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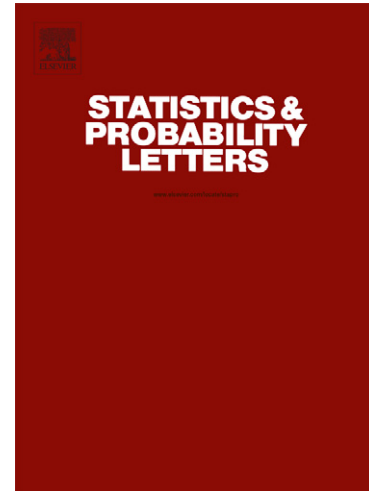
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Can any multivariate Gaussian vector be interpreted as a sample from a stationary random process?

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Running head: multivariate Gaussian vector interpreted as sample from stationary process

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Fundamental parts of the theory in geostatistics is based on the statement of equivalence of the following three assertions (Chilès and Delfiner, 1999, p. 60; Cressie, 1993, p. 84):

- (i) a symmetric real-valued function c on $\mathbb{R}^d$ is positive definite, i.e. $(c(x_j - x_k))_{j,k=1,\dots,n}$ is a positive semi-definite matrix for all $x_j \in \mathbb{R}^d$ and $n \in \mathbb{N}$;
- (ii) a second-order stationary real-valued random field Z in $\mathbb{R}^d$ exists with $\text{Cov}(Z(x+h), Z(x)) = c(h)$ for all $x, h \in \mathbb{R}^d$;
- (iii) a zero-mean stationary Gaussian random field Z in $\mathbb{R}^d$ exists with $\text{Cov}(Z(x+h), Z(x)) = c(h)$ for all $x, h \in \mathbb{R}^d$.

Here, we are interested in a reversed statement of (i): Given a positive semi-definite matrix C , does a positive definite function c exists such that $C = (c(x_j - x_k))_{j,k=1,\dots,n}$ for some $x_j \in \mathbb{R}^d$? Since a multivariate Gaussian distribution is uniquely determined by its mean and the covariance matrix, the question can be formulated also in the following way. Let Z be a real-valued stationary Gaussian random function on $\mathbb{R}^d$ and $x_1, \dots, x_n \in \mathbb{R}^d$ any n points. Then, by definition of a Gaussian random function, the vector

$$Y = (Z(x_1), \dots, Z(x_n)) \tag{1}$$

is a multivariate Gaussian random vector (Chilès and Delfiner, 1999). The question equivalent to the above one is: given a multivariate Gaussian vector Y , is there some space $\mathbb{R}^d$, a stationary random function Z , and some points $x_1, \dots, x_n \in \mathbb{R}^d$, such that (1) holds? An obvious necessary condition is that the expectations, and the variances, are the same for all components of Y . Under this condition and if $d \geq 2$, we give a first positive answer, namely that a hypersurface H and a stationary process Z always exist so that (1) holds. The following theorem is given in terms of positive semi-definite matrices and positive definite functions.

Theorem. An $n \times n$ matrix $C = (C_{jk})_{j,k=1,\dots,n}$ is real-valued, symmetric and positive definite and has identical values on the diagonal if and only if, for all $d \geq 2$, a real-valued positive definite function c on a graph of $\mathbb{R}^d$ and points $x_1, \dots, x_n \in \mathbb{R}^d$ exist, so that

$$C = (c(x_j - x_k))_{j,k=1,\dots,n}. \quad (2)$$

Proof. Let C be a real-valued, symmetric and positive definite matrix with identical values on the diagonal and U be an arbitrary set of n distinct points $t_1 < \dots < t_n$ on the real axis. Without loss of generality we assume that the diagonal of C is identical to 1. First we show that a non-stationary standard Gaussian random function $V = \{V(t), t \in \mathbb{R}\}$ exists that is continuous in quadratic mean such that its covariance function c_V satisfies

$$c_V(t_j, t_k) = C_{jk} \quad \text{for all } 1 \leq j, k \leq n.$$

Let $\eta = (\eta_1, \dots, \eta_n)$ be a Gaussian vector with covariance matrix $(C_{jk})_{j,k=1,\dots,n}$. From η , we define an intermediate random function $\{\epsilon(t), t \in \mathbb{R}\}$ as

$$\epsilon(t) = \eta_1 \mathbb{1}_{(-\infty, t_1)}(t) + \sum_{j=2}^n \left(\eta_{j-1} + \frac{(\eta_j - \eta_{j-1})}{t_j - t_{j-1}}(t - t_{j-1}) \right) \mathbb{1}_{[t_{j-1}, t_j)}(t) + \eta_n \mathbb{1}_{[t_n, \infty)}(t),$$

