Fast and Exact Simulation of Fractional Brownian Surfaces

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Fractional Brownian surfaces are commonly used as models for landscapes and other physical processes in space. This work shows how to simulate fractional Brownian surfaces on a grid efficiently and exactly by embedding them in a periodic Gaussian random field and using the fast Fourier transform. Periodic embeddings are given that are proven to yield positive definite covariance functions and hence yield exact simulations for all possible densities of the simulation grid. Numerical results show these embeddings can sometimes be made more efficient in practice. Further numerical results show how the ideas developed for simulating fractional Brownian surfaces can be used for simulating other Gaussian random fields. The simulation methodology is used to study the behavior of a simple estimator of the parameters of a fractional Brownian surface.

Key Words: Fast Fourier transform; Gaussian random field; Variogram estimation.

1. INTRODUCTION

Fractional Brownian surfaces form a class of Gaussian random fields that are widely used to model a large range of natural processes (Peitgen and Saupe 1988). A fractional Brownian surface Z on $\mathbb{R}^d$ is a nonstationary Gaussian random field with constant mean and, for some $\alpha \in (0, 2)$, $\text{var}\{Z(\mathbf{x}) - Z(\mathbf{y})\} \propto |\mathbf{x} - \mathbf{y}|^\alpha$ for all $\mathbf{x}, \mathbf{y} \in \mathbb{R}^d$. The parameter α controls the roughness of the random field, with larger α corresponding to smoother Z. In particular, the fractal dimension of a fractional Brownian surface is $d + 1 - \alpha/2$ (Cressie 1993, p. 311). For $d = 1$, fractional Brownian surfaces are called fractional Brownian motions. Some authors use the name fractional Brownian motions even for $d > 1$ (Stoksik, Lane, and Nguyen 1995); however, fractional Brownian motion is probably better used to refer to processes on $\mathbb{R}$ with values in $\mathbb{R}^d$.

Fractional Brownian surfaces were used to spectacular effect by Saupe (1988) to simulate artificial landscapes. The simulation methods used by Saupe (1988) are only approx-

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imate, however. The main purpose of this work is to describe a fast and exact approach to simulating fractional Brownian surfaces on square grids for $d = 2$ and, to a lesser extent, $d = 3$.

Note that, as in Saupe (1988), we have defined only the variogram of fractional Brownian surface, $\frac{1}{2}\text{var}\{Z(\mathbf{x}) - Z(\mathbf{y})\}$, and not its covariance function. There is a whole class of nonstationary Gaussian random fields with corresponding variograms proportional to $|\mathbf{x} - \mathbf{y}|^\alpha$; one example is the Gaussian random field with $\text{cov}\{Z(\mathbf{x}), Z(\mathbf{y})\} \propto |\mathbf{x}|^\alpha + |\mathbf{y}|^\alpha - |\mathbf{x}-\mathbf{y}|^\alpha$. For most purposes for which one would simulate fractional Brownian surfaces, as long as the simulated random field has the correct variogram, the exact form of the covariance function does not matter, so this work considers only simulating a Gaussian random field whose variogram is of the required form.

The basic approach used here is to embed a fractional Brownian surface on a bounded region into a periodic random field and then exploit the fast Fourier transform to simulate rapidly the periodic random field on a square grid. The approach is somewhat similar to one taken by Dietrich and Newsam (1993, 1997) and Wood and Chan (1994), but they focused on stationary random fields and their methods generally fail for simulating fractional Brownian surfaces, which are nonstationary. It is worthwhile to describe the basic form of their procedure here, as it will help motivate the material in the next section.

Consider simulating a stationary Gaussian random field Z with $\text{cov}\{Z(\mathbf{x}), Z(\mathbf{y})\} = K(|\mathbf{x}-\mathbf{y}|)$ on a cubic grid in $[0, R]^d$ with spacing h along each coordinate and suppose that $N = 2R/h$ is a highly composite integer. We need some definitions. For a function K on $\mathbb{R}^d$, define $Q_R K$ to be the function on $\mathbb{R}^d$ that equals K on $(-R, R]^d$ and has period $2R$ in each coordinate, so that $K(\mathbf{x}+2R\mathbf{j}) = K(\mathbf{x})$ whenever $\mathbf{j}$ has all integer components. For a function K on $\mathbb{R}^d$, a positive integer N and $h > 0$, define $\mathbf{C}(K; N, h)$ to be the covariance matrix one gets when using K to define the covariances of observations on an N^d cubic grid with spacing h along each coordinate and observations ordered as in Wood and Chan (1994, equation (3.4)). The periodicity of $Q_R K$ implies that the matrix $\mathbf{C}(Q_R K; N, h)$ has a block circulant structure and it follows that its eigenvalues can be found by taking a d-dimensional discrete Fourier transform. This transform can be computed efficiently using the fast Fourier transform since N is highly composite. If all of these eigenvalues are nonnegative, so that $\mathbf{C}(Q_R K; N, h)$ is positive semidefinite, then by simulating a Gaussian random vector with independent components and variances proportional to these eigenvalues [with minor adjustments, see Wood and Chan (1994, proposition 3)] and applying another fast Fourier transform to this random vector, one obtains an exact simulation of the periodic random field with covariance function $Q_R K$ on the cubic grid with spacing h. Any set of these points in a cube of side R provides the desired simulation of a random field with covariance function K. If $\mathbf{C}(Q_R K; R, h)$ is not positive semidefinite, then one needs to be more clever to obtain exact simulations. Both Dietrich and Newsam (1993, 1997) and Wood and Chan (1994) gave the same approach for dealing with this problem for stationary random fields, which is described in Section 4.

