

SPATIAL BOOTSTRAP WITH INCREASING OBSERVATIONS IN A FIXED DOMAIN

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Abstract: Various methods, such as the moving block bootstrap, have been developed to resample dependent data. These contain features that attempt to retain the dependence structure in the data. Asymptotic results for these methods have been based on increasing the number of observations as the observation region increases, combined with restrictions on the range of dependence of the data. In this work, we consider resampling a one-dimensional Gaussian random field observed on a regular lattice, with increasing number of observations within a fixed observation region. We show a consistency result for resampling the variogram when the underlying process has a variogram of the form $\gamma(t) = \theta t + S(t)$, $|S(t)| \leq Dt^2$. For a class of smoother processes, specifically, for a process with variogram of the form $\gamma(t) = \beta t^2 + \theta t^3 + R(t)$, $|R(t)| \leq Dt^4$, we provide a similar result when resampling the second-order variogram. We performed a simulation study in one and two dimensions. We used the Matérn model for the covariance function with varying values of the smoothness parameter ν . We find that the empirical coverage of confidence intervals of the variogram approaches the nominal 95% level as the number of observations increases for models with small ν , but as ν is increased the empirical coverage decreases, with the coverage becoming significantly lower than the nominal level when $\nu \geq 1$. When we consider the second-order variogram, we find that the empirical coverage approaches the nominal level for larger values of ν than for the first-order variogram, with the empirical coverage noticeably lower than the nominal level only when ν is about 2.

Key words and phrases: Fixed domain asymptotics, Gaussian processes, spatial bootstrap, variogram.

1. Introduction

The spatial bootstrap has been studied by a number of researchers, Davison and Hinkley (1997) give a brief overview of methods. Hall (1985) appears to have been the first to use some kind of a block resampling procedure to bootstrap spatial data. Künsch (1989) introduced the block-resampling bootstrap to resample one-dimensional processes for finding the sample mean of weakly stationary observations. With N observations in a line, he suggested forming $N - n + 1$ blocks, each consisting of n consecutive observations, and sampling from these blocks with replacement. Lahiri (1992) considered the

second order properties of the moving block bootstrap procedure of Künsch (1989) and showed that it was second-order correct under appropriate conditions. Liu and Singh (1992) independently proposed a similar method in a paper on bootstrapping m -dependent data, showing consistency of estimates under m -dependence if the size of the blocks $b \rightarrow \infty$ as the sample size $N \rightarrow \infty$, with $b/N \rightarrow 0$. Politis and Romano (1992a) developed the method further and suggested wrapping the data, which we call toroidal wrapping, before performing block resampling. Shi and Shao (1988) and others proposed various versions of the spatial bootstrap. Politis and Romano (1994) studied subsampling, which involves calculating estimates using regions that are smaller than the observation window, and then rescaling the estimates. In his presentation of the block bootstrap, Künsch (1989) provided a way to extend the method to a block of blocks bootstrap method. See also Politis and Romano (1992b) and Bühlmann and Künsch (1995). Loh and Stein (2004) introduced a very similar method, called the marked point bootstrap, for resampling point processes where marks are computed and assigned to observed points before performing the bootstrap. The marks record the contributions made by neighboring points to the estimate of interest. By using the marks in the calculation of bootstrap estimates, the method aims to retain some of the structure inherent in the observations, that might otherwise be partially destroyed by the regular block resampling methods.

Theoretical results that have been obtained are dependent on the underlying process exhibiting only short range dependence. Lahiri (1993) showed that with longer range dependence present, the block resampling method begins to fail, since putting independent blocks together to generate the bootstrapped estimate destroys the long-range dependence present in the original observations. Furthermore, these results consider increasing domain asymptotics, where the observation region or domain increases as the number of observations increases.

In this work, we focus on fixed domain asymptotics and derive consistency results for the block-of-blocks bootstrap in two specific cases. This bootstrap method was introduced by Künsch (1989) and is briefly described in Section 2. It is well known that estimates for dependent data need not be consistent when the domain is fixed (Stein (1999)). We cannot expect resampling methods to work well for estimates that are not consistent. Thus our results are necessarily restricted to certain models and estimated quantities. We consider only Gaussian processes, and for simplicity restrict theoretical results to one dimension.

In Section 3, we work with the variogram γ defined by

$$\gamma(t) = \text{Var}[Z(s_i + t) - Z(s_i)]$$

for distance $t \geq 0$, where $Z(s)$ represents a Gaussian process observed at point s . In particular we consider $t = hL/N$ where h is a fixed positive integer, L the

length of the observation region and N the number of observations. We show a consistency result for resampling the variogram γ of a process that has variogram $\gamma(t) = \theta t + S(t)$, where $|S(t)| \leq Dt^2$, and has a bounded second derivative on $(0, L]$. For a smoother process, higher order differences can remove the long range dependence inherent in the process (Kent and Wood (1997) and Istas and Lang (1997)). In Section 4, we consider a model with variogram $\gamma(t) = \beta t^2 + \theta t^3 + R(t)$, where $|R(t)| \leq Dt^4$ and has a bounded fourth derivative on $(0, L]$. This variogram is proportional to t^2 near the origin and the process is exactly once mean square differentiable. We show a consistency result for the block-of-blocks bootstrap when we consider the second-order variogram, defined as

$$\phi(t) = \text{Var}[Z(s_i + t) - 2Z(s_i) + Z(s_i - t)]. \quad (1)$$

General asymptotic results for bootstrap of dependent data require the observation domain to increase as the number of observations increase, together with some mixing condition for the process. This ensures that the resampling scheme produces replicates that are asymptotically independent, identically distributed. For the case of increasing observations in a fixed observation domain, there is no general analogue to mixing conditions. Furthermore, it is well known (e.g., Stein (1999)) that quantities associated with the process often cannot be consistently estimated. Since randomly selected blocks remain close to each other if the domain has fixed size, it cannot be expected that a general asymptotic result can be proven in the fixed domain setting.

However, there are some quantities related to the random process that can be consistently estimated. For example, Ying (1991) showed that for the process with variogram $\gamma(t) = a[1 - \exp(-\theta t)]$, $a\theta$ can be consistently estimated. A quantity that can be recovered with probability one from observations in a bounded region is called microergodic (Matheron (1971, 1989) and Stein (1999)). For microergodic quantities, it may be possible that bootstrap estimates of standard errors are consistent under the fixed domain setting.

We are not aware of any previous results demonstrating the validity of bootstrapping under fixed domain asymptotics. The results here exploit the fact that first-order and non-overlapping second-order differences of the respective processes we consider are nearly independent. Whether some version of the bootstrap will work for more general microergodic quantities is unknown.

To investigate how well these various bootstrap procedures work in practice, and to investigate their potential validity for processes in two dimensions, we simulated Gaussian processes on the unit interval and the unit square, and examined the empirical coverage of nominal 95% confidence intervals for the

first- and second-order variograms. We used the Matérn model with covariance function given by

$$C(t) = \frac{\sigma}{2^{\nu-1}\Gamma(\nu)} \left(\frac{2\nu^{\frac{1}{2}}t}{\rho}\right)^{\nu} \mathcal{K}_{\nu}\left(\frac{2\nu^{\frac{1}{2}}t}{\rho}\right), \quad (2)$$

where Γ is the Gamma function and \mathcal{K}_{ν} is a modified Bessel function. The parameter ρ is related to the range of the correlation in the process while ν is a smoothness parameter, so that the process is exactly m times mean square differentiable if $m < \nu < m + 1$. We considered values of $\nu = 0.25, 0.5, \dots, 2.0$ and $\rho = 0.01$ and 0.15 .

