Circulant embedding in 2D, Turning bands method

Hauptseminar: Stochastic Simulation and Uncertainty Quantification

Elias Reutelsterz

Department of Mathematics
Technical University of Munich

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Outline

Definition 1.1. (Toeplitz matrix)
An $N \times N$ real-valued matrix $C = (c_{ij}$ is Toeplitz if $c_{ij} = c_{i-j}$ for some real numbers $c_{1-N}, \ldots, c_{N-1}$.

$$C = \begin{pmatrix} c_0 & c_{-1} & \cdots & c_{2-N} & c_{1-N} \\ c_1 & c_0 & c_{-1} & \ddots & c_{2-N} \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ c_{N-2} & \ddots & c_1 & c_0 & c_{-1} \\ c_{N-1} & c_{N-2} & \cdots & c_1 & c_0 \end{pmatrix}$$

which is uniquely defined by the vector $c = [c_{1-N}, \ldots, c_{-1}, c_0, c_1, \ldots, c_{N-1}]^T \in \mathbb{R}^{2N-1}$.

Definition 1.2. (block Toeplitz matrix with Toeplitz blocks - BTTB matrix)
Let $N = n_1 n_2$. An $N \times N$ real-valued matrix C is said to be block Toeplitz with Toeplitz blocks ($BTTB$) if it has the form

$$C = \begin{pmatrix} C_0 & C_{-1} & \cdots & C_{2-n_2} & C_{1-n_2} \\ C_1 & C_0 & \cdots & C_{-1} & C_{2-n_2} \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ C_{n_2-2} & \ddots & C_1 & C_0 & C_{-1} \\ C_{n_2-1} & C_{n_2-2} & \cdots & C_1 & C_0 \end{pmatrix}$$

where C_k are $n_1 \times n_1$ Toeplitz matrices. Let $c_k \in \mathbb{R}^{2n_1-1}$ be the vector containing the entries of the first row and column of C_k. C can be generated from the reduced matrix

$$C_{red} := \left[c_{1-n_2}, ..., c_0, ..., c_{n_2-1}\right]^T \in \mathbb{R}^{(2n_1-1)\times(2n_2-1)}.$$

Definition 1.3. (circulant matrix)
An $N \times N$ real-valued Toeplitz matrix $C = (c_{ij})$ is circulant if each column is a circular shift of the elements of the preceding column.

$$C = \begin{pmatrix} c_0 & c_{N-1} & \cdots & c_2 & c_1 \\ c_1 & c_0 & c_{N-1} & \ddots & c_2 \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ c_{N-2} & \ddots & c_1 & c_0 & c_{N-1} \\ c_{N-1} & c_{N-2} & \cdots & c_1 & c_0 \end{pmatrix}$$

which is uniquely defined by the first column $c_1 = [c_0, c_1, ..., c_{N-1}]^T \in \mathbb{R}^N$.

Definition 1.4. (block circulant matrix with circulant blocks - BCCB matrix)
Let $N = n_1 n_2$. An $N \times N$ real-valued matrix C is block circulant with circulant blocks ($BCCB$) if it is a $BTTB$ matrix of the form

$$C = \begin{pmatrix} C_0 & C_{n_2-1} & \dots & C_2 & C_1 \\ C_1 & C_0 & C_{n_2-1} & \ddots & C_2 \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ C_{n_2-2} & \ddots & C_1 & C_0 & C_{n_2-1} \\ C_{n_2-1} & C_{n_2-2} & \dots & C_1 & C_0 \end{pmatrix}$$

and each of the blocks $C_0, ..., C_{n_2-1}$ is an $n_1 \times n_1$ circulant matrix. Let $c_k \in \mathbb{R}^{n_1}$ be the first column of C_k. Any $BCCB$ matrix C is uniquely determined by the reduced $n_1 \times n_2$ matrix

$$C_{red} = [c_0, ..., c_{n_2-1}],$$

Sample from $\mathcal{N}(0, C)$ with BCCB matrix

Assume $C \in \mathbb{R}^{N \times N}$ is a BCCB matrix, with $n_2 \cdot n_2$ blocks of size $n_1 \times n_1$ and $N = n_1 n_2$ with real, non-negative eigenvalues.
Use IFT for C_{red} to obtain the decomposition $C = WDW^*$ where $D = \mathrm{diag}(\lambda_k)$ with λ_k being the eigenvalues of C_{red} and $W = W_2 \otimes W_1$ where W_1 and W_2 are the $n_1 \times n_1$ and $n_2 \times n_2$ Fourier matrices. Then it holds

$$Z = WD^{1/2}\xi, \qquad \xi \sim C\mathcal{N}(0, 2I_N)$$

where $C = WDW^*$. The resulting real and imaginary parts of $Z = X + iY$ provide two independent samples of $\mathcal{N}(0, C)$

How to apply the BCCB sampling concept to a 2D grid?

