  $\text{span}(\mathbf{V}_1)$  and  $\hat{\Gamma}_0$  be the semi-orthogonal basis for  $\text{span}(\mathbf{V}_0)$ . Then  $\hat{\eta} = \hat{\Gamma}_1^T \hat{\beta}$ ,  $\hat{\Omega}_1 = \hat{\Gamma}_1^T \hat{\Sigma}_{\text{res}} \hat{\Gamma}_1$  and  $\hat{\Omega}_0 = \hat{\Gamma}_0^T \hat{\Sigma}_{\mathbb{Y}} \hat{\Gamma}_0$ , where  $\hat{\Sigma}_{\mathbb{Y}}$  and  $\hat{\Sigma}_{\text{res}}$  are the marginal covariance matrix of  $\mathbb{Y}$  and the residual covariance matrix, respectively. Let  $\log \det(\cdot)$  denote the composite function  $\log \circ \det(\cdot)$ . Then, the coordinate form of the  $\log \mathbf{D}$

$$\log \mathbf{D} = \log \det \left( \Gamma_1^T \left( \mathbf{H}^T \hat{\rho}^{-1}(\theta) \mathbf{H} - \mathbf{H}^T \hat{\rho}^{-1}(\theta) \mathbf{G} \left( \mathbf{G}^T \hat{\rho}^{-1}(\theta) \mathbf{G} \right)^{-1} \mathbf{G}^T \hat{\rho}^{-1}(\theta) \mathbf{H} \right) \Gamma_1 + \Gamma_0^T (\mathbf{H}^T \hat{\rho}^{-1}(\theta) \mathbf{H}) \Gamma_0 \right) \quad (3.13)$$

where  $\mathbf{H} = \mathbf{Y} - \bar{\mathbf{Y}} \otimes \mathbf{1}_n$ , and  $\mathbf{G} = \mathbf{X} - \bar{\mathbf{X}} \otimes \mathbf{1}_n$ .

In order to obtain the parameters of spatial envelope model, the objective function (3.13) can be minimized by the gradient based Grassmann optimization. To do this, first obtain an initial value for  $\hat{\Sigma}_{\mathbf{Y}}^0$ ,  $\hat{\Sigma}_{\text{res}}^0$ , and  $\hat{\beta}_{MLE}$ , the marginal covariance matrix of  $\mathbb{Y}$ , the residual covariance matrix, and the maximum likelihood estimate for  $\beta$  from the fit of the full model

(3.6). Set  $\Theta^1 = \Theta^0$  where  $\Theta = \{\boldsymbol{\theta}, \mathbf{V}_0, \mathbf{V}_1\}$  and  $\mathbf{V}_0$  and  $\mathbf{V}_1$  can be obtained using traditional envelope model and  $\boldsymbol{\theta}$  can be obtained using linear coregionalization model. Then, we estimate  $\mathbf{P}_{\mathbf{V}_1^m}$  by minimizing the objective function (3.13) over the Grassmann manifold  $\mathbb{G}^{(r \times u)}$ , and estimate  $\mathbf{P}_{\mathbf{V}_0^m}$  by  $\hat{\mathbf{P}}_{\mathbf{V}_0^m} = \mathbf{I} - \hat{\mathbf{P}}_{\mathbf{V}_1^m}$ . In order to update the covariance function of material and immaterial parts of the spatial envelope, fix  $\boldsymbol{\theta}^m$  and estimate  $\mathbf{V}_0^m$  and  $\mathbf{V}_1^m$  by  $\hat{\mathbf{V}}_0^m = \hat{\mathbf{P}}_{\mathbf{V}_0^m} \hat{\boldsymbol{\Sigma}}_{\mathbf{Y}}^m \hat{\mathbf{P}}_{\mathbf{V}_0^m}$  and  $\hat{\mathbf{V}}_1^m = \hat{\mathbf{P}}_{\mathbf{V}_1^m} \hat{\boldsymbol{\Sigma}}_{\text{res}}^m \hat{\mathbf{P}}_{\mathbf{V}_1^m}$ . Then, fix  $\mathbf{V}_0^m$  and  $\mathbf{V}_1^m$  and maximize  $L^{(u)}(\boldsymbol{\alpha}, \boldsymbol{\beta}, \mathbf{V}_0^m, \mathbf{V}_1^m, \boldsymbol{\theta}^m)$  over  $\boldsymbol{\theta}$  by solving the following minimization problem using numerical algorithm such as Newton-Raphson method:

$$\hat{\boldsymbol{\theta}}^m = \underset{\boldsymbol{\theta}}{\operatorname{argmin}} \{ r \det(\boldsymbol{\rho}(\boldsymbol{\theta})) + \frac{1}{2} \operatorname{tr} \left( \left( \mathbf{Q}_{(\boldsymbol{\rho}^{-\frac{1}{2}}(\boldsymbol{\theta})\mathbf{G})} \boldsymbol{\rho}^{-\frac{1}{2}}(\boldsymbol{\theta}) \mathbf{H} \right) \mathbf{V}_1^{m\dagger} \left( \mathbf{Q}_{(\boldsymbol{\rho}^{-\frac{1}{2}}(\boldsymbol{\theta})\mathbf{G})} \boldsymbol{\rho}(\boldsymbol{\theta})^{-\frac{1}{2}} \mathbf{H} \right)^T + \boldsymbol{\rho}^{-\frac{1}{2}}(\boldsymbol{\theta}) \mathbf{H} \mathbf{V}_0^{m\dagger} \mathbf{H}^T \boldsymbol{\rho}^{-\frac{1}{2}}(\boldsymbol{\theta}) \right) \}. \quad (3.14)$$