We found that, for the first-order variogram, the empirical coverage of confidence intervals approaches the nominal level as the number of observations increases for models with small ν . We see a gradual drop in empirical coverage as ν is increased, with the coverage becoming substantially lower than the nominal level when $\nu \geq 1$. With the second-order variogram, we find that the empirical coverage of confidence intervals approaches the nominal level with increasing number of observations for larger values of ν , with the empirical coverage becoming noticeably lower than the nominal level only when ν is about 2. Section 5 gives details of our simulation procedure and findings.

2. The Block-of-Blocks Bootstrap Method

As an extension to the block bootstrap method for resampling one-dimensional processes, Künsch (1989) introduced the block-of-blocks bootstrap in order to reduce the effect of joining independent blocks. We describe the procedure below, using a slightly different formulation from that in Künsch (1989).

Suppose Z is a random field with N observed values $Z(s_i)$ at points $s_i, i = 1, \dots, N$, on a regular lattice of length L . Suppose further that a quantity of interest θ can be estimated via a statistic that can be expressed in the form

$$\hat{\theta} = \sum_i Y_i(Z).$$

The quantity $Y_i(Z)$ can include observations of Z other than at s_i , but generally only observations that are near to s_i . Thus each point s_i has a quantity $Y_i(Z)$ associated with it that is a function of values of the process Z near s_i .

The bootstrap procedure consists of first assigning marks $Y_i(Z)$ to each point s_i . The points are then resampled, for example, by deciding in advance the length and number of sampling intervals to use, then picking randomly starting positions for these intervals. The observation points covered by these randomly placed intervals form the bootstrap sample. Often the total length of the sampling intervals is chosen to be equal to the actual length of the observation region,

although this does not necessarily have to be the case. With the resampled points s_1^*, \dots, s_N^* , the bootstrap estimate of θ is given by

$$\hat{\theta}^* = \sum_i Y_i^*(Z). \tag{3}$$

Note that $Y_i^*(Z)$ is the mark computed from the original observations of Z . This is not equal to $Y_i^*(Z^*)$, which would be what is used if the resampled points s_i^* were put back on a lattice and a new estimate computed directly from the new sample.

3. Resampling the Variogram in a Fixed Domain

Here we provide a consistency result for the block-of-blocks bootstrap when we resample for the variogram of a process Z with variogram $\gamma(t) = \theta t + S(t)$, where $|S(t)| \leq Dt^2$ and has a bounded second derivative on $(0, L]$. Specifically, suppose Z is observed at N equally spaced points in the interval $(0, L]$, h fixed. The observation points are denoted by $s_1 = L/N, s_2 = 2L/N, \dots, s_N = L$.

For fixed integer $h > 0$, we consider estimating the quantity $\gamma(hL/N) = \text{Var}[Z(s_{i+h}) - Z(s_i)]$. We write $Z(s_{i+h})$ as Z_{i+h} for short. Note that as N increases, we are estimating the variogram at smaller and smaller distances, specifically the distance between points that are h number of neighbors away.

An unbiased estimate of $\gamma(hL/N)$ is given by

$$\hat{\gamma}\left(\frac{hL}{N}\right) = \frac{1}{(N-h)} \sum_{i=1}^{N-h} (Z_{i+h} - Z_i)^2 = \frac{1}{N-h} \sum_{i=1}^{N-h} Y_i, \tag{4}$$

where $Y_i = (Z_{i+h} - Z_i)^2$. Each point $s_i, i = 1, \dots, N-h$ is assigned the mark Y_i . Set $M = N-h$.

We consider breaking the interval $(0, L-h]$ into B blocks, where M/B is an integer, and resampling the points by sampling these B blocks with replacement. In block bootstrap terminology, we are using fixed rather than moving blocks. It is conceptually straightforward to extend this to the moving block case. Note that the use of blocks here is only to select the points that will be included in the new sample. In computing the bootstrap estimate, the marks Y_i computed from the real sample are used. In the usual block bootstrap, the Z 's corresponding to the resampled points are used to compute new values of Y_i to give the bootstrap estimate. It is this new computation of the Y_i 's that affects the dependence structure. Note also that we do not resample points $N-h+1$ to N , since these points have no marks. The observations at these points are used in the estimate, however, since they are part of the marks assigned to other points.

For the k -th block, $k = 1, \dots, B$, let

$$\hat{\gamma}_k = \frac{B}{M} \sum_{i=1}^{\frac{M}{B}} Y_{k,i},$$

where $Y_{k,i}$ is the i -th value of Y in the k -th block. Thus $\hat{\gamma}_k$ is the average of the Y values in the k -th block. If B blocks are drawn with replacement, the bootstrap estimate of $\gamma(hL/N)$ is given by

$$\hat{\gamma}^* = \frac{1}{B} \sum_{j=1}^B \hat{\gamma}_j^* = \frac{1}{M} \sum_{j=1}^B \sum_{i=1}^{\frac{M}{B}} Y_{j,i}^*.$$

Here, $\hat{\gamma}_j^*$ denotes the average of the Y values of the j -th sampled block, and $Y_{j,i}^*$ the actual Y values of that block.

Let $U_j, j = 1, \dots, B$, be independent with $P(U_j = \hat{\gamma}_k) = 1/B, k = 1, \dots, B$. Thus $\hat{\gamma}^* = \sum U_j/B$ and $E(U_j|Z) = \hat{\gamma}$. Define $\hat{\sigma}_*^2$ as

$$\hat{\sigma}_*^2 = \text{Var}(\hat{\gamma}^*|Z) = \frac{1}{B^2} \sum_{k=1}^B (\hat{\gamma}_k - \hat{\gamma})^2 = \frac{1}{B^4} \sum_{k=1}^B \left(B\hat{\gamma}_k - \sum_{j=1}^B \hat{\gamma}_j \right)^2. \quad (5)$$

We then have the following.

Theorem 1. *With $\hat{\gamma}$ and $\hat{\sigma}_*^2$ defined in (4) and (5) respectively, $\hat{\gamma}$ is unbiased with*

$$\text{Var}(N\hat{\gamma}) = \frac{2\theta^2 L^2 h(2h^2 + 1)}{3N} + O(N^{-2}), \quad (6)$$

$$N[E(N^2\hat{\sigma}_*^2) - \text{Var}(N\hat{\gamma})] = O(B^{-1}) + O(BN^{-1}), \quad (7)$$

$$\text{Var}(N^2\hat{\sigma}_*^2) = O(B^{-2}N^{-1}). \quad (8)$$

Proof. In what follows we suppress the term hL/N and write $\hat{\gamma}$ and γ to denote $\hat{\gamma}(hL/N)$ and $\gamma(hL/N)$ respectively. It is clear that the estimator $\hat{\gamma}$ is unbiased. Furthermore,

$$\begin{aligned} \text{Var}(M\hat{\gamma}) &= \sum_{i=1}^M \text{Var}(Y_i) + 2 \sum_{i<j}^M \text{Cov}(Y_i, Y_j) \\ &= 2M\gamma^2 + 4 \sum_{i<j}^M \text{Cov}(Z_{i+h} - Z_i, Z_{j+h} - Z_j)^2, \end{aligned} \quad (9)$$

using the fact that $Z_{i+h} - Z_i \sim N(0, \gamma)$ and the result that for (U, V) bivariate normal, $\text{Cov}(U^2, V^2) = 2 \text{Cov}(U, V)^2$. For i, j such that $j - i = k \geq 0$,

$$\begin{aligned}
 C_k &\equiv \text{Cov}(Z_{i+h} - Z_i, Z_{j+h} - Z_j) \\
 &= [\gamma(\frac{(k+h)L}{N}) + \gamma(\frac{|h-k|L}{N}) - 2\gamma(\frac{kL}{N})]2^{-1} \\
 &= \begin{cases} O(N^{-2}) & \text{if } k \geq h, \\ \frac{\theta L(h-k)}{N} + O(N^{-2}) & \text{if } k < h. \end{cases} \tag{10}
 \end{aligned}$$

Putting the expressions for γ^2 and C_k into (9) gives (6).