Kaplan and Kuo (1996) described an approach based on periodic embeddings that is suitable for simulating fractional Brownian surfaces. Instead of simulating the fractional

Brownian surface directly, they simulated three sets of random variables, $Z(i+1,j+1) - Z(i+1,j) - Z(i,j+1) + Z(i,j)$ for $i,j = 0,\ldots,n-1$, $Z(i+1,0) - Z(i,0)$ for $i = 0,\ldots,n-1$ and $Z(0,j+1) - Z(0,j)$ for $j = 0,\ldots,n-1$, the first by a two-dimensional periodic embedding and the next two by one-dimensional periodic embeddings. Setting $Z(0,0) = 0$, one can reconstruct $Z(i,j)$ for $i,j = 0,\ldots,n-1$ from these three processes. Kaplan and Kuo (1996) provided evidence that their approach provides accurate simulations of fractional Brownian surfaces, but their method is still not exact for two reasons. The first is that the implied covariance matrices for the periodically extended processes might not be positive semidefinite, which Kaplan and Kuo (1996) treated by setting negative eigenvalues to 0. The second is that the three simulated processes are not independent and their simulation method only approximately captures this dependence.

All other previously suggested practical methods for simulating fractional Brownian surfaces for $d > 1$ at a large number ($> 10^4$, say) of locations are approximate. Chapter 7 of Chilès and Delfiner (1999) provides a good overview of simulation methods for random fields. Approximate methods for simulating fractional Brownian surfaces that have been proposed include discretization of continuous spectral representations (Saupe 1988), turning bands (Yin 1996; Chilès and Delfiner 1999), recursive filters (Bruton and Bartley 1994), wavelets (Zeldin and Spanos 1996), and midpoint displacement methods (Stoksik, Lane, and Nguyen 1995). It is difficult to assess the accuracy of these methods for reproducing the correct joint distributions of the random field for characteristics beyond bivariate distributions. The methods described in this article involve no approximations and produce fractional Brownian surface simulations of over 10^5 observations in $\mathbb{R}^2$ in under 20 seconds of processing time on a Sun Ultra 5.

For $d = 1$, Chilès and Delfiner (1999, p. 515) described how to simulate fractional Brownian motions exactly by periodic embeddings for all $\alpha < 2$. For $\alpha \leq 1$, they showed that periodic embedding directly yields exact simulations. For $1 < \alpha < 2$, they showed that periodic embedding yields exact simulations of the discrete time process $\Delta Z(i) = Z(i+1) - Z(i)$. By setting, for example, $Z(0) = 0$, one can then construct an exact simulation of fractional Brownian motion on a regular grid from the $\Delta Z(i)$s. Stein (2001) described an alternative approach to periodic embeddings of fractional Brownian motions that is more similar to the approach taken here and can also be used to simulate integrated fractional Brownian motions exactly.

Section 2 describes theoretical results showing how fractional Brownian surfaces on bounded regions in two and three dimensions can be embedded in periodic random fields. These results guarantee that simulation of fractional Brownian surfaces can be done on regular grids of arbitrarily small spacing by periodic embeddings for all $\alpha \in (0,2)$ in two and three dimensions. However, for larger α, the periodic embeddings are not as efficient as they might be; Section 3 describes some numerical results showing how to obtain more efficient embeddings for simulations on square grids in two dimensions. Section 4 considers the simulation of stationary Gaussian random fields and, as an example, describes an approach to simulating Gaussian random fields with an exponential covariance function that can be much more efficient than the approach suggested by Dietrich and Newsam (1993, 1997)

and Wood and Chan (1994). Section 5 makes use of the simulation methodology to study the properties of a simple estimator of α for fractional Brownian surfaces observed on a square grid when $\frac{1}{2}\text{var}\{Z(\mathbf{x}) - Z(\mathbf{y})\} = c|\mathbf{x} - \mathbf{y}|^\alpha$ for all $\mathbf{x}, \mathbf{y} \in \mathbb{R}^d$ with (c, α) unknown.

2. THEORETICAL RESULTS

Let $\mathcal{D}_d$ be the class of continuous, isotropic covariance functions for random fields on $\mathbb{R}^d$. More specifically, using $|\cdot|$ for Euclidean distance, $K \in \mathcal{D}_d$ means that K is a continuous function on $[0, \infty)$ and $\sum_{i,j=1}^n \lambda_i \lambda_j K(|\mathbf{x}_i - \mathbf{x}_j|) \geq 0$ for all finite n, all real $\lambda_1, \ldots, \lambda_n$ and all $\mathbf{x}_1, \ldots, \mathbf{x}_n \in \mathbb{R}^d$. The approach used here to simulating fractional Brownian surfaces is to seek a function $K \in \mathcal{D}_d$ of the form