Now, update  $\hat{\boldsymbol{\Sigma}}_{\mathbf{Y}}^m$  and  $\hat{\boldsymbol{\Sigma}}_{\text{res}}^m$  using the new estimate for  $\mathbf{V}_0$ ,  $\mathbf{V}_1$ , and  $\boldsymbol{\theta}$ . Then, check the convergence. If  $\|\Theta^{m+1} - \Theta^m\| < \delta$  where  $\delta$  is a pre-specified tolerance level, then stop the iteration, output the final spatial envelope estimators and estimate  $\boldsymbol{\beta}$  by  $\hat{\boldsymbol{\beta}} = \hat{\mathbf{P}}_{\mathbf{V}_1} \hat{\boldsymbol{\beta}}_{MLE}$ ; otherwise, set  $m := m + 1$  and redo the procedure. Finally, estimate the intercept by  $\hat{\boldsymbol{\alpha}} = \bar{\mathbf{Y}} - \bar{\mathbf{X}} \hat{\boldsymbol{\beta}}^T$ . When the problem reduces to a standard envelope estimation problem, the

fast algorithm for the envelope such as Cook, Forzani, and Su (2016) can be applied.

#### 4. Theoretical Properties

In what follows, we study the asymptotic properties of the spatial envelope parameter estimates. The regression coefficients can be written as  $\boldsymbol{\beta} = \boldsymbol{\Gamma}_1 \boldsymbol{\eta}$ . Furthermore,  $\mathbf{V}_0 = \boldsymbol{\Gamma}_0 \boldsymbol{\Omega}_0 \boldsymbol{\Gamma}_0^T$  and  $\mathbf{V}_1 = \boldsymbol{\Gamma}_1 \boldsymbol{\Omega}_1 \boldsymbol{\Gamma}_1^T$  are the covariance of the immaterial part and material part to the regression, respectively. Therefore, aside from the intercept, the parameters of spatial envelope model in equation (3.6) can be combined into the vector as follows:

$$\boldsymbol{\phi} = \begin{bmatrix} \text{vec}(\boldsymbol{\eta}) \\ \text{vec}(\boldsymbol{\Gamma}_1) \\ \text{vech}(\boldsymbol{\Omega}_1) \\ \text{vech}(\boldsymbol{\Omega}_0) \end{bmatrix} \equiv \begin{bmatrix} \phi_1 \\ \phi_2 \\ \phi_3 \\ \phi_4 \end{bmatrix} \quad (4.1)$$

where the  $\text{vec}(\cdot)$  denotes the vector operator and  $\text{vech}(\cdot)$  denotes vector half operator. For background on these operators, see Seber (2008). Here we focus on the following parameters under the spatial envelope model:

$$\boldsymbol{\psi}(\boldsymbol{\phi}) = \begin{bmatrix} \text{vec}(\boldsymbol{\beta}^*) \\ \text{vech}(\mathbf{V}) \end{bmatrix} = \begin{bmatrix} \text{vec}(\boldsymbol{\eta}^T \boldsymbol{\Gamma}_1^T) \\ \text{vech}((\boldsymbol{\Gamma}_1 \boldsymbol{\Omega}_1 \boldsymbol{\Gamma}_1^T + \boldsymbol{\Gamma}_0 \boldsymbol{\Omega}_0 \boldsymbol{\Gamma}_0^T)) \end{bmatrix} \equiv \begin{bmatrix} \psi_1(\boldsymbol{\phi}) \\ \psi_2(\boldsymbol{\phi}) \end{bmatrix} \quad (4.2)$$



Let

$$\Psi = \begin{bmatrix} \frac{\partial \psi_1}{\partial \phi_1^T} & \cdots & \frac{\partial \psi_1}{\partial \phi_4^T} \\ \frac{\partial \psi_2}{\partial \phi_1^T} & \cdots & \frac{\partial \psi_2}{\partial \phi_4^T} \end{bmatrix} \quad (4.3)$$

denote the gradient matrix. Using this gradient matrix and following Cook, Li, and Chiaromonte (2010), we present the following asymptotic properties of proposed estimators.

**Lemma 1:** Suppose  $\bar{\mathbf{X}} = \mathbf{0}$ , the Fisher information,  $\mathbf{J}$ , for  $\psi(\phi)$  in the model (3.6) is as follows:

$$\begin{aligned} \mathbf{J} &= \begin{bmatrix} \frac{1}{n} \mathbb{X}^T (\mathbf{V}^{-1} \otimes \boldsymbol{\rho}^{-1}(\boldsymbol{\theta})) \mathbb{X} & \mathbf{0} \\ \mathbf{0} & \frac{1}{2} \mathbf{E}_r^T (\mathbf{V}^{-1} \otimes \mathbf{V}^{-1}) \mathbf{E}_r \end{bmatrix} \\ &= \begin{bmatrix} \mathbf{V}^{-1} \otimes \left( \frac{\mathbf{X}^T \boldsymbol{\rho}^{-1}(\boldsymbol{\theta}) \mathbf{X}}{n} \right) & \mathbf{0} \\ \mathbf{0} & \frac{1}{2} \mathbf{E}_r^T (\mathbf{V}^{-1} \otimes \mathbf{V}^{-1}) \mathbf{E}_r \end{bmatrix}. \end{aligned} \quad (4.4)$$

where  $\mathbf{E}_r \in R^{r^2 \times r(r+1)/2}$  is an expansion matrix such that for a matrix  $\mathbf{A}$ ,  $\text{vec}(\mathbf{A}) = \mathbf{E}_r \text{vech}(\mathbf{A})$ , and  $\text{diag}(\mathbf{A})$  is the matrix with the diagonal elements of  $\mathbf{A}$ . The derivation of  $\mathbf{J}$  is provided in the Supplement, section S4.