To find $E(N^2 \hat{\sigma}_*^2)$ we first define $\Delta_k = B\hat{\gamma}_k - \sum_{j=1}^B \hat{\gamma}_j$. We note that $E(\Delta_k) = 0$, so that

$$E(N^2 \hat{\sigma}_*^2) = \frac{N^2}{B^4} \sum_{k=1}^B \text{Var}(\Delta_k). \tag{11}$$

From the expression

$$\frac{M}{B} \Delta_1 = (B-1)(Y_1 + \dots + Y_{\frac{M}{B}}) - (Y_{\frac{M}{B}+1} + \dots + Y_M), \tag{12}$$

we have

$$\begin{aligned}
 \text{Var}\left(\frac{M}{B} \Delta_1\right) &= M(B-1)\text{Var}(Y_1) + 4(B-1)^2 \sum_{l=1}^{\frac{M}{B}-1} \left(\frac{M}{B} - l\right) C_l^2 \\
 &\quad + 4 \sum_{l=1}^{M-\frac{M}{B}-1} \left(M - \frac{M}{B} - 1\right) C_l^2 \\
 &\quad - 4(B-1) \left[\sum_{l=1}^{\frac{M}{B}} l C_l^2 + \sum_{l=\frac{M}{B}+1}^{M-\frac{M}{B}} \frac{M}{B} C_l^2 + \sum_{l=M-\frac{M}{B}+1}^{M-1} (M-l) C_l^2 \right], \tag{13}
 \end{aligned}$$

where C_l is as defined in (10). In the right-hand side of (13), the second and third terms correspond to cross-terms within the respective bracketed terms in (12), and the last term corresponds to cross-terms between terms in the two brackets in (12). Rearranging the terms and noting that for $l \geq h$, the sum of the coefficients of C_l^2 is $O(M^2)$ while C_l^2 is $O(N^{-4})$, we have

$$\begin{aligned}
 \text{Var}\left(\frac{M}{B} \Delta_1\right) &= M(B-1)\text{Var}(Y_1) + 4 \sum_{l=1}^{h-1} \{BM - M - (B^2 - B + 1)l\} C_l^2 \\
 &\quad + O(N^{-2}), \\
 &= 2MB\theta^2 L^2 h(2h^2 + 1)(3N^2)^1 + O(B^2 N^{-2}) + O(N^{-1}).
 \end{aligned}$$

Expressions for $M\Delta_k/B, k = 2, \dots, B-1$, are the same as the above, differing only in the smaller order terms. Putting these into (11) yields

$$E(N^2\hat{\sigma}_*^2) = \frac{2\theta^2 L^2 h(2h^2 + 1)}{3N} + O(N^{-1}B^{-1}) + O(BN^{-2}),$$

which in turn gives (7).

Next, we have

$$\begin{aligned} \text{Var}(\hat{\sigma}_*^2) &= \frac{1}{B^8} \sum_{k=1}^B \text{Var}(\Delta_k^2) + \frac{2}{B^8} \sum_{k,l:k<l}^B \text{Cov}(\Delta_k^2, \Delta_l^2) \\ &= \frac{1}{B^8} \sum_{k=1}^B \text{Var}(\Delta_k^2) + \frac{2}{B^8} \left[\sum_{k=1}^{B-1} \text{Cov}(\Delta_k^2, \Delta_{k+1}^2) \right. \\ &\quad \left. + \sum_{k=1}^{B-2} \text{Cov}(\Delta_k^2, \Delta_{k+2}^2) + \dots + \text{Cov}(\Delta_1^2, \Delta_B^2) \right]. \end{aligned} \quad (14)$$

The quantities $\text{Var}(\Delta_k^2)$, $\text{Cov}(\Delta_k^2, \Delta_{k+1}^2)$ and $\text{Cov}(\Delta_k^2, \Delta_{k+l}^2)$ for $l = 2, \dots, B-1$, have terms of the form $\text{Cov}(Y_i Y_j, Y_u Y_v)$. First consider the case where at least one of $\{u, v\}$ is less than h away from $\{i, j\}$. The covariance terms $\text{Cov}(Y_i Y_j, Y_u Y_v)$ can be classified into four types, represented by $\text{Cov}(Y_i Y_{i'}, Y_{i''} Y_{i'''})$, $\text{Cov}(Y_i Y_{i'}, Y_{i''} Y_j)$, $\text{Cov}(Y_i Y_j, Y_{i'} Y_k)$ and $\text{Cov}(Y_i Y_j, Y_{i'} Y_{j'})$, where i' denotes integers such that $|i - i'| < h$, and similarly for i'', i''' . These are in turn bounded by $\text{Cov}(Y_i^2, Y_i^2)$, $\text{Cov}(Y_i^2, Y_i Y_j)$, $\text{Cov}(Y_i Y_j, Y_i Y_k)$ and $\text{Cov}(Y_i Y_j, Y_i Y_j)$ respectively, where each is $O(N^{-4})$.

Using (12) and similar expressions for $M\Delta_k/B$, we can find the sums of the coefficients of each type for $\text{Var}(M^2\Delta_k^2/B^2)$, $\text{Cov}(M^2\Delta_k^2/B^2, M^2\Delta_{k+1}^2/B^2)$ and $\text{Cov}(M^2\Delta_k^2/B^2, M^2\Delta_{k+l}^2/B^2)$ for $l = 2, \dots, B-1$. For $\text{Var}(M^2\Delta_k^2/B^2)$, the sum of the coefficients corresponding to $\text{Cov}(Y_i Y_{i'}, Y_{i''} Y_{i'''})$, $\text{Cov}(Y_i Y_{i'}, Y_{i''} Y_j)$, $\text{Cov}(Y_i Y_j, Y_{i'} Y_k)$ and $\text{Cov}(Y_i Y_j, Y_{i'} Y_{j'})$ are, respectively, $O(MB)$, $O(M^2B^2)$, $O(M^3B)$ and $O(M^2)$. Similarly, these coefficients are $O(MB + B^4)$, $O(MB^3 + M^2B)$, $O(M^3 + M^2B^2)$ and $O(M^2)$ for $\text{Cov}(M^2\Delta_k^2/B^2, M^2\Delta_{k+1}^2/B^2)$, and $O(MB)$, $O(M^2B)$, $O(M^3)$ and $O(M^2)$ for $\text{Cov}(M^2\Delta_k^2/B^2, M^2\Delta_{k+l}^2/B^2)$, $l = 2, \dots, B-1$. Thus the contribution of these terms to (14) is $O(N^{-5}B^{-2})$.

Repeating the same argument, we find that the contribution of terms $\text{Cov}(Y_i Y_j, Y_u Y_v)$ where both $\{u, v\}$ are both at least h away from $\{i, j\}$ add up to $O(N^{-6}B^{-2})$. Combining these findings gives (8).

Together with the asymptotic normality of $\hat{\gamma}$ (Kent and Wood (1997)), we can further show asymptotic normality of $(\hat{\gamma} - \gamma)/\hat{\sigma}_*$ as B increases with N , N

increasing slightly faster than B :

$$\begin{aligned} \frac{\hat{\gamma} - \gamma}{\hat{\sigma}_*} &= \frac{\hat{\gamma} - \gamma}{\sqrt{\text{Var}(\hat{\gamma})}} \times \left(\frac{\text{Var}(N\hat{\gamma})}{N^2\hat{\sigma}_*^2} \right)^{\frac{1}{2}} \\ &= \frac{\hat{\gamma} - \gamma}{\sqrt{\text{Var}(\hat{\gamma})}} [1 + O_p(N^{\frac{1}{2}}B^{-1}) + O(BN^{-1})]^{\frac{1}{2}} \quad (\text{using Theorem 1}) \\ &= \frac{\hat{\gamma} - \gamma}{\sqrt{\text{Var}(\hat{\gamma})}} + O_p(N^{\frac{1}{2}}B^{-1}) + O_p(BN^{-1}), \end{aligned}$$

where $(\hat{\gamma} - \gamma)/\sqrt{\text{Var}(\hat{\gamma})}$ is asymptotically standard normal (Kent and Wood (1997)). Specifically, $(\hat{\gamma} - \gamma)/\hat{\sigma}_*$ is asymptotically normal if we let $B = N^\alpha$ such that $0.5 < \alpha < 1$ and $N \rightarrow \infty$.