Definition 1.5. (stationary random field)
We say a second-order random field $\{u(x) : x \in \mathbb{R}^d\}$ is stationary if the mean $\mu(x)$ is independent of x (i.e. constant) and the covariance has the form $C(x, y) = c(x - y)$, for a function $c(x)$ known as the stationary covariance.

Example 1.6. (BCCB extension for uniformly spaced grids)
Consider $D = [0, 1]^2$, $n_1 = 3$, $n_2 = 2$, $\Delta x_1 = 1/2$, $\Delta x_2 = 1$ and a stationary random field $\{u(x) : x \in D\}$ with covariance function $c(x)$.

$$\Rightarrow x^{(0)} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}, x^{(1)} = \begin{pmatrix} 1/2 \\ 0 \end{pmatrix}, x^{(2)} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, x^{(3)} = \begin{pmatrix} 0 \\ 1 \end{pmatrix}, x^{(4)} = \begin{pmatrix} 1/2 \\ 1 \end{pmatrix}, x^{(5)} = \begin{pmatrix} 1 \\ 1 \end{pmatrix}$$

Let $C \in \mathbb{R}^{6\times 6}$ denote the covariance matrix.

Covariance matrices for uniformly spaced grids I

$$C = \begin{pmatrix}
c(x^{(0)} - x^{(0)}) & c(x^{(0)} - x^{(1)}) & c(x^{(0)} - x^{(2)}) & c(x^{(0)} - x^{(3)}) & c(x^{(0)} - x^{(4)}) & c(x^{(0)} - x^{(5)}) \\
c(x^{(1)} - x^{(0)}) & c(x^{(1)} - x^{(1)}) & c(x^{(1)} - x^{(2)}) & c(x^{(1)} - x^{(3)}) & c(x^{(1)} - x^{(4)}) & c(x^{(1)} - x^{(5)}) \\
c(x^{(2)} - x^{(0)}) & c(x^{(2)} - x^{(1)}) & c(x^{(2)} - x^{(2)}) & c(x^{(2)} - x^{(3)}) & c(x^{(2)} - x^{(4)}) & c(x^{(2)} - x^{(5)}) \\
c(x^{(3)} - x^{(0)}) & c(x^{(3)} - x^{(1)}) & c(x^{(3)} - x^{(2)}) & c(x^{(3)} - x^{(3)}) & c(x^{(3)} - x^{(4)}) & c(x^{(3)} - x^{(5)}) \\
c(x^{(4)} - x^{(0)}) & c(x^{(4)} - x^{(1)}) & c(x^{(4)} - x^{(2)}) & c(x^{(4)} - x^{(3)}) & c(x^{(4)} - x^{(4)}) & c(x^{(4)} - x^{(5)}) \\
c(x^{(5)} - x^{(0)}) & c(x^{(5)} - x^{(1)}) & c(x^{(5)} - x^{(2)}) & c(x^{(5)} - x^{(3)}) & c(x^{(5)} - x^{(4)}) & c(x^{(5)} - x^{(5)})
\end{pmatrix}$$