**Theorem 1:** Suppose  $\bar{\mathbf{X}} = \mathbf{0}$  and  $\mathbf{J}$  is the Fisher information defined in lemma 1. Let  $\boldsymbol{\Lambda} = \mathbf{J}^{-1}$  be the asymptotic variance of the MLE under the full model. Then

$$\sqrt{n}(\hat{\phi} - \phi) \rightarrow N(\mathbf{0}, \boldsymbol{\Lambda}_0) \quad (4.5)$$

where  $\boldsymbol{\Lambda}_0 = \Psi(\Psi^T \boldsymbol{\Lambda} \Psi)^\dagger \Psi$ . Furthermore,  $\boldsymbol{\Lambda}^{-\frac{1}{2}}(\boldsymbol{\Lambda} - \boldsymbol{\Lambda}_0)\boldsymbol{\Lambda}^{-\frac{1}{2}} \geq 0$ , which

means the asymptotic variance of the parameter estimation under the spatial envelope model is smaller than their estimate under MLE. Proof of this theorem can be found in the Supplement, section S5.

**Corollary 1:** The asymptotic variance (avar) of  $\sqrt{n}\boldsymbol{\beta}^*$  can be written as

$$avar(\sqrt{n}\boldsymbol{\beta}^*) = K_{rp} \left\{ \left( \frac{\mathbf{X}^T \boldsymbol{\rho}(\boldsymbol{\theta})^{-1} \mathbf{X}}{n} \right)^{-1} \otimes \boldsymbol{\Gamma}_1 \boldsymbol{\Omega}_1 \boldsymbol{\Gamma}_1^T + (\boldsymbol{\eta}^T \otimes \boldsymbol{\Gamma}_0) (\Psi_2^T \mathbf{J} \Psi_2)^\dagger (\boldsymbol{\eta} \otimes \boldsymbol{\Gamma}_0^T) \right\} K_{rp}^T \quad (4.6)$$

where  $\Psi_2 = \left( \frac{\partial \psi_1}{\partial \phi_2^T}, \frac{\partial \psi_2}{\partial \phi_2^T} \right)^T$  and  $K_{rp} \in \mathbb{R}^{rp \times rp}$  is the unique matrix such that for a matrix  $\mathbf{A}$ ,  $vec(\mathbf{A}^T) = K_{rp} vec(\mathbf{A})$  i.e.  $K_{rp}$  transforms the  $vec$  of a matrix into the  $vec$  of its transpose. Proof of this theorem can be found in the Supplement, section S6.

To gain further insight into the structure of the spatial envelope, we present the simply version of the asymptotic variance of the  $\boldsymbol{\beta}^*$  for the cases that we have one covariate,  $\boldsymbol{\Omega}_1 = \sigma_1^2 \mathbf{I}_u$ , and  $\boldsymbol{\Omega}_0 = \sigma_0^2 \mathbf{I}_{r-u}$ . Then, the asymptotic variance of the  $\boldsymbol{\beta}^*$  can be shown to be

$$avar(\sqrt{n}\boldsymbol{\beta}^*) = \frac{n\sigma_1^2}{\mathbf{X}^T \boldsymbol{\rho}^{-1}(\boldsymbol{\theta}) \mathbf{X}} \boldsymbol{\Gamma}_1 \boldsymbol{\Gamma}_1^T + \frac{n\sigma_0^2 \sigma_1^2 \|\boldsymbol{\beta}\|^2}{\mathbf{X}^T \boldsymbol{\rho}^{-1}(\boldsymbol{\theta}) \mathbf{X} \sigma_1^2 \|\boldsymbol{\beta}\|^2 + n(\sigma_0^2 - \sigma_1^2)^2} \boldsymbol{\Gamma}_0 \boldsymbol{\Gamma}_0^T. \quad (4.7)$$

For this simplify version, it can be shown that

$$\frac{\mathbf{V}_{SPEN}^{-\frac{1}{2}} \mathbf{V}_{EN} \mathbf{V}_{SPEN}^{-\frac{1}{2}}}{\frac{\mathbf{X}^T \boldsymbol{\rho}^{-1}(\boldsymbol{\theta}) \mathbf{X}}{n\sigma_{\mathbf{X}}^2}} = \mathbf{I}_r + \left( \frac{(\sigma_0^2 - \sigma_1^2)^2 \left( \frac{n\sigma_{\mathbf{X}}^2}{\mathbf{X}^T \boldsymbol{\rho}^{-1}(\boldsymbol{\theta}) \mathbf{X}} - 1 \right)}{(\sigma_0^2 - \sigma_1^2)^2 + \sigma_1^2 \sigma_{\mathbf{X}}^2 \|\boldsymbol{\beta}\|^2} \right) \boldsymbol{\Gamma}_0 \boldsymbol{\Gamma}_0^T, \quad (4.8)$$

---

where  $\mathbf{V}_{SPEN}$  shows the asymptotic variance of the spatial envelope model,  $\mathbf{V}_{EN}$  shows the asymptotic variance of the envelope model, and  $\sigma_{\mathbf{X}}^2$  denotes the variance of the  $\mathbf{X}$  which is an  $n \times 1$  vector. Proof of equation (4.8) can be found in the Supplement, section S7. This results indicates that when the spatial correlation does not exists, i.e.  $\rho(\boldsymbol{\theta}) = \mathbf{I}$ , the asymptotic variance for both model would be equal. On the other hand, for the cases that spatial correlation exists, drawing an analytical conclusion for comparing the asymptotic variance of the two models is very difficult. In this case, the variance of the two models can be compared numerically.

