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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. $\left(c\left(x_{j}-x_{k}\right)\right)_{j, k=1, \ldots, n}$ 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 $\operatorname{Cov}(Z(x+$ $h), Z(x))=c(h)$ for all $x, h \in \mathbb{R}^{d}$;
(iii) a zero-mean stationary Gaussian random field $Z$ in $\mathbb{R}^{d}$ exists with $\operatorname{Cov}(Z(x+h), Z(x))=$ $c(h)$ 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 $C=\left(c\left(x_{j}-x_{k}\right)\right)_{j, k=1, \ldots, n}$ 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 $x_{1}, \ldots, x_{n} \in \mathbb{R}^{d}$ any $n$ points. Then, by definition of a Gaussian random function, the vector

$$
\begin{equation*}
Y=\left(Z\left(x_{1}\right), \ldots, Z\left(x_{n}\right)\right) \tag{1}
\end{equation*}
$$

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 $x_{1}, \ldots, x_{n} \in \mathbb{R}^{d}$, 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 $C=\left(C_{j k}\right)_{j, k=1, \ldots, n}$ 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 $x_{1}, \ldots, x_{n} \in \mathbb{R}^{d}$ exist, so that

$$
\begin{equation*}
C=\left(c\left(x_{j}-x_{k}\right)\right)_{j, k=1, \ldots, n} \tag{2}
\end{equation*}
$$

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 $t_{1}<\ldots<t_{n}$ 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

$$
c_{V}\left(t_{j}, t_{k}\right)=C_{j k} \quad \text { for all } 1 \leq j, k \leq n
$$

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

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

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 $c_{\epsilon}\left(t, t^{\prime}\right),\left(t, t^{\prime}\right) \in \mathbb{R}^{2}$, 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

$$
a(t)=\left(\mathbb{1}_{\left(-\infty, t_{1}\right)}, \ldots, \mathbb{1}_{\left[t_{j-1}, t_{j}\right)}, \ldots, \mathbb{1}_{\left[t_{n}, \infty\right)}\right)(t)
$$

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

$$
b(t)=\left(\begin{array}{cccccc}
1 & 0 & 0 & \cdots & 0 & 0 \\
\frac{t_{2}-t}{t_{2}-t_{1}} & \frac{t-t_{1}}{t_{2}-t_{1}} & 0 & \cdots & 0 & 0 \\
0 & \frac{t_{3}-t}{t_{3}-t_{2}} & \frac{t-t_{2}}{t_{3}-t_{2}} & \ddots & 0 & 0 \\
\vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\
0 & 0 & 0 & \ddots & \frac{t-t_{n-2}}{t_{n-1}-t_{n-2}} & 0 \\
0 & 0 & 0 & \ddots & \frac{t_{n} t}{t_{n}-t_{n-1}} & \frac{t-t_{n-1}}{t_{n}-t_{n-1}} \\
0 & 0 & 0 & \ldots & 0 & 1
\end{array}\right) .
$$

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

$$
c_{\epsilon}\left(t, t^{\prime}\right)=a(t) b(t) C b\left(t^{\prime}\right)^{t} a\left(t^{\prime}\right)^{t} .
$$

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 $x_{1}, \ldots, x_{n} \in \mathbb{R}^{2}$, such that (2) holds. For instance, according to Perrin and Meiring (2003), we can take $x_{j}=\left(t_{j}, \exp \left(t_{j}\right)\right), j=1, \ldots, n$. 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 $6 \times 6$ 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 $x_{1}, \ldots, x_{n} \in \mathbb{R}$ exists for which (2) holds. Let $\alpha$ be an arbitrary angle in $(0, \pi / 3)$ and $\mathbb{R}^{3}$ endowed with the canonical scalar product $\langle,\rangle_{3}$. Let $X_{1}, X_{2}$ and $X_{3}$ be unit vectors in $\mathbb{R}^{3}$ such that

$$
\left\|X_{j}+X_{k}\right\|_{3}=2 \cos \alpha, 1 \leq j \neq k \leq 3
$$

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 $X_{3}$,

$$
\begin{equation*}
X_{4}=\frac{X_{1}+X_{2}}{2 \cos \alpha} \tag{3}
\end{equation*}
$$

$$
\begin{equation*}
X_{6}=\frac{X_{1}+X_{3}}{2 \cos \alpha} \tag{5}
\end{equation*}
$$

$$
\begin{equation*}
X_{5}=\frac{X_{2}+X_{3}}{2 \cos \alpha} \tag{4}
\end{equation*}
$$