Covariance matrices for uniformly spaced grids II

$$
= \begin{pmatrix}
c\begin{pmatrix}0\\0\end{pmatrix} & c\begin{pmatrix}-\frac{1}{2}\\0\end{pmatrix} & c\begin{pmatrix}-1\\0\end{pmatrix} & c\begin{pmatrix}0\\-1\end{pmatrix} & c\begin{pmatrix}-\frac{1}{2}\\-1\end{pmatrix} & c\begin{pmatrix}-1\\-1\end{pmatrix} \\
c\begin{pmatrix}\frac{1}{2}\\0\end{pmatrix} & c\begin{pmatrix}0\\0\end{pmatrix} & c\begin{pmatrix}-\frac{1}{2}\\0\end{pmatrix} & c\begin{pmatrix}\frac{1}{2}\\-1\end{pmatrix} & c\begin{pmatrix}0\\-1\end{pmatrix} & c\begin{pmatrix}-\frac{1}{2}\\-1\end{pmatrix} \\
c\begin{pmatrix}1\\0\end{pmatrix} & c\begin{pmatrix}\frac{1}{2}\\0\end{pmatrix} & c\begin{pmatrix}0\\0\end{pmatrix} & c\begin{pmatrix}1\\-1\end{pmatrix} & c\begin{pmatrix}\frac{1}{2}\\-1\end{pmatrix} & c\begin{pmatrix}0\\-1\end{pmatrix} \\
c\begin{pmatrix}0\\1\end{pmatrix} & c\begin{pmatrix}-\frac{1}{2}\\1\end{pmatrix} & c\begin{pmatrix}-1\\1\end{pmatrix} & c\begin{pmatrix}0\\0\end{pmatrix} & c\begin{pmatrix}-\frac{1}{2}\\0\end{pmatrix} & c\begin{pmatrix}-1\\0\end{pmatrix} \\
c\begin{pmatrix}\frac{1}{2}\\1\end{pmatrix} & c\begin{pmatrix}0\\1\end{pmatrix} & c\begin{pmatrix}-\frac{1}{2}\\1\end{pmatrix} & c\begin{pmatrix}\frac{1}{2}\\0\end{pmatrix} & c\begin{pmatrix}0\\0\end{pmatrix} & c\begin{pmatrix}-\frac{1}{2}\\0\end{pmatrix} \\
c\begin{pmatrix}1\\1\end{pmatrix} & c\begin{pmatrix}\frac{1}{2}\\1\end{pmatrix} & c\begin{pmatrix}0\\1\end{pmatrix} & c\begin{pmatrix}1\\0\end{pmatrix} & c\begin{pmatrix}\frac{1}{2}\\0\end{pmatrix} & c\begin{pmatrix}0\\0\end{pmatrix}
\end{pmatrix}
$$

Covariance matrices for uniformly spaced grids II

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c\begin{pmatrix}0\\0\end{pmatrix} & c\begin{pmatrix}-\frac{1}{2}\\0\end{pmatrix} & c\begin{pmatrix}-1\\0\end{pmatrix} & c\begin{pmatrix}0\\-1\end{pmatrix} & c\begin{pmatrix}-\frac{1}{2}\\-1\end{pmatrix} & c\begin{pmatrix}-1\\-1\end{pmatrix} \\
c\begin{pmatrix}\frac{1}{2}\\0\end{pmatrix} & c\begin{pmatrix}0\\0\end{pmatrix} & c\begin{pmatrix}-\frac{1}{2}\\0\end{pmatrix} & c\begin{pmatrix}\frac{1}{2}\\-1\end{pmatrix} & c\begin{pmatrix}0\\-1\end{pmatrix} & c\begin{pmatrix}-\frac{1}{2}\\-1\end{pmatrix} \\
c\begin{pmatrix}1\\0\end{pmatrix} & c\begin{pmatrix}\frac{1}{2}\\0\end{pmatrix} & c\begin{pmatrix}0\\0\end{pmatrix} & c\begin{pmatrix}1\\-1\end{pmatrix} & c\begin{pmatrix}\frac{1}{2}\\-1\end{pmatrix} & c\begin{pmatrix}0\\-1\end{pmatrix} \\
c\begin{pmatrix}0\\1\end{pmatrix} & c\begin{pmatrix}-\frac{1}{2}\\1\end{pmatrix} & c\begin{pmatrix}-1\\1\end{pmatrix} & c\begin{pmatrix}0\\0\end{pmatrix} & c\begin{pmatrix}-\frac{1}{2}\\0\end{pmatrix} & c\begin{pmatrix}-1\\0\end{pmatrix} \\
c\begin{pmatrix}\frac{1}{2}\\1\end{pmatrix} & c\begin{pmatrix}0\\1\end{pmatrix} & c\begin{pmatrix}-\frac{1}{2}\\1\end{pmatrix} & c\begin{pmatrix}\frac{1}{2}\\0\end{pmatrix} & c\begin{pmatrix}0\\0\end{pmatrix} & c\begin{pmatrix}-\frac{1}{2}\\0\end{pmatrix} \\
c\begin{pmatrix}1\\1\end{pmatrix} & c\begin{pmatrix}\frac{1}{2}\\1\end{pmatrix} & c\begin{pmatrix}0\\1\end{pmatrix} & c\begin{pmatrix}1\\0\end{pmatrix} & c\begin{pmatrix}\frac{1}{2}\\0\end{pmatrix} & c\begin{pmatrix}0\\0\end{pmatrix}
\end{pmatrix}
$$

Roadmap

For a uniformly spaced grid every stationary covariance function leads to a BTTB covariance matrix

