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A Comparison of Block and Semi-Parametric Bootstrap Methods for Variance Estimation in Spatial Statistics

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8 Abstract

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Efron (1979) introduced the bootstrap method for independent data but it can not be easily applied to spatial data because of their dependency. For spatial data that are correlated in terms of their locations in the underlying space the moving block bootstrap method is usually used to estimate the precision measures of the estimators. The precision of the moving block bootstrap estimators is related to the block size which is difficult to select. In the moving block bootstrap method also the variance estimator is underestimated. In this paper, first the semi-parametric bootstrap is used to estimate the precision measures of estimators in spatial data analysis. In the semiparametric bootstrap method, we use the estimation of spatial correlation structure. Then, we compare the semi-parametric bootstrap with a moving block bootstrap for variance estimation of estimators in a simulation study.

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Finally, we use the semi-parametric bootstrap to analyze the coal-ash data.

- 9 Key words: Moving block bootstrap; Semi-parametric bootstrap; Plug-in
- ¹⁰ kriging; Monte-Carlo simulation; Coal-ash data.

11 1. Introduction

In environmental studies the data are usually spatially dependent. Deter-12 mination of the spatial correlation structure of the data and prediction are 13 two important problems in statistical analysis of spatial data. To do so a valid 14 parametric variogram model is often fitted to the empirical variogram of the 15 data. Since there is no closed form for the variogram parameter estimates, 16 they are usually computed numerically. In addition, when data behave as 17 a realization of a non-Gaussian random field, the bootstrap method can be 18 used for statistical inference of spatial data. 19

The bootstrap technique (Efron, 1979; Efron and Tibshirani, 1993) is a very general method to measure the accuracy of estimators, in particular for parameter estimation from independent identically distributed (iid) variables. For spatially dependent data, the block bootstrap method can be used without requiring stringent structural assumptions. This is an important aspect of the bootstrap in the dependent case, as the problem of model misspecification is more prevalent under dependence and traditional statistical methods

are often very sensitive to deviations from model assumptions. A prime ex-27 ample of this issue appears in the seminal paper by Singh (1981), who in 28 addition to providing the first theoretical confirmation of the superiority of 29 the Efron's bootstrap, also pointed out its inadequacy for dependent data. 30 Different variants of spatial subsampling and spatial block bootstrap meth-31 ods have been proposed in the literature; see Hall (1985), Possolo (1991), Liu 32 and Singh (1992), Politis and Romano (1993, 1994), Sherman and Carlstein 33 (1994), Sherman (1996), Politis, Paparoditis and Romano (1998, 1999), Poli-34 tis, Romano and Wolf (1999), Bühlman and Künsch (1999), Nordman and 35 Lahiri (2003) and references therein. Here we shall follow the moving block 36 bootstrap (MBB) methods suggested by Lahiri (2003). 37

On the other hand, the semi-parametric bootstrap (SPB) method has 38 been used by Freedman and Peters (1984) for linear models and Bose (1988) 39 for autoregressive models in time series. In this paper, first, we apply SPB 40 method for estimation of the sampling distribution of estimators in spatial 41 data analysis. Then, the SPB and MBB methods are compared for variance 42 estimation of estimators in a Monte-Carlo simulation study. Finally, the 43 SPB method is used to estimate the bias, variance and distribution of plug-44 in kriging and variogram parameter estimation for the analysis of the coal-ash 45

46 data.

In Section 2, spatial statistics, kriging and plug-in kriging are briefly re-47 viewed. The MBB method is given in Section 3. We use the SPB algorithm 48 for analysis of spatial data in Section 4. Section 5 consists of a Monte-Carlo 49 simulation study for comparison of the SPB and MBB methods for variance 50 estimation of estimators. These estimators are; sample mean, GLS plug-51 in estimator of mean, plug-in kriging and variogram parameters estimator; 52 nugget effect, partial sill and range. In Section 6, we apply the SPB method 53 for estimation of bias, variance and distribution of plug-in kriging and pa-54 rameter variogram estimators for coal-ash data. In the last section, we will 55 end with discussion and results. 56

57 2. Spatial Statistics and Kriging

Usually a random field $\{Z(s) : s \in D\}$ is used for modeling spatial data, where the index set D is a subset of Euclidean space \mathbb{R}^d , $d \geq 1$. Suppose $\mathcal{Z} = (Z(s_1), \ldots, Z(s_N))^T$ denotes N realizations of a second-order stationary random field $Z(\cdot)$ with constant unknown mean $\mu = E[Z(s)]$ and covariogram $\sigma(h) = \operatorname{Cov}[Z(s), Z(s+h)]; s, s+h \in D$. The covariogram $\sigma(h)$ is a positive definite function. At a given location $s_0 \in D$ the best linear ⁶⁴ unbiased predictor for $Z(s_0)$, the ordinary kriging predictor and its variance ⁶⁵ are given by (Cressie, 1993)

$$\hat{Z}(s_0) = \lambda^T \mathcal{Z}, \quad \sigma_k^2(s_0) = \sigma(0) - \lambda^T \sigma + m, \tag{1}$$

66 where

$$\lambda^{T} = (\sigma + \mathbf{1}m)^{T} \Sigma^{-1}, \quad m = (1 - \mathbf{1}^{T} \Sigma^{-1} \sigma) (\mathbf{1}^{T} \Sigma^{-1} \mathbf{1})^{-1}.$$
 (2)

Here, $\mathbf{1} = (1, \dots, 1)^T$, $\sigma = (\sigma(s_0 - s_1), \dots, \sigma(s_0 - s_N))^T$ and Σ is an $N \times N$ matrix whose $(i, j)^{th}$ element is $\sigma(s_i - s_j)$.

