Simulation of Stationary Gaussian Processes in $[0, 1]^d$

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A method for simulating a stationary Gaussian process on a fine rectangular grid in $[0, 1]^d \subset \mathbf{R}^d$ is described. It is assumed that the process is stationary with respect to translations of $\mathbf{R}^d$, but the method does not require the process to be isotropic. As with some other approaches to this simulation problem, our procedure uses discrete Fourier methods and exploits the efficiency of the fast Fourier transform. However, the introduction of a novel feature leads to a procedure that is exact in principle when it can be applied. It is established that sufficient conditions for it to be possible to apply the procedure are (1) the covariance function is summable on $\mathbf{R}^d$, and (2) a certain spectral density on the d-dimensional torus, which is determined by the covariance function on $\mathbf{R}^d$, is strictly positive. The procedure can cope with more than 50,000 grid points in many cases, even on a relatively modest computer. An approximate procedure is also proposed to cover cases where it is not feasible to apply the procedure in its exact form.

Key Words: Circulant; Fast Fourier transform; Positive definite; Toeplitz.

1. INTRODUCTION

We consider the problem of simulating realizations of a stationary Gaussian process on the set

$$\left\{ \left(\frac{j[1]}{n[1]}, \ldots, \frac{j[d]}{n[d]} \right)^T \in \mathbf{R}^d : 0 \leq j[l] \leq n[l] - 1,\ 1 \leq l \leq d \right\} \subset [0, 1]^d \subset \mathbf{R}^d, \quad (1.1)$$

where the $j[l]$ and $n[l]$ are integers with $n[l] \geq 1$ fixed for $1 \leq l \leq d$. It is assumed that we are given a covariance function $\gamma : \mathbf{R}^d \to \mathbf{R}$ that is stationary with respect to translations of $\mathbf{R}^d$, but not necessarily isotropic. The most important cases are $d = 1$ (the line) and $d = 2$ (the plane), but the method also extends to dimension $d > 2$.

This work was motivated by the desire to examine the numerical performance of various estimators of the fractal dimension of rough surfaces (and one-dimensional sections of these surfaces). See, for example, Constantine and Hall (1994) and Hall and

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Wood (1993). In these articles the idea was to view the surface as a realization of a continuous, stationary Gaussian process. Thus numerical study of the estimators depends on the availability of a method for simulating a stationary Gaussian process on a fine grid.

A notable feature of our procedure is that it generates realizations that are *exact in principle*, while it exploits the speed and efficiency of the fast Fourier transform. By "exact in principle" we mean that realizations on the grid (1.1) would have exactly the required multivariate normal distribution if (1) there are no inaccuracies in computer arithmetic and (2) genuinely random and independent numbers, rather than pseudo-random numbers, are used. Exactness in principle is clearly a desirable property for a simulation procedure to have, particularly if there is no sacrifice in speed and efficiency relative to existing approximate methods.

There is a sizeable geostatistics literature on this simulation problem. Our main sources are the helpful reviews given by Ripley (1987, sec. 4.5) and Cressie (1991, sec. 3.6), the references given in these two books, and recent volumes of the journal *Mathematical Geology*. To put our approach in context and to explain why it fills a gap in this literature, we briefly mention earlier proposals without giving any details of the methods concerned.

One possibility is to use the Cholesky factorization of the relevant covariance matrix. This approach, which has been widely used, is exact in principle and does not require stationarity, but it breaks down when the number of grid points is moderately large. Let $\bar{n} = \prod_{l=1}^{d} n[l]$ denote the cardinality of the set (1.1). If $\bar{n}$ is sufficiently large (e.g., $\bar{n} \geq$ 1,200 on many computers), Cholesky factorization of the relevant covariance matrix is not feasible, a consequence of the fact that storage requirements of the Cholesky approach are $O(\bar{n}^2)$. For example, Cholesky factorization of a matrix of order 50,000 $\times$ 50,000 is beyond the capacity of any computer. In contrast, our approach can comfortably deal with $\bar{n} = 50{,}000$ in many cases, even on a relatively modest computer.

A second possibility, which is widely used for simulating isotropic Gaussian processes on $\mathbb{R}^d$, is the *turning bands* method. See Brooker (1985), Christakos (1987), Cressie (1991), Mantoglue (1987), Mantoglue and Wilson (1982), Matheron (1973), and Ripley (1987). As noted by all these authors, however, the turning bands method for simulating isotropic Gaussian processes is approximate because it depends on the application of a central limit theorem. So the turning bands approach is not exact in principle.

A variety of one-dimensional and multidimensional spectral methods have been proposed. However, with one exception that is discussed in the following, all the proposals based on spectral methods that we have seen require one of three types of approximation: the invocation of a central limit theorem, the inexact treatment of edge effects, or approximation of the covariance function with a function that has compact support. Whether such approximations are of consequence from a practical point of view is highly context dependent, but it is clear that if any of the three approximations mentioned is made, then the resulting procedure will not be exact in principle. For further details of approximate procedures based on spectral methods see Borgman, Taheri, and Hagan (1984), Davis, Hagan, and Borgman (1981), Mejia and Rodriguez-Iturbe (1974), Miller and Borgman (1985), Rice (1954, p. 180), Shinozuka (1971), and Shinozuka and Jan (1972).

Another possibility is to use spatial nearest neighbor or autoregressive models; see

Martin (1979, 1990, 1991), Sen (1989, 1990), Sharp and Aroian (1985, 1989), and Smith and Freeze (1979a, 1979b). Assuming that we wish to view the covariance function as prescribed, as is the case here, this kind of approach has the following significant drawback: the resulting autoregressive structure will not be sparse except in very special circumstances. There is also a question over whether it is feasible to implement this kind of approach exactly in principle when the number of grid points is at least moderately large (e.g., $\bar{n} \geq 1{,}200$).

Davis (1987) suggested an approximate approach based on the idea of approximating the square root of the covariance matrix by a matrix polynomial.

Finally, we mention the one-dimensional moving-average approach proposed by Black and Freyberg (1990). This procedure is exact in principle if the relevant covariance matrix is a type of band matrix but not otherwise.

Exactness in principle is a theoretical property of a simulation procedure. Why, then, do we give it weight when most users will probably be more interested in reasonably good distributional accuracy in practice, rather than exactness in theory? The main reason is a practical one. When studying the accuracy of an exact procedure, we only need to consider two issues: inaccuracy in computer arithmetic and the choice of random-number generator. When there are additional sources of error, however, assessment of the accuracy of the procedure is likely to become far more complicated.

We now briefly outline our approach. When $d = 1$ in (1.1), the resulting covariance matrix is Toeplitz, when $d = 2$ it is block Toeplitz, and when $d \geq 3$, it is nested block Toeplitz, assuming that we order the components in an appropriate way. It is well known that any Toeplitz matrix can be embedded in a symmetric circulant matrix. In similar fashion, a (nested) block Toeplitz matrix can be embedded in a (nested) block circulant matrix that is symmetric. The main idea is to simulate from a longer vector whose covariance matrix is the circulant, and then select a subvector whose covariance matrix has the appropriate Toeplitz form. Calculation of the square root of the circulant, assuming it is nonnegative definite, may be performed efficiently using the fast Fourier transform, provided the dimension of the circulant is highly composite.

This embedding idea is implicit in the procedure of Davis and Harte (1987, appendix A), and if the positivity condition they refer to is satisfied, then their procedure is identical to ours. Though our procedure was developed before seeing their article, we can say, with hindsight, that this article extends their algorithm in two ways. First, it considers the general d-dimensional case. Second, we treat the dimension of the circulant as an integer parameter that is chosen to ensure that the circulant is positive definite; the motivation for doing this is given in Proposition 3.2.

Since completing the work in this article, it has come to our attention that Dietrich and Newsam (1993) also adopted the circulant embedding approach and extended it to higher dimensions.

In Section 2 we discuss the one-dimensional case. In Section 3 we move on to the general d-dimensional case. In some circumstances it may be necessary to consider an approximate circulant embedding procedure; this is described in Section 4. In Section 5 we outline the simulation procedure. In Section 6 we describe the results of some numerical experiments, and Section 7 contains proofs.