The Gram matrix of $X_{1}, \ldots, X_{6}$,

$$
\begin{equation*}
\left(C_{j k}\right)=\left(\left\langle X_{j}, X_{k}\right\rangle_{3}\right), 1 \leq j, k \leq 6 \tag{6}
\end{equation*}
$$

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

Lemma. Let $W_{1}, \ldots, W_{6}$ be six complex numbers with modulus equal to 1 . Then, for all $\alpha \in(0, \pi / 3)$ we have

$$
\begin{equation*}
\left|W_{4}-\frac{W_{1}+W_{2}}{2 \cos \alpha}\right|^{2}+\left|W_{5}-\frac{W_{2}+W_{3}}{2 \cos \alpha}\right|^{2}+\left|W_{6}-\frac{W_{1}+W_{3}}{2 \cos \alpha}\right|^{2}>0 \tag{7}
\end{equation*}
$$

Proof. It suffices to show that $\left|W_{1}+W_{2}\right|=\left|W_{1}+W_{3}\right|=2 \cos \alpha$ implies $\left|W_{2}+W_{3}\right| \neq 2 \cos \alpha$. Without lost 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 $\left|W_{1}+W_{2}\right|=\left|W_{1}+W_{3}\right|=2 \cos \alpha$ is equivalent to

$$
\begin{equation*}
\cos \beta=\cos \gamma=2 \cos ^{2} \alpha-1 \tag{8}
\end{equation*}
$$

If $\beta=-\gamma$ then the condition $\left|W_{2}+W_{3}\right|=2 \cos \alpha$ 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 $\alpha \in(0, \pi / 3)$.

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

$$
C_{j k}=c\left(x_{j}-x_{k}\right)=\int_{-\infty}^{\infty} e^{i \omega\left(x_{j}-x_{k}\right)} \mu(d \omega)
$$

for some $x_{1}, \ldots, x_{6} \in \mathbb{R}$. Defining $W_{j}(\omega)=e^{i \omega x_{j}}$ for $1 \leq j \leq 6$, we get

$$
\left\langle X_{j}, X_{k}\right\rangle_{3}=C_{j k}=\int_{-\infty}^{\infty} W_{j}(\omega) \bar{W}_{k}(\omega) \mu(d \omega)=\left\langle W_{j}, W_{k}\right\rangle_{L_{\mathrm{C}}^{2}(\Omega, \mu)} .
$$

Therefore,

$$
\begin{equation*}
\left\|X_{4}-\frac{X_{1}+X_{2}}{2 \cos \alpha}\right\|_{3}^{2}=\left\|W_{4}-\frac{W_{1}+W_{2}}{2 \cos \alpha}\right\|_{L_{\mathbb{C}}^{2}(\Omega, \mu)}^{2}=\int_{-\infty}^{\infty}\left|W_{4}(\omega)-\frac{W_{1}(\omega)+W_{2}(\omega)}{2 \cos \alpha}\right|^{2} \mu(d \omega) . \tag{9}
\end{equation*}
$$

Similar relations hold for $X_{5}$ and $X_{6}$. Define

$$
\begin{aligned}
D(w)= & \left|W_{4}(\omega)-\frac{W_{1}(\omega)+W_{2}(\omega)}{2 \cos \alpha}\right|^{2}+\left|W_{5}(\omega)-\frac{W_{2}(\omega)+W_{3}(\omega)}{2 \cos \alpha}\right|^{2}+ \\
& +\left|W_{6}(\omega)-\frac{W_{1}(\omega)+W_{3}(\omega)}{2 \cos \alpha}\right|^{2} .
\end{aligned}
$$

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 $\mu$ 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 Chilès 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 $c^{\star}$ defined by

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

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 $d=\min \left|x_{k}-x_{i}\right|, 1 \leq i \neq k \leq 6$. 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 $1 \leq i, k \leq 6$

$$
c_{0}\left(x_{k}-x_{i}\right)=c^{\star}\left(x_{k}-x_{i}\right) .
$$

This contradicts our previous counter-example.

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