⁶⁹ In reality, the covariogram is unknown and should be estimated based on ⁷⁰ the observations. An empirical estimator of covariogram is given by

$$\hat{\sigma}(h) = N_h^{-1} \sum_{N(h)} [(Z(s) - \bar{Z})(Z(s+h) - \bar{Z})],$$

⁷¹ where $\bar{Z} = N^{-1} \sum_{i=1}^{N} Z(s_i)$ is the sample mean, $N(h) = \{(s_i, s_j) : s_i - s_j =$ ⁷² $h; i, j = 1, \dots, N\}$ and N_h is the number of elements of N(h). The covari-⁷³ ogram estimator $\hat{\sigma}(h)$ cannot be used directly for kriging predictor equations, ⁷⁴ because it is not necessarily positive definite. The idea is to fit a valid para-⁷⁵ metric covariogram model $\sigma(h; \theta)$ that is closest to the empirical covariogram ⁷⁶ $\hat{\sigma}(h)$. Various parametric covariogram models such as exponential, spheri-⁷⁷ cal, Gaussian, linear are presented in Journel and Huijbregts (1978). For ⁷⁸ example, the exponential covariogram is given by

$$\sigma(h;\theta) = \begin{cases} c_0 + c_1 & ||h|| = 0\\ c_1 \exp(\frac{-||h||}{a}) & ||h|| \neq 0, \end{cases}$$
(3)

where $\theta = (c_0, c_1, a)^T$ are the nugget effect, partial sill and range, respectively. 79 The maximum likelihood (ML), restricted maximum likelihood (REML), or-80 dinary least squares (OLS) and generalized least squares (GLS) methods can 81 be applied to estimate θ . In these methods, $\hat{\theta}$ is computed numerically with 82 the use of iterative algorithms since there is no closed form. For example, 83 Mardia and Marshall (1984) described the maximum likelihood method for 84 fitting the linear model when the residuals are correlated and when the co-85 variance among the residuals is determined by a parametric model containing 86 unknown parameters. Kent and Mardia (1996) introduced the spectral and 87 circulant approximations to the likelihood for stationary Gaussian random 88 fields. Also, Kent and Mohammadzadeh (1999) obtained a spectral approx-89 imation to the likelihood for an intrinsic random field. We will estimate 90 $\operatorname{Var}(\hat{\theta})$ by SPB method. 91

The plug-in kriging predictor and the plug-in kriging predictor variance are determined by using $\hat{\theta}$ instead of θ in the covariogram $\hat{\sigma}(s_i, s_j) = \sigma(s_i, s_j; \hat{\theta})$ 94 as

$$\hat{\hat{Z}}(s_0) = \hat{Z}(s_0; \hat{\theta}); \quad \hat{\sigma}_k^2(s_0) = \sigma_k^2(s_0; \hat{\theta}).$$
 (4)

The plug-in kriging predictor is a non-linear function of \mathcal{Z} because $\hat{\theta}$ is a non linear estimator of θ . As a result, properties of the plug-in kriging predictor and the plug-in kriging predictor variance — such as unbiasedness and variance — are unknown. Mardia, Southworth and Taylor (1999) discussed the bias in maximum likelihood estimators. Under the assumption that $Z(\cdot)$ is Gaussian, Zimmerman and Cressie (1992) show that

$$E[\sigma_k^2(s_0;\hat{\theta})] \le \sigma_k^2(s_0) \le E[\hat{Z}(s_0;\hat{\theta}) - Z(s_0)]^2$$

where $\hat{\theta}$ is ML estimator of θ . We can estimate the variance of the plug-in kriging predictor $\sigma^2(s_0) = \operatorname{Var}[\hat{\hat{Z}}(s_0)]$ using the SPB method.

3. Moving Block Bootstrap

¹⁰⁴ Suppose that the sampling region D_n is obtained by inflating the proto-¹⁰⁵ type set D_0 by the scaling constant λ_n as

$$D_n = \lambda_n D_0,\tag{5}$$

where $\{\lambda_n\}_{n\geq 1}$ is a positive sequence of scaling factors such that $\lambda_n \to \infty$ as $n \to \infty$ and D_0 is a Borel subset of $(-1/2, 1/2)^d$ containing an open neighborhood of the origin. Suppose that $\{Z(s) : s \in \mathbb{Z}^d\}$ is a stationary random field that is observed at finitely many locations $S_n = \{s_1, \ldots, s_{N_n}\}$ given by the part of the integer grid \mathbb{Z}^d that lies inside D_n , i.e., the data are $\mathcal{Z} = \{Z(s) : s \in S_n\}$ for $S_n = D_n \cap \mathbb{Z}^d$. Let $N \equiv N_n$ denote the sample size or the number of sites in D_n such that N and the volume of the sampling region D_n satisfies the relation $N = \operatorname{Vol}(D_0)\lambda_n^d$, where $\operatorname{Vol}(D_0)$ denotes the volume of D_0 .

Let $\{\beta_n\}_{n\geq 1}$ be a sequence of positive integers such that $\beta_n^{-1} + \beta_n/\lambda_n =$ 115 o(1) as $n \to \infty$. Here, β_n gives the scaling factor for the blocks in the 116 spatial block bootstrap method. As a first step, the sampling region ${\cal D}_n$ is 117 partitioned using blocks of volume β_n^d . Let $\mathcal{K}_n = \{k \in \mathbb{Z}^d : \beta_n(k + \mathcal{U}) \subset D_n\}$ 118 denote the index set of all separate complete blocks $\beta_n(k + \mathcal{U})$ lying inside 119 D_n such that $N = K\beta_n^d$, where $\mathcal{U} = (0, 1]^d$ denotes the unit cube in \mathbb{R}^d and 120 $K \equiv K_n$ denotes the size of \mathcal{K}_n . We define a bootstrap version of $\mathcal{Z}_n(D_n)$ 121 by putting together bootstrap replicates of the process $Z(\cdot)$ on each block of 122 D_n given by 123

$$D_n(k) \equiv D_n \cap [\beta_n(k + \mathcal{U})], \quad k \in \mathcal{K}_n.$$
(6)

Let $\mathcal{I}_n = \{i \in \mathbb{Z}^d : i + \beta_n \mathcal{U} \subset D_n\}$ denote the index set of all blocks of volume β_n^d in D_n , with starting points $i \in \mathbb{Z}^d$. Then, $\mathcal{B}_n = \{i + \beta_n \mathcal{U} :$