2. THE ONE-DIMENSIONAL CASE

Suppose that we wish to generate a random vector

$$X = \left(X(0), X\left(\frac{1}{n}\right), \ldots, X\left(\frac{n-1}{n}\right)\right)^T$$

from a zero mean stationary Gaussian process $\{X(t) : t \in \mathbb{R}\}$ with prescribed covariance function γ. Then $X \sim N_n(0, G)$, where

$$G = \begin{bmatrix} \gamma(0) & \gamma\left(\frac{1}{n}\right) & \cdots & \gamma\left(\frac{n-1}{n}\right) \\ \gamma\left(\frac{1}{n}\right) & \gamma(0) & \cdots & \gamma\left(\frac{n-2}{n}\right) \\ \vdots & \vdots & & \vdots \\ \gamma\left(\frac{n-1}{n}\right) & \gamma\left(\frac{n-2}{n}\right) & \cdots & \gamma(0) \end{bmatrix}. \tag{2.1}$$

Note that G is a Toeplitz matrix.

The essence of our simulation approach is indicated in Steps 1 and 2.

Step 1. Embed G in a circulant covariance matrix C $(m \times m)$, where $m = 2^g$ for some integer g, and $m \geq 2(n-1)$.

Step 2. Use the fast Fourier transform twice, as indicated in the following, to generate a random vector $Y = (Y_0, Y_1, \ldots, Y_{m-1})^T \sim N_m(0, C)$. Then, with appropriate construction of C in Step 1, $(Y_0, \ldots, Y_{n-1})^T \sim N_n(0, G)$.

In Step 1 we take C to be the circulant matrix

$$C = \begin{bmatrix} c_0 & c_1 & \cdots & c_{m-1} \\ c_{m-1} & c_0 & \cdots & c_{m-2} \\ \vdots & \vdots & & \vdots \\ c_1 & c_2 & \cdots & c_0 \end{bmatrix}, \tag{2.2}$$

where

$$\begin{aligned} c_j &= \gamma\left(\frac{j}{n}\right) \quad \text{if} \quad 0 \leq j \leq m/2 \\ &= \gamma\left(\frac{m-j}{n}\right) \quad \text{if} \quad m/2 < j \leq m-1 \end{aligned} \tag{2.3}$$

Note that, by construction, C is symmetric and, provided $m \geq 2(n-1)$, the $n \times n$ submatrix in the top left corner of C is equal to G in (2.1).

It may happen that, for a particular m, C in (2.2) fails to be nonnegative definite. In such cases we consider two options:

(a) increase m (motivation for increasing m is given in Proposition 2);

(b) use the nonnegative definite part of C (see Section 4).

In practice we have found that it is usually possible to choose m so that C is nonnegative definite. In such cases the procedure is exact in principle. Occasionally, we have had to resort to option (b). If option (b) is used, then the procedure is approximate. However, in Section 4 we give simple yet fairly tight probabilistic bounds for the error incurred in using option (b).

Suppose now that C in (2.2) is nonnegative definite. We briefly indicate how Step 2 of the simulation procedure is performed. Standard results for symmetric circulant matrices (see Brockwell and Davis 1987) show that $C = Q\Lambda Q^*$, where $\Lambda = \text{diag}\{\lambda_0, \ldots, \lambda_{m-1}\}$ is the diagonal matrix of eigenvalues of C, $Q = \{q_{jk} : 0 \le j, k \le m-1\}$ is the unitary matrix with entries

$$q_{jk} = m^{-1/2} \exp\left(-\frac{2\pi ijk}{m}\right),$$

Q^* is the conjugate transpose of Q, and $i = \sqrt{-1}$.

If we define $Y = Q\Lambda^{1/2}Q^*Z$, where $\Lambda^{1/2} = \text{diag}\{\lambda_0^{1/2}, \ldots, \lambda_{m-1}^{1/2}\}$ and $Z = (Z_0, Z_1, \ldots, Z_{m-1})^T$ is a vector of independent $N(0,1)$ random variables, then $Y \sim N_m(0, C)$, because Q is unitary. Note that the vector X we wish to generate has the same distribution as the subvector of Y indicated in Step 2. In many cases of interest, m will be large, $m = 2^{18}$, for example. Thus the computational problem is to compute $Y = Q\Lambda^{1/2}Q^*Z$ quickly using minimal storage. We proceed as follows.

(S1) Determine the eigenvalues $\lambda_0, \ldots, \lambda_{m-1}$ of C. These are given by the discrete Fourier transform of the sequence $\{c_0, c_1, \ldots, c_{m-1}\}$—that is,

$$\lambda_k = \sum_{j=0}^{m-1} c_j \exp\left(-\frac{2\pi ijk}{m}\right), \quad k = 0, 1, \ldots, m-1. \tag{2.4}$$

(S2) Simulate Q^*Z directly and at the same time determine $W = \Lambda^{1/2}Q^*Z$. Note that Q^*Z may be simulated directly using Proposition 3 (described later).

(S3) Calculate $X = (X(0), X(1/n), \ldots, X((n-1)/n))^T$, where

$$X\left(\frac{k}{n}\right) = \sum_{j=0}^{m-1} \left(W_j/m^{1/2}\right) \exp\left(-\frac{2\pi ijk}{m}\right), \qquad k = 0, 1, \ldots, n-1. \tag{2.5}$$

The important point is that (2.4) and (2.5) may be calculated extremely efficiently using the one-dimensional fast Fourier transform, provided m is highly composite (e.g., if $m = 2^g$ for some integer g). For additional discussion of the fast Fourier transform, see Brockwell and Davis (1987) or NAG (1990).

It turns out that the approach described previously can be extended to the problem of simulating a zero mean scalar-valued stationary Gaussian process $\{X(t) : t \in \mathbf{R}^d\}$ on a grid of the form (1.1). In the one-dimensional case, the Toeplitz matrix G defined in (2.1) is embedded in the circulant matrix C defined in (2.2) and (2.3). In the general d-dimensional case, an analogous construction works: We embed a block Toeplitz matrix in a block circulant matrix; the role of the one-dimensional fast Fourier transform is played by the d-dimensional fast Fourier transform (e.g., NAG 1990). The focus of the remainder of this article is on the general d-dimensional case.

3. MAIN RESULTS

We first introduce some notation. Let Z^d denote the set of d vectors with integer components. Components of members of Z^d will be indicated by square brackets.

For example, if $j \in Z^d$, then $j = (j[1], \ldots, j[d])^T$. We also define division in Z^d in component-wise fashion:

$$\frac{j}{n} = \left(\frac{j[1]}{n[1]}, \ldots, \frac{j[d]}{n[d]}\right)^T, \tag{3.1}$$

which is well defined provided $n[l] \neq 0$, $l = 1, \ldots, d$.

For $m \in Z^d$ with strictly positive components, we define sets

$$I(m) = \{j \in Z^d : 0 \leq j[l] \leq m[l] - 1\,,\ 1 \leq l \leq d\}\,, \tag{3.2}$$

and

$$I^*(m) = \{j \in Z^d : 0 \leq |j[l]| \leq m[l] - 1\,,\ 1 \leq l \leq d\}, \tag{3.3}$$

and write $\overline{m} = \prod_{l=1}^{d} m[l]$. Note that $\overline{m}$ is the number of elements in the set $I(m)$.

Consider an array of complex numbers $\{a(j) : j \in I(m) \subseteq Z^d\}$. When convenient, $\{a(j)\}$ will be interpreted as a column vector of length $\overline{m}$ using the following convention: the multi-index $j \in I(m)$ is related to the index r of the column vector by

$$r = j[1] + m[1]\,j[2] + m[1]\,m[2]\,j[3] + \cdots + m[1]\ldots m[d-1]\,j[d]\,. \tag{3.4}$$

Note that (3.4) defines a bijection between $I(m)$ and $\{0, 1, \ldots, \overline{m} - 1\}$.