$$K(r) = \begin{cases} c_0 - r^\alpha + c_2 r^2, & 0 \leq r \leq 1; \\ K_1(r), & 1 < r \leq R; \\ 0, & r > R, \end{cases} \tag{2.1}$$

where $R \geq 1$, $c_2 \geq 0$ and K_1 has no restrictions beyond making $K \in \mathcal{D}_d$. For a function K on $[0, \infty)$, define $P_R^d K$ to be the function on $\mathbb{R}^d$ such that $P_R^d K(\mathbf{x}) = K(|\mathbf{x}|)$ for $\mathbf{x} \in [-R, R]^d$ and has periodicity $2R$ in each coordinate. Note that P_R^d maps a function on $[0, \infty)$ to a periodic function on $\mathbb{R}^d$, whereas Q_R maps a function on $\mathbb{R}^d$ to a periodic function on $\mathbb{R}^d$. If $K \in \mathcal{D}_d$, then the fact that $K(r) = 0$ for $r \geq R$ implies that $P_R^d K$ is a positive definite function on $\mathbb{R}^d$, which follows from an easy generalization of a result in Feller (1971, p. 631).

Before giving functions of the form (2.1) that are in $\mathcal{D}_d$, let us first consider how we could use such a result to simulate fractional Brownian surfaces on a rectangular grid in a ball of diameter 1. For notational convenience, I will assume that the grid is equally spaced along each axis; the extension to more general rectangular grids is simple. Consider $K \in \mathcal{D}_d$ of the form (2.1) and simulate the Gaussian random field with covariance function $P_R^d K$ on the square grid $2RN^{-1}\mathbf{j}$ for $\mathbf{j} \in \{1, \ldots, N\}^d$ using the fast Fourier transform as described in Section 1. Let A be a subset of these simulated observations contained in a ball of diameter 1. If $\mathbf{x}$ and $\mathbf{y}$ are in A, then $\frac{1}{2}\text{var}\{Z(\mathbf{x}) - Z(\mathbf{y})\} = |\mathbf{x} - \mathbf{y}|^\alpha - c_2|\mathbf{x} - \mathbf{y}|^2$. This is not quite what we want, but extending an idea in Stein (2001) removes the unwanted term $-c_2|\mathbf{x} - \mathbf{y}|^2$. Let $X_1, \ldots, X_d$ be iid $N(0, 2c_2)$ and independent of Z and for $\mathbf{x} = (x_1, \ldots, x_d)$, define $Z^*(\mathbf{x}) = Z(\mathbf{x}) + \sum_{i=1}^d x_i X_i$. Then Z^* is a Gaussian random field with constant mean and for $\mathbf{x}, \mathbf{y} \in A$, $\frac{1}{2}\text{var}\{Z^*(\mathbf{x}) - Z^*(\mathbf{y})\} = |\mathbf{x} - \mathbf{y}|^\alpha$. Thus, for any set of points in a ball of diameter 1, Z^* possesses the defining properties of a fractional Brownian surface. Note that for $\mathbf{x}, \mathbf{y} \in A$, $\text{cov}\{Z^*(\mathbf{x}), Z^*(\mathbf{y})\} = c_0 - |\mathbf{x} - \mathbf{y}|^\alpha + c_2(|\mathbf{x}|^2 + |\mathbf{y}|^2)$, which is not a function of $\mathbf{x} - \mathbf{y}$, so that Z^* is not locally stationary as defined by Matheron (1974) (see also Chilès and Delfiner 1999). It is not clear to me why one might prefer a locally stationary version of fractional Brownian surface. If $\mathbf{0} \in A$, then $Z^*(\mathbf{x}) - Z^*(\mathbf{0})$ is also a fractional Brownian surface on A, in case it is desirable to have a fractional Brownian surface that equals 0 at the origin.

Pasenchenko (1996) showed that $K(r) = (1 - r^\alpha)^+$ is in $\mathcal{D}_2$ for $\alpha \leq 1/2$. This section gives three new results showing that functions of the form given in (2.1) are in $\mathcal{D}_2$ or $\mathcal{D}_3$.

Theorem 1 gives $K \in \mathcal{D}_3$ of the form (2.1) with $R = 2$ for all $\alpha \in (1, 2)$. Theorem 2 gives $K \in \mathcal{D}_3$ of the form (2.1) with $R = 1$ for all $\alpha \leq 1$. Theorem 3 shows that this same class of functions is in $\mathcal{D}_2$ for all $\alpha \leq 1.5$. Smaller values of R are desirable for purposes of simulating fractional Brownian surfaces since the larger R is, the larger the region we must simulate on to yield the realization of fractional Brownian surface in a ball of diameter 1.

We now state the theoretical results. Consider the function

$$V_\alpha(r) = \begin{cases} 1 - \frac{1}{6}\alpha - \frac{1}{6}\alpha^2 - r^\alpha + \frac{\alpha(5+2\alpha)}{18} r^2, & 0 < r \leq 1; \\ \frac{\alpha(2-\alpha)}{18} \frac{(2-r)^3}{r}, & 1 < r \leq 2; \\ 0, & r > 2. \end{cases}$$

Theorem 1. *For* $1 < \alpha < 2$, $V_\alpha \in \mathcal{D}_3$.