3.1. Resampling in the presence of a trend

Theorem 1 still holds if the observed process has a trend, provided the trend is sufficiently smooth. Specifically, suppose $X(t) = \mu(t) + Z(t)$, where Z is a zero mean process with variogram $\gamma(t) = \theta t + S(t)$, $S(t) \leq Dt^2$, with a bounded second derivative on $(0, L]$.

First, we note that $\text{Var}(X_{i+h} - X_i) = \gamma(hL/N)$. Setting $\hat{\gamma} = \sum_{i=1}^{N-h} (X_{i+h} - X_i)^2 / (N - h)$, we find that

$$E(\hat{\gamma}) = \gamma\left(\frac{hL}{N}\right) + \frac{1}{N-h} \sum_{i=1}^{N-h} (\mu_{i+h} - \mu_i)^2.$$

If, for example, the first derivative of μ is bounded, then the second term in the expression above is $O(N^{-2})$. Then $\hat{\gamma}$ is asymptotically unbiased and $\text{Var}(N\hat{\gamma})$ is as given in (6), with the additional terms in μ being $O(N^{-3})$. Furthermore, the steps in the proof leading to Equations (7) and (8) carry through unchanged.

4. Resampling the Second-Order Variogram in a Fixed Domain

Kent and Wood (1997) showed that for processes with variogram given by

$$\gamma(t) = \theta t^\alpha + o(t^\alpha) \quad \text{as } t \rightarrow 0,$$

the fixed domain asymptotic behavior of estimates of α is different for $\alpha < 1.5$ and $\alpha \geq 1.5$. This difference in asymptotic behavior can be attributed to longer range dependence in processes with $\alpha \geq 1.5$. Kent and Wood (1997) also showed that higher order differencing of the data can remove this long range dependence. See also Istas and Lang (1997).

In this section, we show how the idea of differencing to remove dependence can apply to inference via resampling with a specific model where $\alpha = 2$. Specifically, we consider the model for a Gaussian process Z in one dimension, with variogram given by

$$\gamma(t) = \beta t^2 + \theta t^3 + R(t) \quad t \geq 0, \quad (15)$$

where $|R(t)| \leq Dt^4$ and $\gamma(t)$ has a bounded fourth derivative.

We consider estimating the second-order variogram, which we denote by ϕ , defined in (1). For this model, the second-order variogram $\phi(hL/N) = 6C(0) - 8C(hL/N) + 2C(2hL/N)$ has the form

$$\begin{aligned} N^3\phi &= -8\theta h^3 L^3 + 8N^3 R\left(\frac{hL}{N}\right) - 2N^3 R\left(\frac{2hL}{N}\right) \\ &= -8\theta h^3 L^3 + O(N^{-1}), \end{aligned} \quad (16)$$

so that the first term of $N^3\phi$ is independent of N . Note also that (16) does not contain β . An estimator of ϕ is

$$\hat{\phi}\left(\frac{hL}{N}\right) = \frac{1}{M} \sum_{i=1}^M Y_i, \quad (17)$$

where $Y_i = [Z_{i+h} - 2Z_i + Z_{i-h}]^2$, $i = h + 1, \dots, N - h$, and $M = N - 2h$. Using the block-of-blocks bootstrap as in the previous section we get the following.

Theorem 2. *The estimator $\hat{\phi}$ given in (17) is unbiased and*

$$\text{Var}(N^3\hat{\phi}) = \frac{\theta^2 L^6}{105N} P(h) + O(N^{-2}), \quad (18)$$

where $P(h) = 29280h^7 - 47040h^6 + 42336h^5 + 3360h^4 - 17920h^3 + 3360h^2 + 1744h$ is a fixed polynomial in h , so that $N^3\hat{\phi}$ has N^{-1} convergence. Furthermore,

$$N[\mathbb{E}(N^6\hat{\sigma}_*^2) - \text{Var}(N^3\hat{\phi})] = O(B^{-1}) + O(BN^{-1}), \quad (19)$$

$$\text{Var}(N^6\hat{\sigma}_*^2) = O(B^{-2}N^{-1}). \quad (20)$$

Proof. The estimate $\hat{\phi}$ is clearly unbiased. Furthermore,

$$\begin{aligned} \text{Var}(\hat{\phi}) &= \frac{1}{M} \text{Var}(Y_1) + \frac{4}{M^2} \sum_{i < j}^M \text{Cov}(Z_{i+h} - 2Z_i + Z_{i-h}, Z_{j+h} - 2Z_j + Z_{j-h})^2 \\ &= \frac{2}{M} \phi\left(\frac{hL}{N}\right)^2 + \frac{4}{M^2} \sum_{i < j}^M C_{|i-j|}^2, \end{aligned} \quad (21)$$

where

$$C_k = -6\gamma\left(\frac{kL}{N}\right) + 4\gamma\left(\frac{(k+h)L}{N}\right) - \gamma\left(\frac{(k+2h)L}{N}\right) - \gamma\left(\frac{|k-2h|L}{N}\right) + 4\gamma\left(\frac{|k-h|L}{N}\right). \tag{22}$$

Using (15), we can evaluate (22) for the three cases $k = |i - j| < h, h \leq k < 2h$ and $k \geq h$, giving

$$C_k = \begin{cases} -\theta L^3(6k^3 - 12k^2h + 8h^3)N^{-3} + O(N^{-4}) & \text{for } k < h, \\ -\theta L^3(-2k^3 + 12k^2h - 24kh^2 + 16h^3)N^{-3} + O(N^{-4}) & \text{for } h \leq k < 2h, \\ O(N^{-4}) & \text{for } k \geq 2h. \end{cases} \tag{23}$$

There are $M - k$ pairs of Y_i and Y_j such that $j - i = k$, thus there are order M^2 terms with $k \geq 2h$. The sum of the corresponding covariance terms within the double sum in (21) for $k \geq 2h$ is of order N^{-6} , whereas for $k < 2h$,

$$\sum_{i < j: |i-j| < 2h}^M C_{|i-j|}^2 = \frac{\theta^2 L^6}{N^6} \left[\sum_{k=1}^{h-1} (6k^3 - 12k^2h + 8h^3)^2 (M - k) + \sum_{k=h}^{2h-1} (-2k^3 + 12k^2h - 24kh^2 + 16h^3)^2 (M - k) \right] + O(N^{-6}).$$

Putting this together with (16) into (21) gives (18).

For the bootstrap calculations, many of the expressions for the bootstrap variance estimator follow from the previous section. Here, we find that the terms involving C_k for $k \geq 2h$ sum up to a lower order than the terms corresponding to $k < 2h$. Specifically, for (13), there are $O(M^2)$ number of terms involving C_l^2 with $l \geq 2h$, of order $O(N^{-8})$. Thus we find that, for $M/B \geq 2h$,

$$\begin{aligned} \text{Var}\left(\frac{M}{B}\Delta_1\right) &= M(B-1)\text{Var}(Y_1) + \frac{4\theta^2 L^6}{N^6} \sum_{l=1}^{h-1} [MB - M - (B^2 - B + 1)l] \\ &\quad \times [(6l^3 - 12l^2h + 8h^3)^2 + O(N^{-1})] \\ &\quad + \frac{4\theta^2 L^6}{N^6} \sum_{l=h}^{2h-1} [MB - M - (B^2 - B + 1)l] \\ &\quad \times [(-2l^3 + 12l^2h - 24lh^2 + 16h^3)^2 + O(N^{-1})] + O(N^{-6}) \\ &= \frac{MB\theta^2 L^6}{105N^6} P(h) + O(N^{-5}) + O(B^2 N^{-6}), \end{aligned}$$

where $P(h)$ is defined just after (18). Putting this into

$$E(N^6 \hat{\sigma}_*^2) = \frac{N^6}{B^4} \sum_{k=1}^B \text{Var}(\Delta_k)$$

and comparing with $\text{Var}(N^3 \hat{\phi})$ in (18) gives (19).