Suppose that we are given a covariance function $\{\gamma(t) : t \in \mathbf{R}^d\}$ for a stationary real-valued process defined on $\mathbf{R}^d$. Note that γ will have symmetry about the origin in the sense that

$$\gamma(t) = \gamma(-t) \quad \text{for all} \quad t \in \mathbf{R}^d\,, \tag{3.5}$$

but that it need not possess any stronger forms of symmetry. Using the notion of division indicated in (3.1), our simulation problem may be expressed as follows. Generate an array of zero mean Gaussian variables

$$X = \left\{X\left(\frac{j}{n}\right) : j \in I(n)\right\} \tag{3.6}$$

with covariances given by

$$E\left\{X\left(\frac{j}{n}\right) X\left(\frac{k}{n}\right)\right\} = \gamma\left(\frac{j-k}{n}\right), \quad j, k \in I(n)\,. \tag{3.7}$$

In (3.5) and (3.6), $n \in Z^d$ is fixed and has strictly positive components. Note that the spacing between sample points along the lth coordinate axis is given by $n[l]^{-1}$.

The covariance matrix determined by (3.7) has block Toeplitz structure. Our first task is to specify an analog of the embedding matrix C defined in (2.2) and (2.3). Define the matrix $C = \{C_{jk} : j, k \in I(m)\}$, where $C_{jk} = c(j-k)$,

$$c(h) = \gamma\left(\frac{\tilde{h}}{n}\right), \qquad h, \tilde{h} \in I^*(m)\,, \tag{3.8}$$

$\tilde{h} = \tilde{h}(h)$ is given by

$$\begin{aligned} \tilde{h}(h)[l] &= h[l] && \text{if} \quad 0 \le |h[l]| \le m[l]/2 && 1 \le l \le d \\ &= h[l] - m[l] && \text{if} \quad m[l]/2 < h[l] \le m[l] - 1 && 1 \le l \le d \\ &= h[l] + m[l] && \text{if} \quad m[l]/2 < -h[l] \le m[l] - 1 && 1 \le l \le d, \end{aligned} \tag{3.9}$$

and the set $I^*(m)$ is defined in (3.3).

Some care is needed in the construction of C via (3.8)–(3.9), as we now explain. We say that γ is even in the lth coordinate if

$$\gamma(t[1], \ldots, t[l], \ldots, t[d]) = \gamma(t[1], \ldots, -t[l], \ldots, t[d])$$

for all $(t[1], \ldots, t[d])^T \in \mathbf{R}^d$; otherwise, we say that γ is uneven in the lth coordinate. If γ is even in each coordinate, then no problem with construction (3.8)–(3.9) can arise. However, if γ is uneven in the lth coordinate, and $m[l]$ is even, then C will usually not have circulant structure because of conflicting definitions at points $h \in I^*(m)$ with $h[l] = \pm m[l]/2$. This problem cannot occur when $d = 1$, but it can occur when $d > 1$. Two possible resolutions are suggested in the following.

(a) If γ is uneven in the lth coordinate, choose $m[l]$ to be an odd integer. Otherwise choose $m[l]$ to be even. To optimize the efficiency of the fast Fourier transform, we suggest taking $m[l]$ to be of the form

$$\begin{aligned} m[l] &= 2^{g[l]} \quad \text{if} \quad m[l] \text{ is even} \\ &= 3^{g[l]} \quad \text{if} \quad m[l] \text{ is odd.} \end{aligned} \tag{3.10}$$

(b) If γ is uneven in the lth coordinate, still choose $m[l]$ to be of the form $2^{g[l]}$ for some integer $g[l]$ and define $c(\cdot)$ using (3.8) and (3.9), but with the following exceptions:

$$\text{put} \quad c(h) = 0 \quad \text{for all} \quad h \in I^*(m) \quad \text{with} \quad |h[l]| = m[l]/2 \quad \text{for some} \quad l. \tag{3.11}$$

Either way, the resulting matrix C constructed in (3.8)–(3.9) will have block circulant structure. (Resolution (b) was suggested to us by John Kent, personal communication, 1994.) Note that, in view of (3.5), C is symmetric.

The d-dimensional discrete Fourier transform of c in (3.8) is given by

$$\lambda(k) = \sum_{j \in I(m)} c(j) \exp\left\{-2\pi i\, j^T \left(\frac{k}{m}\right)\right\}, \quad k \in I(m). \tag{3.12}$$

For each $j \in I(m)$, define a vector q_j of length $\overline{m}$ using (3.4), with components

$$q_j(k) = \overline{m}^{-1/2} \exp\left\{-2\pi i\, j^T \left(\frac{k}{m}\right)\right\}, \quad k \in I(m). \tag{3.13}$$

Proposition 1. *The following representations hold for C, defined in (3.8)–(3.11).*

$$C = \sum_{j \in I(m)} \lambda(j)\, q_j\, q_j^* = \sum_{j \in F} \lambda(j)\, R_j, \tag{3.14}$$

where λ is defined in (3.12), q_j is defined in (3.13), the asterisk indicates conjugate transpose, and F is a subset of $I(m)$ to be determined. The $\overline{m} \times \overline{m}$ matrices R_j, $j \in F$, are real, symmetric, idempotent and, for each $j, k \in F$, satisfy

$$R_j R_k = 0 \quad \textit{unless} \quad j = k. \tag{3.15}$$

Note that (3.14) and (3.15) imply that the $\lambda(j)$ are the eigenvalues of C. Proposition 1 has a number of useful consequences, one of which is the following. If C is nonnegative definite, then it has a square root

$$C^{1/2} = \sum_{j \in I(m)} \lambda^{1/2}(j)\, q_j\, q_j^* = \sum_{j \in F} \lambda^{1/2}(j)\, R_j\,. \tag{3.16}$$

The argument that establishes the second equality in (3.16) is identical to the argument that establishes the second equality in (3.14). Note that (3.16) implies that if C is nonnegative definite, then $C^{1/2}$ is real, symmetric, and nonnegative definite.

Because, by construction, C is symmetric, it will be an admissible covariance matrix iff it is also nonnegative definite. We now give sufficient conditions for C to be positive definite for $m \in Z^d$ with components sufficiently large.

Proposition 2. *Suppose that*

$$\sum_{j \in Z^d} \left| \gamma\left(\frac{j}{n}\right) \right| < \infty, \tag{3.17}$$

and that the spectral density

$$g(t) = (2\pi)^{-d} \sum_{j \in Z^d} \gamma\left(\frac{j}{n}\right) \exp\left(-2\pi i\, j^T t\right) \tag{3.18}$$

is strictly positive for all $t \in [0,1]^d$. Then there exists an integer $u_0 = u_0(n, \gamma)$ such that for all m that satisfy $\min_{1 \le l \le d} m[l] \ge u_0$, C is positive definite.

Write Q for the $\overline{m} \times \overline{m}$ matrix whose rth column is q_j, where q_j is defined in (3.13), and r and j are identified using (3.4). Define the $\overline{m} \times \overline{m}$ matrix $\Lambda = \operatorname{diag}\{\lambda(j),\ j \in I(m)\}$, with the ordering of the $\lambda(j)$ determined by (3.4). Then it follows from (3.14) and (3.16) that

$$C = Q \Lambda Q^* \quad \text{and} \quad C^{1/2} = Q \Lambda^{1/2} Q^*\,. \tag{3.19}$$

Let $Z = (Z(j),\ j \in I(m))^T$ denote an $\overline{m}$ vector of independent $N(0,1)$ variables. Then (3.19) implies that

$$Y = C^{1/2} Z = Q\, \Lambda^{1/2}\, Q^*\, Z \sim N_{\overline{m}}(0, C), \tag{3.20}$$

provided that C is nonnegative definite. Finally we put

$$X\left(\frac{j}{n}\right) = Y\left(\frac{j}{n}\right), \quad j \in I(n).$$

Efficient calculation of (3.20) may be performed using exactly the same steps as in the one-dimensional case (see (S1)–(S3) in sec. 2), except that the d-dimensional discrete Fourier transform (3.12) is used in place of the one-dimensional discrete Fourier transform (2.4).

We now explain how to simulate Q^*Z directly (see (S2) in sec. 2). Write

$$Q^*Z = S + iT, \tag{3.21}$$

where S and T are vectors of length $\overline{m}$ whose components are real Gaussian random variables with zero mean.