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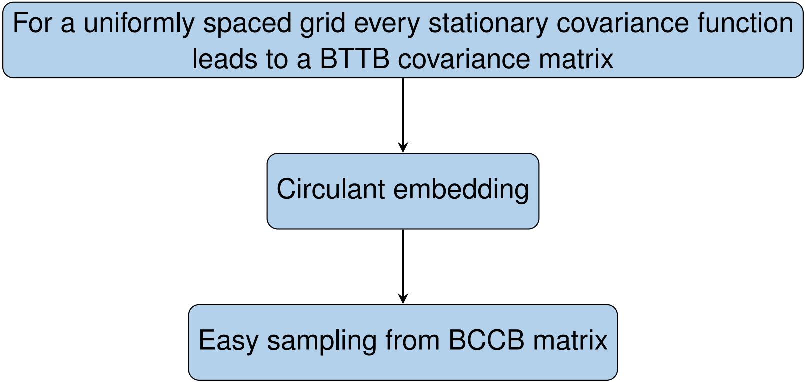
Easy sampling from BCCB matrix

Roadmap


For a uniformly spaced grid every stationary covariance function leads to a BTTB covariance matrix
Circulant embedding
Easy sampling from BCCB matrix

Definition 1.7. (even circulant extension)
Let $C \in \mathbb{R}^{n_1 \times n_1}$ be a Toeplitz matrix generated by $c = [c_{1-n_1}, ..., c_{-1}, c_0, c_1, ..., c_{n_1-1}]^T \in \mathbb{R}^{2n_1-1}$. The even circulant extension is the circulant matrix $\tilde{C} \in \mathbb{R}^{2n_1 \times 2n_1}$ with first column $\tilde{c} = [c_0, c_1, ..., c_{n_1-1}, 0, c_{1-n_1}, ..., c_{-1}]^T \in \mathbb{R}^{2n_1}$. Hence,

$$\tilde{C} = \begin{pmatrix} C & B \\ B & C \end{pmatrix}$$

where C is the original Toeplitz matrix and $B \in \mathbb{R}^{n_1 \times n_1}$.

Example 1.8. (even circulant extension versus minimal circulant extension)

$$C_0 = \begin{pmatrix} 1 & 3 & 4 \\ 2 & 1 & 3 \\ 1 & 2 & 1 \end{pmatrix} \overset{even}{\Rightarrow} \tilde{C}_0 = \begin{pmatrix} 1 & 3 & 4 & 0 & 1 & 2 \\ 2 & 1 & 3 & 4 & 0 & 1 \\ 1 & 2 & 1 & 3 & 4 & 0 \\ 0 & 1 & 2 & 1 & 3 & 4 \\ 4 & 0 & 1 & 2 & 1 & 3 \\ 3 & 4 & 0 & 1 & 2 & 1 \end{pmatrix} \in \mathbb{R}^{6\times 6}$$

$$C_0 = \begin{pmatrix} 1 & 3 & 4 \\ 2 & 1 & 3 \\ 1 & 2 & 1 \end{pmatrix} \overset{minimal}{\Rightarrow} \tilde{C}_0 = \begin{pmatrix} 1 & 3 & 4 & 1 & 2 \\ 2 & 1 & 3 & 4 & 1 \\ 1 & 2 & 1 & 3 & 4 \\ 4 & 1 & 2 & 1 & 3 \\ 3 & 4 & 1 & 2 & 1 \end{pmatrix} \in \mathbb{R}^{5\times 5}$$

Definition 1.9. (even BCCB extension of BTTB matrices)
Given a BTTB matrix $C \in \mathbb{R}^{N\times N}$ where $N = n_1 n_2$, let $\tilde{C}_k$ be the even circulant extension of the Toeplitz block C_k. The even BCCB extension of C is the BCCB matrix

$$\tilde{C} = \begin{pmatrix} \tilde{C}_0 & \tilde{C}_{-1} & \dots & \tilde{C}_{1-n_2} & \tilde{0} & \tilde{C}_{n_2-1} & \dots & \tilde{C}_1 \\ \tilde{C}_1 & \tilde{C}_0 & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots \\ \vdots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots \\ \tilde{C}_{n_2-1} & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots \\ \tilde{0} & \tilde{C}_{n_2-1} & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots \\ \tilde{C}_{1-n_2} & \tilde{0} & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots \\ \vdots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \tilde{C}_{-1} \\ \tilde{C}_{-1} & \tilde{C}_{-2} & \ddots & \ddots & \ddots & \ddots & \tilde{C}_1 & \tilde{C}_0 \end{pmatrix} \in \mathbb{R}^{4N\times 4N},$$

where $\tilde{0}$ is the $2n_1 \times 2n_1$ zero matrix.