To obtain (20), we note that the argument of the two paragraphs after (14) applies here as well. The terms $\text{Cov}(Y_i Y_j, Y_u Y_v)$, where at least one of $\{u, v\}$ is at most $2h$ away from $\{i, j\}$, are bounded by one of $\text{Cov}(Y_i^2, Y_i^2)$, $\text{Cov}(Y_i^2, Y_i Y_j)$, $\text{Cov}(Y_i Y_j, Y_i Y_k)$ or $\text{Cov}(Y_i Y_j, Y_i Y_j)$, which are $O(N^{-12})$. The sums of coefficients corresponding to these terms are of the same order as those in the previous section. This gives (20), after noting that terms $\text{Cov}(Y_i Y_j, Y_u Y_v)$ for u and v both $2h$ or more away from i and j are $O(N^{-14})$ and their total is $o(B^{-2}N^{-1})$.

As in Section 3.1, the bootstrap is consistent in the presence of a trend if the trend is sufficiently smooth. Specifically, if the second derivative of μ is bounded, $\hat{\phi}$ is asymptotically unbiased. Equations (18), (19) and (20) of Theorem 2 remain unchanged.

Note that the second-order variogram ϕ contains θ but not β . Under fixed domain asymptotics ϕ , and thus θ , can be consistently estimated and we showed above that the block-of-blocks bootstrap yielded asymptotically correct inferences under fixed domain asymptotics.

On the other hand, β cannot be consistently estimated using observations in a fixed domain and we do not expect any bootstrap method to yield asymptotically correct inferences for β under fixed domain asymptotics. The results of our simulation study (Section 5, Figure 3) also show that as we consider smoother processes, consistency is achieved only if we difference enough, e.g., by considering the second-order variogram rather than the first-order variogram.

5. Simulation Study

We present here the results of a simulation study to bootstrap a Gaussian random field using the block-of-blocks bootstrap. We performed simulations in one and two dimensions, using equally spaced observations on the unit interval and the unit square. In our simulations we used the Matérn model with covariance function given by (2), with $\rho = 0.01$ and 0.15 and $\nu = 0.25, 0.5, \dots, 2.0$. The values $\nu = 0.5$ and 1.5 correspond to models belonging to those considered in Sections 3 and 4, respectively.

Normally a simulation of a realization of a random field requires performing a Cholesky decomposition of the covariance matrix and, for large data sets, is very computationally intensive. However, for observations on a regular lattice, simulations can be done very quickly using the Fast Fourier Transform.

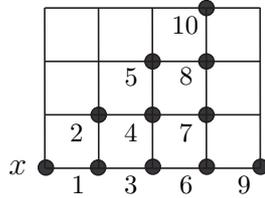


Figure 1. For each point x in the two dimensional simulations, the distances at which the variograms are estimated are the distances to the 10 nearest neighbors as shown here.

Wood and Chan (1994) and Dietrich and Newsam (1997) provide slightly different methods to do this (see also Stein (2002)). We used the method of Dietrich and Newsam (1997).

With a realization of the process, we computed the first and second-order variograms at distances corresponding to the 10 nearest neighbors of the observations. In one dimension, $h = 1, \dots, 10$, while in two dimensions, $h = 1, \sqrt{2}, 2, \sqrt{5}, \sqrt{8}, 3, \sqrt{10}, \sqrt{13}, 4, \sqrt{18}$ (see Figure 1).

The bootstrap method described in Section 2 was then used to resample the observations to obtain bootstrap estimates. For each realization, we obtained $R = 999$ bootstrap samples. With the 999 bootstrap estimates, a nominal 95% confidence interval is then constructed using what Davison and Hinkley (1997) call the basic bootstrap interval.

Specifically, for each realization of a process, we have, for the first order variogram, say, an estimate $\hat{\gamma} = \hat{\gamma}(h/N)$ and R bootstrap estimates $\hat{\gamma}_k^*, k = 1, \dots, R$. If $\hat{\gamma}_{(R+1)(1-\alpha/2)}$ and $\hat{\gamma}_{(R+1)\alpha/2}$ are respectively the $(R+1)(1-\alpha/2)$ th and $(R+1)(\alpha/2)$ th ordered values of $\hat{\gamma}_k^*, k = 1, \dots, R$, the $100(1-\alpha)\%$ basic bootstrap interval is given by

$$[2\hat{\gamma} - \hat{\gamma}_{(R+1)(1-\alpha/2)}, 2\hat{\gamma} - \hat{\gamma}_{(R+1)\alpha/2}]. \tag{24}$$

The above interval is obtained by assuming that the sampling distribution of $\hat{\gamma}^* - \hat{\gamma}$ is similar to that of $\hat{\gamma} - \gamma$, so that the $(1-\alpha/2)$ th and $(\alpha/2)$ th quantiles of $\hat{\gamma} - \gamma$ can be estimated by the $(R+1)(1-\alpha/2)$ th and $(R+1)(\alpha/2)$ th ordered values of $\hat{\gamma}^* - \hat{\gamma}$. The bootstrap procedure is performed 500 times, giving 500 nominal 95% confidence intervals. The empirical coverage of the confidence intervals can then be examined.

We implemented a few modifications to the resampling scheme described in the earlier sections. First, we used overlapping blocks instead of non-overlapping ones. In analogy to the block bootstrap, this means we used moving blocks instead of fixed blocks. Thus, in the one-dimensional simulations, block 1 consists

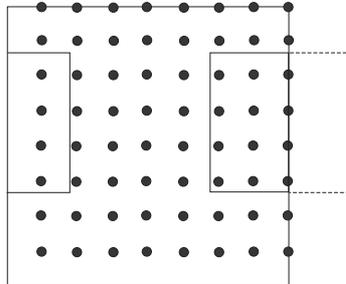


Figure 2. This figure shows how toroidal wrapping is implemented in two dimensions. The dots represent the observation points. The smaller square is a resampling block that does not fully lie within the observation region. The dotted portion is wrapped around and samples the observations on the other side as well.

of observations 1 through N/B , block 2 of observations 2 through $N/B+1$, and so on, and a new sample is obtained by sampling B of these blocks with replacement.

Also, to ensure that every point has equal probability of being selected, we implemented a toroidal wrapping procedure and allow blocks to fall partly outside the observation region. Such blocks are wrapped around so that they also sample points on the other side of the observation region. So, for example, in one dimension, block N consists of observations $N, 1, \dots, N/B - 1$. Figure 2 shows toroidal wrapping implemented in two dimensions. Note that the marks are calculated from the original observations without any toroidal wrapping. The toroidal wrapping is only applied to the resampling of the points. Any other procedure for selecting points with equal probability can be used, if desired. For the simulations in one dimension, we use N equal to 32, 64, 128, 256, 512, 1024, and 2,048, and blocks of length $1/2, 1/4, 1/8$, and $1/16$. In two dimensions, we use $N = 16^2, 32^2, \dots, 1024^2$ and blocks of area $1/2^2, 1/4^2, 1/8^2$, and $1/16^2$.