Proposition 3. *The random vectors S and T satisfy the following.*

1. *$E(S) = E(T) = 0$ and $E(ST^T) = 0$, so that S and T are independent.*
2. *If $j \in I(m)$ and $j[l] = 0$ or $m[l]/2$ for each $l \in \{1, \ldots, d\}$, then for each $k \in I(m)$,*

$$\begin{aligned} \operatorname{cov}\{S(j), S(k)\} &= 1 \quad \text{if} \quad j = k \\ &= 0 \quad \text{otherwise} \end{aligned}$$

   and $T(j) \equiv 0$.
3. *For $j \in I(m)$, define $k = k(j) \in I(m)$ by*

$$\begin{aligned} k[l] = k(j)[l] &= j[l] && \text{if} \quad j[l] = 0 \quad \text{or} \quad m[l]/2 \quad 1 \le l \le d \\ &= m[l] - j[l] && \text{otherwise} \qquad\qquad\quad 1 \le l \le d. \end{aligned}$$

If at least one $j[l]$ is not equal to 0 or $m[l]/2$, then for each $h \in I(m)$

$$\begin{aligned} \operatorname{cov}\{S(j), S(h)\} &= \tfrac{1}{2} \quad \text{if} \quad h = j \quad \text{or} \quad k \\ &= 0 \quad \text{otherwise,} \end{aligned}$$

and

$$\begin{aligned} \operatorname{cov}\{T(j), T(h)\} &= \tfrac{1}{2} \quad \text{if} \quad h = j \\ &= -\tfrac{1}{2} \quad \text{if} \quad h = k \\ &= 0 \quad \text{otherwise.} \end{aligned}$$

4. APPROXIMATE CIRCULANT EMBEDDING

As noted in Section 2, nonnegative definiteness of C can usually be achieved by increasing the components of m (see Proposition 2). However, it occasionally happens that those m for which C is nonnegative definite have components $m[1], \ldots, m[d]$ that are too large to be practicable. In such cases, we propose the following approximate embedding procedure.

Suppose that, for given m, C defined in (3.8)–(3.11) is not nonnegative definite (i.e., some of the eigenvalues of C are strictly negative). Starting from the first term in (3.19), we write

$$C = Q\Lambda Q^* = Q(\Lambda_+ - \Lambda_-)\, Q^* = C_+ - C_-, \tag{4.1}$$

where

$$\Lambda_{\pm} = \text{diag}\{\max(0, \pm\lambda(j)),\ j \in I(m)\}.$$

Then we use the symmetric, nonnegative definite matrix $\rho^2 C_+$, with suitable $\rho \neq 0$, as an approximate embedding matrix. Two choices for ρ are

$$\rho_1 = \frac{\text{tr}(\Lambda)}{\text{tr}(\Lambda_+)} \quad \text{and} \quad \rho_2 = \left\{\frac{\text{tr}(\Lambda)}{\text{tr}(\Lambda_+)}\right\}^{1/2}. \tag{4.2}$$

The choice $\rho = \rho_2$ leads to the correct one-dimensional marginal distributions; the motivation for choosing $\rho = \rho_1$ is given in the following.

Recall the definitions of $Y = \{Y(\frac{j}{n}) : j \in I(m)\}$ and $C = \{C_{jk} : j, k \in I(m)\}$, put $J = I(n)$, and define the subvector $Y(J)$ and the submatrix $C(J)$ by

$$Y(J) = \left\{Y\left(\frac{j}{n}\right) :\ j \in J\right\} \quad \text{and} \quad C(J) = \{C_{jk} :\ j, k \in J\}.$$

The submatrices $C_-(J)$ and $C_+(J)$ are defined similarly. We may write $Y_+(J) = Y(J) + \Delta$, where $Y(J)$ and Δ are independent $N_{\bar{n}}(0, C(J))$ and $N_{\bar{n}}(0, C_-(J))$ respectively, $Y_+(J) \sim N_{\bar{n}}(0, C_+(J))$ and $\bar{n} = \prod_{l=1}^{d} n[l]$. Note that $Y(J)$ is equal in distribution to the array that we wish to simulate. For given $\rho \neq 0$, we may view

$$U = (U(j), j \in J)^T = \rho Y_+(J) - Y(J) \sim N_{\bar{n}}(0, (1-\rho)^2 C(J) + \rho^2 C_-(J))$$

as the random error due to the approximation in the embedding. Using an inequality for multivariate Normal probabilities on rectangles (see Tong 1982, chap. 2), we have, for each $x > 0$,

$$P\left(\max_{j \in J} |U(j)| > x\right) \leq 1 - \left\{2\Phi\left(\frac{x}{\sigma}\right) - 1\right\}^{\bar{n}}, \tag{4.3}$$

where

$$\sigma^2 = \sigma^2(\rho) = \{(1-\rho)^2 \,\text{tr}(\Lambda) + \rho^2 \,\text{tr}(\Lambda_-)\}/\overline{m}. \tag{4.4}$$

By calculating the bound in (4.3) for various values of x, we can obtain a good idea of the distributional error incurred by setting the negative eigenvalues of C to zero. Note that $\sigma^2(\rho)$, and also the right side of (4.3), are minimized when $\rho = \rho_1 = \text{tr}(\Lambda)/\text{tr}(\Lambda_+)$, and that

$$\sigma^2(\rho_1) = \text{tr}(\Lambda)\,\text{tr}(\Lambda_-)/\{\overline{m}\,\text{tr}(\Lambda_+)\}.$$

5. THE SIMULATION PROCEDURE

An explicit specification of simulation procedure is now given. The one-dimensional case is dealt with first. Then we cover the general d-dimensional case.

5.1 THE ONE-DIMENSIONAL CASE ($d = 1$)

We employ the notation in Section 2. It is assumed that n and the covariance function γ are given and that $m = 2^g$ for some integer $g > 0$ to be determined.

5.1.1 Preliminary Step

Find smallest integer g such that C defined in (2.2) and (2.3) is nonnegative definite, and $2^g \geq 2(n-1)$. Store the eigenvalues $\lambda(0), \lambda(1), \ldots, \lambda(m-1)$ corresponding to this choice of g.

If such a g cannot be found, or if it is too large to be practicable, then use the approximate embedding matrix $\rho^2 C_+$ with particular choices of $\rho \neq 0$ and g; see Section 4. In this case, write $\lambda(0), \lambda(1), \ldots, \lambda(m-1)$ for the eigenvalues of $\rho^2 C_+$.

5.1.2 The Procedure

Step 1. Generate independent random variables $U \sim N(0,1)$, $V \sim N(0,1)$; then put

$$a(0) = m^{-1/2}\,\lambda^{1/2}(0)\,U\,, \quad a(m/2) = m^{-1/2}\,\lambda^{1/2}(m/2)\,V\,.$$

Step 2. For $1 \leq j < m/2$, generate independent random variables $U_j \sim N(0,1)$, $V_j \sim N(0,1)$; then put

$$a(j) = (2m)^{-1/2}\,\lambda^{1/2}(j)(U_j + iV_j)\,,$$

and

$$a(m-j) = (2m)^{-1/2}\,\lambda^{1/2}(j)(U_j - iV_j).$$

Step 3. Use the fast Fourier transform to obtain

$$X\left(\frac{k}{n}\right) = \sum_{j=0}^{m-1} a(j)\,\exp\left(-\frac{2\pi i j k}{m}\right), \quad 0 \leq k \leq n-1\,. \tag{5.1}$$

It is straightforward to check that the sequence (5.1) has correlation structure given by (2.1).

5.2 THE d-DIMENSIONAL CASE

The simulation procedure in the general d-dimensional case is based on the same ideas as in the one-dimensional case, but technically it is a little bit more involved. We allow for the possibility that the covariance function γ is uneven in some coordinates, and assume that option (a) (see (3.10), p. 415) rather than (b) (see (3.11), p. 415) is followed. Were option (b) followed instead, the procedure would be identical except that there would be no need to consider the possibility of choosing odd $m[l]$ for some l.

5.2.3 Preliminary Step

Find $g \in Z^d$ to minimize

$$\left(\sum_{l:m[l] \text{ even}} g[l] \right) \log 2 + \left(\sum_{l:m[l] \text{ odd}} g[l] \right) \log 3$$

subject to the constraints $m[l] \geq 2(n[l] - 1)$, $l = 1, \ldots, d$, and $\lambda(j) \geq 0$, $j \in I(m)$, where the $m[l]$ are of the form (3.10) and the $\lambda(j)$ are the eigenvalues of C defined in (3.8)–(3.9).

If such a g cannot be found, or if the components of such a g are too large to be practicable, then use the approximate embedding matrix $\rho^2 C_+$ with suitable choices of $\rho \neq 0$ and g, as indicated in Section 4. In this case, write $\lambda(j)$, $j \in I(m)$ for the eigenvalues of $\rho^2 C_+$.