Sample from $\mathcal{N}(0, C)$ with BTTB matrix I

If the BCCB extension $\tilde{C} \in \mathbb{R}^{4N \times 4N}$ with $N = n_1 n_2$ is non-negative definite, then we can draw samples from it $\tilde{u} \sim \mathcal{N}(0, \tilde{C})$. To recover samples from $\mathcal{N}(0, C)$ we only consider the first half of $\tilde{u}$ because the leading principal submatrix contains the necessary covariance information (cut out the even BCCB extension).

$$\tilde{C} = \begin{pmatrix} S & R \\ R & S \end{pmatrix}, \quad S = \begin{pmatrix} \tilde{C}_0 & \tilde{C}_1^T & \dots & \tilde{C}_{n_2-2}^T & \tilde{C}_{n_2-1}^T \\ \tilde{C}_1 & \tilde{C}_0^T & \tilde{C}_1^T & \ddots & \tilde{C}_{n_2-1}^T \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ \tilde{C}_{n_2-2} & \ddots & \tilde{C}_1 & \tilde{C}_0 & \tilde{C}_1^T \\ \tilde{C}_{n_2-1} & \tilde{C}_{n_2-2} & \dots & \tilde{C}_1 & \tilde{C}_0 \end{pmatrix}$$

Then it holds $\tilde{u}_{1:2N} \sim \mathcal{N}(0, S)$.

Sample from $\mathcal{N}(0, C)$ with BTTB matrix II

Now use the same logic for each of the circulant blocks to cut out the even circulant extension of the respective block

$$S = \begin{pmatrix} \tilde{C}_0 & \tilde{C}_1^T & \dots & \tilde{C}_{n_2-2}^T & \tilde{C}_{n_2-1}^T \\ \tilde{C}_1 & \tilde{C}_0^T & \tilde{C}_1^T & \ddots & \tilde{C}_{n_2-1}^T \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ \tilde{C}_{n_2-2} & \ddots & \tilde{C}_1 & \tilde{C}_0 & \tilde{C}_1^T \\ \tilde{C}_{n_2-1} & \tilde{C}_{n_2-2} & \dots & \tilde{C}_1 & \tilde{C}_0 \end{pmatrix}, \quad \tilde{C}_i = \begin{pmatrix} C_i & B_i \\ B_i & C_i \end{pmatrix},$$

Then we obtain with $\tilde{u}_{(2n_1 \cdot i+1):(n_1 \cdot (2i+1))} \sim \mathcal{N}(0, C_i)$ the resulting $u \sim \mathcal{N}(0, C)$ as follows:

$$u = \mathrm{vec}(V) \in \mathbb{R}^{n_1 n_2}, \quad V = \begin{pmatrix} \tilde{u}_1 & \tilde{u}_{2n_1+1} & \dots & \tilde{u}_{(2n_2-2)n_1+1} \\ \tilde{u}_2 & \tilde{u}_{2n_1+2} & \dots & \ddots \\ \vdots & \vdots & \vdots & \vdots \\ \tilde{u}_{n_1} & \tilde{u}_{3n_1} & \dots & \tilde{u}_{(2n_2-1)n_1} \end{pmatrix}$$

Example images sample from $\mathcal{N}(0, C)$ with BTTB matrix

Example 1.10. Consider $u(x)$ a mean-zero Gaussian random field with stat. covariance

$$c(x) = \exp\left(-\frac{|x_1|}{l_1} - \frac{|x_2|}{l_2}\right)$$

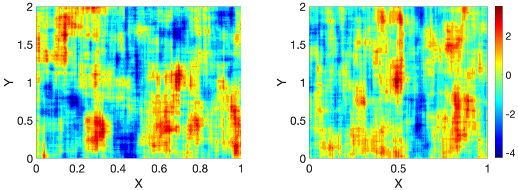
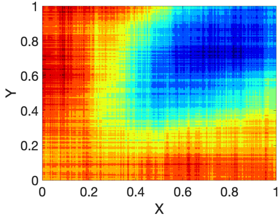


Figure 1 Two realisations with $l_1 = 1/5$, $l_2 = 1/10$ on a uniformly spaced grid

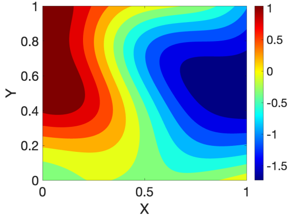
The covariance matrix C is BTTB and its even BCCB extension $\tilde{C}$ is non-negative definite with $\lambda_{min} = 0$.