 $i \in \mathcal{I}_n$ gives a collection of cubic blocks that are overlapping and contained 126 in D_n . For the MBB method, for each $k \in \mathcal{K}_n$, one block is resampled at 127 random from the collection \mathcal{B}_n independently of the other resampled blocks, 128 giving a version $\mathcal{Z}_n^*(D_n(k))$ of $\mathcal{Z}_n(D_n(k))$ using the observations from the 129 resampled blocks. The bootstrap version $\mathcal{Z}_n^*(D_n)$ of $\mathcal{Z}_n(D_n)$ is now given by 130 concatenating the resampled blocks of observations $\{\mathcal{Z}_n^*(D_n(k)) : k \in \mathcal{K}_n\}$. 131 Now the bootstrap version of a random variable $T_n = t_n(\mathcal{Z}_n(D_n); \theta)$ is 132 given by $T_n^* = t_n(\mathcal{Z}_n^*(D_n); \hat{\theta}_n)$. For example, the bootstrap versions of $T_n =$ 133 $\sqrt{N}(\overline{Z}_n - \mu)$, where $\overline{Z}_n = N^{-1} \sum_{i=1}^N Z(s_i)$ and $\mu = E[Z(0)]$ is given by 134 $T_n^* = \sqrt{N}(\bar{Z}_n^* - \hat{\mu}_n)$, where $\bar{Z}_n^* = N^{-1} \sum_{i=1}^N Z^*(s_i)$, $\hat{\mu}_n = E_*(\bar{Z}_n^*)$, and E_* 135 denotes the conditional expectation given \mathcal{Z} . 136

Lahiri (2003) shows that the MBB method can be used to derive a con-137 sistent estimator of the variance of the sample mean, and more generally, 138 of statistics that are smooth functions of the sample mean. Suppose that 139 $\hat{\theta}_n = H(\bar{Z}_n)$ be an estimator of a parameter of interest $\theta = H(\mu)$, where H is 140 a smooth function. Then, the bootstrap version of $\hat{\theta}_n$ is given by $\theta_n^* = H(\bar{Z}_n^*)$, 141 and the bootstrap estimator of $\sigma_n^2 = N \operatorname{Var}(\hat{\theta}_n)$ is given by $\hat{\sigma}_n^2 \equiv \hat{\sigma}_n^2(\beta_n) =$ 142 $N\operatorname{Var}_*(\theta_n^*)$. He shows that under a weak dependence condition for the ran-143 dom field $\{Z(s): s \in \mathbb{Z}^d\}$, like a strong mixing condition, then $\hat{\sigma}_n^2 \longrightarrow_p \sigma_{\infty}^2$ as 144

¹⁴⁵ $n \longrightarrow \infty$, where $\sigma_{\infty}^2 \equiv \lim_{n \longrightarrow \infty} N \operatorname{Var}(\hat{\theta}_n) = \frac{1}{\operatorname{Vol}(D_0)} \sum_{i \in \mathbb{Z}^d} EW(0)W(i)$, with ¹⁴⁶ $W(i) = \sum_{|\alpha|=1} D^{\alpha} H(\mu)(Z(i) - \mu)^{\alpha}$, H is continuously differentiable and the ¹⁴⁷ partial derivatives $D^{\alpha} H(\cdot)$, $|\alpha| = 1$, satisfy Holder's condition. Nordman and ¹⁴⁸ Lahiri (2003) and Lahiri (2003) determined the optimal block size by com-¹⁴⁹ puting $\operatorname{Bias}[\hat{\sigma}_n^2(\beta_n)] = \beta_n^{-2} \gamma_2^2 + o(\beta_n^{-1})$ and $\operatorname{Var}[\hat{\sigma}_n^2(\beta_n)] = N^{-1} \beta_n^d \gamma_1^2 + (1+o(1))$ ¹⁵⁰ and minimizing $\operatorname{MSE}[\hat{\sigma}_n^2(\beta_n)] = N^{-1} \beta_n^d \gamma_1^2 + \beta_n^{-2} \gamma_2^2 + o(N^{-1} \beta_n^d + \beta_n^{-2})$ to obtain

$$\beta_n^{opt} = N^{\frac{d}{d+2}} [2\gamma_2^2/d\gamma_1^2]^{\frac{1}{d+2}} (1+o(1)), \tag{7}$$

151 where $\gamma_1^2 = (\frac{2}{3})^d \cdot \frac{2\sigma_{\infty}^4}{(\text{Vol}(D_0))^3}$ and $\gamma_2 = -\frac{1}{\text{Vol}(D_0)} \sum_{i \in \mathbb{Z}^d} |i| \sigma_W(i)$ with $\sigma_W(i) =$ $\operatorname{Cov}(W(0), W(i)), i \in \mathbb{Z}^d \text{ and } |i| = i_1 + \dots + i_d \text{ for } i = (i_1, \dots, i_d) \in \mathbb{Z}^d.$ The 152 $\operatorname{Bias}[\hat{\sigma}_n^2(\beta_n)]$ shows that the MBB estimator $\hat{\sigma}_n^2(\beta_n)$ is an underestimator of 153 $\sigma_n^2.$ Lahiri, Furukawa and Lee (2007) suggested a nonparametric plug-in 154 rule for estimating optimal block sizes in various block bootstrap estimation 155 problems. The optimal block size determination is difficult and sometimes 156 impossible. On the other hand, when using the MBB method the variance 157 estimator $\hat{\sigma}_n^2(\beta_n)$ is underestimated. Therefore, we use the SPB method for 158 spatial data analysis. 159

¹⁶⁰ 4. Semi-Parametric Bootstrap

Suppose $\mathcal{Z} = (Z(s_1), \cdots, Z(s_N))^T$ are observations of a random field 161 $\{Z(s): s \in D \subset \mathbb{R}^d\}$ with decomposition $Z(s) = \mu(s) + \delta(s)$, where $\mu(\cdot) =$ 162 $E[Z(\cdot)]$ and the error term $\delta(\cdot)$ is a zero-mean stationary random field having 163 $N \times N$ positive-definite covariance matrix $\Sigma \equiv (\sigma(s_i - s_j))$. The Cholesky 164 decomposition allows Σ to be decomposed as the matrix product $\Sigma = LL^T$, 165 where L is a lower triangular $N \times N$ matrix. Let $\epsilon \equiv (\epsilon(s_1), \ldots, \epsilon(s_N))^T =$ 166 $L^{-1}(\mathcal{Z} - \mu)$, be a vector of uncorrelated random variables with zero mean 167 and unit variance from an unknown cumulative distribution $F(\varepsilon)$, where the 168 mean $\mu = (\mu(s_1), \ldots, \mu(s_N))^T$. In the SPB method, we need an empirical 169 distribution $F_N(\varepsilon)$ to estimate $F(\varepsilon)$. The SPB algorithm is described by the 170 following steps: 171

172 **Step 1.** Estimation and removal of mean structure.