For given $m \in Z^d$ with strictly positive components, define $m^\dagger \in Z^d$ as follows:

$$m^\dagger[l] = \text{int}(m[l]/2) + 1\,, \qquad 1 \leq l \leq d\,,$$

where int(.) denotes "integer part." Write $\overline{m}^\dagger = \prod_{l=1}^d m^\dagger[l]$, and define the bijection $p^\dagger : \{0, 1, \ldots, \overline{m}^\dagger - 1\} \to I(m^\dagger)$ as the inverse of the map (3.4), with $m^\dagger$ replacing m.

5.2.4 The Procedure

Step 0. Put $r = -1$.

Step 1. Set $r = r + 1$, $j = p^\dagger(r) \in I(m^\dagger)$, determine the set

$$A(j) = \{l \in \{1, \ldots, d\} : 0 < j[l] < m^\dagger[l]/2\}\,,$$

and obtain $\chi(j)$, the cardinality of $A(j)$. If $\chi(j) > 0$, go to Step 3.

Step 2. Generate $U \sim N(0, 1)$, put

$$a(j) = (\overline{m})^{-1/2}\, \lambda^{1/2}(j)\, U\,,$$

and go to Step 6.

Step 3. Label the $2^{\chi(j)}$ subsets of $A(j)$ in pairs of complementary subsets in some convenient way, to obtain $B(1), B^c(1), \ldots, B(2^{\chi(j)-1}), B^c(2^{\chi(j)-1})$ say. Put $s = 0$.

Step 4. Put $s = s + 1$ and determine $j_1, j_2 \in I(m)$ as follows:

$$\begin{aligned} j_1[l] &= j[l] && \text{if} \quad l \notin B(s) \quad 1 \leq l \leq d \\ &= m[l] - j[l] && \text{if} \quad l \in B(s) \quad 1 \leq l \leq d\,, \end{aligned}$$

$$\begin{aligned} j_2[l] &= j[l] && \text{if} \quad l \notin B^c(s) \quad 1 \leq l \leq d \\ &= m[l] - j[l] && \text{if} \quad l \in B^c(s) \quad 1 \leq l \leq d\,. \end{aligned}$$

Step 5. Generate independent random variables $U \sim N(0,1)$, $V \sim N(0,1)$; then put

$$a(j_1) = (2\overline{m})^{-1/2} \lambda^{1/2}(j_1)(U + iV)$$
$$a(j_2) = (2\overline{m})^{-1/2} \lambda^{1/2}(j_1)(U - iV)$$

and return to Step 4 if $s < 2^{x(j)-1}$.

Step 6. If $r < \overline{m}^{\dagger} - 1$, return to Step 1.

Step 7. Use the d-dimensional fast Fourier transform to calculate

$$X\left(\frac{k}{n}\right) = \sum_{j \in I(m)} a(j) \exp\left\{-2\pi i j^T \left(\frac{k}{m}\right)\right\}, \quad k \in I(n). \tag{5.2}$$

Then the array (5.2) has zero mean and covariance structure given by (3.7).

5.3 MISCELLANEOUS PRACTICAL REMARKS

Provided we have a subroutine for calculating the d-dimensional fast Fourier transform, the simulation procedure is straightforward to program, particularly when $d = 1$.

Note that some authors divide by $\overline{m}^{-1/2}$ or $\overline{m}^{-1}$ in the definition of the discrete Fourier transform. See, for example, the NAG (1990) Subroutine Library in the C06 section for an example of the former definition.

6. NUMERICAL RESULTS

In Subsection 6.1 we present several one-dimensional and two-dimensional examples, including details of central processing unit (CPU) timings. In Subsection 6.2 we present a comparison in accuracy and CPU timing of the circulant method and the Gibbs sampler in the case of the Ornstein–Uhlenbeck process.

6.1 EXAMPLES WITH CPU TIMINGS

Figures 1 and 2 present single realizations based on the covariance functions

$$\gamma(t) = \exp\{-c|t|^{\alpha}\}, \quad t \in \mathbb{R} \tag{6.1}$$

in the one-dimensional case, and

$$\gamma(t) = \exp\{-c\|t\|^{\alpha}\}, \quad t = (t[1], t[2])^T \in \mathbb{R}^2 \tag{6.2}$$

with $\|t\| = \sqrt{t[1]^2 + t[2]^2}$, in the two-dimensional case.

Table 1 gives CPU times in seconds on a Sparcstation 10/52 running Solaris 2.2. T_1 is the time used in calculating the eigenvalues, T_2 is the time used in the simulation step, and $T = T_1 + T_2$ is the total CPU time. If more than one vector is simulated with a given covariance function, the total CPU time, T, will be approximately $T_1 +$

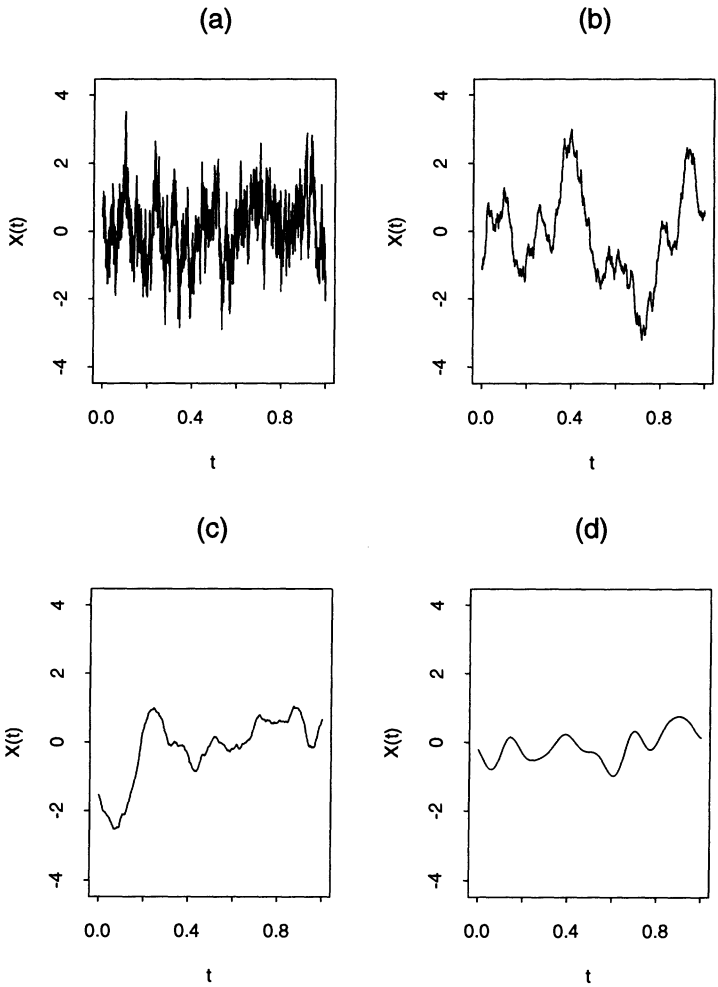

Figure 1. Gaussian Processes With n = 50,000, c = 100, and α = 1.0 (a), 1.5 (b), 1.9 (c), and 2.0 (d).

(number of vectors required) $\times T_2$. The asterisk in Table 1 indicates that the approximate circulant embedding approach was used; see Section 4. For both $d = 1$ and 2, it was necessary to use an approximate embedding when $\alpha = 2$. We considered two embeddings corresponding to $g = 17$ and $g = 20$. When $d = 1$, the corresponding values of $\sigma^2(\rho_1)$, defined in (4.2) and (4.4), were 5.29×10^{-9} and 3.40×10^{-9}. The values of $\sigma^2(\rho_1)$ when $d = 2$ were of the same order of magnitude. Note that there is a trade-off between a (much) smaller CPU time ($g = 17$) on the one hand, and a (slightly) smaller value of $\sigma^2(\rho_1)$, indicating a (slightly) smaller error due to the approximation, when $g = 20$. In general, if we calculate the bound in (4.3) for various values of x, the trade-off can be made in a sensible and informed way.