Consider the function

$$F_\alpha(r) = \begin{cases} 1 - \frac{1}{2}\alpha - r^\alpha + \frac{1}{2}\alpha r^2, & 0 \leq r \leq 1; \\ 0, & r > 1. \end{cases}$$

Theorem 2. *For* $0 < \alpha \leq 1$, $F_\alpha \in \mathcal{D}_3$.

Theorem 3. *For* $0 < \alpha \leq 1.5$, $F_\alpha \in \mathcal{D}_2$.

The proof of Theorem 2 is given in the Appendix. Theorems 1 and 3 have considerably longer proofs, which can be found at http://www.amstat.org/publications/jcgs/toc_01.html#mstein.

To give an indication of the practicality of running simulations of fractional Brownian surfaces using periodic embeddings, I simulated the periodic random field with covariance function $P_1^2 F_{1.5}$ on a 1024×1024 square grid with spacing $1/512$ in S-Plus. Since $2^{1/2}(363-1)/512 < 1$, this simulation yields a realization of a fractional Brownian surface on a 363×363 grid for a total of 131,769 observations. This simulation took 18.6 seconds of processing time on a Sun Ultra 5. The initial calculation of the eigenvalues of the covariance matrix of the covariance matrix took an additional 10.6 seconds, but this calculation does not need to be repeated when simulating multiple realizations of the same random field.

For α very near to 2, one can run into numerical problems using V_α due to the fact that r^α and r^2 are nearly equal. When simulating the periodic random field with covariance function $P_1^2 V_\alpha$ on a 1024×1024 square grid with spacing $1/512$ in S-Plus, there are clear numerical instabilities in the computed minimum eigenvalues of the covariance matrices for $\alpha > 1.9994$, including negative values for some α. I have no evidence of numerical problems for $\alpha < 1.9994$ for this sample size, but that is no guarantee that there are none.

3. EMPIRICAL IMPROVEMENTS

Theorems 1–3 provide a guarantee that $P_1^d F_\alpha$ and $P_2^d V_\alpha$ yield positive semidefinite covariance matrices for any possible set of observation locations. As already noted, we would prefer to have R in (2.1) as close to 1 as possible. For $d = 2$, Theorem 3 shows that F_α, for which $R = 1$, is in $\mathcal{D}_2$ for $\alpha \leq 1.5$, so no improvement is possible. However,

Table 1. Minimum values of R to make $\mathbf{C}(P_R^2 V_{\alpha R}; 1024, R/512)$ positive semidefinite. Values determined numerically to three decimal places.

α	1.60	1.65	1.70	1.75	1.80	1.85	1.90	1.95	1.99
R	1.001	1.009	1.026	1.052	1.087	1.128	1.172	1.219	1.273

for $\alpha > 1.5$, we might hope to improve on V_α, for which $R = 2$. Consider the following generalization of V_α:

$$V_{\alpha R}(r) = \begin{cases} c_0 - r^\alpha + c_2 r^2, & 0 \le r \le 1; \\ \dfrac{\beta(R-r)^3}{r}, & 1 < r \le R; \\ 0, & r > R, \end{cases}$$

where c_0, c_2 and β are chosen so that $V_{\alpha R}$ is twice differentiable on $(0, \infty)$, which implies

$$\begin{aligned} \beta &= \frac{\alpha(2-\alpha)}{3R(R^2-1)}, \\ c_2 &= \frac{1}{2}\alpha - \frac{\alpha(2-\alpha)(R+2)(R-1)}{6R(R+1)} \quad \text{and} \\ c_0 &= 1 - \frac{1}{2}\alpha + \frac{\alpha(2-\alpha)(R-1)(2R^2-R+2)}{6R^2(R+1)}. \end{aligned}$$

Note that $V_{\alpha 2} = V_\alpha$. Furthermore, it is straightforward to show that for every $\alpha > 0$, $V_{\alpha R}$ converges uniformly to F_α on $[0, \infty)$ as $R \downarrow 1$, so we can reasonably define $V_{\alpha 1} = F_\alpha$. Theorem 1 proves that $V_{\alpha 2} \in \mathcal{D}_3$ for all $\alpha \in (1, 2)$. It is possible that $V_{\alpha R}$ is in $\mathcal{D}_2$ or $\mathcal{D}_3$ for some $\alpha > 1$ and some $R < 2$. Rather than pursue further theoretical results, let us just numerically investigate when $\mathbf{C}(P_R^2 V_{\alpha R}; N, 2RN^{-1})$ is positive semidefinite. I only present results here for $N = 1024$. Calculations in S-Plus indicate that $\mathbf{C}(P_1^2 V_{\alpha 1}; 1024, 1/512)$ (i.e, $N = 1024$ and $R = 1$) is positive semidefinite if and only if $\alpha \le \alpha_0$, where $\alpha_0 \approx 1.599$. Further calculations suggest that if $\mathbf{C}(P_R^2 V_{\alpha R}; 1024, R/512)$ is positive semidefinite for some $R \ge 1$ and some $\alpha < 2$, so is $\mathbf{C}(P_R^2 V_{\alpha' R'}; 1024, R'/512)$ whenever $\alpha' \le \alpha$ and $R' \ge R$. For various $\alpha \ge \alpha_0$, Table 1 gives numerically determined minimum values of R to make $\mathbf{C}(P_R^2 V_{\alpha R}; 1024, R/512)$ positive semidefinite. These values are all quite a bit smaller than 2, the value guaranteed to work by Theorem 1. Keep in mind that these results are only for a 1024×1024 grid and one should expect that somewhat larger values of R will be needed for larger grids.