The trend or mean structure $\mu(\cdot)$ is estimated by the median polish algorithm (Cressie, 1993) or generalized additive models (Hastie, and Tibshirani, 1990) and is removed to obtain $R(s_i) = Z(s_i) - \hat{\mu}(s_i); \quad i = 1, ..., N.$

176 **Step 2.** Estimation and removal of correlation structure.

Estimate the spatial dependence structure of residual $R(s_i)$ by the covariance matrix $\hat{\Sigma}$. Note that, $\hat{\Sigma}$ is an $N \times N$ symmetric positive definite matrix whose (*i*, *j*)th element is an estimate of the covariogram $\hat{\sigma}(s_i - s_j) = \sigma(s_i - s_j; \hat{\theta})$. Then $\hat{\epsilon} \equiv (\hat{\epsilon}(s_1), \dots, \hat{\epsilon}(s_N))^T = \hat{L}^{-1}\mathcal{R}$ is a vector of uncorrelated residuals, where, \hat{L} is a lower triangular $N \times N$ matrix from Cholesky decomposition $\hat{\Sigma} = \hat{L}\hat{L}^T$ and $\mathcal{R} \equiv (R(s_1), \dots, R(s_N))^T$ is the vector of residuals.

183 Step 3. Computation of empirical distribution $F_N(\varepsilon)$.

Suppose that $\tilde{\epsilon} \equiv (\tilde{\epsilon}(s_1), \dots, \tilde{\epsilon}(s_N))^T$ is a vector of standardized values $\hat{\epsilon}$, where $\tilde{\epsilon}(s_i) = (\hat{\epsilon}(s_i) - \bar{\epsilon})/s_{\hat{\epsilon}}$ and $\bar{\hat{\epsilon}}$, $s_{\hat{\epsilon}}$ denote the sample mean and standard deviation of the residuals, repectively. The empirical distribution function formed from standardized uncorrelated residuals $\{\tilde{\epsilon}(s_1), \dots, \tilde{\epsilon}(s_N)\}$ is $F_N(\varepsilon) = N^{-1} \sum_{i=1}^N I(\tilde{\epsilon}(s_i) \leq \varepsilon)$, where $I(\tilde{\epsilon}(\cdot) \leq \varepsilon)$ is the indicator function equal to 1 when $\tilde{\epsilon}(\cdot) \leq \varepsilon$ and equal to 0 otherwise.

190 Step 4. Resampling and Bootstrap sample.

Efron's (1979) bootstrap algorithm is used for the vector of standardized uncorrelated residuals $\tilde{\epsilon}$. We generate N iid bootstrap random variables $\epsilon^*(s_1), \ldots, \epsilon^*(s_N)$ having common distribution $F_N(\varepsilon)$. In other words, $\epsilon^* \equiv$ $(\epsilon^*(s_1), \ldots, \epsilon^*(s_N))^T$ is a simple random sample with replacement from the standardized uncorrelated residuals $\{\tilde{\epsilon}(s_1), \ldots, \tilde{\epsilon}(s_N)\}$. The bootstrap sample $\mathcal{Z}^* \equiv (Z^*(s_1), \cdots, Z^*(s_N))^T$ can be determined using an inverse transform $\mathcal{Z}^* = \hat{\mu} + \hat{L}\epsilon^*$, where $\hat{\mu} = (\hat{\mu}(s_1), \ldots, \hat{\mu}(s_N))^T$ estimates the mean structure. If $\hat{T} = t(\mathcal{Z}; \hat{\mu}, \hat{\theta})$ is a plug-in estimator of $T = t(\mathcal{Z}; \mu, \theta)$, where $\hat{\theta}$ is the plug-in estimator of θ , then, the SPB version of \hat{T} is given by $T^* = t(\mathcal{Z}^*; \hat{\mu}, \hat{\theta})$.

²⁰¹ Step 6. Bootstrap estimators.

The bootstrap estimators of the bias, variance and distribution of T are given by

Bias_{*}(
$$T^*$$
) = $E_*(T^*) - \hat{T}$,
Var_{*}(T^*) = $E_*[(T^*) - E_*(T^*)]^2$,
 $G_*(t) = P_*(T^* \le t)$,

where E_* , Var_{*} and P_* denote the bootstrap conditional expectation, variance and probability given \mathcal{Z} .

206 Step 7. Monte-Carlo approximation.

When the above bootstrap estimators have no closed form, the precision measures of T^* may be evaluated by Monte-Carlo simulation as follows. We repeat Steps 4 and 5, B (e.g., B = 1000) times to obtain bootstrap replicates T_1^*, \ldots, T_B^* . Then the Monte-Carlo approximations of the bootstrap estimators in step 6 are given by

$$\widehat{\text{Bias}}_{*}(T^{*}) = \frac{1}{B} \sum_{b=1}^{B} T_{b}^{*} - \hat{T}, \qquad (8)$$

$$\widehat{\operatorname{Var}}_{*}(T^{*}) = \frac{1}{B} \sum_{b=1}^{B} (T_{b}^{*} - \frac{1}{B} \sum_{b=1}^{B} T_{b}^{*})^{2}, \qquad (9)$$

$$\widehat{G}_{*}(t) = \frac{1}{B} \sum_{b=1}^{B} I(T_{b}^{*} \le t).$$
(10)

212 5. Simulation Study

In this section, we conduct a simulation study to compare the MBB and 213 SPB estimator of $\sigma^2 = \operatorname{Var}(T)$, where T is a statistic of interest. We consider 214 four examples for T: the sample mean; GLS plug-in mean estimator; plug-215 in kriging; and covariogram parameters estimator. Let $\{Z(s) : s \in \mathbb{Z}^2\}$ be 216 a zero mean second-order stationary Gaussian process with the exponential 217 covariogram (3) using parameter values $\theta_1 = (1, 1, 1)^T$ (weak dependence) 218 and $\theta_2 = (0, 2, 2)^T$ (strong dependence). We generate realizations of the 219 Gaussian random field $Z(\cdot)$ over three rectangular regions $D = n \times n$; n =220 6, 12, 24 as spatial sample $\mathcal{Z} = (Z(s_1), \ldots, Z(s_N))^T$ where $N = n^2$. 221