## 5. Prediction

Prediction at an unsampled location is often a major objective of a spatial analysis. Let  $\mathbb{Y}_{new}$  be the  $vec(\mathbf{Y}_{new})$  of the new multivariate response and  $\mathbb{X}_{new}$  be the predictor vector at an unsampled location. The model then can be written as:

$$\begin{pmatrix} \mathbb{Y}_{new} \\ \mathbb{Y} \end{pmatrix} = \begin{pmatrix} \boldsymbol{\alpha} \otimes \mathbf{1}_{n_{new}} + \mathbb{X}_{new}\boldsymbol{\beta}^* \\ \boldsymbol{\alpha} \otimes \mathbf{1}_n + \mathbb{X}\boldsymbol{\beta}^* \end{pmatrix} + \begin{pmatrix} \boldsymbol{\epsilon}_{new} \\ \boldsymbol{\epsilon} \end{pmatrix} \sim N \left( \boldsymbol{\alpha} \otimes \mathbf{1}_N + \begin{pmatrix} \mathbb{X}_{new} \\ \mathbb{X} \end{pmatrix} \boldsymbol{\beta}^*, \boldsymbol{\Sigma} \right). \quad (5.1)$$

---

where  $N = n + n_{new}$  and  $\Sigma$  is as follows

$$\Sigma = \begin{pmatrix} \Sigma_{11} & \Sigma_{12} \\ \Sigma_{21} & \Sigma_{22} \end{pmatrix} = \begin{pmatrix} (\mathbf{V}_0 + \mathbf{V}_1) \otimes \boldsymbol{\rho}_{new,new}(\boldsymbol{\theta}) & (\mathbf{V}_0 + \mathbf{V}_1) \otimes \boldsymbol{\rho}_{new,\mathbf{Y}}(\boldsymbol{\theta}) \\ (\mathbf{V}_0 + \mathbf{V}_1) \otimes \boldsymbol{\rho}_{\mathbf{Y},new}(\boldsymbol{\theta}) & (\mathbf{V}_0 + \mathbf{V}_1) \otimes \boldsymbol{\rho}_{\mathbf{Y},\mathbf{Y}}(\boldsymbol{\theta}) \end{pmatrix}. \quad (5.2)$$

The conditional distribution  $\mathbf{Y}_{new}|\mathbf{Y}$  is

$$\mathbf{Y}_{new}|\mathbf{Y}, \boldsymbol{\alpha}, \boldsymbol{\eta}, \mathbf{V}_0, \mathbf{V}_1, \boldsymbol{\theta} \sim N(\boldsymbol{\mu}_1 + \Sigma_{12}\Sigma_{22}^{-1}(\mathbf{Y} - \boldsymbol{\mu}_2), \Sigma_{11} - \Sigma_{12}\Sigma_{22}^{-1}\Sigma_{21}), \quad (5.3)$$

where  $\boldsymbol{\mu}_1 = \boldsymbol{\alpha} \otimes \mathbf{1}_{n_{new}} + \mathbb{X}_{new}\boldsymbol{\beta}^*$  and  $\boldsymbol{\mu}_2 = \boldsymbol{\alpha} \otimes \mathbf{1}_n + \mathbb{X}\boldsymbol{\beta}^*$ . Using the method described in section 3, one can estimate the parameters of the model and then from the conditional distribution (5.3) the  $E(\mathbf{Y}_{new}|\mathbf{Y})$  can be estimated.

## 6. Simulation

In this section, we carry out a simulation study to evaluate the finite sample performance of the proposed spatial envelope model and to compare it with the traditional multivariate linear regression (MLR), linear coregionalization model (LCM; Zhang, 2007), and envelope (Cook, Li, and Chiaromonte, 2010).

The data  $\{(\mathbf{X}_1, \mathbf{Y}_1), \dots, (\mathbf{X}_n, \mathbf{Y}_n)\}$  are generated from the model

$$\mathbf{Y} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\epsilon}, \quad (6.1)$$

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where  $\mathbf{Y}_i \in \mathbb{R}^5$ ,  $\mathbf{X}_i \in \mathbb{R}^6$ , and the structural dimension  $u = 2$ . The matrix  $(\mathbf{\Gamma}_1; \mathbf{\Gamma}_0)$  is obtained by orthogonalizing an  $5 \times 5$  matrix generated from uniform  $(0, 1)$  variables. The elements of  $\boldsymbol{\eta}$  follow standard normal distribution, and  $\boldsymbol{\beta} = \mathbf{\Gamma}_1 \boldsymbol{\eta}$ . We generate  $\boldsymbol{\Sigma}_{\mathbf{Y}} = (\mathbf{\Gamma}_1 \boldsymbol{\Omega}_1 \mathbf{\Gamma}_1^T + \mathbf{\Gamma}_0 \boldsymbol{\Omega}_0 \mathbf{\Gamma}_0^T) \otimes \boldsymbol{\rho}(\boldsymbol{\theta})$  where  $\boldsymbol{\Omega}_1 = [\{(-0.9)^{|i-j|}\}]$  and  $\boldsymbol{\Omega}_0 = [\{(-0.5)^{|i-j|}\}]$ . For the spatial correlation function  $\boldsymbol{\rho}(\boldsymbol{\theta})$ , we use the following Matern covariance function:

$$\boldsymbol{\rho}(h; \boldsymbol{\theta}) = \frac{1}{2^{\theta_2-1} \Gamma(\theta_2)} \left( \frac{\|h\|}{\theta_1} \right)^{\theta_1} \kappa_{\theta_2} \left( \frac{\|h\|}{\theta_1} \right),$$