4. STATIONARY RANDOM FIELDS

The idea behind the definition of F_α of adding a quadratic term in distance to a covariance function to help embed a random field model in a periodic model can be used to aid in the simulation of Gaussian random fields other than fractional Brownian surfaces. For example, suppose one wants to simulate a stationary Gaussian random field with covariance function K on a square grid on $[0, 1]^2$ with spacing n^{-1}, where n is some highly

composite integer. Dietrich and Newsam (1993, 1997) and Wood and Chan (1994) recommended essentially the same approach, which I summarize here. If all of the eigenvalues of $\mathbf{C}(Q_1 K; 2n, n^{-1})$ are nonnegative, then proceed as described in Section 1 and simulate the periodic random field on this grid. Any set of points in a square of side 1 provides the desired simulation of a random field with covariance function K. If $\mathbf{C}(Q_1 K; 2n, n^{-1})$ has negative eigenvalues, then pick some $R > 1$ for which Rn is an integer and compute the eigenvalues of $\mathbf{C}(Q_R K; 2Rn, n^{-1})$. Theoretical results in Wood and Chan (1994) and Dietrich and Newsam (1997) essentially prove that if K is integrable and positive definite on $\mathbb{R}^d$, for any given spacing n^{-1}, $\mathbf{C}(Q_R K; 2Rn, n^{-1})$ is positive semidefinite for R sufficiently large. Once one finds an R such that $\mathbf{C}(Q_R K; 2Rn, n^{-1})$ is positive semidefinite and $2Rn$ is highly composite, one can then use the fast Fourier transform to carry out the simulation. However, it may sometimes be necessary to take R quite large to make $\mathbf{C}(Q_R K; 2Rn, n^{-1})$ positive semidefinite.

To get an idea of the possible extent of this problem, consider simulating a random field on $\mathbb{R}^2$ with covariance function $B_\theta(\mathbf{x}) = e^{-\theta|\mathbf{x}|}$ for some $\theta > 0$ on a square grid on $[0, 1]^2$. Numerical calculations suggest that $\mathbf{C}(Q_1 B_\theta; 1024, 1/512)$ is positive semidefinite if and only if $\theta \geq \theta_0$, where $\theta_0 \approx 6.047$. When $\theta \geq \theta_0$, we can then directly simulate on a 1024×1024 square grid with spacing $1/512$ and obtain a simulation of a Gaussian random field with covariance function B_θ on a 513×513 square grid with spacing $1/512$. Rather than work out how large R would need to be for various $\theta < \theta_0$ in order to simulate a Gaussian random field with covariance function B_θ with spacing $1/512$ on $[0, 1]^2$, we can more easily calculate what spacing we can achieve on $[0, 1]^2$ if we are only willing to simulate the extended periodic random field on a 1024×1024 square grid. Specifically, since simulating under B_θ on a 1024×1024 square grid with spacing h is the same as simulating under B_{θ_0} on a 1024×1024 square grid with spacing $h\theta_0/\theta$, our numerical results suggest that $\mathbf{C}(Q_R B_\theta, 1024, R/512)$ is positive semidefinite for $R \geq \theta_0/\theta$ and not otherwise. Setting $R = \theta_0/\theta$ and simulating the Gaussian random vector with covariance matrix $\mathbf{C}(Q_R B_\theta, 1024, R/512)$ then yields a simulation of a Gaussian random field with covariance function B_θ on a square grid on $[0, 1]^2$ with spacing $\theta_0/(512\theta)$. The smaller the value of θ, the larger this spacing is. For example, if $\theta = 1$ then the spacing is approximately 0.0118 and we only get to use $85^2/1024^2 \approx 0.69\%$ of the simulated observations.

In many situations, it suffices to simulate only the joint distribution of all increments of the random field Z correctly, where an increment is any linear combination $\sum_{i=1}^n \lambda_i Z(\mathbf{x}_i)$ for which $\sum_{i=1}^n \lambda_i = 0$. For example, if the mean of a stationary random field is assumed unknown, then all commonly used estimators of the covariance function are functions of increments of the observations (Zimmerman and Cressie 1992). Consider the function $\widetilde{B}_\theta$ on $[0, \infty)$ defined by

$$\widetilde{B}_\theta(r) = \begin{cases} c_0 + e^{-\theta r} + c_2 r^2, & r \leq 1; \\ 0, & r > 1, \end{cases}$$

where c_0 and c_2 are chosen so that $\widetilde{B}_\theta$ is differentiable at $r = 1$, yielding $c_0 = -e^{-\theta}\left(1 + \frac{1}{2}\theta\right)$ and $c_2 = \frac{1}{2}\theta e^{-\theta}$. Numerical evidence suggests that for observations on a 1024×1024 square grid with spacing $1/512$ and covariances given by $P_1^2 \widetilde{B}_\theta$, the resulting covariance matrix is