To apply the MBB method, we identify the above rectangular regions Das $[-3,3) \times [-3,3), [-6,6) \times [-6,6)$ and $[-12,12) \times [-12,12)$, the scaling constants $\lambda = 6, 12, 24$ respectively and the prototype set $D_0 = [-\frac{1}{2}, \frac{1}{2}) \times$ $[-\frac{1}{2}, \frac{1}{2})$. For example, for the sample size $N = \lambda^2 = 144$ and $\beta = 2$, there are $K = |\mathcal{K}| = 36$ subregions in the partition (6), given by $D(k) = [2k_1, 2k_1 + 227 \ 2) \times [2k_2, 2k_2 + 2); \ k \in \mathcal{K} = \{(k_1, k_2)^T \in Z^2, -3 \le k_1, k_2 < 3\}$. To define the MBB version of the random field $Z(\cdot)$ over D we randomly resample 36 times, with replacement from the collection of all observed moving blocks

$$\mathcal{B}(i) = [i_1, i_1 + 2) \times [i_2, i_2 + 2); \quad i \in \mathcal{I} = \{(i_1, i_2)^T \in \mathbb{Z}^2, -6 \le i_1, i_2 < 4\}$$

The MBB sample $\mathcal{Z}^* = \mathcal{Z}^*(D) = (Z^*(s_1), \dots, Z^*(s_N))^T$ is given by concatenating the K-many resampled blocks to size β of observations $\{\mathcal{Z}^*(D(k)) : k \in \mathcal{K}\}$.

To define the SPB version of the random field $Z(\cdot)$ over D, we apply 233 steps 2–4 in SPB method. First, the covariance matrix Σ is estimated 234 using the plug-in estimator of the covariogram $\hat{\sigma}(h;\theta) = \sigma(h;\hat{\theta})$, where 235 $\hat{\theta} = (\hat{c}_0, \hat{c}_1, \hat{a})^T$ is an estimator of θ (e.g. ML estimator). Let \hat{L} be the 236 Cholesky decomposition of $\hat{\Sigma}$, then $\hat{\epsilon} = \hat{L}^{-1} \mathcal{Z}$ is a vector of uncorrelated val-237 ues. Hence, the bootstrap vector $\epsilon^* = (\epsilon^*(s_1), \ldots, \epsilon^*(s_N))^T$ is generated as a 238 simple random sample with replacement from $\{\tilde{\epsilon}(s_1), \ldots, \tilde{\epsilon}(s_N)\}$, where $\tilde{\epsilon}(\cdot)$ 239 denotes standardized uncorrelated values of $\hat{\epsilon}(\cdot)$. Finally, the SPB sample 240 $\mathcal{Z}^* = (Z^*(s_1), \dots, Z^*(s_N)))^T$ is given by the inverse transform $\mathcal{Z}^* = \hat{L}\epsilon^*$. 241 Suppose that $T = t(\mathcal{Z})$ is the statistic of interest, then the MBB and SPB 242

versions of T are given by $T^* = t(\mathcal{Z}^*)$. The MBB and SPB estimators $\hat{\sigma}^2 =$ Var_{*}(T^*) of $\sigma^2 = \text{Var}(T)$ are approximated based on B = 1000 bootstrap replicates (9). For each region D and covariance structure, we compute the variance estimator $\hat{\sigma}^2$ and approximate the normalized bias, variance and mean squared error(MSE)

NBias
$$(\hat{\sigma}^2) = E(\hat{\sigma}^2/\sigma^2) - 1,$$

NVar $(\hat{\sigma}^2) = Var(\hat{\sigma}^2/\sigma^2),$
NMSE $(\hat{\sigma}^2) = E[(\hat{\sigma}^2/\sigma^2) - 1]^2,$

by its empirical version based on 10000 simulations. In MBB method, the variance estimator is determined as $\hat{\sigma}^2 = \hat{\sigma}^2(\beta^{opt})$, where the optimal block size β^{opt} is based on minimal NMSE over various block sizes β .

251 Example 1. The Sample mean

In this example, we compare the MBB and SPB estimators $\hat{\sigma}_1^2 = N \text{Var}_*(\bar{Z}^*)$ of $\sigma_1^2 = N \text{Var}(\bar{Z}) = N^{-1} \mathbf{1}^T \Sigma \mathbf{1}$, where the sample mean $\bar{Z} = N^{-1} \sum_{i=1}^N Z(s_i)$ is the OLS estimator of mean μ and \bar{Z}^* is a bootstrap sample mean. We consider version T_1^* of the sample mean $T_1 = \sqrt{N}\bar{Z}$ based on a bootstrap sample \mathcal{Z}^* by $T_1^* = \sqrt{N}\bar{Z}^*$. The MBB and SPB estimators $\hat{\sigma}_1^2 = N \text{Var}_*(\bar{Z}^*)$ are approximated based on B = 1000 bootstrap replicates (9). The covariogram models that we considered are exponential, spherical and unknown.

Table 1 shows approximates of the NBias, NVar and NMSE for MBB estimators $\hat{\sigma}_1^2$ for various block sizes β based on the exponential covariogram model. The asterisk (*) denotes the minimal value of the NMSE. From Table 1, the optimum block size β^{opt} can be determined based on minimal value of the NMSE. For example, for θ_1 and n = 6, 12, 24 the optimum block size is $\beta^{opt} = 2, 3, 6$ and for θ_2 and $n = 6, 12, 24, \beta^{opt} = 3, 4, 8$. We have used the optimum block sizes β^{opt} for MBB method in Table 2. To conserve space, we will not further mention the determination of β^{opt} as in Table 1.

Tables 2-4 show true values of σ_1^2 , estimates of the NBias, NVar and NMSE for MBB (based on β^{opt}) and SPB estimators $\hat{\sigma}_1^2$ based on exponential covariogram, spherical covariogram with parameter values $\theta_2 = (0, 2, 2)^T$ and $\theta_3 = (0, 2, 4)^T$ and unknown covariogram.

Example 2. The GLS plug-in mean estimate

Let $\hat{\mu} = \mathbf{1}^T \Sigma^{-1} \mathcal{Z} / \mathbf{1}^T \Sigma^{-1} \mathbf{1}$ be the GLS estimator of mean μ with variance $1/\mathbf{1}^T \Sigma^{-1} \mathbf{1}$. We compare MBB and SPB estimators of $\sigma_2^2 = N \operatorname{Var}(\hat{\mu})$, where $\hat{\mu} = \mathbf{1}^T \hat{\Sigma}^{-1} \mathcal{Z} / \mathbf{1}^T \hat{\Sigma}^{-1} \mathbf{1}$ is GLS plug-in estimator of μ . We define a version T_2^* of the GLS plug-in mean $T_2 = \sqrt{N}\hat{\mu}$ based on a bootstrap sample \mathcal{Z}^* by $T_2^* = \sqrt{N}\mu^*$, where $\mu^* = \mathbf{1}^T \hat{\Sigma}^{-1} \mathcal{Z}^* / \mathbf{1}^T \hat{\Sigma}^{-1} \mathbf{1}$.