where $\mathbb{1}_A$ denotes the indicator function for the set A . Then $\{\epsilon(t), t \in \mathbb{R}\}$ is a measurable Gaussian random function, continuous in quadratic mean. To compute its covariance function $c_\epsilon(t, t')$, $(t, t') \in \mathbb{R}^2$, let us re-write $\epsilon(t)$ in a matrix form

$$\epsilon(t) = a(t)b(t)\epsilon$$

with $a(t)$ the $n \times 1$ matrix

$$a(t) = (\mathbb{1}_{(-\infty, t_1)}, \dots, \mathbb{1}_{[t_{j-1}, t_j)}, \dots, \mathbb{1}_{[t_n, \infty)})(t)$$

and $b(t)$ the $n \times n$ matrix

$$b(t) = \begin{pmatrix} 1 & 0 & 0 & \dots & 0 & 0 \\ \frac{t_2-t}{t_2-t_1} & \frac{t-t_1}{t_2-t_1} & 0 & \dots & 0 & 0 \\ 0 & \frac{t_3-t}{t_3-t_2} & \frac{t-t_2}{t_3-t_2} & \ddots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \ddots & \frac{t-t_{n-2}}{t_{n-1}-t_{n-2}} & 0 \\ 0 & 0 & 0 & \ddots & \frac{t_n-t}{t_n-t_{n-1}} & \frac{t-t_{n-1}}{t_n-t_{n-1}} \\ 0 & 0 & 0 & \dots & 0 & 1 \end{pmatrix}.$$

Then the covariance of $\epsilon(t)$ equals

$$c_\epsilon(t, t') = a(t)b(t)Cb(t')^t a(t')^t.$$

where t is the transpose operator.

The random function V is now defined as

$$V(t) = \frac{\epsilon(t)}{\sqrt{c_\epsilon(t, t)}}.$$

Then, Theorem 1 in Perrin and Meiring (2003) guarantees the existence of a positive definite function c on a graph of $\mathbb{R}^2$ and points $x_1, \dots, x_n \in \mathbb{R}^2$, such that (2) holds. For instance, according to Perrin and Meiring (2003), we can take $x_j = (t_j, \exp(t_j))$, $j = 1, \dots, n$. The remaining assertions of the theorem are obvious. In particular, the graph on $\mathbb{R}^2$ can be trivially extended to a graph on $\mathbb{R}^d$. ■

Hence, a necessary and sufficient condition that a Gaussian random vector can be interpreted as a sample from a stationary random function on a graph of $\mathbb{R}^d$, $d \geq 2$, is that the expectations are the same for all components and the covariance matrix has identical components on the diagonal.

We conclude with a counter example, that $d = 1$ does not work in general. To be specific, there exists a 6×6 real-valued, symmetric and positive semi-definite matrix C that has identical values on the diagonal, such that for no continuous positive definite function c on $\mathbb{R}$ a set of n points $x_1, \dots, x_n \in \mathbb{R}$ exists for which (2) holds. Let α be an arbitrary angle in $(0, \pi/3)$ and $\mathbb{R}^3$ endowed with the canonical scalar product $\langle \cdot, \cdot \rangle_3$. Let X_1, X_2 and X_3 be unit vectors in $\mathbb{R}^3$ such that

$$\|X_j + X_k\|_3 = 2 \cos \alpha, \quad 1 \leq j \neq k \leq 3.$$

This means that the angle between X_j and X_k , $1 \leq j \neq k \leq 3$, is strictly smaller than $2\pi/3$. Note that the intersections of X_1, X_2, X_3 with the unit sphere are the vertices of an equilateral triangle; hence such vectors X_1, X_2 and X_3 always exist. Further three vectors X_4, X_5, X_6 are defined as linear combinations of X_1, X_2 and X_3 ,

$$X_4 = \frac{X_1 + X_2}{2 \cos \alpha} \tag{3}$$

$$X_5 = \frac{X_2 + X_3}{2 \cos \alpha} \tag{4}$$

$$X_6 = \frac{X_1 + X_3}{2 \cos \alpha}. \tag{5}$$

The Gram matrix of $X_1, \dots, X_6$,

$$(C_{jk}) = (\langle X_j, X_k \rangle_3), \quad 1 \leq j, k \leq 6, \tag{6}$$

has identical values on the diagonal and is symmetric and positive definite. The latter follows from the fact that $a^\top C a = \|\sum_{j=1}^6 a_j X_j\|^2 \geq 0$ for any $a = (a_1, \dots, a_6) \in \mathbb{R}^6$.