Example images for padding

Example 1.11. Consider $u(x)$ a mean-zero random field with stationary covariance function $c(x) = \exp(-x^T A x)$ for $x \in \mathbb{R}^2$ and $A = \begin{pmatrix} 4 & 0 \\ 0 & 4 \end{pmatrix}$ and the space $[0,1]^2$ for $n_1 = n_2 = 257$. The BCCB extension has dimension $4N \times 4N$, where $N = (n_1 + m_1)(n_2 + m_2)$, m_1 is the padding of the circulant extension in each block and m_2 the padding in the BCCB extension.



(a) Padding $m_{1,2} = 0$, $\lambda_{min} = -80$



(b) Padding $m_{1,2} = 2056$, $\lambda_{min} = -8 \cdot 10^{-12}$

Outline

Lemma 2.1. (Bochner)
A function $c : \mathbb{R}^d \to \mathbb{C}$ is non-negative definite and continous if and only if

$$c(x) = \int_{\mathbb{R}^d} \exp(iv^T x) dF(v)$$

for some measure F on $\mathbb{R}^d$ that is finite (i.e. $F(\mathbb{R}^d) < \infty$).

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for some measure F on $\mathbb{R}^d$ that is finite (i.e. $F(\mathbb{R}^d) < \infty$).

Lemma 2.2. (Wiener-Khintchine)
The following are equivalent:

(i) There exists a stationary random field $\{u(x) : x \in \mathbb{R}^d\}$ with stationary covariance function $c(x)$ that is mean-square continuous.

(ii) The function $c : \mathbb{R}^d \to \mathbb{R}$ can be written in spectral form, that is

$$c(x) = \int_{\mathbb{R}^d} \exp(iv^T x) dF(v)$$

for some measure F on $\mathbb{R}^d$ with $F(\mathbb{R}^d) < \infty$.

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(ii) The function $c : \mathbb{R}^d \to \mathbb{R}$ can be written in spectral form, that is

$$c(x) = \int_{\mathbb{R}^d} \exp(iv^T x) dF(v)$$

for some measure F on $\mathbb{R}^d$ with $F(\mathbb{R}^d) < \infty$.

Here notice that for the Fourier transform $\hat{c}$ of a covariance function $c : \mathbb{R} \to \mathbb{R}$ it holds

$$c(x) = \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}^d} \exp(iv^T x) \hat{c}(v) dv = \int_{\mathbb{R}^d} \exp(iv^T x) f(v) dv$$

So the density satisfies $f(v) = \hat{c}(v)/\sqrt{2\pi}$.

Definition 2.3. (isotropic random field)
A stationary random field $\{u(x) : x \in \mathbb{R}^d\}$ is isotropic if the stationary covariance $c(x)$ is invariant to rotations. Then μ is constant and $c(x) = c^0(r)$, where $r := \|x\|_2$, for a function $c^0 : \mathbb{R}^+ \to \mathbb{R}$ known as the isotropic covariance.

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A stationary random field $\{u(x) : x \in \mathbb{R}^d\}$ is isotropic if the stationary covariance $c(x)$ is invariant to rotations. Then μ is constant and $c(x) = c^0(r)$, where $r := \|x\|_2$, for a function $c^0 : \mathbb{R}^+ \to \mathbb{R}$ known as the isotropic covariance.

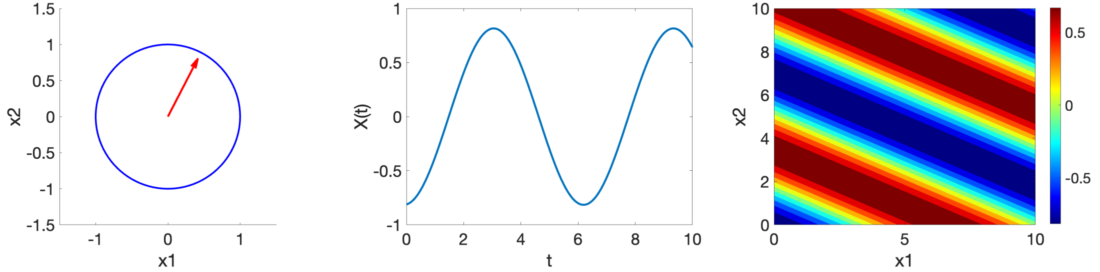
Lemma 2.4. (isotropic covariance)
Let $\{u(x) : x \in \mathbb{R}^d\}$ be an isotropic random field with a mean-square continuous covariance function $c^0(r)$. There exists a finite measure F^0 on $\mathbb{R}^+$, known as the radial spectral distribution, such that

$$c^0(r) = \Gamma(d/2) \int_0^\infty \frac{J_p(rs)}{(rs/2)^p} dF^0(s), \qquad p = \frac{d}{2} - 1$$

where $\Gamma(z) = \int_0^\infty t^{z-1} \exp(-t) dt$ for $Re(z) > 0$.
and $J_p(z) = \sum_{r=0}^\infty \frac{(-1)^r (\frac{x}{2})^{2r+p}}{\Gamma(p+r+1) r!}$ called Bessel function.