5.1. Results

Figure 3 shows the results of our simulation study in one dimension, specifically, plots of the empirical coverage of nominal 95% confidence intervals for the first-order and second-order variograms for the Matérn process with $\rho = 0.15$ and ν from 0.25 to 2.0. The results for $\rho = 0.01$ are very similar and are not shown. We only show plots for representative values of N and B , specifically, $N = 128$ with $B = 4$, $N = 512$ with $B = 8$, and $N = 2,048$ with $B = 16$. We did not include plots for $N = 32$ as the empirical coverages attained for this N are uniformly poor, especially for large r .

When estimating the first-order variogram, we find that the empirical coverage of nominal 95% confidence intervals approaches the nominal level as N

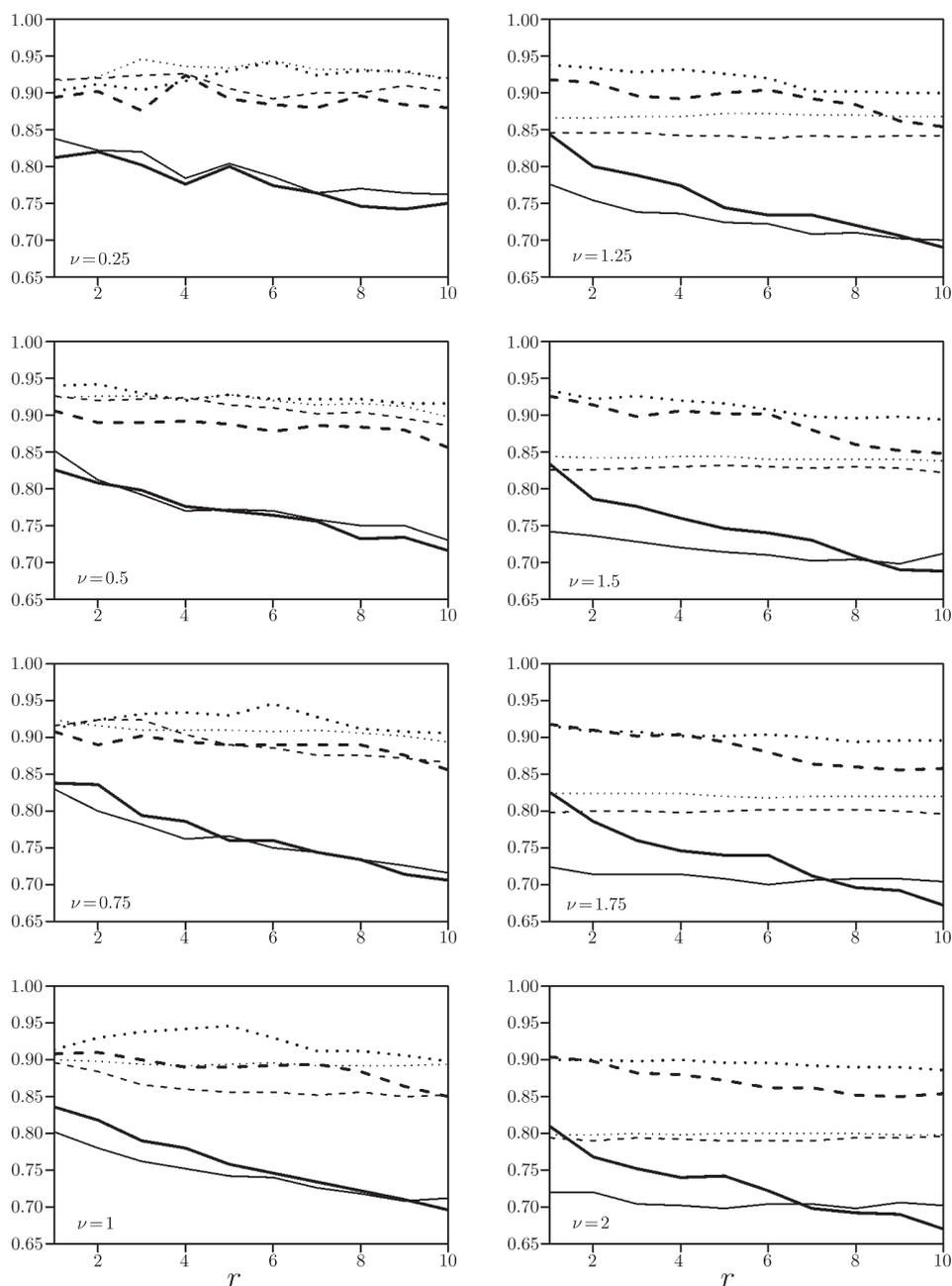


Figure 3. Plots of empirical coverage of nominal 95% confidence intervals for the first-order variogram γ (thin lines) and second-order variogram ϕ (thick lines), obtained by resampling using the block-of-blocks bootstrap method for the Matérn models in one dimension, for $\rho = 0.15, \nu = 0.25, 0.5, \dots, 2$. Different numbers of observations N and block sizes $1/B$ were considered: $N = 128, B = 4$ (solid), $N = 512, B = 8$ (dashed) and $N = 2,048, B = 16$ (dotted).

and B get larger, with N/B increasing, for small ν , specifically, $\nu = 0.25, 0.5$ and 0.75 . This holds for both $\rho = 0.01$ and 0.15 . As we increase ν further, we find a gradual degradation, with the empirical coverage becoming noticeably less than 95% for all N when ν is about 1 and larger, especially so when $\rho = 0.15$. Furthermore, there is little or no improvement in coverage probabilities when N increases from 512 to 2,048.

From the results in the previous sections, we expect, for the $\nu = 1.5$ model, that the empirical coverage will be closer to the nominal level when we consider the second-order variogram for larger values of N . We find from Figure 3 that this is indeed the case. Again, we see a gradual drop in empirical coverage as ν is increased to 2. For $\nu = 2$, we find that the empirical coverage of 95% confidence intervals for the second-order variogram does not approach the 95% level as the number of observations is increased.

We also examine how the empirical coverage probabilities of nominal 95% confidence intervals vary when B is varied, with N fixed. In general, we find that for a particular value of N , empirical coverage improves as B increases. With small B , the bootstrap samples tend to be more alike, so that bootstrap estimates do not have the appropriate variance. However, we find that the empirical coverage may drop if B is increased too much. Figure 4 shows the empirical coverage of nominal 95% confidence intervals for the second-order variogram for $N = 32$ (left), and $N = 2,048$ (right), with the Matérn $\nu = 1.5, \rho = 0.15$ model. The right plot shows the common situation of empirical coverage increasing as B increases. The left plot shows an example of empirical coverage dropping when B gets too large.

This drop in empirical coverage when B is too large is slightly more pronounced in our simulations in two dimensions. Figure 5 shows plots of the empirical coverage of nominal 95% confidence intervals for ϕ of the Matérn $\nu = 1.5, \rho = 0.15$ model, with $N = 32^2$ and 512^2 . Notice that empirical coverage drops when the smallest block sizes were used.

Figure 6 shows plots of the empirical coverage of nominal 95% bootstrap confidence intervals of the first- and second-order variograms in the two-dimensional case, with different combinations of the number of observations N and block area $1/B^2$: $N = 32^2$ with $B = 2$, $N = 128^2$ with $B = 4$, and $N = 512^2$ with $B = 8$. In two dimensions, we see that we require larger sample sizes for the asymptotics to become apparent. Note that the actual empirical coverages attained in the one- and two-dimensional simulations are difficult to compare. For example, it is not clear whether $N = 128$ in the one-dimensional case should be compared with $N = 128$ or $N = 128^2$ in two dimensions. It is also not clear whether to make comparisons using block width or number of blocks.