Lemma. Let $W_1, \dots, W_6$ be six complex numbers with modulus equal to 1. Then, for all $\alpha \in (0, \pi/3)$ we have

$$\left| W_4 - \frac{W_1 + W_2}{2 \cos \alpha} \right|^2 + \left| W_5 - \frac{W_2 + W_3}{2 \cos \alpha} \right|^2 + \left| W_6 - \frac{W_1 + W_3}{2 \cos \alpha} \right|^2 > 0. \tag{7}$$

Proof. It suffices to show that $|W_1 + W_2| = |W_1 + W_3| = 2 \cos \alpha$ implies $|W_2 + W_3| \neq 2 \cos \alpha$. Without loss of generality we may assume that $W_1 = 1$. Let $W_2 = \cos \beta + i \sin \beta$ and $W_3 = \cos \gamma + i \sin \gamma$ for some $\beta, \gamma \in [0, 2\pi)$. Then $|W_1 + W_2| = |W_1 + W_3| = 2 \cos \alpha$ is equivalent to

$$\cos \beta = \cos \gamma = 2 \cos^2 \alpha - 1. \quad (8)$$

If $\beta = -\gamma$ then the condition $|W_2 + W_3| = 2 \cos \alpha$ yields that $\cos^2 \beta = \cos^2 \alpha$. Together with Eq. (8) this implies that $|\cos \alpha| \in \{1/2, 1\}$. Similarly, the assumption $\beta = \gamma$ implies $|\cos \alpha| = 1$. We conclude that the left hand side of Eq. (7) is strictly positive for $\alpha \in (0, \pi/3)$. $\blacksquare$

Now, we show that no stationary random function with continuous covariance c exists such that (2) holds for C defined in (6). Assume that such a real-valued random function exists. Bochner's theorem states that c can be written as

$$c(u) = \int_{-\infty}^{\infty} e^{i\omega u} \mu(d\omega)$$

where μ is a finite positive measure ($0 < \mu(\mathbb{R}) < \infty$) and $c(u) = c(-u)$. Hence, for all $1 \leq j \leq k \leq 6$,

$$C_{jk} = c(x_j - x_k) = \int_{-\infty}^{\infty} e^{i\omega(x_j - x_k)} \mu(d\omega)$$

for some $x_1, \dots, x_6 \in \mathbb{R}$. Defining $W_j(\omega) = e^{i\omega x_j}$ for $1 \leq j \leq 6$, we get

$$\langle X_j, X_k \rangle_3 = C_{jk} = \int_{-\infty}^{\infty} W_j(\omega) \bar{W}_k(\omega) \mu(d\omega) = \langle W_j, W_k \rangle_{L^2_{\mathbb{C}}(\Omega, \mu)}.$$

Therefore,

$$\left\| X_4 - \frac{X_1 + X_2}{2 \cos \alpha} \right\|_3^2 = \left\| W_4 - \frac{W_1 + W_2}{2 \cos \alpha} \right\|_{L^2_{\mathbb{C}}(\Omega, \mu)}^2 = \int_{-\infty}^{\infty} \left| W_4(\omega) - \frac{W_1(\omega) + W_2(\omega)}{2 \cos \alpha} \right|^2 \mu(d\omega). \quad (9)$$

Similar relations hold for X_5 and X_6 . Define

$$\begin{aligned} D(\omega) &= \left| W_4(\omega) - \frac{W_1(\omega) + W_2(\omega)}{2 \cos \alpha} \right|^2 + \left| W_5(\omega) - \frac{W_2(\omega) + W_3(\omega)}{2 \cos \alpha} \right|^2 + \\ &\quad + \left| W_6(\omega) - \frac{W_1(\omega) + W_3(\omega)}{2 \cos \alpha} \right|^2. \end{aligned}$$

Eqs. (3)-(5) and (9) yield that $\int D(\omega) \mu(\omega)$ is identically zero, whereas the preceding lemma states that $D(\omega)$ is positive for all $\omega \in \mathbb{R}$. Since μ is a positive measure, we obtain the required contradiction.

Now, models that are the sum of a continuous covariance function and a nugget effect are of major interest both from a practical and a theoretical point of view, see section 2.3.1 in Chiles and Delfiner (1999) and Gneiting and Sasvári (1999). Hence it is important to note that the counter-example is still valid when we allow for nugget-effect covariances c^* defined by

$$c^*(u) = \theta c(u) + (1 - \theta) \mathbb{1}_{u=0}(u),$$

where $\theta \in [0, 1]$ and c is a continuous covariance. Assume a nugget-effect covariance $c^\star$ exists such that (2) holds for C defined in (6). Let $d = \min |x_k - x_i|, 1 \leq i \neq k \leq 6$. Then $d > 0$ and

$$c_0(u) = \theta c(u) + (1 - \theta) \left(1 - \frac{|u|}{d}\right) \mathbb{1}_{0 \leq |u| \leq d}(u)$$

is a continuous covariance such that for all $1 \leq i, k \leq 6$

$$c_0(x_k - x_i) = c^\star(x_k - x_i).$$

This contradicts our previous counter-example. ■

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