Definition 2.5. (turning bands random field)
Let $\{X(t) : t \in \mathbb{R}\}$ denote a 1D stationary stochastic process and $e \sim U(\mathbb{S}^{d-1})$ a random vector uniformly distributed on the surface of the unit ball $\mathbb{S}^{d-1} := \{x \in \mathbb{R}^d : \|x\|_2 = 1\}$.
Then the turning bands random field is defined as

$$\{v(x) := X(x^T e) : x \in \mathbb{R}^d\}$$



(a) Sample of e

(b) $X(t)$ for Bessel covariance

(c) $X(x^T e)$ for $x \in (0, 10)^2$

Definition 2.6. (turning bands operator)
Let $c^0(r)$ be an isotropic covariance function of a random field on $\mathbb{R}^d$ with radial spectral distribution $F^0(s)$. The turning bands operator T_d is defined by

$$c_X(t) = T_d c^0(t) := \int_0^\infty \cos(st)dF^0(s) = \int_{-\infty}^\infty \exp(ist)dF(s)$$

$T_d c^0(t)$ is the covariance function of a 1D stationary process with radial spectral distribution $F(s) = F^0(s)/2$.

Lemma 2.7. (isotropic covariance of turning bands random field)
Consider an isotropic covariance function $c^0(r)$ in $\mathbb{R}^d$ and a mean-zero process $\{X(t) : t \in \mathbb{R}\}$ with stationary covariance $T_d c^0(t)$. Then, the turning bands random field $v(x)$ has isotropic covariance $c^0(r)$.

Lemma 2.7. (isotropic covariance of turning bands random field)
Consider an isotropic covariance function $c^0(r)$ in $\mathbb{R}^d$ and a mean-zero process $\{X(t) : t \in \mathbb{R}\}$ with stationary covariance $T_d c^0(t)$. Then, the turning bands random field $v(x)$ has isotropic covariance $c^0(r)$.

Proof:

(i)

Lemma 2.8. (stationary covariance of turning bands random field)
If the process $X(t)$ has mean zero and stationary covariance $c_X(t)$, the turning bands random field $v(x) = X(x^T e)$ has mean zero and stationary covariance $\mathbb{E}[c_X(x^T e)]$ where $e \sim U(\mathbb{S}^{d-1})$.

(ii) Computation $\mathbb{E}[c_X(x^T e)] = c^0(r)$

Turning bands method summary

Goal: sample $\{u(x) : x \in \mathbb{R}^d\}$ with mean zero and isotropic covariance $c^0(r)$

$\rightarrow$ $\{v(x) = X(x^T e) : x \in \mathbb{R}^d\}$ has covariance $c_0(r)$ as well if $c_X(t) = T_d c^0(t)$

$\rightarrow$ sample from $\{X(t) : t \in \mathbb{R}\}$ in 1D via circulant embedding or quadrature

$\rightarrow$ for $u(x)$ Gaussian use central limit theorem

Lemma 2.9. Suppose that $X_j(t)$ for $j = 1, ..., M$ are iid copies of $X(t)$ and that $e_j \sim U(\mathbb{S}^{d-1})$. Further suppose $X_j(t)$ and e_j are pairwise independent (where $X_j(t)$ is treated as an $\mathbb{R}^{\mathbb{R}}$ random variable)
Define

$$v_M(x) := \frac{1}{\sqrt{M}} \sum_{j=1}^{M} X_j(x^T e_j)$$

where M is the number of bands. As $M \to \infty$ the central limit theorem implies convergence in distribution of $v_M(x)$ to the mean-zero Gaussian random field with isotropic covariance $c^0(r)$.
In practice deterministic uniformly spaced bands $e_j \in \mathbb{S}^{d-1}$ are used.