In Tables 2 and 3, true and estimated correlations are compared for single realizations generated using covariance functions (6.1) and (6.2). As pointed out by a referee, there does in some cases appear to be a small but noticeable deterioration in accuracy as

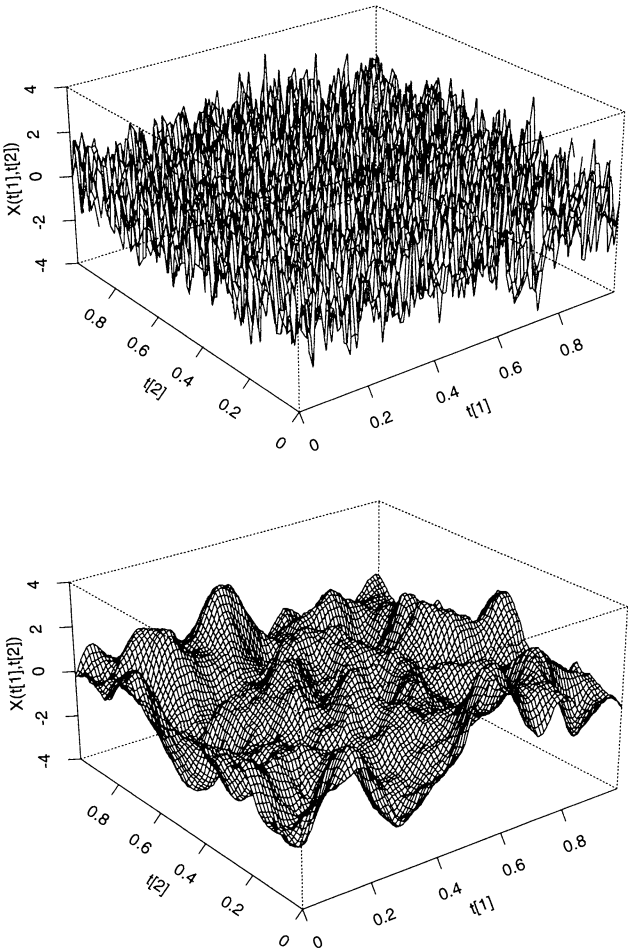

Figure 2. Gaussian Surfaces With n = (100,100), c = 100, and α = 1.0 (top) and 1.9 (bottom).

distance increases. This is to be expected on purely statistical grounds, but perhaps not to the extent observed in some of the examples. However, considerable reassurance is provided by Figure 3.

From the point of view of the simulation procedure, there is no particular advantage in choosing $n[1] = n[2]$ when $d = 2$, but it does make calculation of the estimated correlations somewhat easier.

6.2 Comparison With Gibbs Sampler

The circulant embedding method proposed here and the Gibbs sampler (see Tanner 1993) have domains of application that are to a large extent complementary. The circulant approach requires normality and stationarity, whereas the Gibbs sampler requires "nice"

Table 1. CPU Timings in Seconds With $c = 100$ in All Cases

d, n	α	g	T_1	T_2	T
	.5	17	4.189	6.563	10.752
	1.0	17	4.030	6.525	10.556
1, 50000	1.5	17	4.155	6.772	10.927
	1.9	17	4.507	6.360	10.867
	*2.0	17	4.595	6.577	11.172
	*2.0	20	44.140	56.820	100.960
	1.0	(8, 8)	2.911	3.736	6.647
	1.5	(8, 8)	2.871	3.631	6.502
2, (100, 100)	1.9	(8, 8)	2.978	3.701	6.679
	*2.0	(8, 8)	3.036	3.630	6.666
	*2.0	(10, 10)	57.827	70.941	128.768
	1.0	(9, 9)	14.065	16.416	30.481
	1.5	(9, 9)	13.808	16.711	30.519
2, (250, 250)	1.9	(9, 9)	13.745	16.419	30.164
	*2.0	(9, 9)	13.784	16.179	29.963
	*2.0	(10, 10)	60.778	67.875	128.653

NOTE: An * indicates that an approximate embedding was used.

conditional dependence structure. However, there is an important case in which both can be applied: the Ornstein–Uhlenbeck process, which corresponds to a covariance function of the form $\gamma(t) = \sigma^2\psi^{|t|}$, $t \in \mathbb{R}$, where $\sigma^2 > 0$ and $\psi \in (0, 1)$ are parameters. The numerical comparison that follows was suggested by a referee.

We consider the problem of generating a Gaussian random vector $X \sim N_n(0, \Sigma)$, where $\Sigma = (\Sigma_{pq}) = (\psi^{|p-q|})$ and $\psi \in (0, 1)$. The viability of the Gibbs sampler in this application depends on the band structure of $\Sigma^{-1} = (\Sigma^{pq})$, which is given by

Table 2. Comparison Between True and Estimated Correlations With Covariance Function (6.1), $c = 100$, and $n = 50{,}000$

	$\alpha = .5$		$\alpha = 1.0$		$\alpha = 1.5$	
t	True	Estimated	True	Estimated	True	Estimated
n^{-1}	.6394	.6365	.9980	.9977	1.0000	1.0000
$2n^{-1}$	.5313	.5284	.9960	.9954	1.0000	1.0000
$3n^{-1}$	.4609	.4549	.9940	.9931	1.0000	.9999
$4n^{-1}$	.4088	.4019	.9920	.9908	.9999	.9999
$5n^{-1}$	.3679	.3560	.9900	.9885	.9999	.9999
$6n^{-1}$	.3344	.3224	.9881	.9863	.9999	.9998
$7n^{-1}$	.3063	.2982	.9861	.9840	.9998	.9998
$8n^{-1}$	.2823	.2755	.9841	.9818	.9998	.9998
$9n^{-1}$	.2614	.2519	.9822	.9796	.9998	.9997
$10n^{-1}$	.2431	.2346	.9802	.9775	.9997	.9997

Table 3. Comparison Between True and Estimated Correlations With Covariance Function (6.2) and $c = 100$

		$\alpha = 1.0$		$\alpha = 1.5$		$\alpha = 1.9$	
n	$\|\|t\|\|$	True	Estimated	True	Estimated	True	Estimated
	$(n[1])^{-1}$	.368	.371	.905	.904	.984	.977
	$\sqrt{2}(n[1])^{-1}$	.243	.241	.845	.839	.970	.957
	$2(n[1])^{-1}$	.135	.139	.754	.755	.943	.930
	$\sqrt{5}(n[1])^{-1}$	.107	.112	.716	.709	.929	.912
	$\sqrt{8}(n[1])^{-1}$	.059	.071	.621	.610	.892	.872
	$3(n[1])^{-1}$	.050	.046	.595	.599	.880	.864
(100,100)	$\sqrt{10}(n[1])^{-1}$	.042	.038	.570	.564	.868	.848
	$\sqrt{13}(n[1])^{-1}$	.027	.032	.504	.491	.834	.812
	$4(n[1])^{-1}$	.018	.026	.449	.458	.802	.783
	$\sqrt{17}(n[1])^{-1}$	.016	.018	.433	.430	.791	.770
	$\sqrt{18}(n[1])^{-1}$	.014	.016	.417	.398	.781	.759
	$\sqrt{20}(n[1])^{-1}$	.011	.014	.388	.376	.761	.739
	$(n[1])^{-1}$	.670	.668	.975	.970	.997	.992
	$\sqrt{2}(n[1])^{-1}$	.568	.567	.958	.948	.995	.984
	$2(n[1])^{-1}$	.449	.450	.931	.920	.990	.978
	$\sqrt{5}(n[1])^{-1}$	.409	.410	.919	.903	.987	.970
	$\sqrt{8}(n[1])^{-1}$	.323	.320	.887	.865	.980	.957
	$3(n[1])^{-1}$	.301	.303	.877	.861	.978	.959
(250,250)	$\sqrt{10}(n[1])^{-1}$	.282	.281	.867	.846	.976	.951
	$\sqrt{13}(n[1])^{-1}$	.236	.234	.841	.814	.969	.938
	$4(n[1])^{-1}$	.202	.200	.817	.797	.962	.935
	$\sqrt{17}(n[1])^{-1}$	.192	.192	.809	.784	.960	.928
	$\sqrt{18}(n[1])^{-1}$	.183	.180	.802	.770	.958	.921
	$\sqrt{20}(n[1])^{-1}$	.167	.164	.787	.757	.953	.915

$$\begin{aligned}
\Sigma^{pq} &= (1-\psi^2)^{-1} && \text{if} && p = q = 0 \quad \text{or} \quad n-1 \\
&= (1-\psi^2)^{-1}(1+\psi^2) && \text{if} && p = q = 1, \ldots, n-2 \\
&= -\psi(1-\psi^2)^{-1} && \text{if} && |p-q| = 1 \\
&= 0 && \text{otherwise} && \qquad (6.3)
\end{aligned}$$