positive definite for all $\theta > 0$. Simulating on this 1024×1024 square grid yields a simulation of a random field Z with isotropic covariance function $\widetilde{B}_\theta$ on a 363×363 square grid with spacing $1/512$. Since $c_2 > 0$ for all $\theta > 0$, taking X_1, X_2 iid $N(0, 2c_2)$ and independent of Z, $Z(\mathbf{x}) + x_1 X_1 + x_2 X_2$ gives a correct simulation of all increments of a stationary Gaussian random field with covariance function B_θ on the 363×363 square grid with spacing $1/512$. For $\theta \geq \theta_0$, this region is roughly half the size obtained by simulating on a 1024×1024 square grid under $Q_1 B_\theta$, which yields a correct simulation on a 513×513 grid. Note, however, that if one were interested in simulating on a grid inside a ball, both approaches would yield correct simulations in balls of diameter at most 1, so that the methods would be equally efficient for $\theta \geq \theta_0$. For θ small, using $P_1^2 \widetilde{B}_\theta$ can be vastly superior. For example, again assume $\theta = 1$ and consider simulating on the densest possible grid on $[0, 1]^2$ using a simulation of a periodic random field on a 1024×1024 square grid. Using $P_1^2 \widetilde{B}_\theta$ with $\theta = 512/362$ and then taking a linear transformation of coordinates yields a simulation under B_1 on a 363×363 grid on $[0, 1]^2$, whereas, as we have already noted, using the approach suggested by Dietrich and Newsam (1993, 1997) and Wood and Chan (1994) for exact simulations yields only an 85×85 grid.

In circumstances in which adding a quadratic term to an isotropic covariance function does not yield an efficient periodic embedding, it may be possible to generalize the idea behind the definition of $V_{\alpha R}$ in which a given isotropic covariance function is altered beyond distance 1 so that it is 0 beyond distance R and is smooth at both 1 and R. Whether, as for $V_{\alpha R}$, extensions of the form $\beta(R - r)^3/r$ will be generally useful is unknown, although I have experimented with extensions of many other forms that do not work as well as $V_{\alpha R}$ for embedding fractional Brownian surfaces in periodic random fields.

5. SIMULATION STUDY OF PARAMETER ESTIMATION

Suppose Z is a random field on $\mathbb{R}^d$ with variogram $\frac{1}{2}\text{var}\{Z(\mathbf{x}) - Z(\mathbf{y})\} = \gamma(\mathbf{x} - \mathbf{y})$ for all $\mathbf{x}, \mathbf{y} \in \mathbb{R}^d$. For a fractional Brownian surface, $\gamma(\mathbf{x}) = c|\mathbf{x}|^\alpha$ for some $\alpha \in (0, 2)$ and some $c > 0$. This section reports the results of a small simulation study on the behavior of a simple estimator of (c, α) when a fractional Brownian surface is observed on a square grid. The simulations are all on $\mathbb{R}^2$ with $\alpha \leq 1.5$, so that, by Theorem 3, F_α can be used for the periodic embedding.

Suppose a fractional Brownian surface Z with variogram parameters (c, α) is observed at (hj_1, hj_2) for $j_1, j_2 = 1, \ldots, n$. For a positive integer $k < n$, define

$$\widehat{\gamma}(hk) = \frac{1}{4n(n-k)} \sum_{j_1=1}^{n} \sum_{j_2=k+1}^{n} \{Z(hj_1, hj_2) - Z(hj_1, h(j_2 - k))\}^2 + \frac{1}{4n(n-k)} \sum_{j_1=1}^{n} \sum_{j_2=k+1}^{n} \{Z(hj_1, hj_2) - Z(h(j_1 - k), hj_2)\}^2. \quad (5.1)$$

Noting that $\log\{\gamma(hk)\} = \log c + \alpha \log(hk)$ and following Kent and Wood (1997), a simple

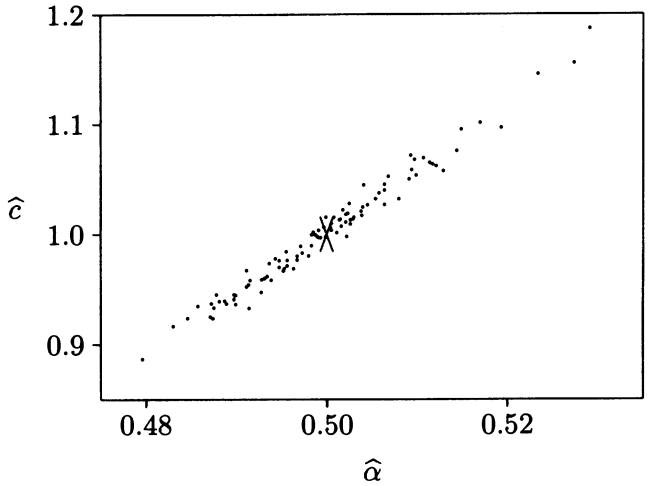

Figure 1. Values of $(\widehat{c}, \widehat{\alpha})$ based on 100 simulations of fractional Brownian surfaces on a 363 × 363 square grid with $(c, \alpha) = (1, 0.5)$ (marked by ╳ on plot).

estimate of α is given by

$$\widehat{\alpha} = \frac{\log \widehat{\gamma}(2h) - \log \widehat{\gamma}(h)}{\log 2}, \tag{5.2}$$

which then suggests estimating c by

$$\widehat{c} = \frac{\widehat{\gamma}(h)}{h^{\widehat{\alpha}}}. \tag{5.3}$$

Chan and Wood (2000) studied similar estimates of α for locally self-similar random fields on $\mathbb{R}^2$, but they did not consider averaging the variogram across directions as in (5.1). They proved a number of theorems about the asymptotic properties of estimators of the fractal dimension of random fields. They also carried out a simulation study, but their results are sometimes misleading due to the approximate methods they used to carry out the simulations. Zhu and Stein (2002) compared a broad array of estimators of α using the exact simulation methods given here.