Example 2.10. (isotropic exponential $d = 3$)

The Gaussian random field $u(x)$ with isotropic covariance $c^0(r) = e^{-r/l}$ is created by the Gaussian process with covariance $c_X(t) = (1 - t/l)e^{-t/l} \overset{5.5}{=} \frac{d}{dt}(tc^0(t))$. The following plots show the convergence with different M for a Gaussian random field with $l = 0.01$:

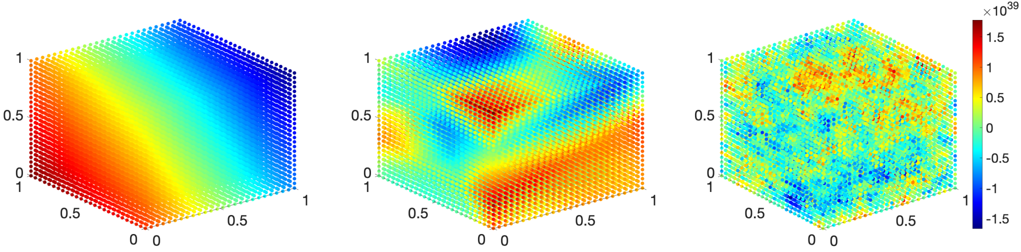


Figure 4 Approximations with $M = 2$, $M = 10$, $M = 100$

Outline

Qualitative comparison

Method supports:	Circulant embedding	Turning bands
Dimension $d > 2$	$\sim$	✓
Unisotropic covariance function	✓	✗
Exact sampling	✓ $\mid$ $\tilde{C}$ p.s.d.	✗

Literature

[1] Gabriel J. Lord, Catherine E. Powell, and Tony Shardlow. *An Introduction to Computational Stochastic PDEs*. Cambridge Texts in Applied Mathematics. Cambridge University Press, 2014.

Example 5.1. (symmetric BCCB matrices)
Consider $n_1 = 3$, $n_2 = 3$ and

$$C = \begin{pmatrix} C_0 & C_1^T & C_1 \\ C_1 & C_0 & C_1^T \\ C_1^T & C_1 & C_0 \end{pmatrix}$$

with circulant blocks

$$C_0 = \begin{pmatrix} 1 & 0.2 & 0.2 \\ 0.2 & 1 & 0.2 \\ 0.2 & 0.2 & 1 \end{pmatrix}, \qquad C_1 = \begin{pmatrix} 0.5 & 0.2 & 0.1 \\ 0.1 & 0.5 & 0.2 \\ 0.2 & 0.1 & 0.5 \end{pmatrix}$$

Sample result example: $[1.08, -1.94, 2.12, -0.34, -1.33, 3.06, -0.33, -0.19, 0.66]^T$

Appendix II

Definition 5.2. (two-dimensional IDFT)
The two-dimensional inverse discrete Fourier transform of $\hat{V} \in \mathbb{C}^{n_1 \times n_2}$ is the matrix $V \in \mathbb{C}^{n_1 \times n_2}$ with entries

$$v_{i,j} := \frac{1}{n_1 n_2} \sum_{m=1}^{n_2} \left(\sum_{l=1}^{n_1} \hat{v}_{lm} \omega_1^{-(i-1)(l-1)} \right) \omega_2^{-(j-1)(m-1)},$$

for $i = 1, ..., n_1$ and $j = 1, ..., n_2$.

Lemma 5.3. (Fourier representation of BCCB matrices)
Let C be an $N \times N$ real-valued BCCB matrix, where $N = n_1 n_2$. Then $C = WDW^*$, where W is the two-dimensional Fourier matrix and D is a diagonal matrix with diagonal $d = \text{vec}(\Lambda)$ where

$$\Lambda := \sqrt{N} \cdot \text{array}(W^* c_{red}), \qquad c_{red} := \text{vec}(C_{red}).$$

Appendix III

Definition 5.4. (radial spectral density)
If the radial spectral distribution F^0 has a radial spectral density f^0, then

$$dF^0(s) = \omega_d s^{d-1} f^0(s) ds$$
$$f^0(s) = \frac{1}{(2\pi)^{d/2}} \int_0^\infty \frac{J_p(rs)}{(rs)^p} c^0(r) r^{d-1} dr$$

Appendix IV

Example 5.5. (three dimensions)
The turning bands operator takes a particular simple form in dimension $d = 3$. We have $J_{1/2}(r) = \sqrt{2/(\pi r)}\sin(r)$ and $\Gamma(3/2) = \sqrt{\pi}/2$. Hence,

$$\frac{d}{dt}\left(\Gamma(3/2)t\frac{J_{1/2}(ts)}{(ts/2)^{1/2}}\right) = \frac{d}{dt}\left(\frac{1}{s}\sin(ts)\right) = \cos(ts)$$

$$\int_0^\infty \frac{d}{dt}\left(\Gamma(3/2)t\frac{J_{1/2}(ts)}{(ts/2)^{1/2}}\right)dF^0(s) = \int_0^\infty \cos(ts)dF^0(s)$$

it follows

$$\frac{d}{dt}(tc^0(t)) = T_3c^0(t)$$