277 Example 3. Plug-in kriging

To compare MBB and SPB variance estimators of $\sigma_3^2 = \text{Var}[\hat{Z}(s_0)]$, we define the T_3^* version of plug-in ordinary kriging predictor $T_3 = \hat{Z}(s_0) = \hat{\lambda}^T \mathcal{Z}$, based

		$ heta_1$	=(1,1,1)	$(1)^{T}$	θ_2	=(0,2,2)	$(2)^{T}$
n	β	NBias	NVar	NMSE	NBias	NVar	NMSE
6	2	-0.569	0.039	0.362^{*}	-0.853	0.008	0.736
	3	-0.624	0.057	0.446	-0.844	0.013	0.725^{*}
	2	-0.561	0.011	0.326	-0.864	0.002	0.750
12	3	-0.475	0.033	0.258^{*}	-0.786	0.009	0.626
	4	-0.452	0.063	0.267	-0.732	0.021	0.557^{*}
	6	-0.563	0.080	0.397	-0.751	0.033	0.597
	2	-0.575	0.003	0.333	-0.874	0.001	0.764
	3	-0.463	0.009	0.233	-0.790	0.003	0.626
24	4	-0.369	0.018	0.174	-0.710	0.008	0.512
	6	-0.320	0.053	0.155^{*}	-0.595	0.029	0.383
	8	-0.328	0.087	0.195	-0.541	0.058	0.351^{*}
	12	-0.507	0.102	0.359	-0.648	0.064	0.484

Table 1: Approximates of the NBias, NVar and NMSE for MBB estimators $\hat{\sigma}_1^2 = \hat{\sigma}_1^2(\beta)$ based on exponential covariogram. The asterisk (*) denotes the minimal value of MSE.

$\theta_1 = (1,1,1)^T$				$\theta_2 = (0,2,2)^T$								
Method	n	σ_1^2	β^{opt}	NBias	NVar	NMSE		σ_1^2	β^{opt}	NBias	NVar	NMSE
MBB	6	5.279	2	-0.572	0.039	0.366		19.994	3	-0.846	0.014	0.729
SPB				-0.254	0.295	0.359				-0.327	0.367	0.474
MBB	12	6.311	3	-0.471	0.033	0.254		32.074	4	-0.740	0.021	0.569
SPB				-0.059	0.239	0.242				-0.067	0.343	0.347
MBB	24	6.890	6	-0.310	0.054	0.150		40.598	8	-0.558	0.057	0.369
SPB				0.012	0.142	0.143				0.039	0.193	0.195

Table 2: True values of σ_1^2 and approximates of the NBias, NVar and NMSE for MBB and SPB estimators $\hat{\sigma}_1^2$ based on exponential covariogram.

Table 3: True values of σ_1^2 and approximates of the NBias, NVar and NMSE for MBB and SPB estimators $\hat{\sigma}_1^2$ based on spherical covariogram.

			θ	$_{2} = (0, 2,$	$(2)^{T}$			θ_{i}	g = (0, 2, 4)	$(4)^{T}$	
Method	n	σ_1^2	β^{opt}	NBias	NVar	NMSE	σ_1^2	β^{opt}	NBias	NVar	NMSE
MBB	6	4.728	2	-0.398	0.078	0.236	14.069	3	-0.703	0.051	0.546
SPB				-0.042	0.231	0.232			-0.302	0.275	0.366
MBB	12	5.072	3	-0.285	0.053	0.134	17.046	4	-0.493	0.063	0.306
SPB				-0.046	0.048	0.048			-0.122	0.120	0.135
MBB	24	5.249	4	-0.188	0.029	0.064	18.638	6	-0.313	0.057	0.155
SPB				-0.026	0.011	0.012			-0.048	0.020	0.022

			we	ak depen	dence		strong dependence						
Method	n	σ_1^2	β^{opt}	NBias	NVar	NMSE		σ_1^2	β^{opt}	NBias	NVar	NMSE	
MBB	6	2.593	2	-0.125	0.124	0.140		35.637	3	-0.927	0.004	0.863	
SPB				-0.026	0.101	0.102				-0.620	0.353	0.737	
MBB	12	3.896	3	-0.032	0.031	0.032		78.315	4	-0.880	0.006	0.781	
SPB				-0.011	0.013	0.013				-0.482	0.465	0.697	
MBB	24	4.681	4	-0.006	0.009	0.009		126.930	8	-0.754	0.024	0.592	
SPB				-0.003	0.004	0.004				-0.422	0.349	0.527	

Table 4: True values of σ_1^2 and approximates of the NBias, NVar and NMSE for MBB and SPB estimators $\hat{\sigma}_1^2$ based on unknown covariogram.

Table 5: True values of σ_2^2 and approximates of the NBias, NVar and NMSE for MBB and SPB estimators $\hat{\sigma}_2^2$.

			θ	$_{1} = (1, 1, 1)$	$(1)^T$			θ_2	e = (0, 2, 2)	$(2)^{T}$	
Method	n	σ_2^2	β^{opt}	NBias	NVar	NMSE	σ_2^2	β^{opt}	NBias	NVar	NMSE
MBB	6	5.700	2	-0.574	0.044	0.374	16.355	2	-0.749	0.031	0.592
SPB				-0.341	0.201	0.317			-0.274	0.406	0.481
MBB	12	6.242	3	-0.434	0.046	0.235	27.771	4	-0.643	0.045	0.458
SPB				-0.108	0.202	0.214			-0.116	0.286	0.299
MBB	24	6.504	4	-0.329	0.025	0.133	36.802	6	-0.521	0.043	0.315
SPB				-0.039	0.123	0.124			0.006	0.166	0.166

				$\theta_1 = (1,1,1)^T$					$\theta_2 = (0,$	$(2,2)^{T}$		
Method	n	s_0	σ_3^2	β^{opt}	NBias	NVar	NMSE	 σ_3^2	β^{opt}	NBias	NVar	NMSE
MBB	6	(3.5, 3.5)	0.496	2	-0.386	0.404	0.553	1.530	2	-0.510	0.133	0.393
SPB					-0.297	0.414	0.503			-0.372	0.168	0.306
MBB	12	(6.5, 6.5)	0.415	3	-0.212	0.252	0.297	1.436	4	-0.215	0.114	0.160
SPB					-0.128	0.265	0.282			-0.111	0.087	0.099
MBB	24	(12.5, 12.5)	0.381	8	-0.036	0.132	0.133	1.385	8	-0.068	0.059	0.063
SPB					-0.018	0.115	0.115			0.001	0.036	0.036

Table 6: True values of σ_3^2 and approximates of the NBias, NVar and NMSE for MBB and SPB estimators $\hat{\sigma}_3^2$.

on a bootstrap sample \mathcal{Z}^* by $T_3^* = Z^*(s_0) = \hat{\lambda}^T \mathcal{Z}^*$.