To study the behavior of these estimates for $\alpha = 0.5$, 1, and 1.5 and $c = 1$, for each of these α values I did 100 simulations on a 512×512 square grid with spacing $1/256$ of the periodic random field with covariance function $P_1^2 F_\alpha$. From each simulation, I extracted observations on a 182×182 grid, which, since $2^{1/2}(182 - 1)/256 < 1$, are all contained in a ball of diameter 1. I then calculated $\widehat{\gamma}(1/256)$, $\widehat{\gamma}(2/256)$, $\widehat{\alpha}$ and $\widehat{c}$; Figures 1–3 plot the results for the three values of α. There are a number of noteworthy patterns. First, for all α, $\widehat{c}$, and $\widehat{\alpha}$ are highly correlated. Second, the relative variation in $\widehat{c}$ is much greater than that in $\widehat{\alpha}$ for all α. Theorem 1 in Section 6.7 of Stein (1999) suggests that the restricted maximum likelihood estimators of c and α should also have these properties. More specifically, this result suggests that as the number of observations N on a square grid tends to infinity, the correlation of the restricted maximum likelihood estimators of α and c tends to 1 and that

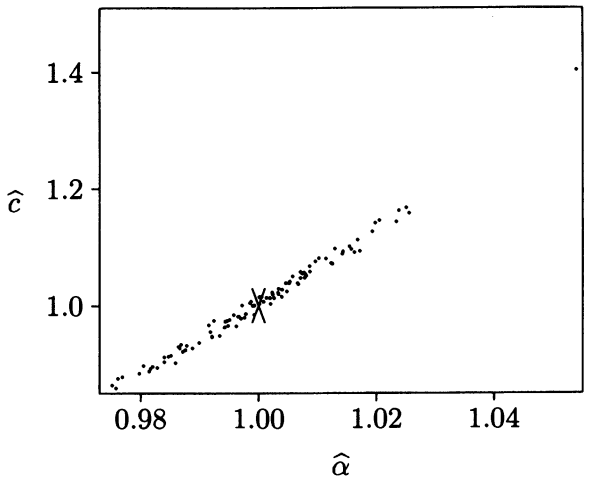

Figure 2. Values of $(\widehat{c}, \widehat{\alpha})$ based on 100 simulations of fractional Brownian surfaces on a 363 × 363 square grid with $(c, \alpha) = (1,1)$ (marked by ╳ on plot).

the asymptotic variances for these estimators are of order N^{-1} and $N^{-1} \log^2 N$ for α and c, respectively. Additional patterns in evidence are a clear increase in the variability of $\widehat{c}$ as α increases and a much larger relative variation in $\widehat{\alpha}$ when $\alpha = 1.5$ than when $\alpha = 0.5$ or 1. The difficulty in estimating α based on the empirical variogram when $\alpha = 1.5$ should be expected in light of theoretical results in Chan and Wood (2000). For larger α, one obtains better estimates by looking at sums of squares of second order differences rather than the first order differences used here (Chan and Wood 2000; Zhu and Stein 2002).

As Kent and Wood (1997) suggested for processes on $\mathbb{R}$, one could use the empirical variogram at distances other than h and $2h$ to estimate α and c. In two dimensions, one can

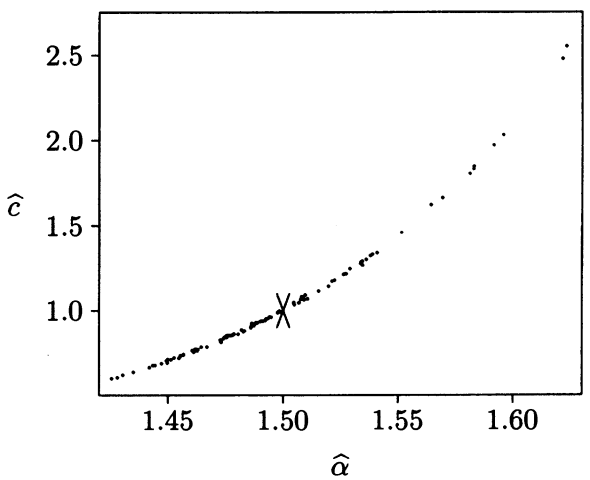

Figure 3. Values of $(\widehat{c}, \widehat{\alpha})$ based on 100 simulations of fractional Brownian surfaces on a 363 × 363 square grid with $(c, \alpha) = (1,1.5)$ (marked by ╳ on plot).