By one loop of the Gibbs sampler, we mean simulation of $X(j)$ conditional on $\{X(k) = x(k) : \ k = 0, 1, \ldots, n-1, \ k \neq j\}$ for $j = 0, 1, \ldots, n-1$, using the updated X values at each stage. (For simplicity, we have worked with $X(j)$ rather than $X(\frac{j}{n})$ in this example.) From (6.3) these conditional distributions are given by

$$X(0)|\text{ rest } \sim N(\psi x(1), 1-\psi^2),$$

$$X(n-1)|\text{ rest } \sim N(\psi x(n-2), 1-\psi^2),$$

and, for $j = 1, \ldots, n-2$,

$$X(j)|\text{ rest } \sim N(\psi\{x(j-1)+x(j+1)\}/(1+\psi^2), (1-\psi^2)/(1+\psi^2)).$$

Two starting options were considered: (a) generate the $X(j)$ independently with the correct $N(0,1)$ marginal distributions, and (b) use a common $N(0,1)$ starting value. Two options for sweeping through a loop were considered: (c) in a fixed sequence, given by the ordering $0, 1, \ldots, n-1$, and (d) in a random order $\pi_0, \ldots, \pi_{n-1}$, where $(\pi_0, \ldots, \pi_{n-1})$ is a random permutation of $(0, 1, \ldots, n-1)$ that is generated independently for each loop. All four combinations were tried, but difference in both CPU timing and speed of convergence were found to be fairly minor. In the results presented, options (a) and (c) were used.

The CPU time for one loop of the Gibbs sampler is $O(n)$, but independent of ψ. For the values of n we considered, one run of the circulant embedding procedure, including

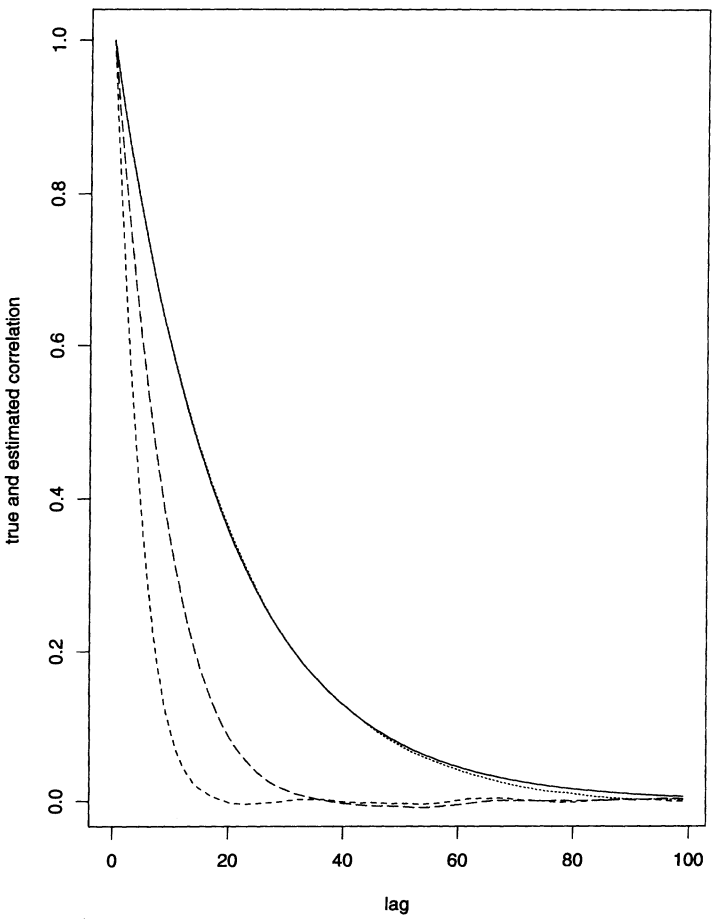

Figure 3. Comparison Between the Circulant Method and the Gibbs Sampler Method, ψ = .95. — true; · · · circulant method; - - - Gibbs sampling, 10; – – – Gibbs sampling, 50. True and estimated variance: true, 1.000; circulant method, .997; Gibbs sampling, 10, .305; Gibbs sampling, 50, .547.

both applications of the fast Fourier transform, corresponded to approximately seven loops of the Gibbs sampler.

We used the closeness of the estimated correlations to their true values as an informal (and fairly crude) measure of the degree of convergence achieved by the Gibbs sampler. We found that the larger the value of ψ, the slower the convergence. With $n = 2^{19}$, we found that when $\psi \leq .6$, convergence had occurred by the 10th loop of the Gibbs sampler; when $\psi = .8$, convergence occurred at around the 50th loop; but when $\psi = .95$, the Gibbs sampler was still a long way from convergence by the 50th loop. See Figure 3 for details of the case with $n = 2^{19}$ and $\psi = .95$. The corresponding CPU times for the circulant embedding approach, Gibbs sampler with 10 loops, and Gibbs sampler with 50 loops, were 107.253 seconds, 154.1863 seconds, and 804.4591 seconds.

7. PROOFS

Before going on to prove Propositions 3.1–3.3, we mention some elementary properties of the rth roots of unity. For any positive integer r, define the rth roots of unity

$$w_u = \exp\left(\frac{2\pi i u}{r}\right), \quad u = 0, 1, \ldots, r-1.$$

Then $w_u^r = 1$ for each integer u, and for each integer v

$$\begin{aligned} \sum_{u=0}^{r-1} w_u^v &= r \quad \text{if} \quad v = 0 (\text{mod } r) \\ &= 0 \quad \text{otherwise.} \end{aligned} \tag{7.1}$$

By considering the real and imaginary parts of (7.1) separately, it is also seen that

$$\begin{aligned} \sum_{u=0}^{r-1} \cos\left(\tfrac{2\pi u v}{r}\right) &= r \quad \text{if} \quad v = 0 (\text{mod } r) \\ &= 0 \quad \text{otherwise} \end{aligned} \tag{7.2}$$

and

$$\sum_{j=0}^{n-1} \sin\left(\frac{2\pi u v}{r}\right) = 0 \tag{7.3}$$

for each integer v. The following Lemma, which extends (5.2) and (5.3), will be used in the proofs of Propositions 1 and 3.

Lemma 1. *For any $h \in Z^d$*

$$\begin{aligned} \sum_{j \in I(m)} \cos\left\{2\pi h^T \left(\tfrac{j}{m}\right)\right\} &= \overline{m} \quad \textit{if } h[l] = 0 (\textit{mod } m[l]), \quad 1 \leq l \leq d \\ &= 0 \quad \textit{otherwise,} \end{aligned} \tag{7.4}$$

and

$$\sum_{j \in I(m)} \sin\left\{2\pi h^T \left(\frac{j}{m}\right)\right\} = 0. \tag{7.5}$$

Proof: Note that (7.4) and (7.5) are the real and imaginary parts of

$$\sum_{j\in I(m)} \exp\left\{2\pi i h^T\left(\frac{j}{m}\right)\right\} = \sum_{j\in I(m)} \prod_{l=1}^{d} \exp\left\{2\pi i \frac{h[l]\, j[l]}{m[l]}\right\}$$
$$= \prod_{l=1}^{d} \left[\sum_{j[l]=0}^{m[l]-1} \exp\left\{2\pi i \frac{h[l]\, j[l]}{m[l]}\right\}\right], \qquad (7.6)$$

and (7.4) and (7.5) follow after using (7.1) on each factor of (7.6). □

Proof of Proposition 3.1: Choose any $k_1, k_2 \in I(m)$. Then, by the definition of q_j in (3.13),

$$\sum_{j\in I(m)} \lambda(j)\, q_j(k_1)\, q_j^*(k_2) = \overline{m}^{-1} \sum_{j\in I(m)} \lambda(j) \exp\left\{2\pi i\, (k_2 - k_1)^T\left(\frac{j}{m}\right)\right\}.$$

Substituting for $\lambda(j)$ using (3.12), we obtain

$$\overline{m}^{-1} \sum_{j\in I(m)} \sum_{h\in I(m)} c(h) \exp\left\{2\pi i\, (k_2 - k_1 - h)^T\left(\frac{j}{m}\right)\right\}$$
$$= \overline{m}^{-1} \sum_{h\in I(m)} c(h) \sum_{j\in I(m)} \exp\left\{2\pi i\, (k_2 - k_1 - h)^T\left(\frac{j}{m}\right)\right\}$$
$$= c(k_1 - k_2) \equiv C_{k_1 k_2},$$

which proves the first equality in (3.14). Note that in the penultimate step, we used Lemma 1.