The MBB and SPB estimators $\hat{\sigma}_2^2 = N \text{Var}_*(\mu^*)$ and $\hat{\sigma}_3^2 = \text{Var}_*[Z^*(s_0)]$ are approximated based on B = 1000 bootstrap replicates (9). Tables 5 and 6 show true values of σ_2^2 and σ_3^2 , estimates of the NBias, NVar and NMSE for MBB (based on β^{opt}) and SPB estimators $\hat{\sigma}_2^2$ and $\hat{\sigma}_3^2$ based on exponential covariogram for each region D and covariogram parameters θ_1 and θ_2 .

²⁸⁶ Example 4. Covariogram parameters estimator

Let $\hat{\theta} = (T_4, T_5, T_6) = (\hat{c}_0, \hat{c}_1, \hat{a})$ be the MLEs of the covariogram parameters $\theta = (c_0, c_1, a)$. Note that the estimator of $\hat{\theta}$ is computed numerically based

			θ	$_{1} = (1, 1, 1)$	$(1)^{T}$			θ	$_{2} = (0, 2,$	$(2)^{T}$	
Method	n	σ_2^2	β^{opt}	NBias	NVar	NMSE	σ_2^2	β^{opt}	NBias	NVar	NMSE
MBB	6	0.639	2	-0.547	0.240	0.539	0.026	3	-0.037	0.141	0.142
SPB				-0.114	0.237	0.250			-0.072	0.129	0.134
MBB	12	0.378	4	-0.091	0.312	0.321	0.011	4	-0.055	0.100	0.103
SPB				-0.083	0.220	0.227			0.073	0.092	0.097
MBB	24	0.198	6	-0.102	0.291	0.301	0.003	8	-0.148	0.010	0.032
SPB				0.069	0.193	0.198			0.040	0.003	0.005

Table 7: True values of σ_4^2 and approximates of the NBias, NVar and NMSE for MBB and SPB estimators $\hat{\sigma}_4^2$.

on the spatial sample \mathcal{Z} as $T_i = t_i(\mathcal{Z})$; i = 4, 5, 6 and has no closed form, so $\sigma_i^2 = \operatorname{Var}(T_i)$ is unknown. We define a version $T_i^* = t_i(\mathcal{Z}^*)$ of the estimator T_i based on bootstrap samples \mathcal{Z}^* . The MBB and SPB estimators $\hat{\sigma}_i^2 = \operatorname{Var}_*(T_i^*)$ are approximated based on B = 1000 bootstrap replicates (9). Tables 7–9 show true values of σ_i^2 , estimates of the NBias, NVar and NMSE for MBB (based on β^{opt}) and SPB estimators $\hat{\sigma}_i^2$ based on exponential covariogram for each region D and covariogram parameters θ_1 and θ_2 .

296 **Results**

²⁹⁷ Tables 1–9 show that the MBB variance estimations $\hat{\sigma}^2$ are underestimated.

	$\theta_1 = (1,1,1)^T$					$\theta_2 = (0, 2, 2)^T$						
Method	n	σ_2^2	β^{opt}	NBias	NVar	NMSE		σ_2^2	β^{opt}	NBias	NVar	NMSE
MBB	6	0.863	2	-0.655	0.233	0.662		0.686	2	-0.363	0.764	0.896
SPB				-0.120	0.258	0.272				-0.297	0.689	0.777
MBB	12	0.409	3	-0.118	0.288	0.302		0.246	4	-0.309	0.702	0.797
SPB				-0.084	0.181	0.188				-0.273	0.507	0.581
MBB	24	0.203	4	-0.145	0.2775	0.298		0.078	6	-0.294	0.624	0.710
SPB				-0.074	0.139	0.144				0.220	0.358	0.406

Table 8: True values of σ_5^2 and approximates of the NBias, NVar and NMSE for MBB and SPB estimators $\hat{\sigma}_5^2$.

Table 9: True values of σ_6^2 and approximates of the NBias, NVar and NMSE for MBB and SPB estimators $\hat{\sigma}_6^2$.

			$\theta_1 = (1,1,1)^T$				$\theta_2 = (0, 2, 2)^T$						
Method	n	σ_2^2	β^{opt}	NBias	NVar	NMSE			σ_2^2	β^{opt}	NBias	NVar	NMSE
MBB	6	0.471	2	-0.714	0.459	0.969			1.477	3	-0.377	0.761	0.903
SPB				-0.616	0.447	0.826					-0.247	0.594	0.655
MBB	12	0.258	4	-0.552	0.312	0.616			0.592	6	-0.302	0.702	0.793
SPB				-0.434	0.195	0.383					-0.206	0.488	0.530
MBB	24	0.162	8	-0.400	0.278	0.438			0.151	8	-0.260	0.639	0.707
SPB				-0.260	0.145	0.213					0.117	0.384	0.398

Tables 2–9 show that the MBB and SPB variance estimations $\hat{\sigma}^2$ are asymptotically unbiased and consistent. Tables 2–9 also indicate that the SPB estimators are preferable to the MBB versions, especially for stronger dependence structure and larger sample sizes. In Tables 5–9, true values of $\sigma_i^2 = \operatorname{Var}(T_i); i = 2, \dots, 6$ have no closed form and they can be approximated based on Monte-Carlo simulation by 10000 times replicates.