look in directions other than parallel to the axes of the grid (Chan and Wood 2000, Zhu and Stein 2002). For example, define

$$\widehat{\gamma}(2^{1/2}h) = \frac{1}{4(n-1)^2}\sum_{j_1=2}^{n}\sum_{j_2=2}^{n}\left\{Z(hj_1,hj_2) - Z(h(j_1-1),h(j_2-1))\right\}^2 + \frac{1}{4(n-1)^2}\sum_{j_1=2}^{n}\sum_{j_2=1}^{n-1}\left\{Z(hj_1,hj_2) - Z(h(j_1-1),h(j_2+1))\right\}^2$$

and consider estimating α and $\log c$ by fitting a line by least squares to the three pairs of points $(\log h, \log\widehat{\gamma}(h))$, $(\log(2^{1/2}h), \log\widehat{\gamma}(2^{1/2}h))$ and $(\log(2h), \log\widehat{\gamma}(2h))$. Since $\log(2^{1/2}h)$ is halfway between $\log h$ and $\log(2h)$, the estimate of α is still given by (5.2) but the estimate of c is changed from (5.3). For these three values of α, the estimates of c are slightly improved when $\widehat{\gamma}(2^{1/2}h)$ is used, but the variances decrease by less than 1% in all three cases.

APPENDIX

The proof of Theorem 2 is given. If K is a continuous function on $[0,\infty)$ and $\int_0^\infty r^{d-1}K(r)dr < \infty$, then $K \in \mathcal{D}_d$ if and only if the isotropic spectral density f on $[0,\infty)$ given by

$$f(u) = \frac{1}{2^{(d-2)/2}\Gamma(d/2)}\int_0^\infty J_{d/2}(ur)(ur)^{d/2}\frac{K(r)}{r}dr$$

is nonnegative for all $u \geq 0$ (Yaglom 1987, sec. 22.1), where J_ν is an ordinary Bessel function of order ν. For $d = 3$, this simplifies to

$$f(u) = \frac{1}{2\pi^2}\int_0^\infty \frac{\sin(ur)}{ur}r^2K(r)dr,$$

so it suffices to show that

$$f_\alpha(u) = \frac{1}{2\pi^2}\int_0^\infty \frac{\sin(ur)}{ur}r^2F_\alpha(r)dr$$

is nonnegative for all $u > 0$. Repeated integration by parts yields

$$\widetilde{f}_\alpha(u) = \frac{2\pi^2}{\alpha}u^5f(u) = 3u\cos u - 3\sin u + (\alpha+1)u^{2-\alpha}\int_0^u v^{\alpha-1}\sin v\,dv.$$

Now,

$$\frac{\partial}{\partial u}\widetilde{f}_\alpha(u) = -(2-\alpha)u\sin u + (\alpha+1)(2-\alpha)u^{1-\alpha}\int_0^u v^{\alpha-1}\sin v\,dv \qquad \text{(A.1)}$$

and

$$\frac{\partial^2}{\partial u^2}\widetilde{f}_\alpha(u) = \alpha(2-\alpha)\sin u + (1-\alpha^2)(2-\alpha)u^{-\alpha}\int_0^u v^{\alpha-1}\sin v\,dv. \qquad \text{(A.2)}$$

As a function of u, the local minima of $\int_0^u v^{\alpha-1} \sin v \, dv$ for $u \geq 0$ are at the multiples of 2π and, for every positive integer n,

$$\begin{aligned}\int_0^{2n\pi} v^{\alpha-1} \sin v \, dv &= \sum_{k=1}^{n} \int_{2(k-1)\pi}^{2k\pi} v^{\alpha-1} \sin v \, dv \\ &= \sum_{k=1}^{n} \int_{2(k-1)\pi}^{(2k-1)\pi} \left\{ v^{\alpha-1} - (\pi + v)^{\alpha-1} \right\} \sin v \, dv,\end{aligned}$$

which is nonnegative for all $\alpha \in (0, 1]$. Thus, $\int_0^u v^{\alpha-1} \sin v \, dv \geq 0$ for all $\alpha \in (0, 1]$ and all $u > 0$. It follows from (A.1) that, for every $\alpha \in (0, 1]$, $\widetilde{f}_\alpha$ is nondecreasing on $[(2n-1)\pi, 2n\pi]$ for all positive integers n. From (A.2), for every $\alpha \in (0, 1]$, $\widetilde{f}_\alpha$ is convex on $[2n\pi, (2n+1)\pi]$ for all nonnegative integers n. Furthermore, $(\partial/\partial u)\widetilde{f}_\alpha(0) = 0$ for every $\alpha \in (0, 1]$. Now, for every $\alpha \in (0, 1]$, $\widetilde{f}_\alpha$ is continuously differentiable and, for all nonnegative integers n, $(\partial/\partial u)\widetilde{f}_\alpha(2n\pi) \geq 0$ and $\widetilde{f}_\alpha$ is convex on $[2n\pi, (2n+1)\pi]$. Thus, $\widetilde{f}_\alpha$ is nondecreasing on $[2n\pi, (2n+1)\pi]$ for all nonnegative integers n. Thus, $\widetilde{f}_\alpha$ is nondecreasing on $[0, \infty)$ for every $\alpha \in (0, 1]$, which, together with $\widetilde{f}_\alpha(0) = 0$, implies Theorem 2.

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