where  $\boldsymbol{\theta} = (\theta_1, \theta_2)$ ,  $\theta_1 > 0$  is the range parameter,  $\theta_2$  is the smoothness parameter,  $\Gamma(\cdot)$  is the Gamma function, and  $\kappa_{\theta_2}$  is the modified Bessel function of the second kind of order  $\theta_2$  (Abramowitz and Stegun, 1964). We assume  $\boldsymbol{\epsilon}$  follows a normal distribution with mean 0 and covariance  $\boldsymbol{\Sigma}$ . Three different cases for the covariance  $\boldsymbol{\Sigma}_{\mathbf{Y}}$  are investigated. For first scenario,  $\boldsymbol{\Sigma} = (\mathbf{\Gamma}_1 \boldsymbol{\Omega}_1 \mathbf{\Gamma}_1^T + \mathbf{\Gamma}_0 \boldsymbol{\Omega}_0 \mathbf{\Gamma}_0^T)$ . This density serves as a benchmark where the errors are independent from each other. For the second scenario, let  $\boldsymbol{\rho}(\boldsymbol{\theta})$  be a Matern covariance function with  $\theta_1 = 1$  and  $\theta_2 = 0.5$ ; This case represents a spatial correlation in the data with a short range of dependency. This case is an example of weak spatial correlation. Finally, let  $\boldsymbol{\rho}(\boldsymbol{\theta})$  to be a Matern covariance function with  $\theta_1 = 5$  and  $\theta_2 = 0.5$ ; This case represents a spatial correlation in the data with a long range of dependency. This case is an example of strong spatial correlation.

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Sample size is 100, 225, and 400. There are two different ways to generate these samples. One is based on  $10 \times 10$ ,  $15 \times 15$  and  $20 \times 20$  evenly spaced grids on  $[0, 1]^2$ , respectively. Another way is to randomly choose 100, 225, and 400 locations from a  $101 \times 101$  grid on  $[0, 1]^2$ . We use both sampling procedures to check whether the spatial distribution of the observations has any impact on the proposed estimation. All results reported here are based on 200 replications from the simulation model in each scenario. In order to compare the different estimators, we use *Leave One Out Cross-Validation* (LOCV) method, which provides a convenient approximation for the prediction error under squared-error loss

$$MSPE = \frac{\sum_{i=1}^n (\hat{\mathbf{Y}}^{(-i)}(s_i) - \mathbf{Y}(s_{i,obs}))^2}{n}, \quad (6.2)$$

where  $\mathbf{Y}(s_{i,obs})$  is the observe value for response in location  $s_i$  and  $\hat{\mathbf{Y}}^{(-i)}(s_i)$  is the predicted values of  $\mathbf{Y}(s_i)$  computed with the  $i$ th row of the data removed. The Matlab package *Envlp* was used for all our simulation studies. Tables 1 and 2 summarize the results of these simulations. These tables provide the LOCV for different methods and different error distributions.

From the summary of all three different error distributions, one can see that for the standard normal errors, where the observations are independent from each other, the spatial envelope provides comparable results to the envelope method and both performs better than MLR and LCM. In

Table 1: Prediction accuracy comparison based on the mean (standard deviation) of leave one out cross-validation (LOCV) for all 200 data sets from equally spaced samples. Smaller LOCV shows better performance.

$\epsilon$	n	MLR	LCM	Envelope	Spatial Envelope
1	100	19.02 (1.537)	20.01 (1.754)	13.71 (1.547)	14.28 (1.644)
	225	18.49 (1.153)	19.75 (1.659)	11.49 (1.124)	12.51 (1.234)
	400	18.27 (0.828)	19.02 (1.002)	10.37 (0.812)	10.87 (0.989)
2	100	102.79 (35.570)	22.54 (3.246)	91.98 (36.379)	20.21 (1.988)
	225	101.57 (32.495)	20.46 (2.897)	89.24 (33.083)	18.34 (1.450)
	400	99.98 (32.185)	18.89 (2.051)	88.95 (31.855)	17.68 (1.056)
3	100	117.79 (48.834)	24.19 (4.125)	119.08 (47.852)	21.36 (2.353)
	225	103.22 (39.065)	21.78 (3.278)	104.73 (39.023)	20.76 (2.012)
	400	99.08 (37.718)	19.45 (3.001)	100.39 (36.896)	18.10 (1.651)

Table 2: Prediction accuracy comparison based on the mean (standard deviation) of leave one out cross-validation (LOCV) for all 200 data sets from random location samples. Smaller LOCV shows better performance.

$\epsilon$	n	MLR	LCM	Envelope	Spatial Envelope
1	100	20.12 (1.613)	21.01 (1.863)	14.32 (1.699)	14.98 (1.722)
	225	19.34 (1.231)	19.68 (1.542)	13.12 (1.234)	13.19 (1.201)
	400	17.83 (0.804)	18.22 (1.101)	11.73 (0.718)	12.37 (0.819)
2	100	104.02 (36.702)	23.32 (4.111)	93.02 (30.433)	19.21 (2.004)
	225	102.41 (34.521)	21.41 (3.758)	91.34 (27.211)	17.34 (1.352)
	400	100.39 (30.822)	19.20 (3.201)	89.21 (25.581)	16.68 (1.110)
3	100	116.34 (45.089)	25.21 (4.821)	97.01 (43.021)	20.79 (2.115)
	225	108.15 (34.211)	22.35 (3.555)	95.52 (31.774)	18.92 (1.944)
	400	101.54 (32.102)	20.44 (2.998)	90.94 (30.234)	17.03 (1.234)



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error distributions 2 and 3 where there exists spatial dependency in the data, the spatial envelope method performed almost equally as well as they did in the cases without spatial dependency while original envelope loses its efficiency. In addition, spatial envelope outperformed LCM in both independent and dependent cases. Since spatial envelope takes the spatial correlation among observations into consideration, it provides more accurate results compared to the original envelope model. Furthermore, spatial envelope only uses the material part of the data which leads to a more efficient results compared to LCM which uses both material and immaterial part of the data. Therefore, we can conclude that the proposed spatial envelope model provided consistent estimates with good prediction accuracy in all error distributions considered. This result is consistent for both sampling methods which indicates the spatial distribution of the observations has minimal impact on the estimation.

As in Cook, Li, and Chiaromonte (2010), it is possible for an objective function defined on Grassmann manifolds to have multiple local optimal points. One way to check this is to run the simulation with different starting values and compare the results. In our numerical experiment, we have not find the local optima to be a problem for our method.