To prove the second equality in (3.14), we argue as follows. For each $j \in I(m)$, define

$$A(j) = \{l \in \{1, \ldots, d\} : 0 < j[l] < m[l]/2 \quad \text{or} \quad m[l]/2 < j[l] \leq m[l] - 1\}, \qquad (7.7)$$

and consider the following subsets of $I(m)$:

$$E_0 = \{j \in I(m) : A(j) = \phi\}, \qquad E_l = \{j \in I(m) : \min\{A(j)\} = l\},$$
$$E_l^{(1)} = \{j \in E_l : 0 < j[l] < m[l]/2\}, \quad E_l^{(2)} = E_l \backslash E_l^{(1)}, 1 \leq l \leq d. \qquad (7.8)$$

By construction, the $2d + 1$ sets E_0, $E_1^{(1)}$, $E_1^{(2)}, \ldots, E_d^{(1)}$, $E_d^{(2)}$ are disjoint and their union is $I(m)$. We now define a function $\hat{h} : I(m) \to I(m)$ as follows: for $j \in I(m)$, $\hat{h}(j) \in I(m)$ is given by

$$\hat{h}(j)[l] = j[l] \quad \text{if} \quad l \notin A(j)$$
$$= m[l] - j[l] \quad \text{if} \quad l \in A(j).$$

There are two points to note. First, symmetry in the construction of C in (3.8)–(3.11) implies that $\lambda(j) = \lambda(\hat{h}(j))$ for all $j \in I(m)$. Second,

$$\hat{h}(E_0) = E_0, \quad \hat{h}\left(E_l^{(1)}\right) = E_l^{(2)}, \quad \hat{h}\left(E_l^{(2)}\right) = E_l^{(1)}, \quad 1 \leq l \leq d.$$

It follows that the middle term in (3.14) may be written

$$\sum_{j \in F} \lambda(j)\, R_j\,,$$

where $F = E_0 \cup E_1^{(1)} \cup E_2^{(1)} \ldots \cup E_d^{(1)}$, and

$$\begin{aligned} R_j &= q_j\, q_j^* && \text{if} \quad j \in E_0 \\ &= q_j\, q_j^* + q_{\hat{h}(j)}\, q_{\hat{h}(j)}^* && \text{if} \quad j \in F \backslash E_0. \end{aligned}$$

It is easily checked that for each $j \in E_0$, the components of q_j are real; and for each $j \in F\backslash E_0$, $q_{\hat{h}(j)}^T = q_j^*$. Hence, R_j must be real and symmetric for each $j \in F$. Idempotence and (3.15) follow from the following easy consequence of Lemma 1: for any $j, k \in I(m)$,

$$\begin{aligned} q_j^*\, q_k &= 1 \quad \text{if} \quad \text{j = k} \\ &= 0 \quad \text{otherwise.} \end{aligned}$$

□

Proof of Proposition 3.2: Suppose that $m \in Z^d$ has $m[l] > 2$ for $l = 1, \ldots, d$, and write

$$B(m) = \left\{ j \in Z^d : -\text{int}\left(\frac{m[l]-1}{2}\right) \le j[l] \le \text{int}\left(\frac{m[l]}{2}\right),\ 1 \le l \le d \right\},$$

where int(.) denotes "integer part." The complement of $B(m)$ in Z^d is written $B^c(m)$.

Suppose that

$$\inf_{t \in [0,1]^d} g(t) = (2\pi)^{-d}\, \eta > 0\,.$$

Then (3.17) implies that there exists an $u_0 = u_0(n, \gamma)$ such that for all m which satisfy $\min\{m[1], \ldots, m[d]\} \ge u_0$,

$$\sum_{j \in B^c(m)} \left| \gamma\left(\frac{j}{n}\right) \right| < \eta/2\,.$$

Now if we consider the function $k : I(m) \to I^*(m)$ defined by

$$\begin{aligned} k(j)[l] &= j[l] && \text{if} \quad 0 \le j[l] \le m[l]/2 && 1 \le l \le d,\ j \in I(m) \\ &= j[l] - m[l] && \text{if} \quad m[l]/2 < j[l] \le m[l] - 1 && 1 \le l \le d,\ j \in I(m), \end{aligned}$$

and note the properties indicated in (3.5), (3.8), and (3.9), then it follows that $\lambda(j)$ may be rewritten as

$$\sum_{k \in B(m)} \gamma\left(\frac{k}{n}\right) \exp\left\{ -2\pi i\, j^T \left(\frac{k}{m}\right) \right\}$$

for each $j \in I(m)$; and so

$$\begin{aligned} \left| (2\pi)^d\, g\left(\frac{j}{n}\right) - \lambda(j) \right| &\le \left| \sum_{k \in B^c(m)} \gamma\left(\frac{k}{n}\right) \exp\left\{ -2\pi i j^T \left(\frac{k}{m}\right) \right\} \right| \\ &\le \sum_{k \in B^c(m)} \left| \gamma\left(\frac{k}{m}\right) \right| \le \eta/2\,, \end{aligned}$$

provided $\min\{m[1], \ldots, m[d]\} \geq u_0$. Thus

$$\min_{j \in I(m)} \lambda(j) \geq (2\pi)^d \inf_{t \in [0,1]^d} g(t) - \eta/2 = \eta/2 > 0$$

when $\min\{m[1], \ldots, m[d]\} \geq u_0$. □

Proof of Proposition 3.3: Using (3.13) and (3.21), we may write

$$S(k) = (\overline{m})^{-1/2} \sum_{j \in I(m)} \cos\left\{2\pi j^T \left(\frac{k}{m}\right)\right\} Z(j),$$

and

$$T(k) = (\overline{m})^{-1/2} \sum_{j \in I(m)} \sin\left\{2\pi j^T \left(\frac{k}{m}\right)\right\} Z(j),$$

where $\{Z(j), j \in I(m)\}$ is a collection of independent $N(0,1)$ random variables. Clearly $E(S) = E(T) = 0$; and for $k_1, k_2 \in I(m)$,

$$\begin{aligned} E\{S(k_1)T(k_2)\} &= (\overline{m})^{-1} \sum_{j \in I(m)} \cos\left\{2\pi j^T \left(\frac{k_1}{m}\right)\right\} \sin\left\{2\pi j^T \left(\frac{k_2}{m}\right)\right\} \\ &= (2\overline{m})^{-1} \sum_{j \in I(m)} \sin\left\{2\pi j^T \left(\frac{k_1 + k_2}{m}\right)\right\} \\ &\quad + \sin\left\{2\pi j^T \left(\frac{k_2 - k_1}{m}\right)\right\} \\ &= 0, \end{aligned}$$

by Lemma 1 and the fact that $\sin\theta \cos\phi = \{\sin(\theta + \phi) + \sin(\theta - \phi)\}/2$. Other trigonometric identities yield

$$E\{S(k_1)S(k_2)\} = (2\overline{m})^{-1} \sum_{j \in I(m)} \cos\left\{2\pi j^T \left(\frac{k_1 + k_2}{m}\right)\right\} + \cos\left\{2\pi j^T \left(\frac{k_2 - k_1}{m}\right)\right\}$$

and

$$E\{T(k_1)T(k_2)\} = (2\overline{m})^{-1} \sum_{j \in I(m)} \cos\left\{2\pi j^T \left(\frac{k_2 - k_1}{m}\right)\right\} - \cos\left\{2\pi j^T \left(\frac{k_1 + k_2}{m}\right)\right\},$$

and (2) and (3) of Proposition 3 then follow easily from Lemma 1. □

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