We do find the same qualitative behavior of the empirical coverage as in the one-dimensional case: as N and B are increased, with N/B increasing, the

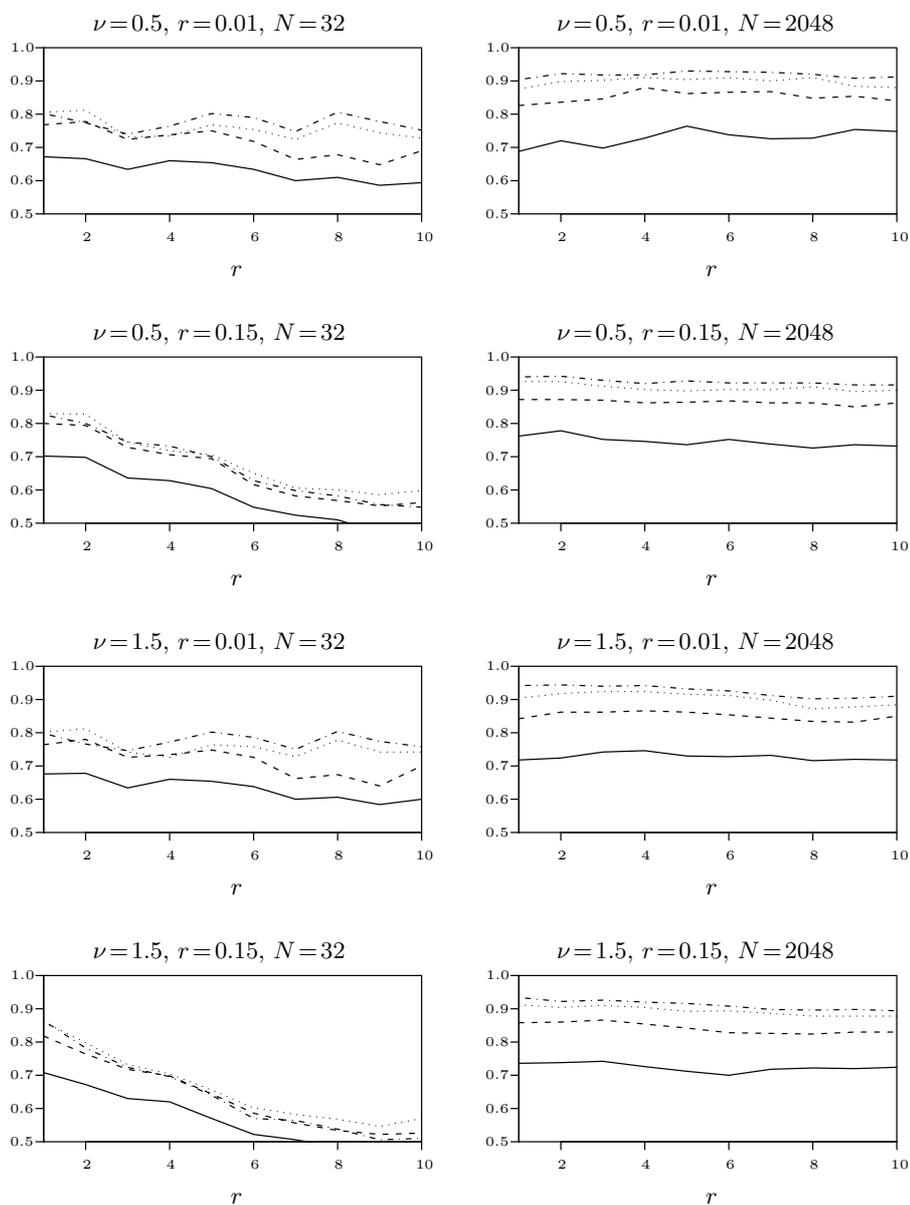


Figure 4. Plots of empirical coverage of nominal 95% confidence intervals for the second-order variogram ϕ , obtained by resampling using the block-of-blocks bootstrap method for the Matérn model with $\nu = 1.5, \rho = 0.15$ in one dimension. The numbers of observations N are 32 (left) and 2,048 (right). For each plot, the different lines correspond to different block size $1/B$: $B = 2$ (solid), $B = 4$ (dashed), $B = 8$ (dotted), and $B = 16$ (dotted and dashed).

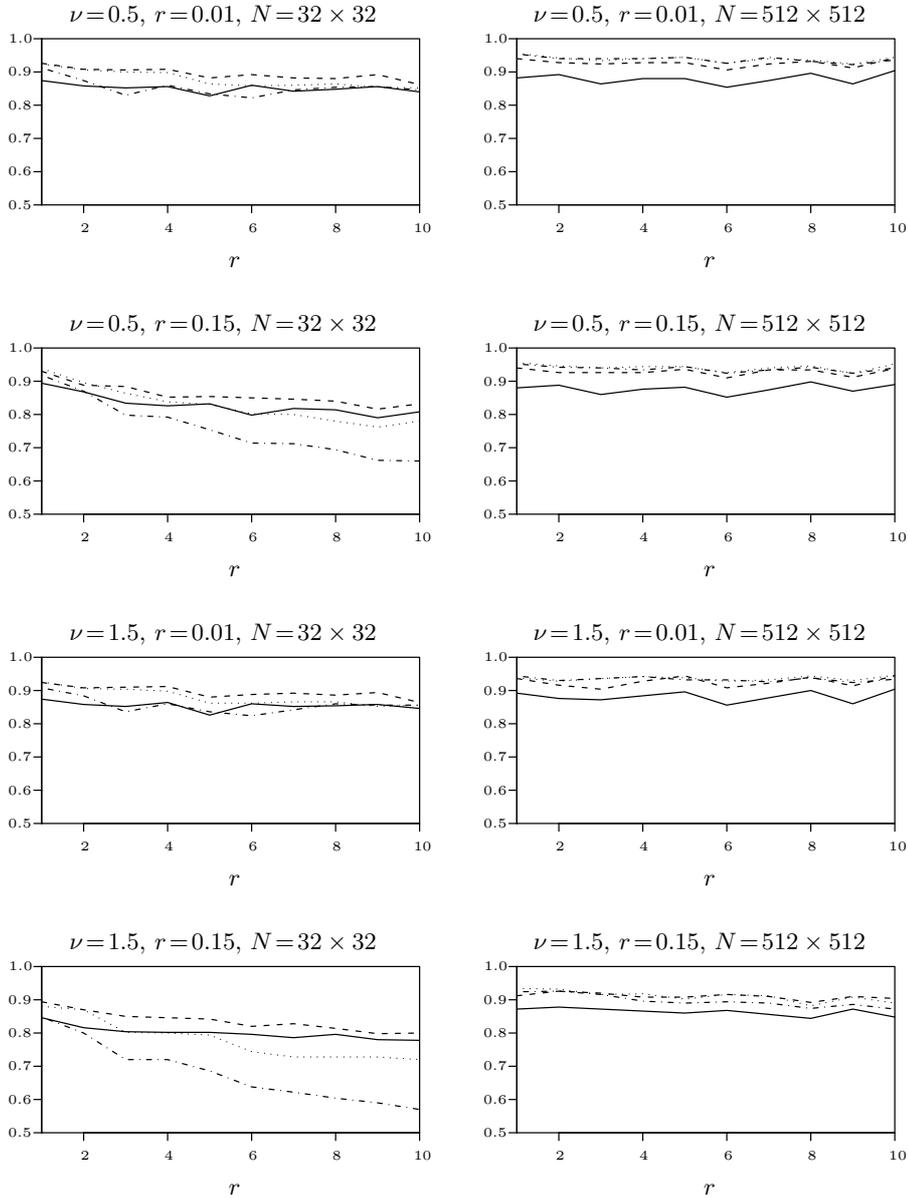


Figure 5. Plots of empirical coverage of nominal 95% confidence intervals for the second-order variogram ϕ , obtained by resampling using the block-of-blocks bootstrap method for the Matérn model with $\nu = 1.5, \rho = 0.15$ in two dimensions. The numbers of observations N are 32×32 (left) and 512×512 (right). For each plot, the different lines correspond to blocks with area $1/B^2$: $B = 2$ (solid), $B = 4$ (dashed), $B = 8$ (dotted), and $B = 16$ (dotted and dashed).