In order to investigate the accuracy of the asymptotic variance of  $avar(\sqrt{n}\beta^*)$

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that is presented in (4.7), we used the following simulation. The purpose of this simulation is to show that the variation of the spatial envelope estimator approaches its asymptotic variance derived in (4.7) when the sample size increases. The data is generated following model (6.1) with five responses and one covariate i.e.  $\mathbf{Y}_i \in \mathbb{R}^5$ ,  $\mathbf{X}_i \in \mathbb{R}$ , and the structural dimension  $u = 1$ . In addition, we let  $\boldsymbol{\Omega}_1 = 5\mathbf{I}_u$ ,  $\boldsymbol{\Omega}_0 = \mathbf{I}_{5-u}$  and  $\boldsymbol{\eta} = 1$ . The sample size  $n$  is 100, 225, 400, and 900, randomly chosen from a  $101 \times 101$  grid on  $[0, 1]^2$ . For each sample size, 100 replications are performed to compute the estimation variance for the elements in  $\hat{\boldsymbol{\beta}}$ . For the spatial correlation, we used the Matern covariance function with  $\theta_1 = 2$  and  $\theta_2 = 0.5$ .

Figure 1 shows the simulation results of the asymptotic variance for a randomly selected element of  $\hat{\boldsymbol{\beta}}$ . The left panel of the figure 1 shows the asymptotic variance for the independent case and the right panel shows the same results for the spatially correlated data for the envelope and the spatial envelope. The blue line shows the estimated standard deviation of the envelope estimator and the black line denotes the estimated standard deviation of the spatial envelope estimator. From this figure, one can see that for the standard normal errors, where the observations are independent of each other, the variance of the spatial envelope and the envelope method are very similar. On the other hand, where there exists spatial dependency in

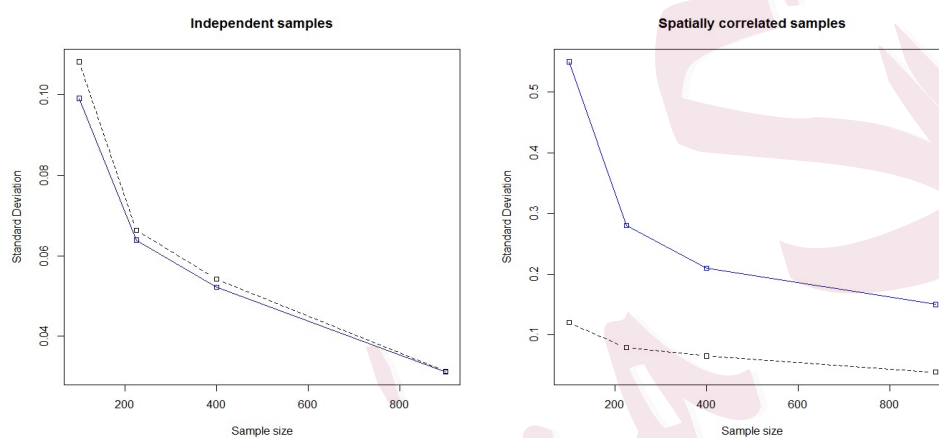


Figure 1: Simulation results of the asymptotic variance for a randomly selected element of  $\hat{\beta}$  for the envelope and the spatial envelope for the independent case (**left panel**) and for the spatially correlated data (**right panel**). The blue solid line shows the estimated standard deviation of the envelope estimator and the black dash line denotes the estimated standard deviation of the spatial envelope estimator.

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the data, the spatial envelope method outperformed the envelope method.

## 7. Application

In this section, we apply the proposed methodology to the air pollution data in the Northeastern United States. It is worth mentioning that the main purpose of this data analysis is to provide an insight that how the proposed approach can be used to find the reduced response space in multivariate spatial data analysis. This data has drawn much attention from both statisticians and scientists in other areas. Researchers looked at this data from different points of view including, but not restricted to, climate change (Phelan et al., 2016), health science (Kioumourtzoglou et al., 2016), and air quality (Battye et al., 2016). These studies showed that relationships exist between air pollution and meteorological factors, such as wind, temperature and humidity. Most of the existing studies focus on one of these pollutants, but since correlation exists among these pollutants, it is beneficial to study them simultaneously.

The pollutants and weather data that we used in this study include the average levels of the following variables in January 2015. We choose a group of ambient air pollutants monitored by EPA because they present a high threat to human health. Specifically, we have 8 response variables:

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ground level ozone, sulfur dioxide ( $SO_2$ ), carbon monoxide ( $CO$ ), nitrogen dioxide ( $NO_2$ ), nitrogen monoxide ( $NO$ ), lead, PM 2.5, and PM 10. PM 10 includes particles less than or equal to 10 micrometers in diameter. Similarly, PM 2.5 includes particles less than or equal to 2.5 micrometers and is also called fine particle pollution. This data also includes the following meteorological variables: wind, temperature, and relative humidity as predictors. Along with this information, latitude and longitude of the monitoring locations are used to model the spatial structure in the data. Our study area consists of 9 states in the Northeast of the United States: Connecticut, Maine, Massachusetts, New Hampshire, New Jersey, New York, Pennsylvania, Rhode Island, and Vermont. This dataset is available at [http://aqsdr1.epa.gov/aqsweb/aqstmp/airdata/download\\_files.html#Daily](http://aqsdr1.epa.gov/aqsweb/aqstmp/airdata/download_files.html#Daily). Figure 2 shows the study area and the location of 270 air monitoring sites.