304 6. Analysis of Coal-Ash Data

In this section, we apply the SPB method to analyze the coal-ash data (Cressie, 1993) from Greene County, Pennsylvania. These data are collected with sample size N = 206 at locations $\{Z(x, y) : x = 1, ..., 16; y = 1, ..., 23\}$ with west coordinates greater than 64 000 ft; spatially this defines an approximately square grid, with 2500 ft spacing (Cressie, 1993; Fig. 2.2). Our goal is estimation of bias, variance and distribution of plug-in kriging predictor and variogram parameters estimator by SPB method.

The SPB algorithm is used to estimate and remove the correlation structure. To estimate the correlation structure of the residuals, first, the spherical 314 semi-variogram

$$\gamma(h;\theta) = \begin{cases} 0 & ||h|| = 0\\ c_0 + c_1(\frac{3}{2}\frac{||h||}{a} - \frac{1}{2}(\frac{||h||}{a})^3) & 0 < ||h|| \le a \\ c_0 + c_1 & ||h|| \ge a \end{cases}$$
(11)

315 is fitted to the empirical semi-variogram estimation of coal-ash data with

 $\hat{\theta} = (\hat{c}_0, \hat{c}_1, \hat{a}) = (0.817, 0.815, 15.787).$ Figure 1(a) shows the fitted spherical



Figure 1: (a) Spherical semi-variogram model $\hat{\gamma}(h; \theta)$ fitted to the empirical semivariogram $\hat{\gamma}(h)$ before removal correlation structure. (b) Empirical semi-variogram $\hat{\gamma}(h)$ for standardized residuals after removal correlation structure.

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semi-variogram. The covariance matrix can be estimated as $\hat{\Sigma} = \sigma(h; \hat{\theta}) =$ 317 $\sigma(0;\hat{\theta}) - \gamma(h;\hat{\theta})$. Then, the uncorrelated residuals $\hat{\epsilon} = \hat{L}^{-1}R$ are used to 318 compute the standardized uncorrelated residuals $\tilde{\epsilon}(s_i) = (\hat{\epsilon}(s_i) - \bar{\hat{\epsilon}})/s_{\hat{\epsilon}}; i =$ 319 $1, \ldots, N$. Figure 1(b) shows the fit of a linear semi-variogram to the em-320 pirical semi-variogram estimate of the standardized residuals. The linear 321 semi-variogram model in Figure 1(b) shows that the standardized residuals 322 $(\tilde{\epsilon}(s_1),\ldots,\tilde{\epsilon}(s_N))$ are uncorelated. Finally, the bootstrap samples are deter-323 mined by $\mathcal{Z}^* = \hat{\mu} + \hat{L}\epsilon^*$, where the bootstrap vector ϵ^* is generated by simple 324 random sampling with replacement from the standardized uncorrelated resid-325 uals vector $\tilde{\epsilon}$. 326

Now suppose that the plug-in ordinary kriging $T_1 = \hat{\hat{Z}}(s_0)$ and variogram 327 parameter estimators $\hat{\theta} = (T_2, T_3, T_4) = (\hat{c}_0, \hat{c}_1, \hat{a})$ are the estimators of in-328 terest, where $T_i = t_i(\mathcal{Z})$. For example, if $s_0 = (5, 6)$ is a new location then, 329 $\hat{Z}(s_0) = \hat{\lambda}^T Z = 10.696$ and also $\hat{\theta} = (\hat{c}_0, \hat{c}_1, \hat{a}) = (0.817, 0.815, 15.787)$. The 330 SPB version T_i^* of T_i is $T_i^* = t_i(\mathcal{Z}^*)$, where \mathcal{Z}^* is the SPB sample. We es-331 timate the precision measures $Bias(T_i)$ and $Var(T_i)$ and distribution $G_{T_i}(t)$ 332 by SPB method and B bootstrap replicates $T_{i,1}^*, \ldots, T_{i,B}^*$; i = 1, 2, 3, 4 in 333 relations (8)-(10). Table 10 shows estimates of SPB bias and variance for 334 plug-in kriging and estimates of variogram parameters based on B = 1000335

T_i^*	Bias_*	Var_*
$Z^*(s_0)$	-0.901	0.706
c_0^*	0.002	0.017
c_1^*	0.066	0.037
a^*	-5.829	21.602

 Table 10: Estimates of SPB bias and variance for plug-in kriging and variogram parameters

 for coal-ash data.

bootstrap replicates. Figure 2 shows the histogram of plug-in kriging and variogram parameters estimator based on B = 1000 bootstrap replicates.

338 7. Discussion and Results

Spatial data analysis is based on the estimate of correlation structure, for example, kriging predictor. The estimation of correlation structure is based on parametric covariogram models. Unfortunately, the estimates of covariogram parameters have no closed form and so are computed numerically. If we can estimate the correlation structure as well, then we will use knowledge of the covariogram model which describes the dependence structure in the SPB method. For spatial data the MBB method is usually used to estimate



Figure 2: Histogram of (a) plug-in kriging and variogram parameters estimator:(b) nugget effect, (c) partial sill and (d) range for coal-ash data.

the precision measures of the estimators. However, as already pointed out, the MBB method has limitations and weaknesses. We now summarize some advantages of the SPB method as compared with the MBB method:

The precision of the MBB estimators is related to the optimal block size 349 β_n^{opt} in (7) which depends on unknown parameters which are difficult to 350 estimate. In our simulations it is clear that the optimal block size differs 351 for various estimators or precision measures. Note also that the optimal 352 block size determination is impossible for estimators that have no closed 353 form (e.g. covariogram parameters estimator). For some data sets we may 354 not be able to find the block size that satisfies $N = K \beta_n^d$. In other words, 355 there is not always complete blocking and then $N_1 = K \beta_n^d < N$ is the total 356 number of data-values in the resampled complete blocks. As a result, $N-N_{\rm 1}$ 357 observations are ignored. 358

Establishing the consistency of MBB estimators and estimation of block size requires that the random field satisfies strong-mixing conditions. In the MBB method, our simulations indicate that the variance estimators $\hat{\sigma}^2$ are underestimated. Moreover, our simulations show that the MBB and SPB variance estimations $\hat{\sigma}^2$ are asymptotically unbiased and consistent. In this study, the SPB estimators are more accurate than the MBB estimator, for variance estimation of estimators in spatial data analysis, especially for stronger dependence structure and larger sample sizes. In the SPB method, we use the estimation of spatial correlation structure, therefore the SPB method will perform better than the MBB method. We are studying on comparison of estimation of distribution, spatial prediction interval and confidence interval by SPB and MBB methods.

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