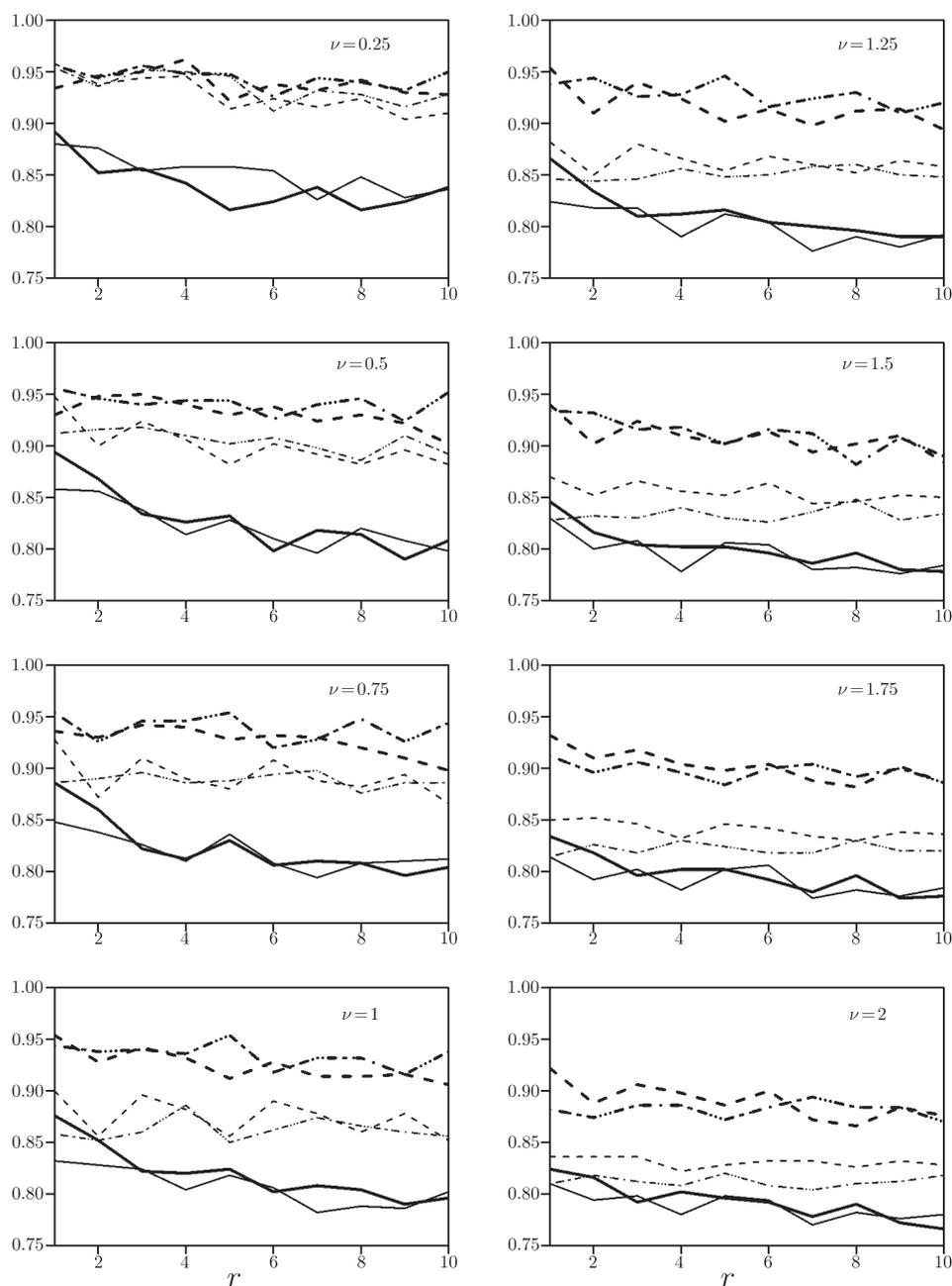


Figure 6. Plots of empirical coverage of nominal 95% confidence intervals for the 1st order variogram γ (thin lines) and 2nd order variogram ϕ (thick lines), obtained by resampling using the block-of-blocks bootstrap method in two dimensions for the Matérn model with $\rho = 0.15$ and $\nu = 0.25, 0.5, \dots, 2$. Different numbers of observations N and block areas $1/B^2$ were considered: $N = 32 \times 32, B = 2$ (solid), $N = 128 \times 128, B = 4$ (dashed), $N = 512 \times 512, B = 8$ (dotted and dashed).

empirical coverage increases toward the nominal level provided $\nu < 1$ for the first-order variogram, and $\nu < 2$ for the second-order variogram. This once again suggests that consistency is achieved only if we difference enough. The results in Chan and Wood (2000) show different asymptotic behavior of increment-based estimators in one and two dimensions for a related setting. However, it is difficult to say anything conclusive about differences between the one- and two-dimensional cases from our simulation study.

6. Conclusion

In spatial statistics, asymptotics can be considered in the context of an increasing or fixed domain as the number of observations increases. As far as we are aware, there has not been any asymptotic results for the spatial bootstrap under the fixed-domain setting. In this work, we showed that the block-of-blocks bootstrap gives asymptotically consistent results in the fixed domain case, when appropriate quantities are considered. Specifically, we considered two Gaussian processes, one with variogram of the form $\gamma(t) = \theta t + S(t)$, $|S(t)| \leq Dt^2$ and the other of the form $\gamma(t) = \beta t^2 + \theta t^3 + R(t)$, $|R(t)| \leq Dt^4$, and showed that the block-of-blocks bootstrap gives consistent results for the variogram and second-order variogram respectively. The results here are not specific to the block-of-blocks bootstrap and should apply to other similar resampling schemes.

In our simulations with Matérn processes, we find that as the smoothness parameter ν is increased, the empirical coverage of nominal 95% confidence intervals for the variogram decreased. For ν about 1 and larger, the coverage of confidence intervals was noticeably lower than the nominal level even for large N . For confidence intervals of the second-order variogram, however, the nominal level is attained as N is increased, for larger values of ν , with the degradation becoming noticeable at a higher value of ν than for the first-order variogram.

Following Matheron (1971), Stein (1999) defines the principal irregular term as the first term in the expansion of the covariance function $C(t)$ in t about 0 that is not an even power of t . For example, for the processes considered in Section 3 and 4, the principal irregular terms are θt and θt^3 respectively. For the Matérn model, the principal irregular term has power given by 2ν . With the second-order variogram in Section 4, we removed the βt^2 term in the expansion of the covariance function by taking second differences and were able to make consistent inferences for the principal irregular term under fixed-domain asymptotics.

Kent and Wood (1997) considered estimating α in $\gamma(t) = \theta t^\alpha + o(t^\alpha)$. They showed that estimates for α obtained from first differences of the process are $n^{1/2}$ -consistent only if $\alpha \in (0, 1.5)$, but when second differences are used, $n^{1/2}$ -consistent estimates are obtained for $\alpha \in (0, 2)$. Our simulations suggest a similar

result for the bootstrap: the bootstrap can work reasonably well for a high enough order of the variogram relative to the smoothness of the process.

Covariance functions with similar high frequency behavior of their spectral densities yield very similar predictions (Stein (1999)). The high frequency behavior is in turn related to the principal irregular term in the expansion of the covariance function in t about 0. We showed here that the bootstrap estimate is consistent for the standard error of the principal irregular term estimate, but not necessarily for the empirical variogram.

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