The preliminary analysis using Moran's I and plots of the empirical variogram determined that spatial correlation does exist in this data. The results of the preliminary analysis can be found in the Supplement, section S8. Cross-validation showed that the best choice for the structural dimension is 3. The Matern's covariance parameters,  $\theta_1$  and  $\theta_2$ , are estimated to be 0.51 and 0.91, respectively. This estimates shows the existence of spatial dependency in the data. The corresponding direction estimates ( $\hat{\Gamma}_1$ ) from

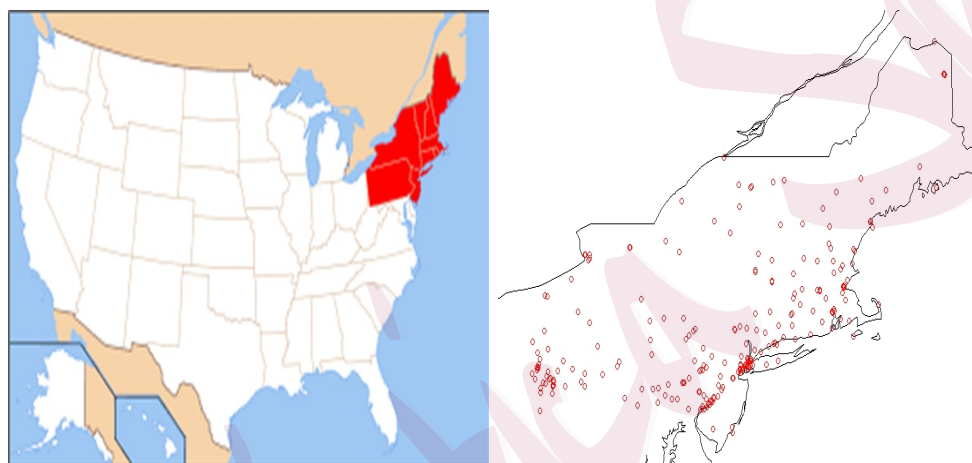


Figure 2: **Left:** Study area in the United States of America. States of interest are shaded in red. **Right:** Location of different sites in the study area. It can be seen that there is a higher number of sites in places with larger population compare to other places in the study area.

the spatial envelope are in Table 3. It is worth mentioning that the  $\hat{\Gamma}_1$  is not unique and it can be any orthonormal basis of the envelope subspace. The estimated regression coefficients and their standard deviation can be found in the Supplement, section S9.

Table 3: The corresponding direction estimates using spatial envelope for the air pollution data in northeastern United States of America.

Variable	Direction 1	Direction 2	Direction 3
Ozone	-0.0464	0.0432	-0.0080
Carbon monoxide	0.2840	-0.3717	-0.0179
Lead	-0.0739	0.0872	0.0008
Nitrogen dioxide	-0.5089	0.2612	-0.4639
Nitrogen monoxide	-0.3056	-0.1137	0.2757
Sulfur dioxide	-0.5335	0.0241	-0.2981
PM10	-0.3257	-0.8667	-0.0506
PM2.5	-0.4106	0.1394	0.7855

By checking the estimated basis coefficients of the minimal subspace (directions) and the regression coefficients, we can see Sulfur dioxide, Nitrogen dioxide, PM 10, and PM 2.5 dominate each of the three directions, respectively. Using fossil fuels creates sulfur dioxide, nitrogen monoxide, and nitrogen dioxide. The nitrogen monoxide will also become nitrogen

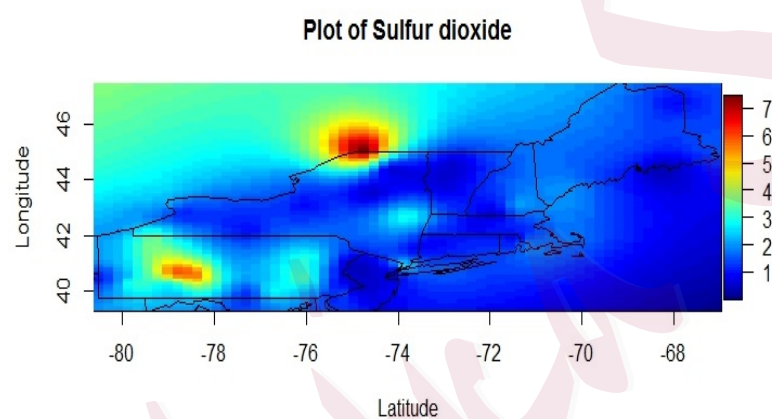


Figure 3: Prediction plot of the Sulfur dioxide for the study area. As it can be seen, the Sulfur dioxide is moderately high for the most part of the study area. Sulfur dioxide is extremely high in Johnstown where there exists a lot of defense manufacturing.



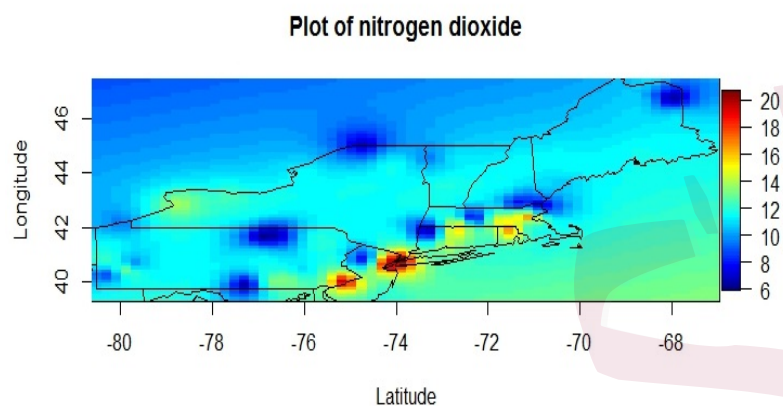


Figure 4: Prediction plot of the Nitrogen dioxide for the study area. The Nitrogen dioxide is high in Newark, New York, Philadelphia, and Rhode Island which are all highly populated areas.

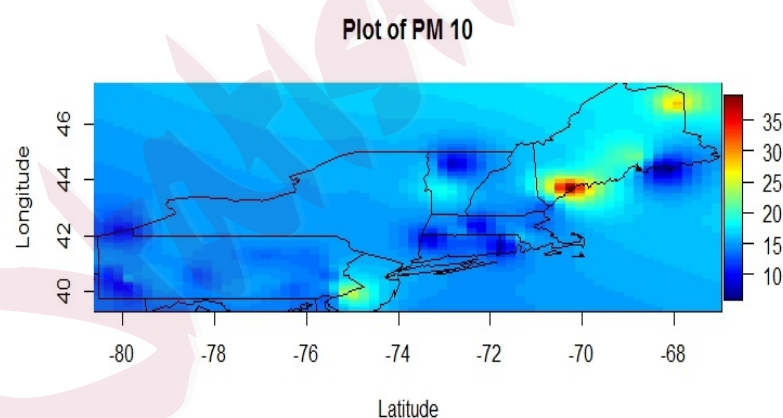


Figure 5: Prediction plot of the PM 10 for the study area. The PM 10 is high for most part of the study area especially in Philadelphia and August.

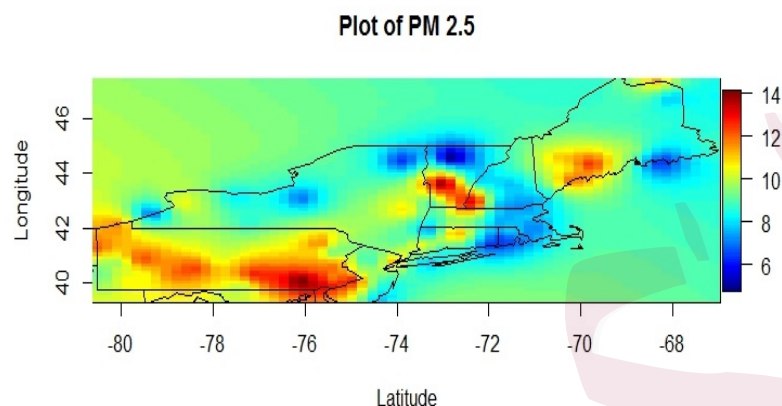


Figure 6: Prediction plot of the PM 2.5 for the study area. The PM 2.5 is moderately high in almost every place in the study area especially in Pennsylvania state, Augusta, and middle of Vermont state.

dioxide in the atmosphere. Existence of the particles in the air leads to reduction in visibility and causes the air to become hazy when levels are elevated. Furthermore, since these particles can travel deeply into the human lungs, they can cause health problem such as lung cancer. The main source of these particles in the air is from pollutants emitted from power plants, industries and automobiles.

Figure 3 to 6 shows the prediction plots for the three pollutants with the largest impact. Figure 3 shows the prediction plot of the Sulfur dioxide for the study area. The Sulfur dioxide is moderately high for the most part of the study area. In addition, Sulfur dioxide is extremely high in

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Johnstown where there exists a lot of defense manufacturing. Figure 4 shows the prediction plot of the Nitrogen dioxide for the study area. The Nitrogen dioxide is high in Newark, New York, Philadelphia, and Rhode Island which are all highly populated areas. Figure 5 shows the prediction plot of the PM 10 for the study area. The PM 10 is high for most part of the study area especially in Philadelphia and Augusta. Figure 6 shows the prediction plot of the PM 2.5 for the study area. The PM 2.5 is moderately high in almost every place in the study area especially in Pennsylvania state, Augusta, and middle of Vermont state. Prediction plots of the other variables can be found in Supplement, section S10.

The square root of the leave one out cross-validation for MLR, LCM, envelope, and spatial envelope are 7.537, 3.562, 4.876, and 1.978, respectively. This result shows that spatial envelope outperforms other methods and provides more accurate prediction. In summary, we find out that the most important pollutants in January are particulates, sulfur, and nitrogen, and other pollutants have minimal effect. These statistical conclusions support the environmental chemical claim that in the cold weather, due to the fossil burning and inversion, sulfur dioxide, nitrogen dioxide, and particulate matters are the most important pollutants (Byers, 1959; Læg Reid, Bockman, and Kaarstad, 1999).

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## 8. Conclusion

Air pollution has a serious impact on human health. Research has greatly improved the understanding of each particular pollutant and their relationship with weather conditions. However, there are relatively few studies about the effects of meteorological variables on several pollutants together. Motivated by an analysis of air pollution in the northeastern United States, we proposed a new parsimonious multivariate spatial model. Emphasis of this work is placed on inference and constructing a method that can provide more efficient estimation for the parameters of interest than traditional maximum likelihood estimators through capturing the spatial structure in the data.

Our model is flexible enough to characterize complex dependency and cross-dependency structures of different pollutants. From a simulation study and real data analysis, we showed that the proposed spatial envelope model outperforms multivariate linear regression, envelope, and linear coregionalization models. This new approach provides more efficient estimation for regression coefficients compared to the traditional maximum likelihood approach.

The method presented in this paper is for a multivariate spatial response with separable covariance matrix. This framework can be also extended to

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the cases that the covariance matrix is non-separable. Furthermore, current work assumes the normality in the derivations of the estimators. Confirming that the normality assumption is satisfied is more important for the spatial random fields than when working with envelope models. The violation of the normality assumption brings computational and theoretical challenges Diggle, Tawn, and Moyeed (1998); Liu et al. (1992). Incorporating the envelope idea with a multivariate non-Gaussian spatial random field, which is beyond the scope of this paper, is a very interesting and challenging topic. The mis-specification of the spatial structure is also a very interesting and challenging topic. Investigation of the potential cost of mis-specifying the spatial correlation structure is also an interesting topic. The mis-specification can affect the estimation of the coefficient and prediction. Another possible extension of current methodology is for the case with spatiotemporal responses. The investigation for these more general cases is under way.

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